

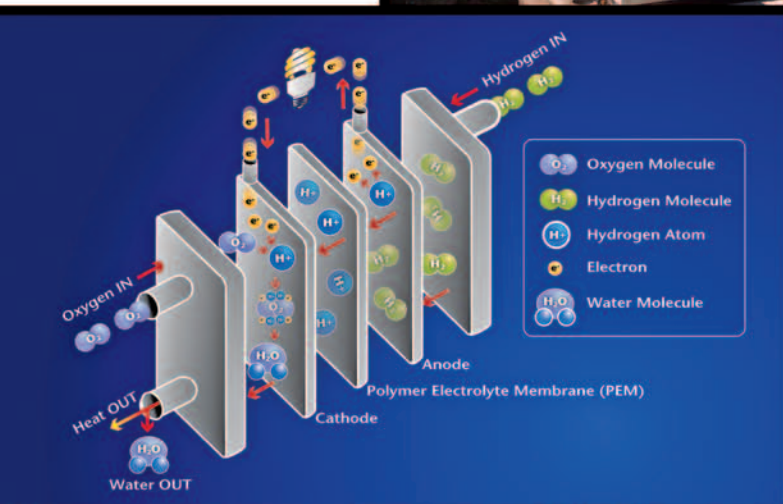
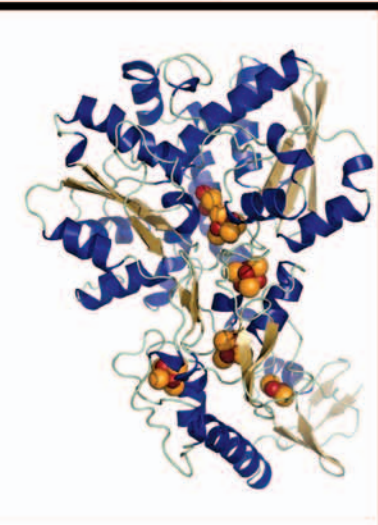
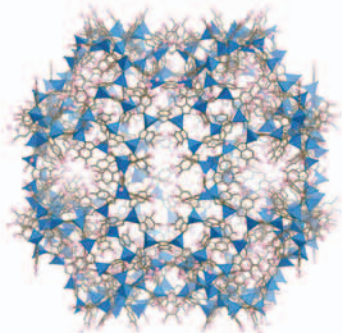
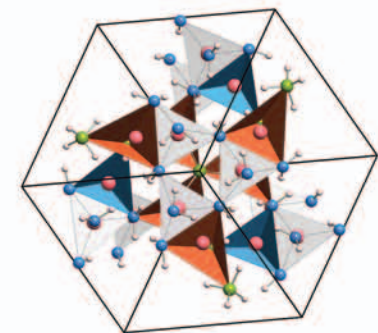


U.S. DEPARTMENT OF  
**ENERGY**



June 9–13, 2008  
Arlington, Virginia

# Hydrogen Program 2008 Annual Merit Review and Peer Evaluation Report



## **About the Cover**

*(From top to bottom) Photo of young interest in hydrogen-fuel-cell technology, courtesy of Christy Cooper; illustrations of structures of two potential hydrogen storage materials:  $\text{Li}_4\text{BN}_3\text{H}_{10}$  and ZIF-100; illustration of [FeFe] hydrogenase catalyst system for light-driven hydrogen generation; photo of hydrogen fuel cell forklift in airport service, courtesy of Hydrogenics (NREL PIX 15987); photo of UTC Power PC-25 fuel cells, courtesy of UTC Power Corporation; schematic of a polymer electrolyte membrane fuel cell; photo of a Chevrolet Equinox fuel cell vehicle in service with the U.S. Postal Service, courtesy of the U.S. Postal Service, Richard Maher, photographer (NREL PIX 15988).*

# **DOE Hydrogen Program**

## **2008 Annual Merit Review and Peer Evaluation Report**

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## PROLOGUE

Dear Colleague:

This document summarizes the comments provided by the peer reviewers at the U.S. Department of Energy (DOE) Hydrogen Program's FY 2008 Annual Merit Review and Peer Evaluation meeting, held on June 9-13, 2008 in Washington, D.C. In response to direction from the Under Secretary of Energy, this review process provides evaluations of the Program's projects in applied research, development and demonstration, and analysis of hydrogen, fuel cells and infrastructure technologies. All four Offices that support the President's Hydrogen Fuel Initiative, Energy Efficiency and Renewable Energy (EERE), Fossil Energy (FE), Nuclear Energy (NE), and Science (SC), participated in the meeting to provide the hydrogen community a view of the breadth and depth of DOE's efforts under the Initiative. Overview presentations were given by all four Offices during the opening plenary session; projects from EERE, FE, and NE were presented and peer reviewed, and the hydrogen production related projects from SC were presented.

The recommendations of the reviewers have been taken into consideration by DOE Technology Development Managers in the generation of future work plans. The table below lists the projects presented at the review, evaluation scores and the major actions to be taken during the upcoming fiscal year (October 1, 2008 to September 30, 2009). The projects have been grouped according to Program Element (Production, Delivery, Storage, Fuel Cells, etc.) and then by the five evaluation criteria. The weighted scores are based on a 4-point scale. To furnish all principal investigators (PIs) with direct feedback, all evaluations and comments are provided to each presenter; however, the authors of the individual comments remain anonymous. The PI of each project is instructed to fully consider these summary evaluation comments, as appropriate, in their FY 2009 plans.

I would like to express my sincere appreciation to the reviewers. You make this report possible, and we rely on your comments to help make project decisions for the new fiscal year.

We look forward to your participation in the FY 2009 Hydrogen and Vehicle Technologies Programs' joint Annual Merit Review and Peer Evaluation meeting, which is presently scheduled for May 18-22, 2009 at the Crystal Gateway Marriott and Crystal City Marriott hotels in Arlington, VA. Thank you for participating in the FY 2008 Annual Merit Review and Peer Evaluation meeting.

Sincerely,



JoAnn Milliken  
DOE Hydrogen Program Manager  
Office of Energy Efficiency and Renewable Energy

## Hydrogen Production and Delivery:

Project Number	Project Title; Presenting Organization; PI Name	Final Score	Continue	Discontinue	Other	Summary Comment
PD-01	Low-Cost Hydrogen Distributed Production System Development; H2Gen Inno. Inc.; Frank Lomax	3.2	X			This project supports DOE cost targets for distributed natural gas reforming hydrogen production. Reviewers observed that the hydrogen output and efficiency of the prototype plant are good, albeit the hydrogen output capacity is a little short of the target. Future work will focus on hydrogen from ethanol through catalyst and micro-reactor life-testing on fuel-grade ethanol. Techno-economic analyses of H2Gen SMR and ethanol reforming systems will continue.
PD-02	Bio-derived Liquids Reforming; PNNL; David King	2.8	X			The researchers understand the role of variables such as space velocity, catalyst, and steam/carbon ratio in reforming and in achieving project goals for sugar and alcohol reforming. The improvements are significant steps towards achieving the research objectives. However much work still needs to be done to improve catalyst activity and to obtain the right balance of selectivity, conversion and reactivation. Project will continue catalyst modifications and performance characterizations, and H2A analyses for both ethanol reforming and APR systems.
PD-03	Analysis of Ethanol Reforming System Configurations; DTI; Brian James	3.4	X			The project focuses on an economic comparison of distributed reforming of bio-derived liquids (focus on ethanol). Excellent progress has been made on this project. The various distributed ethanol reforming technologies and process configurations have been defined and fully analyzed for cost and energy efficiencies, identifying all the key cost leverages. Project will conclude with a report of analysis of all bio-derived liquids pathways as discussed.
PD-04	Pressurized Steam Reforming of Bio-Derived Liquids for Distributed Hydrogen Production; ANL; Shabbir Ahmed	2.5	X			The project objective is to reduce compression costs and therefore the cost of hydrogen production. Membrane technology is being investigated for the removal of oxygen, carbon dioxide and hydrogen. However, the project may not be technically feasible unless new membrane technology to remove carbon dioxide becomes available to facilitate reaching the targets of this project. Next steps include a Go/No Go decision on the use of Pd-based H <sub>2</sub> membranes, and systems analyses to evaluate the feasibility of alternative fuel processor designs using pressurized reforming.

Project Number	Project Title; Presenting Organization; PI Name	Final Score	Continue	Discontinue	Other	Summary Comment
PD-05	Investigation of Reaction Networks and Active Sites in Bio-Ethanol Steam Reforming Over Cobalt-Based Catalysts; Ohio State U; Umit Ozkan	3.0	X			Non-precious metal catalyst development is necessary to achieve long-term DOE cost targets. Good progress has been made in catalyst formulation and testing and the application of the H2A model to obtain preliminary cost data. Should test the catalyst for more than 100 hours. Further testing of impurity effects under realistic H <sub>2</sub> O/EtOH ratios is warranted. Next steps include long-term (> 100 hrs) time-on-stream experiments and accelerated deactivation and regeneration studies.
PD-07	Integrated Hydrogen Production, Purification & Compression System; Linde; Satish Tamhankar	3.2	X			The project approach combines good engineering and pilot scale testing with the complex integration of the membrane reactor and thermal compressor systems. The heat exchanger shown is novel and should be investigated for synergies in other parts of the Hydrogen Program. However, the issues with membrane stability, startups and shutdowns, and the ability to recover hydrogen from permeate and retentate streams remain. Project will complete proof-of-concept performance tests, and economic assessment. Based on results, a decision will be made regarding construction of a prototype unit.
PD-08	Zeolite Membrane Reactor for Water-Gas-Shift Reaction for Hydrogen Production; Arizona State U; Jerry Y.S. Lin	3.1	X			Materials development in the photo-electrochemical arena is clearly relevant, especially if such materials show improvements over photovoltaics / electrolyzer systems. The technology seems to be technically feasible. A cost analysis is needed to validate the potential for significant cost reductions in hydrogen production. Research would benefit from partnering with industry. Project will continue CVD modifications of membrane materials and H2A analysis of technology will be initiated.
PD-10	Low Cost, High Pressure Hydrogen Generator; Giner Electrochemical Systems LLC; Monjid Hamdan	2.9			X	This Project is completed. Lower-cost materials and fabrication methods for cell components were developed, and systems innovations reduced the cost of components. The initial DSM membrane performance reported very high efficiencies. Future work should focus on understanding the membrane durability, testing the membrane in a stack, and cost reduction.
PD-11	Hydrogen Generation from Electrolysis: 100 kg H <sub>2</sub> /day Trade Study; Proton Energy Systems; Stephen Porter	2.4			X	This Project is completed. The challenges identified were not new or surprising. Final results do not meet Department of Energy 2012 targets in terms of energy efficiency, hydrogen cost or capital costs. Future work should include membrane and catalyst work to enhance efficiency.

**PROLOGUE**

<b>Project Number</b>	<b>Project Title; Presenting Organization; PI Name</b>	<b>Final Score</b>	<b>Continue</b>	<b>Discontinue</b>	<b>Other</b>	<b>Summary Comment</b>
PD-12	Development of Water Splitting Catalysts Using a Novel Molecular Evolution Approach; ASU; Neal Woodbury	2.9	X			The milestones and technical barriers are clearly laid out for the project. Although they have not yet shown water splitting, they have shown catalyst activity. Significant focus was on development of a high volume process to screen different structures. Work will continue toward the goals of understanding the activity mechanisms of the catalysts and water splitting.
PD-13	Development of Solar Powered Thermochemical Production of Hydrogen from Water; STCH Collaboration; Nate Siegel	2.9	X			The overall objective of this project is to select one or two cost competitive solar powered hydrogen production cycles for large scale demonstration. This group has considerable technical ability and a strong team that is working together. The research team will examine material durability as the project progresses.
PD-14	Solar-Driven Photocatalytically-Assisted Water Splitting; UCF/FSEC; Ali T-Raissi	2.7	X			The project is updating the sulfur-ammonia cycle through the use of a photocatalysis assisted reaction. Progress has been demonstrated on the catalyst. In the second year of this project, the investigators will complete economic analysis with a particular emphasis on the solar field size.
PD-16	Hydrogen Delivery Infrastructure Analysis; ANL; Marrienne Mintz	3.1	X			Delivery represents a significant portion of the consumers' cost of hydrogen; it is necessary that we understand the costs associated with the various options. Importantly, the project showed the significant cost reductions available through flattening the hydrogen demand profile. As new delivery technologies and scenarios are developed, they will be added to the model.
PD-17	A Combined Materials Science/Mechanics Approach to the Study of Hydrogen Embrittlement of Pipeline Steels; U of Illinois; Sofronis Petros	3.7	X			Embrittlement is a serious failure mode of steel pipelines for a hydrogen infrastructure; and this study aims at a science-based approach to obtain mechanistic insights into why failures occur. The work has generated considerable insights on the mechanism of steel pipeline failures due to hydrogen transport. The researchers used pipeline samples supplied by manufacturers (Air Products, Air Liquide, OSM steels) to provide a basis for further work. The project ends in FY2009.
PD-18	Materials Solutions for Hydrogen Delivery in Steel Pipeline; Secat/ORNL; Doug Stalheim	3.1	X			This project explores the potential to use commercially available steel materials. Understanding the embrittlement mechanisms will be critical to extrapolate the focused studies. Expanding the number of samples that are tested will help to define whether the test results of the subject materials will be similar for materials fabricated by other manufacturers and whether microstructure improvement needs can be accommodated. The project ends in FY2009.



Project Number	Project Title; Presenting Organization; PI Name	Final Score	Continue	Discontinue	Other	Summary Comment
PD-19	Composite Technology for Hydrogen Pipelines; ORNL; Barton Smith	3.2	X			This project appears to have significant potential to reduce the cost of hydrogen pipelines to meet the DOE targets. Composites experience in the natural gas industry provides a good basis for this work. Surface treatments and associated testing will yield valuable data on the ability to improve the permeability of polymer pipelines. A strong collaboration with pipe, liner, and coupling manufacturers will be pursued moving forward into next year.
PD-20	Hydrogen Permeability and Pipeline Integrity/Fiber Reinforced Composite Pipeline; SRNL; Thad Adams	3.3	X			The hydrogen permeation and integrity part of this project is finished. Test samples from actual weldment were prepared and tested for hydrogen solubility, diffusivity, & permeability at sub-atmospheric pressure and moderate temperatures. This data is valuable in evaluating pipeline costs. The pressure testing of fiber-reinforced polymer and joint types to determine hydrogen leakage rates is a good approach.
PD-21	Innovative Hydrogen Liquefaction Cycle; Gas Equipment Engineering Corporation; Martin Shimko	3.2	X			The project's approach is good and advances hydrogen liquefaction technology toward the goal of reducing energy requirements. Liquid hydrogen significantly reduces delivery costs downstream of production. GECCO will develop catalytic heat exchangers and validate dual hydrogen expander designs.
PD-22	High Pressure, Low Temperature Hydrogen Tube Trailers; LLNL; Salvador Aceves	3.0	X			This method could provide significantly cheaper and stronger overwrap materials by assuming the material is kept at low temperature and environmentally protected from water and air. There are many variables surrounding the glass fibers (humidity, temperature, time at temperature) that must be addressed. The proposed concept has the potential to lower the vessel cost by 25% and to reach the delivery target of \$1/kg. Testing must clearly show the projected advantages next year.
PD-23	Reversible Liquid Carriers for an Integrated Production, Storage and Delivery of Hydrogen; APCI; Bernard Toseland	2.8	X			This project addresses hydrogen carriers for both onboard and off board hydrogen regeneration, but its potential to meet hydrogen production, delivery, and storage targets is not well defined. The evaluation of dehydrogenation reactors appears competent and thorough. Testing will continue next year.
PD-24	Coatings for Centrifugal Compression; ANL; George Fenske	3.3	X			This project is very important for successful pipeline delivery of hydrogen. The approach has logically identified, evaluated, and characterized critical tribological performance of materials. However, hydrogen impurities could have a significant impact on materials selected. Coordination with commercial partners and additional compressor manufacturers in particular will occur next year.

**PROLOGUE**

<b>Project Number</b>	<b>Project Title; Presenting Organization; PI Name</b>	<b>Final Score</b>	<b>Continue</b>	<b>Discontinue</b>	<b>Other</b>	<b>Summary Comment</b>
PD-25	Sulfur-Iodine Thermochemical Cycle; SNL/GA/CEA; Paul Pickard	3.0	X			The production of hydrogen through the sulfur-iodide thermochemical cycle has shown significant progress with the construction of the integrated testing unit. Three separate excellent research groups (GA, Sandia National Laboratories, and CEA) are each responsible for one of the three steps and also collaborate with each other well. This approach will continue as the integrated test unit commences operation.
PD-26	Hybrid Sulfur Thermochemical Process Development; SRNL; Bill Summers	3.0	X			The project has identified the key challenges and is focused on research to overcome the challenges. Critical technical issues included sulfur crossover through the membrane, a membrane with improved ion conductivity, a better and longer lasting catalyst, and good flow field/diffusion media for sulfur dioxide transport. Significantly improved membranes that reduce sulfur crossover and enable higher temperature operations have been identified and tested, and catalyst work will continue.
PD-27	Laboratory-Scale High Temperature Electrolysis System; INL/ANL/Ceramatec; Ed Harvego	2.6	X			The project's approach depends on availability of high temperature nuclear heat, and it is a very long range goal. The project is going in the right direction regarding durability, but plans for scale-up should be slowed until durability problems are solved. Future work should focus on increasing the SOEC stack durability.
PD-28	Alternative Thermochemical Cycles; ANL; Michelle Lewis	3.2	X			Thermochemical water splitting for hydrogen production supports the Hydrogen Fuel Initiative. Overall, very good work has been done toward the development of this "Copper-Chloride" cycle, but it's not clear what the yields and selectivities were for the engineering lab scale hydrolysis reactor. This project is in the early stages and significant development for each unit operation and in understanding the detailed cycle chemistry is needed.
PD-29	Indirectly Heated Biomass Gasification; NREL; Richard Bain	3.7	X			The objective of this project is to experimentally update the technical and economic performance of an integrated biomass gasification-based hydrogen production process based on steam gasification. This project has a strong integration of technical evaluation, process modeling, and economic modeling. Future work will focus on catalyst development and evaluation.
PD-30	One Step Biomass Gas Reforming-Shift Separation Membrane Reactor; GTI; Michael Roberts	2.9	X			The long-term objective of this project is to determine the technical and economic feasibility of using the gasification membrane reactor to produce hydrogen from biomass. Membrane material development will be a key, but locating the membrane in or after the cyclone could compromise performance. The investigators will examine optimum membrane location.

Project Number	Project Title; Presenting Organization; PI Name	Final Score	Continue	Discontinue	Other	Summary Comment
PD-31	A Novel Slurry Based Biomass Reforming Process; UTRC; Thomas Vanderspurt	2.5	X			The objectives of this project are to illustrate, through an initial feasibility analysis on a 2000 ton/day (dry) biomass plant design, that there is an economical path towards the Department of Energy's (DOE's) 2012 cost and efficiency targets. The project did not demonstrate significant progress. The focus over the next year should be on catalyst development.
PD-32	Hydrogen From Water in a Novel Recombinant Oxygen-Tolerant Cyanobacteria System; J Craig Venter Institute; Qing Xu	3.3	X			The project goals are well-aligned with DOE program targets. The metagenomic approach for identification of novel hydrogenase-related sequences is logical, and builds upon progress in the investigators' labs. The progress towards goals was excellent, with successful reconstruction and identification of a novel environmental nickel-iron hydrogenase and stable expression in a heterologous host. The multi-pronged approach ensures casting a wide net for knowledge of optimizing hydrogenase activity. Work on this project toward an oxygen insensitive hydrogenase/organism will continue.
PD-33	Maximizing Light Utilization Efficiency and Hydrogen Production in Microalgal Cultures; UC Berkeley; Tasios Melis	3.7	X			The focus on construction of a minimal photosynthetic antenna complex is good, and the usage of molecular biology toolkits for introducing altered hydrogenase-related gene cassettes into heterologous or homologous host strains is appropriate. The progress towards goals was excellent - a dramatic improvement over the last four years - with efficiency targets achieved ahead of schedule (already completed 2010 milestones). Work on this project toward an ideally efficient microorganism will continue.
PD-34	Use of Biological Materials and Biologically Inspired Materials for Hydrogen Catalysts; Montana State University; Trevor Douglas	3.1	X			The focus on improving hydrogenase stability and on enzymes and catalyst supports is good. The approach demonstrates a good synergism between enzymology and protein structure-function with materials composite synthesis and design. The project will continue and will be encouraged to more clearly define its benchmarks for hydrogen production, with respect to improvements in enzyme stability, enzyme activity, and metrics for sol-gel encapsulants or supported/caged matrices.
PD-35	Photoelectrochemical Hydrogen Production: DOE PEC Working Group Overview & UNLV-SHGR Program Subtask; MV Systems; Eric Miller	3.5	X			The photoelectrochemical working group is an important effort aimed at coordinating research from a dozen institutions. This project shows good integration of theory, synthesis, surface science, and electrochemistry with exceptionally strong collaborations that have leveraged unique abilities. This project will be encouraged to focus on discovering and characterizing new classes of photoelectrochemical materials rather than just extending the findings from other groups.

**PROLOGUE**

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PD-36	Photoelectrochemical Water Splitting; NREL; John Turner	3.9	X			The reviewers consider this group to be a consistent bright spot in the photoelectrochemical hydrogen field since 1991 and the research program is critical for progress towards DOE goals and objectives. The project provides a good basis to understand the limitations of various material classes along with a good mix of theory and wet chemistry techniques that start with a known material, use theory to suggest improvements, and then make theoretically suggested materials prior to testing the new material. This project will continue so that work in this important area, and by this working group, can progress.
PD-37	Critical Research for Cost-effective Photoelectrochemical Production of Hydrogen; Midwest Optoelectronics; Liwei Xu	3.5	X			This project provides a good balance with respect to other material discovery oriented projects in this technology area. The project addresses a number of important applied issues associated with development of photoelectrochemical-hydrogen technology and leverages Midwest's expertise in the manufacture of multi-junction thin film photovoltaic devices. The project will continue and will be encouraged to show the advantages of this concept (a solar cell immersed in an electrolyte) over an external solar cell/electrolyzer system and provide information on economics of a system.
PD-38	Development and Optimization of Cost Effective Materials for PEC Hydrogen Production; U. of CA Santa Barbara; Eric McFarland	3.6	X			This project is advancing many areas of understanding and technology in photoelectrochemical hydrogen production and has made progress in understanding $\alpha\text{Fe}_2\text{O}_3$ that may also be useful when developing other low gap oxide materials or for using $\alpha\text{Fe}_2\text{O}_3$ in a tandem system. The project will continue and will be encouraged to work toward finding an adequate photoelectrochemical material prior to engineering a complete system.
PD-39	Scale-up of Hydrogen Transport Membranes for IGCC and FutureGen Plants; Eltron Research Inc.; Doug Jack	3.4	X			The project was recognized for its relevance to the FutureGen project and Hydrogen Fuel Initiative. Additionally, the project is making progress in addressing the DOE/FE technical targets for hydrogen separation. The investigators should clearly define technology transfer and partner relationships and should conduct lifecycle testing under real-world syngas conditions.



Project Number	Project Title; Presenting Organization; PI Name	Final Score	Continue	Discontinue	Other	Summary Comment
PD-40	Cost-Effective Method for Producing Self-Supporting Pd Alloy Membrane for Use in the Efficient Production of Coal-derived Hydrogen; Southwest Research Institute; Kent Coulter	3.2			X	The first contract with SwRI was completed March 31, 2008. A second contract investigating ternary Pd alloy membranes was also presented. This project began May 2007 and will be completed May 2010. Overall, the project was scored favorably. Collaborations with project partners were well established; however technology transfer efforts need to be more clearly defined. It is suggested that the project review historical DOE project data so as not to duplicate efforts previously performed.
PD-41	Experimental Demonstration of Advanced Palladium Membrane Separators for Central High-Purity Hydrogen Production; United Technologies; Sean Emerson	3.0	X			This project is developing a sulfur-, halide-, and ammonia-resistant hydrogen separation membrane. The project team has very strong experimental testing and modeling capabilities. It was suggested to test the membranes in contaminant containing gas streams and to review prior work on Pd membranes for additional insight.
PD-42	Integration of a Structural Water Gas Shift Catalyst with a Vanadium Alloy Hydrogen Transport Device; Western Res. Ins. & U of Wyoming Res. Corp.; Thomas Barton	3.3	X			The project is well focused on reducing capital and membrane costs by incorporating two unit operations into one for water gas shift. The project was noted for its testing facilities which included an on-site gasifier for experimentation under syngas conditions. It is recommended that additional lab-scale experimentation be completed prior to scale-up and that investigation of vanadium membrane fabrication be conducted.
PD-43	High Flux Metallic Membranes for Hydrogen Recovery & Membrane Reactors; REB Research & Consulting; Robert Buxbaum	3.6	X			This project scored favorably and was noted for its strong collaborative efforts and research partners. The project was also noted for its capability in potential commercialization. It is suggested that greater importance be placed on impurity tolerance of the membranes and that additional discussion is needed on cost targets.
PDP-01	Fundamentals of a Solar-thermal Mn <sub>2</sub> O <sub>3</sub> /MnO Thermochemical Cycle to Split Water; CU; Al Weimer	2.8	X			The objective of this project is to research and develop a cost effective Mn <sub>2</sub> O <sub>3</sub> /MnO solar-thermal thermochemical cycle through theoretical and experimental investigation. The investigators were commended for their strong technical background and collaboration efforts. This project has achieved significant results with little funding. Future work should focus on material and energy balances and cost analysis.

**PROLOGUE**

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PDP-02	Novel Low-Temperature Proton Transport Membranes; ORNL; Andrew Payzant	3.0	X			If successful, this research could provide an improved method for hydrogen purification using non-PM membranes. The reviewers thought the project had a good approach, was well run, worth doing, and had a competent PI. However, they indicated that the results were modest with very low hydrogen fluxes to-date, and that targets, milestones and performance metrics for the project were lacking. Project will continue R&D to improve hydrogen flux and stability of membranes. Performance milestones and metrics will be identified.
PDP-03	Ultra-thin Proton Conduction Membranes for H <sub>2</sub> Stream Purification with Protective Getter Coatings; SNL; Margaret Welk	2.9	X			Project is developing a membrane that could lead to cost, operability and footprint advantages over PSA. Success has been reported for building a support with fine pore structure to enable synthesis of an ultra thin proton conducting membrane. Reviewers recommended that the membranes be tested under real in-service operating conditions; and that clear Go-No-Go decision points be added to the project. Future work will focus on optimization of membrane structures. Success metrics and decision points will be identified. Life-time testing and testing under in-service conditions will take place in FY2010.
PDP-04	Renewable Electrolysis Integrated System Development and Testing; NREL; Kevin Harrison	3.1	X			The project is very relevant to the DOE Hydrogen program and uses a sound experimental approach along with good collaborations and technical transfer. The power electronic development has been solid. The wind to hydrogen system was completed in early FY07, but there was little data generation due to mechanical failures. Future work should include significant data generation from the system, validation of the system models with the data, and a cost analysis to determine the savings potential of the advanced power supply.
PDP-07	Photobiological Hydrogen Research; Florida International University; George Philippidis	2.6			X	Congressionally directed project. Although still somewhat in its infancy, this work has great potential for numerous applications - the "top-down" approach of reconstructing a functional hydrogen-producing gene cassette in a heterologous host is not particularly innovative but seems feasible. It is not clear why they have not yet achieved the goal of obtaining an active enzyme. The progress towards goals was good, with some specific milestones achieved in a timely fashion. The project will continue and will be encouraged to update their techniques for testing successful transformation.

Project Number	Project Title; Presenting Organization; PI Name	Final Score	Continue	Discontinue	Other	Summary Comment
PDP-11	Enabling Hydrogen Embrittlement Modeling of Structural Steels; SNL; Brian Somerday	3.5	X			Progress has been made in the basic understanding of embrittlement, but more is needed before methods of overcoming the barriers can be suggested. They have made significant progress in measuring the properties of pipeline steels in high-pressure hydrogen gas using fracture mechanics methods. Barriers to further progress will be appropriately addressed next year.
PDP-14	Advanced Alkaline Electrolysis; GE Global Res.; Dana Swalla	3.1			X	This project will be completed December 2008. The use of high volume low cost plastic manufacturing was an innovative approach to fabricating low cost electrolyzers. There was considerable focus on durability of the plastics used. However, the project did not demonstrate that cells/stacks can be made using this method. The cost analysis was not detailed enough and used some inappropriate assumptions.
PDP-15	Photoelectrochemical Generation of Hydrogen Using Heterostructural Titania Nanotube Arrays; U of Nev. Reno; Mano Misra	3.1			X	Congressionally directed project. This project includes a good mix of science, system design, and engineering. However, even optimization of TiO <sub>2</sub> as a hydrogen producing photoelectrode, will not result in a useful system since its band gap is too large to use much of the solar spectrum. They have developed a good level of expertise in the area of synthesizing TiO <sub>2</sub> nanotube arrays and related structures but are committed to the idea that they can empirically find a way to lower the band gap of TiO <sub>2</sub> through doping, alloying or sensitization, despite the numerous unsuccessful attempts to do this over the past 30 years. The researchers will continue to be encouraged to look beyond TiO <sub>2</sub> for a useable photoelectrochemical material.
PDP-16	Distributed Bio-Oil Reforming; NREL; Bob Evans	3.2	X			This project is developing methods of hydrogen production from bio-oil, taking into account the complexity of the fuel, its difficulty in handling, and other factors. Reviewers approved the project focus on effects of different feedstocks on bio-oil quality and composition, and suggested that certain bio-crops may be better aligned with this technology than others. Project will continue the development of a compact, low capital cost, low/no maintenance reforming system, as well as catalyst optimization and long-term testing.
PDP-18	Solar Thermochemical Hydrogen (STCH) Production -H <sub>2</sub> A Analysis; TIAX; Kurt Roth	3.3	X			The objective of this project is to evaluate which solar-thermochemical hydrogen (STCH) cycles have the potential to meet the DOE central production cost target of \$3.00/kg. The level of collaboration and the ability to provide a consistent method of cost analysis were noted as significant achievements. This project will continue to compile cost data input for the STCH projects.

**PROLOGUE**

<b>Project Number</b>	<b>Project Title; Presenting Organization; PI Name</b>	<b>Final Score</b>	<b>Continue</b>	<b>Discontinue</b>	<b>Other</b>	<b>Summary Comment</b>
PDP-19	Ocean Thermal Plantships for Production of Ammonia as the Hydrogen Carrier; ANL; Chandrakant Panchal	3.2			X	This project has been completed. A solid approach was taken for the evaluation of this technology. Proposed future work would need to be quantified prior to beginning a new project.
PDP-21	Photoelectrochemical Hydrogen Production; U. Arkansas Little Rock; Malay Mazumber	2.2			X	Congressionally directed project. The objective is to modify the surface of TiO <sub>2</sub> to absorb more of the visible portion of the solar spectrum and split water; however, this objective has been extensively researched over the past 30 years and has achieved very little. TiO <sub>2</sub> will not work as a useful water photoelectrolysis system since its band gap is too large to be efficient. Fundamental science to help understand charge transfer or surface chemistry of oxide semi-conductors will be useful but this project is mainly empirical. The researchers will continue to be encouraged to look beyond TiO <sub>2</sub> for a useable photoelectrochemical material.
PDP-22	Distributed Reforming of Renewable Liquids via Water Splitting using Oxygen Transport Membrane (OTM); ANL; Balu Balachandran	2.9	X			The project aims to develop an oxygen transport membrane (OTM) for distributed reforming of bio-derived liquids to produce hydrogen. Reviewers found the project approach sound and the concept to be a potentially cost effective, renewable hydrogen process relevant to the overall objectives. Recommendations to project team included addressing flux and heat management issues and 3rd party analysis of costs. Project will continue to optimize OTM for hydrogen production and chemical stability, and will refine the H <sub>2</sub> A techno-economic analysis of process.
PDP-25	Carbon Molecular Sieve Membrane as Reactor/Separator for Water Gas Shift Reaction; Media and Process Technology Inc.; Paul Liu	3.0	X			The project focus is on increased production efficiency and cost reductions through a WGS/membrane reactor which combines low and high temperature shift reactions and hydrogen purification and separation, which eliminates the need for an extra water gas shift step. The testing of the system has yet to be completed. The modeled 90 percent hydrogen recovery and 99 percent purity needs to be demonstrated experimentally. Next steps will include completion of a pilot testing unit, in-house pilot demonstration of the system, and completion of H <sub>2</sub> A analysis of the process.



Project Number	Project Title; Presenting Organization; PI Name	Final Score	Continue	Discontinue	Other	Summary Comment
PDP-26	Biological Systems for Hydrogen Photoproduction; NREL; Maria Ghirardi	3.8	X			The project goals include optimizing photosynthetic water-splitting biological hydrogen production and increasing catalyst stability while improving oxygen tolerance. Excellent, cutting edge, molecular and physiological approach. The partnership between various universities, an international institution, and a national lab is good. This project will continue to work toward efficient, cost-effective biological hydrogen production.
PDP-27	Fermentative and Electrohydrogenic Approaches to Hydrogen Production; NREL; Pin-Ching Maness	3.5	X			The progress towards goals was excellent, with pathway engineering targets achieved ahead of schedule. This project takes a very good approach, particularly the inhibitors. The project will continue and the researchers will be encouraged to complement their current approach with the addition of genomics and genetic-based techniques, possibly through collaborations.
PDP-34	Theory of Oxides for Photoelectro-chemical Hydrogen Production; NREL; John Turner	3.6	X			This project is an important demonstration of how an effective mix of theory and experiment can be used to design new multi-element semiconductors that move toward DOE program goals. As work is completed to more accurately correlate the theories to experiments, theoretical methods as part of material research will move the research forward at an increased pace. The work clearly demonstrates that the search for improved optical response semiconductors that are thermodynamically able to split water can be dramatically enhanced by using a DFT based materials search. This project will continue.

### Hydrogen Storage:

ST-01	Analyses of Hydrogen Storage Materials and On-Board Systems; TIAX; Stephen Lasher	3.1	X			The project is important in that it provides an early indication of storage system cost. The limits of the analyses need to be well communicated. It is critical to disseminate key findings among the hydrogen storage R&D community.
ST-02	System Level Analysis of Hydrogen Storage Options; Argonne; Rajesh Ahluwalia	3.3	X			The project provides systems analyses of key storage system performance (e.g. capacity and transient performance). The limits of the analyses need to be well communicated. It is critical to disseminate key findings among the hydrogen storage R&D community.

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ST-03	Best Practices for Characterizing Hydrogen Storage Properties of Materials; H2 Technology Consulting LLC; Karl Gross	3.4	X			It is recommended that the Best Practices document also cover measurement issues of adsorbent materials. It is critical to disseminate the final revised document among the hydrogen storage R&D community. This project is expected to be completed in FY2009.
ST-04	DOE Chemical Hydrogen Storage Center of Excellence (CoE) Overview; LANL; Kevin Ott	3.6	X			This is a well working CoE, with good interaction/coordination among the partners. The team should refine theory work with experimental feedback; continue effort on release kinetics and efficient spent fuel regeneration, and initiate cost analyses to assess the spent fuel regeneration schemes in FY2009.
ST-05	Chemical Hydrogen Storage R&D at Pacific Northwest National Laboratory; PNNL; Chris Aardahl	3.8	X			This project is part of the Chemical Hydrogen Storage Center of Excellence and includes a strong team with interaction among theory, applied science and engineering. The project should continue to address hydrogen discharge issues including complexity of the solid fuel. The project should continue effort on spent fuel regeneration including lithium ammonia borane. <b>Include cost analysis to assess regeneration schemes.</b>
ST-06	Chemical Hydrogen Storage R&D at Los Alamos National Laboratory; LANL; Anthony Burrell	3.7	X			This project is part of the Chemical Hydrogen Storage Center of Excellence and is a good mix of theory, synthesis/characterization, and mechanistic and kinetic studies. The project should continue to improve hydrogen discharge parameters including hydrogen purity & liquid fuel range. LANL should incorporate cost analyses to assess regeneration schemes and investigate methods to avoid spent fuel solidification.
ST-07	Amineborane-Based Chemical Hydrogen Storage; U of Penn.; Larry Sneddon	3.4	X			This project is part of the Chemical Hydrogen Storage Center of Excellence. UPenn should emphasize efficient spent fuel regeneration and consider the effect of additives in the spent fuel. UPenn should also note spent fuel morphology and avoid formation of solid phases.
ST-08	Chemical Hydrogen CoE - Novel Approaches to Hydrogen Storage: Conversion of Borates to Boron Hydrides; Rohm and Haas; Suzanne Linehan	2.9	X			This project is part of the Chemical Hydrogen Storage Center of Excellence. Rohm & Haas should evaluate and validate reaction conditions and products in both synthesis schemes. Greenhouse gas footprint should be minimized for the carbothermal route.

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ST-09	Main Group Element and Organic Chemistry for Hydrogen Storage and Activation; UA; David Dixon	3.5	X			This project is part of the Chemical Hydrogen Storage Center of Excellence. UA should validate theory work with input from experimentalists to establish simulation models that best represent the experimental results. Emphasize obtaining results from carbene and amino(imidazolo)-boranes and discontinue if results are not promising.
ST-10	Solutions for Chemical Hydrogen Storage: Hydrogenation/ Dehydrogenation of B-N Bonds; U of Washington; Karen Goldberg	3.0	X			This project is part of the Chemical Hydrogen Storage Center of Excellence. UWA should investigate dehydrogenation and rehydrogenation temperatures for materials with BN and CC bonds to arrive at the most favorable CBN materials they are starting to investigate.
ST-11	Chemical Hydrogen Storage using Ultra-High Surface Area Main Group Materials & The Development of Efficient Amine-Borane Regeneration Cycles; UC Davis; Philip Powers	2.9	X			This project is part of the Chemical Hydrogen Storage Center of Excellence. UC Davis should address the Argonne ammonia borane spent fuel regeneration analyses findings and coordinate with LANL on the path forward. The approach should address the reduction step with metal hydride in the ammonia borane spent fuel regeneration scheme. Collaboration with UA should be increased to guide spent fuel regeneration efforts.
ST-12	Hydrogen Storage in Metal-Organic Frameworks; UCLA; Omar Yaghi	3.3	X			Professor Yaghi is an innovator in this approach to designing sorbent materials. UCLA should continue to emphasize increasing volumetric capacity and hydrogen binding energy to increase net capacity at near ambient temperatures and nominal pressure.
ST-13	Carbide-Derived Carbons with Tunable Porosity Optimized for Hydrogen Storage; U of Penn./Drexel Univ.; Jack Fischer and Yury Gogotsi	2.7			X	The project is nearly complete. The carbide-derived carbon (CDC) materials and activation procedures produce some of the best understood "amorphous carbons" under study. The R&D is focused on tuning pore size to increase binding energy.
ST-14	Effects and Mechanisms of Mechanical Activation on Hydrogen Sorption/Desorption of Nanoscale Lithium Nitrides; U of Connecticut; Leon Shaw	2.1			X	This project will have a Go/No Go decision at the end of the first quarter of FY2009 based on progress at meeting set milestones. The reviewers commented that there is benefit to understanding the inter/intraphasic reaction mechanisms. However further understanding is needed than provided and the approach used should be reevaluated. Closer collaboration with other groups is recommended.

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ST-15	DOE Hydrogen Sorption Center of Excellence (HSCoE): Overview; NREL; Mike Heben	3.1	X			The Hydrogen Sorption Center of Excellence has made progress in improving volumetric capacity and hydrogen binding energy. The HSCoE needs to stress increasing the net available volumetric capacity at near ambient temperature while improving hydrogen uptake & discharge kinetics.
ST-16	A Biomimetic Approach to New Adsorptive Carbonaceous Hydrogen Storage Materials; Texas A&M; Joe Zhou	3.3	X			This is a new project in the Hydrogen Sorption Center of Excellence emphasizing Metal Organic Frameworks (MOFs). The approach should stress improving volumetric capacity along with net capacity at close to room temperature. Increased collaborations with relevant theory groups is recommended.
ST-17	Hydrogen Storage by Spillover; U of Michigan; Ralph Yang	3.3	X			This project is part of the Hydrogen Sorption Center of Excellence. Efforts should be expanded to improve hydrogen uptake/discharge kinetics along with net available volumetric capacity. The reproducibility of the MOF synthesis needs to be improved. Increased collaborations with relevant theory projects that are associated with understanding spillover are recommended.
ST-18	Theoretical Models of H <sub>2</sub> -SWNT Systems for Hydrogen Storage and Optimization of SWNT; Rice U.; Boris Yakobson	3.2	X			This project is part of the Hydrogen Sorption Center of Excellence. For the theory portion of the project, NREL should place more emphasize on spillover work and increased collaborations with experimentalists. For the project's experimental work, there should be decreased overlap with other efforts within the HSCoE and restructure to be more relevant to the program.
ST-19	NREL Research as Part of the Hydrogen Sorption Center of Excellence; NREL; Anne Dillon	2.8	X			This project is part of the Hydrogen Sorption Center of Excellence. For NREL's experimental work, there should be reduced emphasis on "exotic" synthetic materials and increased effort on more synthetically viable materials. Also, improved communications between the experimental and theory groups to improve and validate theoretical predictions is recommended. NREL should increase spillover efforts to improve synthesis reproducibility, net capacity and hydrogen kinetics.
ST-20	Single-Walled Carbon Nanohorns for Hydrogen Storage and Catalyst Supports; ORNL; David Geohegan	3.1	X			This project is part of the Hydrogen Sorption Center of Excellence. ORNL should increase coordination of theory and experimental work within their project and with other theory work in the HSCoE. ORNL should reduce emphasis on "exotic" synthetic materials and increase efforts on more synthetically viable materials. Also they should work more closely with the theory groups to validate theoretical predictions.

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ST-21	Hydrogen Storage through Nanostructured Polymeric Materials; Argonne; D.J. Liu	2.8	X			This project is part of the Hydrogen Sorption Center of Excellence. Polymer adsorbents is an area that needs to be explored. ANL should provide predictive rationale for designing hydrogen bonding sites in the polymers. ANL needs to increase emphasis on net volumetric capacity and transient performance. Increase ANL's theory collaboration within the HSCoE.
ST-22	Enabling Discovery of Materials With a Practical Heat of H <sub>2</sub> Adsorption; Air Products; Alan Cooper	2.8	X			This project is part of the Hydrogen Sorption Center of Excellence. APCI should increase coordination of theory and experimental work with theory work in the HSCoE. APCI should closely collaborate with the theory work to validate theoretical predictions. APCI should provide more leadership within the HSCoE to address system application performance needs (e.g. net available volumetric capacity, transient performance, energetics).
ST-23	Enhanced Hydrogen Dipole Physisorption: Henry's Law and isosteric heats in microporous sorbents; CalTech; Channing Ahn	3.2	X			This project is part of the Hydrogen Sorption Center of Excellence. CalTech should continue to focus on elucidating the interrelationships among: pore size & distribution, enthalpies, temperature & pressure effects and how they collectively influence hydrogen uptake and release. CalTech should expand collaborations to include experts in other fields, such as catalysis.
ST-24	Carbon Aerogels for Hydrogen Storage; LLNL; Ted Baumann	3.0	X			This project is part of the Hydrogen Sorption Center of Excellence. LLNL should continue to emphasize net available volumetric capacity and hydrogen uptake and discharge kinetics. LLNL should increase collaborations with theoretical and experimental spillover research groups.
ST-25	Characterization of Hydrogen Adsorption by NMR; U of North Carolina; Yue Wu	3.3	X			This project is part of the Hydrogen Sorption Center of Excellence. UNC should compare NMR results with neutron scattering results where available. UNC should consider isotopic studies to evaluate spillover in pores and lower the measurement temperature range capability to allow evaluation of heterogeneous pore size distributions as well as more weakly bound hydrogen species.
ST-26	Hydrogen Storage Materials with Binding Intermediate between Physisorption and Chemisorption; UC-Santa Barbara; Juergen Eckert	2.8	X			This project has resulted in several metal/organic linker combinations to evaluate for higher hydrogen binding energy as well as chemical modifications to increase surface area. Recommendations include reevaluation of approaches to increase H-binding energy and to increase net available volumetric capacity.

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ST-27	A Synergistic Approach to the Development of New Hydrogen Storage Materials, Part I; UC Berkeley/LBNL; Jeffrey Long	2.9	X			This project has several PIs at UCB and LBNL. The porous polymers project develops a rational approach to increasing volumetric capacity and hydrogen binding energy. The MOF work should continue to stress net available volumetric capacity at higher temperatures.
ST-29	Metal Hydride Center of Excellence; SNL; Lennie Klebanoff	3.2	X			The Metal Hydride Center of Excellence was praised for the material down-select performed in FY2007. The reviewers recommended closer coordination between the materials CoEs and the new Engineering CoE. The MHCoE should continue to stress net available volumetric capacity while taking into account the temperature, pressure and kinetics requirements of the application and sorption energetics.
ST-30	Thermodynamically Tuned Nanophase Materials for Reversible Hydrogen Storage; HRL Laboratories; Ping Liu	3.2	X			This project is part of the Metal Hydride Center of Excellence and was found to be highly focused on sorption kinetics and thermodynamics, two key issues with metal hydrides. The work on incorporating destabilized metal hydrides into scaffolds was thought to be innovative and promising. The work should be more closely coordinated with the theory group to include appropriate destabilized systems for investigation.
ST-31	Chemical Vapor Synthesis and Discovery of H <sub>2</sub> Storage Materials: Li-Al-Mg-N-H System; Univ. of Utah; Zak Fang	3.0	X			This project is part of the Metal Hydride Center of Excellence. The mechanistic studies are well aligned with DOE's objectives. However there is concern over ammonia release from amides and reviewers strongly recommended a down-select this year based on the ammonia concentration released during desorption. The chemical vapor synthesis work is promising and further collaborations are encouraged.
ST-32	Reversible Hydrogen Storage Materials – Structure, Chemistry and Electronic Structure; U of Illinois; Ian Robertson	3.0	X			This project is part of the Metal Hydride Center of Excellence. The experimental work, particularly the imaging of catalyst dispersion in hydrogen storage materials, is highly relevant to the program. However the role and relevance of the computational theory work is uncertain. It is recommended that collaborations be expanded and that the theory work be realigned with other efforts in the MHCoE.
ST-33	First-Principles Modeling of Hydrogen Storage in Metal Hydride Systems; Univ. of Pittsburgh/Georgia Tech; Karl Johnson	3.4	X			This project is part of the Metal Hydride Center of Excellence. The computational work of this project is valuable and the predictions have been widely used by the hydrogen storage R&D community. A stronger tie with the experimentalists is recommended. Updating the library of phases for inclusion in the predictions, specifically for carbon-containing phases, is recommended.

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ST-34	Development and Evaluation of Advanced Hydride Systems for Reversible Hydrogen Storage; Jet Propulsion Laboratory; Bob Bowman	3.3	X			This project is part of the Metal Hydride Center of Excellence and is of high importance. The identification of the $[\text{B}_{12}\text{H}_{12}]^{-1}$ species as an intermediate in the $\text{Mg}(\text{BH}_4)_2$ desorption pathway is a significant finding. Specific recommendations include ensuring the mechanistic findings are being employed in the material development efforts and offering the project's NMR analysis capabilities to the other CoEs and independent projects.
ST-35	Complex Hydrides for Hydrogen Storage Studies of the $\text{Al}(\text{BH}_4)_3$ System; ORNL; Gilbert Brown	2.9	X			This project is part of the Metal Hydride Center of Excellence. The materials being investigated in this project are highly relevant and the work on identifying mechanisms is important. However it was not clear that the mechanistic work is being effectively transferred and followed up on by the appropriate experimentalists. Overall the project should be better focused and needs to define a clear future work plan focused on specific materials.
ST-36	Discovery and Development of Metal Hydrides for Reversible On-board Storage; SNL; Ewa Ronnebro	3.4	X			This project is part of the Metal Hydride Center of Excellence and its work is highly relevant. The project has a good mix of experiment and theory. The progress in finding additives to moderate the conditions required to rehydrogenate $\text{Ca}(\text{BH}_4)_2$ is a significant improvement. It is recommended that enthalpy measurements on $\text{Ca}(\text{BH}_4)_2$ polymorphs be completed and compared with predictions as soon as possible. The impact on gravimetric and volumetric properties should be considered early on in the work of incorporating hydrogen storage material into nanoframeworks.
ST-37	Effect of Trace Elements on Long-Term Cycling and Aging Properties of Complex Hydrides for Hydrogen Storage; UNR; Dhanesh Chandra	3.0	X			This project is part of the Metal Hydride Center of Excellence. The investigation of impurity effects on long-term cycling and identification of vapor pressures and volatile products for hydrogen storage materials is very important to the program. However it is recognized that the selection of hydrogen storage materials for investigation is problematic since no material currently possesses all the properties required for on-board hydrogen storage. Recommendations include resolution of unanswered questions, such as $\text{H}_2 + \text{O}_2$ versus $\text{H}_2 + \text{H}_2\text{O}$ results, and testing of more promising materials.

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ST-38	Fundamental studies of advanced high-capacity reversible metal hydrides/ Recharging of Light Metal Hydrides Through Supercritical Fluid Hydrogenation; Univ. of Hawaii; Craig Jensen	3.2	X			This project is part of the Metal Hydride Center of Excellence and is highly relevant and focused on key issues for metal hydride materials. The research team is highly qualified with strong collaborations. It is recommended to reduce the number of material types being investigated and to put more emphasis on development of regeneration of spent alane in supercritical fluids.
ST-39	Aluminum Hydride Regeneration; BNL; Jason Graetz	3.3	X			This project is part of the Metal Hydride Center of Excellence. BNL has made significant progress on developing the adduct formation method as a route for spent alane regeneration. While it is recognized that this work is in an early stage and focused on development of regeneration processes, it is recommended that the new Hydrogen Storage Engineering Center of Excellence be engaged early and that cost estimations for regeneration be conducted.
ST-40	Fundamental Reactivity Testing and Analysis of Hydrogen Storage Materials & Systems; SRNL; Don Anton	3.2	X			The determination of the chemical and environmental reactivity of hydrogen storage materials is important. However without any current material meeting all requirements for on-board hydrogen storage, the selection of material for testing is problematic. Additionally the UN test methods for the classification of goods for shipment may not be the most appropriate tests for use. It is recommended that appropriate quantitative analytical test methods be utilized.
ST-41	Quantifying & Addressing the DOE Material Reactivity Requirements with Analysis & Testing of Hydrogen Storage Materials & Systems; UTRC; Dan Mosher	3.4	X			This project's objective of performing risk analysis of hydrogen storage materials and systems is of high importance. An appropriate and professional approach is being taken in this project. It is recommended that the project coordinate and interact with codes and standards development efforts.
ST-42	Chemical and Environmental Reactivity Properties of Metal Hydrides within the Context of Systems; Sandia-Livermore; Dan Dedrick	3.4	X			The work of this project is highly relevant and important to the Hydrogen Program. The approach and methodology are well-developed. It is recommended that the project coordinate and interact with codes and standards development efforts, especially in the later stages.



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STP-04	Purdue Hydrogen Systems Laboratory; Purdue University; Jay Gore	3.0			X	This is a Congressionally-direct project. For off-board reversible approaches, Purdue should provide transparent arguments that support estimates of regeneration energy requirements (and greenhouse gas emissions). Purdue should increase collaborations with the Chemical Hydrogen Storage CoE as appropriate.
STP-05	Development of Regenerable, High-Capacity Boron Nitrogen Hydrides For Hydrogen Storage; RTI; Ashok Damle	2.5			X	The project has a go/no-go decision point in the third quarter of FY 2009 based on efficient spent fuel regeneration and release parameters. RTI should focus on regeneration of ammonia borane from spent fuel and evaluate their approach of direct re-hydrogenation of spent fuel due to unfavorable thermodynamics.
STP-06	Neutron Characterization in support of the Hydrogen Sorption Center of Excellence; NIST; Dan Neumann	3.5	X			This project is part of both the Hydrogen Sorption and Metal Hydride Centers of Excellence. If appropriate, NIST should use their capabilities to characterize "controversial samples or materials." This would allow erroneous claims of unusually high capacity to be disproved sooner, and accurate claims to be recognized and advanced. NIST should continue to increase collaborations across the DOE hydrogen storage portfolio.
STP-08	Optimizing the Binding Energy of Hydrogen on Nanostructured Carbon Materials through Structure Control and Chemical Doping; Duke U; Jie Liu	2.5	X			This project is part of the Hydrogen Sorption Center of Excellence. The project would be strengthened by addressing carbon microchemistry, surface activity/basicity, and other relevant characterization to the materials under study. Duke should increase collaborations with HSCoE theory groups as appropriate and with HSCoE experimental efforts to reduce overlap and leverage resources.
STP-11	Advanced Boron and Metal Loaded High Porosity Carbons; Penn State; Mike Chung	2.9	X			This project is part of the Hydrogen Sorption Center of Excellence. The Penn State project should increase the effectiveness of its internal collaborations and ties across the HSCoE. Penn State should leverage HSCoE resources to obtain near room temperature net capacity measurements of its most promising materials to determine the effectiveness of the incorporated boron. Penn State should also emphasize net volumetric capacity.
STP-12	Nanoengineering the Forces of Attraction in a Metal-Carbon Array for H <sub>2</sub> Uptake at Ambient Temperatures; Rice University; James Tour and Carter Kittrell	3.0	X			The project is addressing increasing hydrogen binding energy; a key strategy towards enabling near room temperature storage of hydrogen at nominal pressure. The Tour group should increase collaborations particularly for measurement of H <sub>2</sub> storage properties such as hydrogen binding energy and net gravimetric and volumetric capacity.

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STP-16	Catalyzed Nano-Framework Stablized High Density Reversible Hydrogen Storage Systems; UTRC; Dan Mosher	3.1	X			This project is part of the Metal Hydride Center of Excellence. While the project is in its early stages, it is considered to have great potential at improving sorption kinetics. The nanoframework structures are expected, however, to negatively impact gravimetric and volumetric capacities. It is recommended that the team coordinate with the aerogel activities from the Hydrogen Sorption Center of Excellence.
STP-18	Thermodynamically Tuned Nanophase Materials for Reversible Hydrogen Storage: Structure & Kinetics of Nanoparticle and Model System Materials; Stanford U; Bruce Clemens	3.3	X			This project is part of the Metal Hydride Center of Excellence. The work is well planned with a very good approach for determining thermodynamic and kinetic effects. It is recommended that the selection of materials be based on systems under investigation within the MHCoe.
STP-19	Alane Electrochemical Recharging; SRNL; Ragaïy Zidan	3.2	X			This project is part of the Metal Hydride Center of Excellence. Good progress has been made in this highly focused project. The development of an electrochemical process for the regeneration of spent alane is important. Increased collaboration with other partners and detailed cost estimates for the process are recommended.
STP-20	LiMgN Sorption Kinetics and Solid State Hydride System Engineering for the MHCOE; SRNL; Don Anton	3.1	X			This project is part of the Metal Hydride Center of Excellence. Two lines of work were presented for this project. The LiMgN work, while it was preliminary, is well planned and logical. It is recommended that ammonia release be quantified for this material in the early stages of this research. The effort on forecourt heat rejection analysis is essentially complete and it is recommended that if any further analysis is required, it be carried out by either the Hydrogen Storage Engineering Center of Excellence or by other analysis groups.
STP-21	Synthesis of Nanophase Materials for Thermodynamically Tuned Reversible Hydrogen Storage; California Institute of Tech; Channing Ahn	3.1	X			This project is part of the Metal Hydride Center of Excellence. The work in this project is highly relevant to the MHCoe activities and carefully carried out. However work should be focused on one area versus multiple lines of research. The collaborations are strong although closer ties with computational modelers is encouraged.

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STP-24	Center for Hydrogen Storage Research at Delaware State University; Delaware State University; Andrew Goudy	2.4			X	This is a Congressionally-direct project. Reviewers recommended improved alignment of the project with DOE goals. For example, the emphasis should consider the net available capacity of the materials under study, taking into account the energetics and temperature and pressure required for suitable hydrogen uptake/release kinetics.
STP-26	Novel Metal Perhydrides; Michigan Tech Univ.; Jim Hwang	2.5			X	Due to funding delays, the research for this project is in its early stages. The project has a go/no-go decision point in third quarter FY 2009 based on storage capacity. It is recommended that surface hydride structure studies be conducted to validate the density functional theory models employed. Also, validation of the hydrogen uptake/release modeling results via direct measurements is needed.
STP-27	Glass Microspheres for Hydrogen Storage; Alfred; Jim Shelby	2.3			X	In second quarter of FY 2009 this project has an end of phase I go/no-go decision point based on storage capacity. Work should focus on high-pressure filling and cycling of hydrogen and determination of volumetric and gravimetric storage capacity as well as uptake/discharge kinetics.
STP-28	Electron-Charged Graphite-Based Hydrogen Storage Material; Gas Technology Institute; Chinbay Fan	2.8	X			GTI has demonstrated initial success in increasing uptake at room temperature using electron-charged graphite. However the baseline material hydrogen uptake is low. GTI should estimate net volumetric capacity of the materials. DOE will continue to monitor their progress in 2009 and pursue independent verification.
STP-29	Polymer-Based Activated Carbon Nanostructures for H <sub>2</sub> Storage; State University of New York; Israel Cabasso	2.7	X			PI will continue to make high surface area materials with a narrow pore size distribution. Project should focus on estimating net available volumetric capacity and increasing the hydrogen bonding energy to enable near room-temperature storage at nominal pressure.
STP-32	An Integrated Approach for Hydrogen Production and Storage in Complex Hydrides of Transitional Elements; U of Arkansas; Abhijit Bhattacharyya	2.7			X	This is a Congressionally-direct project. This effort includes two different lines of effort, one on polymeric materials and one on glancing angle deposited thin film materials. The reviewers found the practicality of the thin film work questionable due to the materials being investigated and the need to use a quartz crystal microbalance. The polymeric materials were considered to be more promising. Focusing on the polymeric materials, stronger collaborations and avoiding duplication of work carried out by others are recommended.

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STP-33	Hydrogen Fuel Cells and Storage Technology Project; UNLV; Clemens Heske	2.5			X	This is a Congressionally-direct project. The work includes efforts on hydrogen storage materials and fuel cell membranes. The fuel cell membrane work was considered more promising by the reviewers. The reviewers expressed concerns that the materials would not be able to meet DOE targets or are duplicative of other efforts within the Hydrogen Storage Program. More extensive collaborations are recommended.
STP-34	Modular Storage Systems; Limnia (formerly FST); Scott Redmond	1.6			X	This is a Congressionally-direct project completed in FY 2007. Reviewers stated that a more detailed analysis should have been conducted to improve the storage performance. Actual experimental data for the cassette device is needed to provide detailed evaluation of the concept.

**Fuel Cells:**

FC-01	Advanced Cathode Catalysts and Supports for PEM Fuel Cells; 3M Company; Mark Debe	3.7	X			Work will continue on improving mass activity, durability, and water management of nanostructured thin film technology over baseline by increasing catalyst surface area and identifying new catalyst compositions, structures, and processes; reducing losses in overpotential and improving anode cell reversal tolerance; and optimizing GDL interfaces.
FC-02	Non-Platinum Bimetallic Cathode Electrocatalysts; ANL; Debbie Myers	3.1	X			This project exhibits strong experimental and modeling work. Some testing at the MEA level may be appropriate to screen catalysts.
FC-03	Advanced Cathode Catalysts; LANL; Piotr Zelenay	2.8	X			LANL will re-assess metrics for various catalysts and integrate MEA level testing into research plan. The project scored low in the area of future planning- the reviewers advised that it would be appropriate for the project to begin down-selecting the catalyst approach in order to focus resources on achieving performance targets.
FC-04	Development of Alternative and Durable High Performance Cathode Supports for PEM Fuel Cells; PNNL; Yong Wang	2.6	X			PNNL will focus on developing a fundamental understanding of interfacial interactions in Pt/C and Pt/WC catalysts and will continue investigation of other conductive metal oxide-modified XC-72 materials. The PI should focus on <i>in situ</i> rather than <i>ex situ</i> testing.
FC-05	Highly Dispersed Alloy Cathode Catalyst for Durability; UTC Power; Sathya Motupally	3.1	X			UTC will continue with investigation of Pd <sub>3</sub> Co/Pt, Ir/Pt core/shell durability testing and scale-up optimization, new synthesis and characterization of Ir <sub>x</sub> Co <sub>y</sub> alloy cores, and validation of modeling results on core/shell stability and durability.

Project Number	Project Title; Presenting Organization; PI Name	Final Score	Continue	Discontinue	Other	Summary Comment
FC-06	Fuel Cell Systems Analysis; ANL; Rajesh Ahluwalia	3.2	X			Start-stops, transients, variation in operating environment, and other dynamics will be modeled and reported. Alternate humidification devices will be modeled and explored with the system model.
FC-07	Mass Production Cost Estimation for Direct H <sub>2</sub> PEM Fuel Cell Systems for Automotive Applications; DTI; Brian James	3.1	X			The cost estimate will be refined by bottom-up analysis of the balance-of-plant components. DTI will analyze the cost-saving potential of components identified in the sensitivity analysis. The 2008 technology update will include optimization of power density vs. catalyst loading, consideration of alternative catalyst alloys and application methods, and coating for bipolar plates.
FC-08	Direct Hydrogen PEMFC Manufacturing Cost Estimation for Automotive Applications; TIAX; Jayanti Sinha	2.9	X			The project scored poorly in approach because TIAX focuses on an MEA technology that has only been tested in the lab and not in the field. However, the PI uses the Argonne National Laboratory's model as a reference fuel cell system, and complements the DTI cost analysis, which assumes a more conventional fuel cell system architecture. The PI has explored conventional Pt on carbon catalysts in prior work and will include the results of the prior work in their comprehensive report of the 2007 technology that the cost estimates are based on.
FC-09	Microstructural Characterization of PEM Fuel Cell MEAs; ORNL; Karren More	3.7	X			Expansion of facilities will continue, including the capability to rotate a specimen within the column of the TEM. In addition, recommendations include reducing the effort to study carbon corrosion, focusing, instead, on developing capabilities to reveal surface structure and surface composition of catalysts that determine activity and stability under high voltage; performing statistical analysis on the samples imaged; collaborating with researchers with strong modelling capability, and further developing the 3D technique.
FC-10	Applied Science for Electrode Cost, Performance, and Durability; LANL; Christina Johnston	3.0	X			LANL will examine proton conductivity pathways from the catalyst to the membrane; evaluate carbon support properties and correlate to performance; investigate interaction of carbon with ionomer, depending on pre-treatment with solvents; and explore layered and gradient structures for improved catalyst utilization. Reviewers scored the project low in technology transfer and collaboration. Work with commercial partners and better dissemination of results will be considered and encouraged.
FC-11	Low-cost Co-Production of Hydrogen and Electricity; Bloom Energy Corp.; Fred Mitlitsky	2.4			X	Congressionally directed. The hydrogen impurity analysis needs to extend beyond CO and CO <sub>2</sub> , and particularly address S compounds.

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FC-12	Improved, Low-Cost, Durable Fuel Cell Membranes; Arkema; James Goldbach	2.7	X			Arkema will determine whether actual M43 MEA performance correlates with <i>ex situ</i> data. Morphology will be studied by ORNL. Other families of polyelectrolytes will be tested.
FC-13	Membranes and MEA's for Dry, Hot Operating Conditions; 3M; Steven Hamrock	3.4	X			3M will continue to pursue multiple approaches for changing the nature of the acid group to develop lower-equivalent weight, higher-conductivity membranes and to study the degradation pathways for these approaches. Reviewers recommend downselection of the approaches to focus resources; downselection will occur in FY2010.
FC-14	New Polyelectrolyte Materials for High Temperature Fuel Cells; LBNL; John Kerr	2.9	X			In the planned work, the investigators were primarily concerned with MEA testing and mechanical and chemical stability. However, based on reviewer suggestions, the PI will focus on developing materials with a path to meeting the 2015 conductivity targets.
FC-15	Lead Research and Development Activity for DOE's High Temperature, Low Relative Humidity Membrane Program; University of Central Florida; James Fenton	3.0	X			A key recommendation for this project is resolution of issues germane to the conductivity test protocol. An MEA test protocol prepared by UCF will be disseminated to appropriate parties for comment in FY08 and FY09.
FC-16	Advanced Materials for Proton Exchange Membranes; Virginia Tech; James McGrath	3.0	X			Stability and durability issues of these materials will be addressed during the next year. The PI will identify the chemistry and morphology needed to meet the DOE objectives before pursuing scale-up.
FC-17	Protic Salt Polymer Membranes: High-Temperature Water-Free Proton-Conducting Membranes; Arizona State University; Dominic Gervasio	2.4	X			Recommendations include a more systematic approach to understand and enable improvements in conductivity and fuel cell performance. Membranes using ammonia as a proton shuttle are unlikely to be stable or surpass current systems.
FC-18	Fluoroalkyl-phosphonic-acid-based Proton Conductors; Clemson University; Stephen Creager	3.2	X			ASU plans to study non-water mechanisms of proton transport by performing conductivity studies on materials with lower water content, which is reasonable for this project. Also, work directed at refining monomer and ionomer synthesis will continue.

Project Number	Project Title; Presenting Organization; PI Name	Final Score	Continue	Discontinue	Other	Summary Comment
FC-19	Rigid Rod Polyelectrolytes: Effect on Physical Properties Frozen-in Free Volume: High Conductivity at low RH; Case Western Reserve University; Morton Litt	3.2	X			The PI will explore several new approaches for making a high molecular weight, water-insoluble polymer. When a water-insoluble polymer is obtained, attention will be directed at developing reasonable mechanical properties.
FC-20	Nanocapillary Network Proton Conducting Membranes for High Temperature Hydrogen/Air Fuel Cells; Case Western Reserve University; Peter Pintauro	3.2	X			The PI will seek collaborations with other groups that can provide information and/or assistance. The planned future work will increase membrane conductivity at higher temperatures and lower RH.
FC-21	Novel Approaches to Immobilized Heteropoly Acid (HPA) Systems for High Temperature, Low Relative Humidity Polymer-Type Membranes; Colorado School of Mines; Andrew Herring	3.1	X			The investigators plan to complete investigation of the Si-linked design space for polyPOMs and develop more mechanically stable polyPOMs. Reviewers were generally supportive of these plans.
FC-22	New Proton Conductive Composite Materials with Co-continuous Phases Using Functionalized and Crosslinkable VDF/CTFE Fluoropolymers; Penn State; Serguei Lvov	2.3	X			During the next year, Penn State will further modify the terpolymer using inorganic proton conductors. In addition, the effects of new inorganic additives upon conductivity, structure, and particle size will be determined.
FC-23	High Temperature Membrane with Humidification-Independent Cluster Structure; FuelCell Energy, Inc.; Ludwig Lipp	3.0	X			Future activities will include development of a better MEA interface for these novel composite membranes.

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FC-24	Dimensionally Stable Membranes; Giner Electrochemical Systems, LLC; Cortney Mittelsteadt	3.2	X			The suggested future work on both a reinforcement layer and the polyelectrolyte is good. However, more work will also be done with commercially available ionomeric materials.
FC-25	Poly(cyclohexadiene)-Based Polymer Electrolyte Membranes for Fuel Cell Applications; University of Tennessee; Jimmy Mays	2.5	X			It is unclear how the PI will improve conductivity at high temperatures and low relative humidities by adding inorganics, or even what inorganics will be added. The focus on degradation studies is important. The <i>ex situ</i> (i.e., Fenton's test) and the <i>in situ</i> tests proposed are important at this stage and should be done as soon as possible.
FC-26	PEM Fuel Cell Durability; LANL; Rod Borup	2.8	X			LANL will consider collaborating with a system integrator or stack developer to improve technology transfer. In addition, LANL will focus on an improved understanding of GDL hydrophobicity through the GDL aging characterization and GDL accelerated stress test development tasks.
FC-27	Nitrided Metallic Bipolar Plates; ORNL; Peter Tortorelli	3.4	X			ORNL will continue to refine and optimize the nitriding surface treatment process once feasibility is proven.
FC-28	Next Generation Bipolar Plates for Automotive PEM Fuel Cells; GrafTech International Ltd.; Orest Adrianowycz	3.4	X			Graftech will focus on manufacturability and cost. Future plans include continuous incorporation of new plates into stack systems to evaluate performance.
FC-29	Effects of Impurities on Fuel Cell Performance and Durability; Clemson University; James Goodwin	2.6	X			The project could use some higher impact impurities than ethylene and ethane to study. Future focus on halogenated compounds that might be in H <sub>2</sub> produced from chlor-alkali processes, cleaning solvents, etc., may be of more immediate support of DOE goals.
FC-30	Effects of Fuel and Air Impurities on PEM Fuel Cell Performance; LANL; Fernando Garzon	3.2	X			Cyclic voltammetry measurements will be made <i>in situ</i> with potentiostats to characterize the catalyst surface. High frequency resistance measured by A.C. impedance spectroscopy will be a sensitive probe.
FC-31	The Effects of Impurities on Fuel Cell Performance and Durability; University of Connecticut; Trent Molter	3.1	X			The focus on key organic species is excellent, but selected organics should be chosen carefully. The choice of the standard MEA on which to carry out the impurity effect studies should be revised.



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FC-32	Subfreezing Start/Stop Protocol for an Advanced Metallic Open-Flowfield Fuel Cell Stack; Nuvera Fuel Cells, Inc.; James Cross	3.1	X			Nuvera has made it a priority to install and commission an environmental chamber, which will address reviewers' concerns regarding use of ambient gases in Nuvera's test protocol. In addition, Nuvera will develop a 2D model to afford startup procedure optimization and further investigate MEAs and GDLs.
FC-33	Visualization of Fuel Cell Water Transport and Performance Characterization Under Freezing Conditions; Rochester Institute of Technology; Satish Kandlikar	3.4	X			Future work will include evaluation of the improved GDL and channel properties with combinatorial <i>in situ</i> multi-channel and freeze-thaw experiments.
FC-34	Water Transport in PEM Fuel Cells: Advanced Modeling, Material Selection, Testing, and Design Optimization; CFD Research Corp.; Vernon Cole	2.9	X			Future work will include <i>ex situ</i> characterization studies (GDL microstructure, transport properties, freezing point) and GDL-channel transport experiments.
FC-35	Water Transport Exploratory Studies; LANL; Rod Borup	3.2	X			Project will proceed as planned, including neutron imaging of NSTF catalyst systems at start-up, transient operation, segmented cell operation, freeze measurement, characterization, and model development. LANL is encouraged to report GDL material properties and consider investigating PTFE migration due to water transport, changes to the water contact angle due to carbon oxidation, and pore structure changes due to freezing.
FC-36	Neutron Imaging Study of the Water Transport in Operating Fuel Cells; NIST; David Jacobson	3.8	X			DOE considers this project to be high priority, as neutron radiography is the only way that researchers can image water inside an operating fuel cell.

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FC-37	Development of Thermal and Water Management System for PEM Fuel Cells; Honeywell; Zia Mirza	2.3	X			Because humidification devices will not meet automotive requirements, the water management effort will be brought to a conclusion. Final humidifier testing will add value by providing data to validate DOE's humidifier models that may be helpful for guiding future humidifier development. Honeywell's data in thermal management has led Argonne National Laboratory to conclude that commercial metal foams are not good candidates for automotive radiators because the radiators would be bulky and require much higher pumping power. In the coming year, Honeywell will validate Argonne's modeling results that show advanced automotive (louver fins, 25 fins/inch) and microchannel radiators are more compact than standard automotive radiators in fuel cell applications.
FC-38	Low-Cost Manufacturable Microchannel Systems for Passive PEM Water Management; PNNL; Ward TeGrotenhuis	2.7	X			Final testing in this project will provide data for modeling and optimizing the humidifier device in a fuel cell system. However, even if the device shows potential, there are still recognized integration issues to be addressed.
FC-39	Development and Demonstration of a New Generation High-Efficiency 1-10 kW Stationary PEM Fuel Cell Power System; Intelligent Energy; Durai Swamy	2.8	X			A go decision was made on August 6, 2008 to complete the engineering design on the Hestia PSA (and not continue the MesoPure). AER development will continue in parallel. Subsequently, validation of the technologies vs. efficiency and other targets will be conducted.
FC-40	International Stationary Fuel Cell Demonstration; Plug Power; John Vogel	3.6			X	The project will conclude with demonstration of the units and performance and decommissioning data reported back to DOE.
FC-41	Intergovernmental Stationary Fuel Cell System Demonstration; Plug Power; Rhonda Staudt	2.9	X			The project's relevance, approach, accomplishments, collaborations, and future work are solid. In the coming year, a prototype will be built, sited, installed, and commissioned. Field operation and support will commence.
FC-42	Stationary PEM Fuel Cell Power Plant Verification; UTC Power; Eric Strayer	3.1	X			UTC will continue to focus on low cost technology. Durability of greater than 20,000 hours will be validated through scale-up and demonstration.

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FC-43	Diesel Fueled SOFC System for Class 7/Class 8 On-Highway Truck Auxiliary Power; Cummins; Dan Norrick	3.1	X			Although some reviewers suggested that there is no path apparent to reach DOE efficiency targets, other reviewers commented that much remains to be done in this project, and the proposed future work should address all issues.
FC-44	Solid Oxide Fuel Cell System Development for Auxiliary Power in Heavy Duty Vehicle Applications; Delphi; Gary Blake	3.0	X			Planned future work is completion the SOFC APU hardware design and build, followed by test fixture design and system testing.
FC-45	DMFC Prototype Demonstration for Consumer Electronic Applications; MTI MicroFuel Cells, Inc.; Chuck Carlstrom	2.6	X			MTI's technology is applicable to small portable power systems. The energy density advantage over lithium batteries is slight, although the technology has some advantages associated with balance-of-plant. Demonstration of the next generation system with higher energy density and cartridges will be performed.
FC-46	DMFC Power Supply for All-Day True-Wireless Mobile Computing; PolyFuel; Brian Wells	2.7			X	This project is ending this year. Remaining tasks include: improving overall system power to meet the 15 W target and durability tests on complete units.
FC-47	Fuel Cell Research at the University of South Carolina; University of South Carolina; John Van Zee	2.5			X	Congressionally directed. Catalyst support durability was not addressed at all, but should be. Reviewers felt that this project contained four largely unrelated projects with no interconnection.
FC-48	Novel PEMFC Stack Using Patterned Aligned Carbon Nanotubes as Electrodes in MEA; ANL; Di-Jia Liu	2.5			X	This project completes at the end of the fiscal year and, therefore, will not be continued. The final task of the project is to complete a durability study on carbon nanotube-based fuel cells to determine whether reviewers are correct that the nanotubes provide no durability benefit as compared to conventional carbon supports.
FC-49	Detection of Trace Platinum Group Element Particulates with Laser Spectroscopy; Montana State; Stuart Snyder	1.9			X	The plan for this Congressionally-directed project is to calibrate the system for platinum detection and continue analyzing fuel cell water for platinum and palladium. There is an urgent need to prove that Pd/Pt loss to fuel cell water is a problem before continuing project.

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FCP-01	Light-weight, Low Cost PEM Fuel Cell Stacks; Case Western Reserve University; Jesse Wainright	2.8	X			Reviewers were concerned about the low current densities and recommended focusing on the engineering concepts, rather than building full systems. The next steps in this project are to continue single-cell testing, refine the CFD model, and fabricate a first-generation sub-stack.
FCP-02	Platinum Group Metal Recycling Technology Development; BASF; Lawrence Shore	2.7	X			This project is in its last year. Remaining tasks include determining the Pt yield from two competing reactor designs and improving the economic model.
FCP-03	Platinum Recycling Technology Development; Ion Power, Inc.; Stephen Grot	3.1			X	This project ends this year. In FY09, Ion Power will focus on lowering the platinum group metal (PGM) content in the diffusion media to 0.05 wt.% PGM.
FCP-04	Component Benchmarking Subtask Reported: USFCC Durability Protocols and Technically-assisted Industrial and University Partners; LANL; Tommy Rockward	3.1	X			LANL has provided high quality support to the fuel cell R&D community and will continue to serve industrial and university partners.
FCP-05	Low Cost, Durable Seals For PEM Fuel Cells; UTC Power Corporation; Jason Parsons	3.0	X			The project completes within a year and proceeds with downselection of next generation candidates, accelerated <i>ex situ</i> durability testing, and prototype development. UTC should also include <i>in situ</i> fuel cell testing.
FCP-08	Research & Development for Off-Road Fuel Cell Applications; IdaTech; Richard Lawrance	2.7	X			In the next year, performance testing of the system on a dynamometer, on a golf course, and with end-users will be conducted before the researchers design a second prototype and demonstrate the vehicles.
FCP-09	Market Opportunity Assessment of Direct Hydrogen PEM Fuel Cells in Federal and Portable Markets; Battelle Memorial Institute; Kathya Mahadevan	3.0			X	The project has reached planned conclusion.

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### Technology Validation:

TV-01	Hydrogen to the Highways; DaimlerChrysler; Ron Grasman	3.3	X			This project is a key element in determining whether the program's hydrogen and fuel cell activities are on course to achieve established research and development targets. Adding vehicles to government fleets will demonstrate the technology to early adopter markets. DOE will work with technology validation project teams on ways to take advantage of the hydrogen infrastructure investments after the projects are completed.
TV-02	Hydrogen Fuel Cell Vehicle & Infrastructure Demonstration Program Review; Ford; Greg Frenette	3.2	X			This project has direct relevance to the Hydrogen Program's Multi-Year Program Plan and will help DOE achieve its goals. DOE will work with technology validation project teams on ways to take advantage of the hydrogen infrastructure investments after the projects are completed.
TV-03	Controlled Hydrogen Fleet and Infrastructure Demonstration and Validation Project; Chevron; Dan Casey	3.3	X			Acquiring "real world" operational data and experience is vital to making appropriate adjustments to the hydrogen program's research and development projects. DOE will work with technology validation project teams on ways to take advantage of the hydrogen infrastructure investments after the projects are completed.
TV-04	Hydrogen Vehicle and Infrastructure Demonstration and Validation; General Motors; Roz Sell	3.7	X			This project strongly supports the Hydrogen Fuel Initiative and the technology validation aspects of the Multi-Year Program Plan for vehicle and infrastructure demonstration and evaluation. DOE will work with technology validation project teams on ways to take advantage of the hydrogen infrastructure investments after the projects are completed.
TV-05	Controlled Hydrogen Fleet & Infrastructure Analysis; NREL; Keith Wipke	3.5	X			This project is vital to determining whether the Program's hydrogen and fuel cell activities are on course to achieve established research and development targets. This project represents a good summary of the state of hydrogen technology when applied to automotive transportation and will be continued.
TV-06	Validation of an Integrated Hydrogen Energy Station; Air Products; Ed Heydorn	3.5	X			The concept of an integrated electricity and hydrogen production facility is an innovative concept and promises to encourage the use of hydrogen fueling stations even when the vehicle usage might be low, at the start of deployment.
TV-07	California Hydrogen Infrastructure Project; Air Products; Ed Heydorn	3.4	X			Very relevant to have a major hydrogen producer involved in designs and fabrication of hydrogen infrastructure projects. DOE will work with the team to develop plans to allow the hydrogen stations to be used after the project ends.

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TV-08	Hawaii Hydrogen Center for Development and Deployment of Distributed Energy Systems; Hawaii Natural Energy Inst.; Richard Rocheleau	3.1	X			The project presentation clearly demonstrates and supports the President's Hydrogen Fuel Initiative. DOE will work with the project partners to better focus the project on the development of the refueling station and operation of the buses at the Volcanoes National Park.
TV-09	Cryogenic Capable Pressure Vessels for Vehicular Hydrogen Storage; LLNL; Salvador Aceves	2.8			X	The project focuses on one of the key objectives which is to improve on-board hydrogen storage options available to the OEMs. DOE will work with LLNL to have them move towards more realistic packaging for DOE's next vehicle demonstration.
TVP-01	Florida Hydrogen Initiative; Florida Hydrogen Initiative; Pam Portwood	2.5	X			At least two of the four projects discussed are expected to have little or no benefit in terms of contributing to achievement of DOE's Hydrogen goals, targets and objectives. DOE will discuss with the project partners the termination of the diesel reformation project as diesel to hydrogen reformation is highly unattractive from an efficiency and cost standpoint. Additionally, it does not fit within the context of the Florida Hydrogen Initiative.
TVP-02	Technology Validation: Fuel Cell Bus Evaluations; NREL; Leslie Eudy	3.1	X			Making real operational data available for all to view and use is excellent. Will work with NREL to expand the data base to include all fuel cell buses in operation.

**Safety, Codes, and Standards:**

SA-01	Hydrogen Codes and Standards; NREL; Robert Burgess	3.9	X			This project is critical to the continued support of research and development associated with domestic and international hydrogen standards.
SA-02	Materials Compatibility; SNL; Brian Somerday	3.9	X			This project investigates the hydrogen compatibility of materials for multiple applications including storage, transport and system components.
SA-03	Hydrogen Safety Tools: Software and Hardware; PNNL; Linda Fassbender	3.7	X			This project promotes safety education and information sharing related to the safe handling of hydrogen.
SA-04	Hydrogen Fuel Quality; LANL; Tommy Rockward	3.4	X			This project will provide the specifications on tolerable fuel constituents for the development of an international hydrogen quality standard.
SA-06	Hydrogen Safety Panel; PNNL; Steven Weiner	3.5	X			This project is critical to the safe execution of DOE hydrogen projects and information sharing on hydrogen use and practices.
SAP-01	Codes & Standards for the Hydrogen Economy; Regulatory Logic; Gary Nakarado	3.6	X			This project aims to promote and maintain harmonization among Codes and Standards Development Organizations.

Project Number	Project Title; Presenting Organization; PI Name	Final Score	Continue	Discontinue	Other	Summary Comment
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### Education:

ED-01	Hydrogen Knowledge and Opinions Assessment; ORNL; Rick Schmoyer	2.8	X			The project measures important overall key activity metrics. The subprogram will consider stronger ties to other education projects. The survey methodology may be outdated (use of telephone land line survey) but methodology for follow-up surveys must be consistent over time to retain statistical validity.
ED-02	Hydrogen Safety: First Responder Education; PNNL; Marylynn Placet	3.5	X			The project objectives are highly consistent with Hydrogen Fuel Initiative and DOE program objectives. The project has a sound approach; the large number of reviewers and the inclusion of a steering committee shows strong collaborative effort. The effort demonstrated success and clear progress. The subprogram, will consider greater focus on near-term hydrogen applications.
ED-03	Hydrogen Education for Code Officials; NREL; Melanie Caton	3.1	X			The project strategy and goals are reasonable and well-thought out; the use of e-learning modules is especially effective. The subprogram will consider additional collaboration with partners and a more detailed course rollout plan.
ED-04	Increasing "H2IQ": A Public Information Program; The Media Network; Henry Gentenaar	3.3	X			The project is well thought-out and is important for providing objective and consistent information. The project has demonstrated good, simple messaging and contemporary multi-media marketing strategies. The subprogram will consider more specific quantifiable metrics and more active collaborations.
ED-05	H2 and You: A Public Education Initiative by the Hydrogen Education Foundation; Hydrogen Education Foundation; Patrick Serfass	3.4	X			The project is important for dispelling myths and correcting misinformation. Assembling a steering committee of public and private sector partners is a good approach. DOE will coordinate more closely with the project steering committee to align the "hydrogen message."
ED-07	H2 Educate! Hydrogen Education for Middle Schools; NEED; Mary Spruill	3.7	X			This is an aggressive, well thought-out program. There has been considerable success in reaching teachers despite funding issues over the project duration. Project strengths include partnerships, effective use of resources, and alignment with science education standards. The subprogram will consider more frequent content updates.

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**Systems Analysis:**

AN-01	HyTrans Model: Analyzing the Transition to Hydrogen-Powered Transportation; ORNL; David Greene	3.5	X			Future work will address the reviewers' suggestions: (a) obtain additional industrial data to establish how federal procurement of smaller PEM fuel cells will bring about the viability of larger PEM fuel cells used in automobiles; and (b) evaluating alternatives such as the plug-in vehicle (both electric hybrid and hydrogen hybrid) and the H2 internal combustion vehicle.
AN-02	GREET WTW Analysis Results and Comparison of Advanced Vehicle Technologies; ANL; Michael Wang	3.6	X			Argonne National Laboratory's future work will address the reviewers' suggestion regarding increasing validation of assumptions through discussion with industry experts and other experts. Work will be focused on developing well to wheel analysis for renewable pathways and plugin vehicles.
AN-04	Macro-System Model; NREL; Mark Ruth	3.5	X			Additional work will address the reviewers' suggestions of better documentation of assumptions, resolving questions on the efficiency of the distributed steam methane reformers, and seeking additional input from experts as needed. The Macro-System Model will incorporate other renewable hydrogen production pathways.
AN-05	Analysis of the Hydrogen Production and Delivery Infrastructure as a Complex Adaptive System; RCF, Inc.; George Tolley	3.4	X			RCF will address the reviewers' suggestion to use different discount rates and include additional scenarios such as hydrogen co-produced in stationary fuel cell system. The project will be completed in FY 2009.
AN-06	Hydrogen Technology Analysis: H2A Production Model Update; NREL; Darlene Steward	3.9	X			NREL will incorporate the reviewers' suggestion of providing better documentation of the assumptions for the H2A. Reviewers concluded the model is necessary for the Hydrogen Program to calculate a standardized cost of hydrogen but the model should be further peer reviewed.
AN-07	Water Resource Analysis for Hydrogen Infrastructure; LLNL; Rich White	2.9	X			Sandia will address the recommendation to provide the documentation of the rationale for selecting hydrogen pathways for analysis and the rationale for comparing hydrogen pathways' water requirements with biofuels and gasoline pathways.
AN-08	HyDRA: Hydrogen Demand and Resource Analysis Tool; NREL; Witt Sparks	3.2	X			NREL will add renewable hydrogen information as the reviewers suggested. Infrastructure information for electrical systems, railroad and natural gas pipeline infrastructure and carbon sequestration sites will be included in the model. The tool is interactive and enables users to understand and analyze a variety of scenarios relevant to production, transport, and uses of hydrogen fuel.



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AN-09	Lessons Learned for Fueling Infrastructure; NREL; Marc Melaina	3.3			X	The project will be completed at the end of FY08 and provides insights to infrastructure deployment and expansion. Understanding lessons from previous successful and unsuccessful efforts to introduce new alternative fuels is important for developing a successful strategy to introduce hydrogen as a transportation fuel.
AN-10	Hydrogen and Fuel Cell Analysis: Lessons Learned from Stationary Power Generation; U Missouri-Rolla; Scott Grasman	2.9	X			The project has just begun and therefore the reviewers did not see many results. The project will continue to be funded through FY 2009. Future documentation will describe the approach and results in more detail as suggested by the reviewers.
AN-11	Hydrogen Quality Issues for Fuel Cell Vehicles; ANL; Romesh Kumar	3.1	X			Future work will focus on alternative hydrogen separation technologies in addition to PSA as appropriate. Additional hydrogen production pathways will be included in the assessment of quality impacts on fuel cell durability and production costs.
AN-12	Update on Platinum Availability and Assessment of Platinum Leasing Strategies for Fuel Cell Vehicles; TIAX; Matt Kromer	3.5			X	This project will be completed by the end of FY08. Project addresses the concern of platinum availability for widespread fuel cell vehicle deployment and investigates cost mitigation opportunities especially with recent price increases in platinum.
AN-13	Evaluation of the Potential Large-Scale Use and Production of Hydrogen in Energy and Transportation Applications; University of Illinois-Urbana-Champaign; Don Wuebbles	3.5	X			In FY 2009 the project team will assess additional hydrogen pathways for environmental impacts, based on the reviewers' suggestion. This project will create awareness about hydrogen emissions during production, hydrogen reactions with hydroxyl radicals in the atmosphere, hydrogen's effect on the ozone layer, increased soil acidity, and, overall, the impact of the emissions on climate.
AN-14	Potential Environmental Impacts of Hydrogen-Based Transportation and Power Systems; Tetra Tech; Thomas Grieb	3.0	X			Future work will address the reviewers' suggestions of selecting a more defensible baseline scenario for comparison and incorporating renewable hydrogen production pathways in the environmental assessment. Study of hydrogen dynamics in the troposphere and stratosphere is very important and should include fossil and renewable hydrogen production sources.
ANP-01	Hydrogen Technology Analysis: H2A Stationary Power Production Model; NREL; Michael Penev	3.2	X			NREL will develop a more systematic plan of investigation of the various fuel cell categories. This model will be part of a scenario analysis to investigate synergies of stationary power generation with hydrogen production for the transportation sector.

**PROLOGUE**

<b>Project Number</b>	<b>Project Title; Presenting Organization; PI Name</b>	<b>Final Score</b>	<b>Continue</b>	<b>Discontinue</b>	<b>Other</b>	<b>Summary Comment</b>
ANP-04	Hydrogen Infrastructure Analyses; SNL; Anthony McDaniel	2.6	X			The project score was low since the project just began and few results were available or presented. The project will be funded through FY 2009 and will address the reviewers' suggestions related to increasing collaboration with other market transition studies funded by the program and include industrial stakeholders early in the project.

**Manufacturing:**

MF-02	Fuel Cell MEA Manufacturing R&D; NREL; Mike Ulsh	3.1	X			The goals of this project were noted as being directly in line with Hydrogen Program objectives. In the future, the project will focus on making more quantitative, rather than qualitative results, to address reviewer comments.
MF-04	Rapid Manufacturing of Carbon Composite High Pressure Storage Cylinders; Profile Composites; Geoff Wood	3.4			X	Congressionally directed project. Although good progress has been made on the process steps, the project fails to identify how the cycle time reductions relate to overall cost reductions. Additional work could be done to upgrade quality control activities and work to ensure the transfer of technology.
MF-05	Technologies for Mass-Manufacturable Manifolds and Durable Seals for PEM Fuel Cells in Transportation Applications; UTC Power; Patricia Cosentino	3.1			X	Congressionally directed project. The progress claims were not backed up by data. It was not clear which fabrication process resulted in the 90 percent cost reduction.
MF-06	Develop Low-Cost MEA3 Process; DuPont Fuel Cells; Dennis Kountz	2.8			X	Congressionally directed project. DuPont achieved demonstrable performance improvements in a DMFC system. However, this would have been more valuable using a more fundamental approach that would provide information to the DOE Hydrogen Program. The performance results were not made clear.
MF-07	NIST Fuel Cell Manufacturing Research Project Metrology for Fuel Cell Manufacturing; NIST; Eric Stanfield	2.9	X			The project is likely to provide pre-competitive information that the fuel cell industry can use to help achieve the Hydrogen Program goals. Reviewers also noted that NIST is following a logical path to identifying and evaluating non-contact measurement techniques, which will continue in FY09.

Project Number	Project Title; Presenting Organization; PI Name	Final Score	Continue	Discontinue	Other	Summary Comment
MFP-01	Innovative Inkjetting and Spray Deposition for Low-Cost, High-Performance Fuel Cell Catalyst Coated Membrane Manufacturing; Cabot Corp.; Hanwei Lei	2.5			X	Congressionally directed project. There was no analytical assessment of cost, performance, or durability. Therefore, results are inconclusive.
MFP-02	Novel Manufacturing Process for PEM Fuel Cell Stacks; Protonex Corp.; Michael McCarthy	3.2			X	Congressionally directed project. Protonex developed, designed, and manufactured multiple fuel cell stacks and systems demonstrating small-volume manufacturing potential. However, it is not clear if the project's claim of achieving a 25 percent reduction in manufacturing time resulted in the cost target being met. It was not clear how the claim was determined.
MFP-03	Manufacturable Chemical Hydride Fuel System Storage for Fuel Cell Systems; Millennium Cell; Richard Mohring	3.1			X	Congressionally directed project. While the project overcame some technical barriers, there is no plan to scale up the technology to high-volume applications. The future of the effort to commercialize is therefore unclear.
MFP-04	Non-Destructive Testing and Evaluation Methods; ASME Standards Technology; Jim Ramirez	3.2			X	Congressionally directed project. Modal Acoustic Emission (MAE) definitely shows potential for the non-destructive evaluation (NDE) of flaws in pressure vessels. A quantitative comparison with other technologies should be done next year. Statistical data showing fault detection effectiveness should also be developed.

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## INTRODUCTION

This report is a summary of comments from the Peer Review Panel at the FY 2008 DOE Hydrogen Program Annual Merit Review, held on June 9-13, 2008, at the Gateway Crystal Marriott in Arlington, Virginia. The work evaluated in this document supports the Department of Energy (DOE), and the results of this merit review and peer evaluation are major inputs utilized by the DOE in making its funding decisions for following fiscal years.

The objectives of this meeting were to:

- Review and evaluate FY 2008 accomplishments and FY 2009 plans for DOE laboratory programs and industry/university cooperative agreements and R&D that supports development.
- Provide an opportunity for program participants (hydrogen production manufacturers, hydrogen storage manufacturers, fuel cell manufacturers, etc.) to shape the DOE sponsored R&D program so that the highest priority technical barriers are addressed. The meeting also serves to facilitate technology transfer.
- Foster interactions among the national laboratories, industry, and universities conducting the R&D.

The Peer Review process followed the guidelines of the Peer Review Guide developed by EERE. The Peer Review Panel members, listed in Table 1, attended the meeting and provided comments on the projects presented. These panel members are peer experts from a variety of hydrogen and fuel cell related backgrounds including national laboratories, hydrogen production manufacturers, hydrogen storage manufacturers, fuel cell manufacturers, universities, and other U.S. Government agencies. Each member was screened from a conflict of interest (COI) perspective per the Peer Review Guide. A complete list of the meeting participants is presented as Appendix A to this report.

**Table 1: Peer Review Panel Members**

No.	Last Name, First Name, Organization
1	Abdel-Baset, Tarek, Chrysler Corporation
2	Aceves, Salvador, LLNL
3	Adams, Jesse, DOE Golden Field Office
4	Adams, Mike
5	Adjemian, Kev, Nissan Motor Company
6	Adzic, Radoslav, BNL
7	Ahmed, Shabbir, ANL
8	Ahn, Channing, CalTech
9	Akiba, Etsuo, AIST
10	Anderson, Michelle, Office of Naval Research
11	Armstrong, Tim, Oak Ridge National Laboratory
12	Bakke, Paul, DOE
13	Balachandran, Balu, Argonne National Laboratory
14	Balema, Viktor, Sigma-Aldrich Corp.

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15	Baturina, Olga, Naval Research Laboratory
16	Bavarian, Farshad, Chevron
17	Benard, Pierre, Hydrogen Research Institute
18	Benjamin, Thomas, Argonne National Laboratory
19	Birdsall, Jackie
20	Blair, Larry, Consultant (retired from DOE)
21	Bluestein, Linda, DOE/EERE Vehicles Program
22	Bocarsly, Andrew, Princeton University
23	Bonhoff, Klaus
24	Bordeaux, Chris
25	Borup, Rod, LANL
26	Bose, Arun, NETL
27	Bowman, Bob, JPL-retired
28	Buxbaum, Robert, REB Research and Consulting
29	Cai, Mei, GM
30	Casey, Daniel, ChevronTexaco
31	Choate, Bill, BCS
32	Choudhury, Biswajit, DuPont Fuel Cells
33	Christensen, John, Consultant
34	Chu, Deryn, US Army Research Laboratory
35	Collins, Bill, UTC Power/Fuel Cells
36	Conte, Mario, Italian National Agency - ENEA
37	Cooper, Alan, Air Products
38	Costa, Stephen, DOT/Volpe Center
39	Cox, Philip, PolyFuel
40	Curry-Nkansah, Maria, BP
41	Debe, Mark, 3M
42	Domnez, Alkan, NIST
43	Douglas, Trevor, Montana State
44	Driscoll, Daniel, NETL
45	Eisman, Glenn, RPI
46	Erdle, Erich, Retired from Daimler
47	Ernst, Bill
48	Fairlie, Matthew, Retired from Stuart
49	Fenton, Jim, UCF
50	Filiou, Constantina, EC
51	Freund, Deborah, Federal Motor Carrier Safety Administration
52	Gangi, Jennifer, Fuel Cells 2000
53	Gayle, Frank, NIST
54	Ge, Qingfeng
55	Gencer, Mehmet, IMET Corporation
56	Gittleman, Craig, GM
57	Glass, Robert, LLNL

58	Goudy, Andrew, Delaware State U.
59	Grassilli, Leo, Navy
60	Gross, Tom, Consultant
61	Gruber, Jill, DOE
62	Haberman, David, IF, LLC
63	Hamernyik, Erin, WSU
64	Hamrock, Steve, 3M
65	Hardis, Jonathan
66	Heben, Mike, NREL
67	Herring, Andy, Colorado School of Mines
68	Hershkowitz, Frank, ExxonMobil
69	Hirano, Shinichi, Ford Motor Company
70	Hirose, Katsuhiko, Toyota
71	Holladay, Jamie, PNNL
72	Hoskin, Aaron
73	Hua, Thanh, ANL
74	Imam, Ashraf, Naval Research Laboratory
75	James, Brian, Directed Technologies, Inc.
76	Jena, Puru, Virginia Commonwealth U.
77	Jensen, Craig, U of Hawaii
78	Johnston, Christina
79	Jorgensen, Scott, GM R&D
80	Kegerreis, Jim, ExxonMobil
81	Kerr, John, LBNL
82	King, David PNNL
83	King, Merrill, NASA
84	Kirschner, Neil, DOE/NETL
85	Kopasz, John, Argonne National Laboratory
86	Koval, Carl, UC- Boulder
87	Kroposki, Benjamin, National Renewable Energy Laboratory
88	Kumar, Romesh, Argonne National Laboratory
89	Kung, Stephen (for Carl Sink)
90	Kuriyama, Nobuhiro, AIST
91	Lasher, Stephen, TIAX
92	Laskin, Jay, Consultant
93	Lipp, Ludwig, FuelCell Energy
94	Lott, Melissa, Alliance Technical Services
95	Maeland, Arnulf
96	Markovic, Nenad, ANL
97	Maroni, Victor, ANL
98	Masten, David, GM
99	McFarland, Eric
100	McGrath, James, Virginia Tech

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101	McKenny, Kurtis, TIAX
102	McQueen, Shawna, Energetics
103	Mehall, Mark, Ford
104	Meier, Paul, ConocoPhillips
105	Melis, Tasios, UC Berkeley and LBNL
106	Mettes, Jacob, Power and Energy
107	Meyers, Jeremy, University of Texas at Austin
108	Miller, Bob, Air Products
109	Miller, Eric, University of Hawaii
110	Miller, Michael, SwRI
111	Mohtadi, Rana, Toyota Technical Center
112	Moore, Tom, Consultant
113	More, Karren, ORNL
114	Moreland, Greg, SENTECH, Inc.
115	Motyka, Theodore, Savannah River National Laboratory
116	Muradov, Nazim
117	Myers, Deborah, Argonne National Laboratory
118	Nakamura, Yumiko, AIST, Japan
119	Nguyen, Kevin, Chevron
120	Nguyen, Yen-Loan
121	Olson, Greg, Consultant
122	Padro, Cathy, Los Alamos National Lab
123	Parkinson, Bruce, Colorado State University
124	Parks, George, Conoco Philips
125	Paster, Mark, Consultant (retired DOE)
126	Patel, Pinakin, FuelCell Energy, Inc.
127	Paul, Dilo
128	Pecharsky, Vitalij, Ames lab
129	Petrovic, John, Petrovic & Associates
130	Pez, Guido, Air Products & Chemicals
131	Pivovar, Bryan, LANL
132	Podolski, Walter, ANL
133	Quah, Micheal, Concurrent Technologies
134	Ramani, Vijay, Illinois Institute of Technology
135	Rambach, Glenn, Quantum Sphere
136	Reilly, Jim, BNL
137	Richards, Mark, Versa Power
138	Roan, Vernon, University of Florida
139	Sandrock, Gary, Consultant
140	Schmetz, Edward
141	Siegal, Don, Ford
142	Skolnik, Ed, Energetics, Inc.
143	Steward, Darlene, NREL

144	Stubos, Athanasios
145	Sudik, Andrea, Ford
146	Thomas, George, DOE (consultant)
147	Thorn, David, LANL
148	Tran, Doanh, Chrysler Corporation
149	Tumas, William, LANL
150	Vanderborgh, Nicholas, Consultant (retired from LANL)
151	Vanderveen, Keith, SNL
152	Von-wild, Juergen, BMW
153	Wagner, Fred, Energetics
154	Waldecker, Jim , Ford Motor Company
155	Weatherwax, Sharlene, DOE
156	Weiner, Steve, PNNL
157	Wesson, Rose, NSF
158	Wheeler, Doug, DJW Technology
159	Wichert, Robert, US Fuel Cell Council
160	Williams, Mark, ex-NETL, consultant
161	Wipke, Keith, NREL
162	Wolfe, Barb, New West Technologies
163	Wolverton, Chris, Northwestern Univ.
164	Yancey, Lea, DOE
165	Zawodzinski, Tom, Case Western
166	Zelenay, Piotr, LANL
167	Ziegler, Dick, SENTECH, Inc.

## SUMMARY OF PEER REVIEW PANEL'S CROSS-CUTTING COMMENTS AND RECOMMENDATIONS

The Peer Review Panel members provided a number of comments and recommendations that apply to the Annual Merit Review and peer review process, as well as overall management of the DOE Hydrogen Program. These comments are provided in Appendix C of this report. DOE will utilize these comments to improve both the program and future review meetings.

## ANALYSIS METHODOLOGY

As shown above, **167** panel members participated in the merit review process. A total of **232** projects were reviewed at the meeting and a total of **1025** evaluation forms were received from the Peer Review Panel (not every panel member reviewed every project). These panel members were asked to provide numeric scores (on a scale of 1 to 4, with 4 being the highest) for five aspects of the research on their Evaluation Form, a sample of which can be found as Appendix C.

## INTRODUCTION

The five criteria and weights were:

- Relevance to overall DOE objectives (20%);
- Approach to performing the research and development (20%);
- Technical accomplishments and progress toward achieving the project and DOE goals (40%);
- Technology transfer and collaborations with industry, universities, and other laboratories (10%); and
- Approach to and relevance of proposed future research (10%).

All the individual criterion scores from various reviewers were averaged together to obtain average scores for each of the five above-mentioned criterion for every project. These average scores were then weighted and combined to produce a final overall score for that project. In this manner, a project's final overall score can be compared to other projects. Following is the formula used to calculate the weighted average overall score:

$$\text{Final Score} = \text{Score1} * 0.20 + \text{Score2} * 0.20 + \text{Score3} * 0.40 + \text{Score4} * 0.10 + \text{Score5} * 0.10$$

A few new projects were reviewed, where the third criterion (Technical Accomplishments) did not apply because of the project's recent startup. In this case, the other four criteria were scaled proportionally in the weighting calculation and the following formula was used:

*Criterion 3/ Technical Accomplishments weighted at 40% not included; therefore, weighting value for remaining scores = (weight +40/60\*weight)*

$$\text{Final Score} = \text{Score1} * (0.20 + (40/60) * 0.20) + \text{Score2} * (0.20 + (40/60) * 0.20) + \text{Score4} * (0.10 + (40/60) * 0.10) + \text{Score5} * (0.15 + (40/60) * 0.15)$$

$$\text{So, Final Score} = \text{Score1} * 0.33 + \text{Score2} * 0.33 + \text{Score4} * 0.17 + \text{Score5} * 0.17$$

A maximum final overall score of 4 signifies that the project satisfied the above mentioned five criteria to the fullest possible extent, while a minimum score of 1 implies that the project did not satisfactorily meet any of the requirements of the five criteria mentioned above.

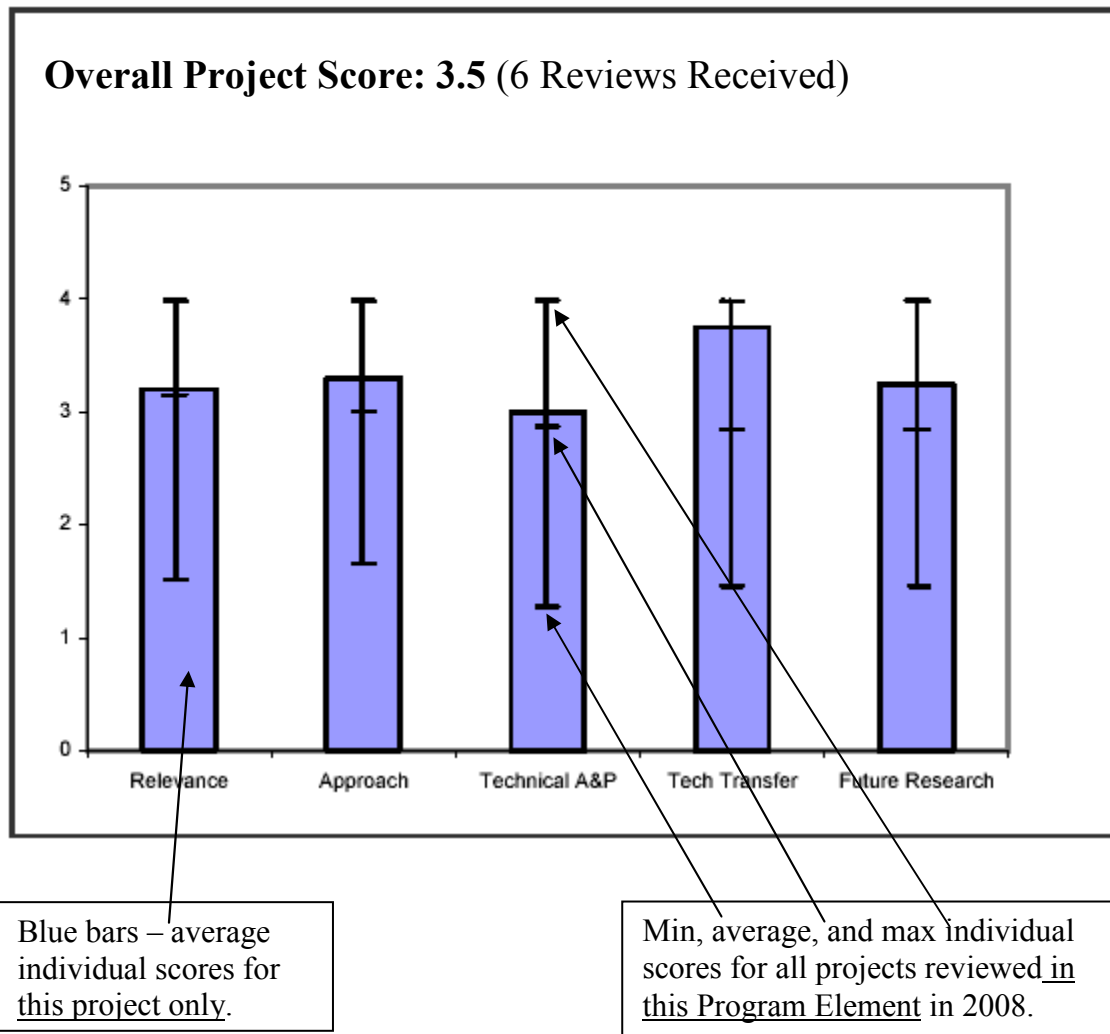
Reviewers were also asked to provide qualitative comments on the five research aspects, as well as the specific strengths and weaknesses of the project, and any recommendations for additions or deletions to the work scope.

These comments, along with the quantitative scores, were placed into a database for easy retrieval and analysis. These comments are summarized in the following sections of this report.

## ORGANIZATION OF THE REPORT

This report is organized in seven sections, in an effort to group projects according to the program elements in which they fall in DOE Hydrogen Program planning. A brief description of the general type of research being performed in each category is presented at the beginning of each major report section.

The remaining pages of each section present the results of the analysis for each of the projects discussed at the merit review. A summary of the qualitative comments is provided, as well as graphs showing overall score and how the particular project compared with all other projects presented within each program category. An example of a graph is provided below:



The project comparisons illustrated in the report are criteria based. Each rectangular blue bar in the chart represents that project's score for that particular criterion of the project. The displayed score for each criterion of a project was obtained by averaging the individual reviewer scores for that particular criterion of the project.



## INTRODUCTION

This project's score for each particular criterion (each blue bar) was then compared with the maximum, minimum and average score for that same criterion of all the presented projects (across all sub sections of the Hydrogen program). The maximum, minimum and average scores for a criterion across all the presented projects is graphically displayed by the black line bars which overlay the blue rectangular bars.

For clarification purposes consider that only three projects were presented and reviewed. The hypothetical projects were scored by reviewers as displayed in the table below:

	Relevance	Approach	Technical A&P	Tech Transfer	Future Research
Project 1	4	2	1	4	3
Project 2	1	4	4	3	2
Project 3	2	3	2	1	4
Max	4	4	4	4	4
Min	1	2	1	1	2
Average	2.3	3.0	2.3	2.6	3.0

In this case, the chart for project 2 would contain a blue rectangular bar with a value of 1 (reflecting the score obtained by project 2 for the relevance criterion) and a black line bar with max, min and average values of 4, 1, and 2.3 respectively for the relevance criteria. Below is a sample calculation for the Project 1 weighted score.

$$\text{Final Score} = 4*0.20 + 2*0.20 + 1*0.40 + 4*0.10 + 3*0.10 = 2.3$$

2008

**Hydrogen Production and Delivery**

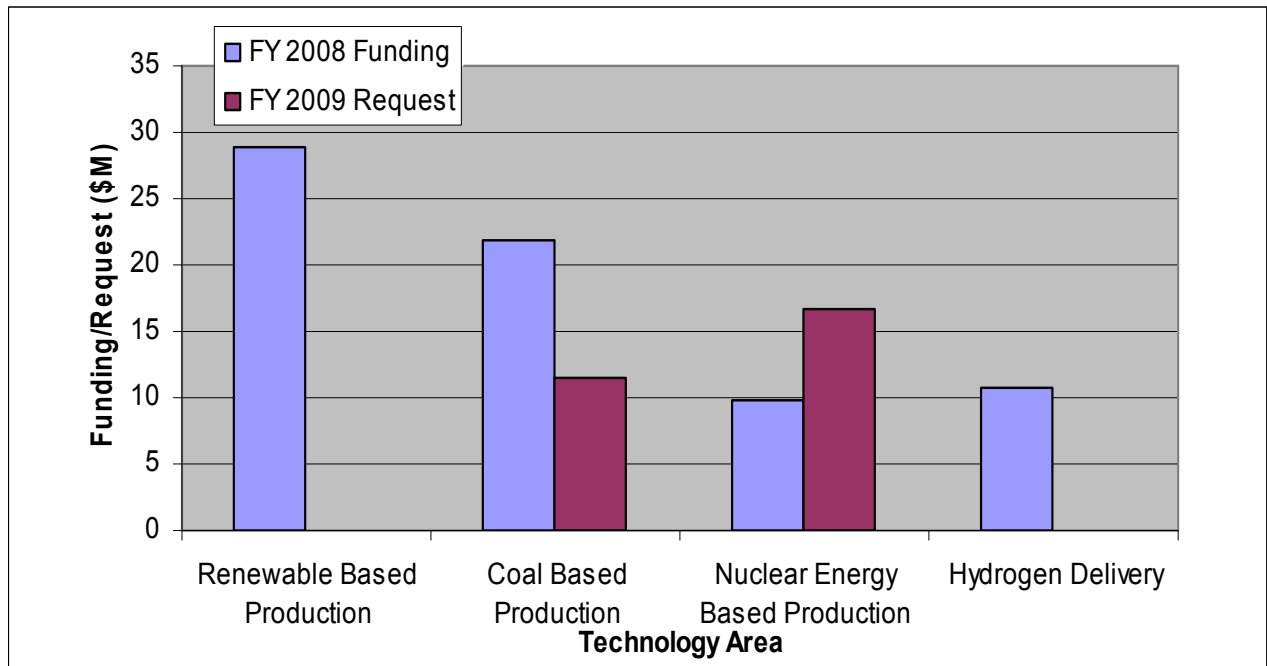
**Summary of Annual Merit Review Hydrogen Production and Delivery Subprogram**

**Summary of Reviewer Comments on Hydrogen Production and Delivery Subprogram:**

This review session evaluated hydrogen production and delivery research from all DOE activities working on the President’s Hydrogen Fuel and Advanced Energy Initiatives, including: the Offices of Fossil Energy, Nuclear Energy, and Energy Efficiency and Renewable Energy. The production and delivery projects are generally considered to be well-aligned with the goals and objectives of the Hydrogen Program.

The production projects include diverse energy sources and technologies for hydrogen production including natural gas reforming, water electrolysis, bio-derived renewable liquids reforming, biomass gasification, solar-driven thermochemical cycles, nuclear-driven thermochemical cycles, photoelectrochemical direct water splitting, biological hydrogen production, and hydrogen production from coal. The delivery projects reviewed included the next stage of development of the H2A Delivery analysis models, and several of the key hydrogen delivery research efforts such as pipeline embrittlement, new fiber reinforced polymer pipeline and linings, and compressor research. Overall, the projects were judged to have made considerable progress in reducing both projected capital and operating costs and in improving material properties. Reviewer concerns and recommendations varied considerably by project and are summarized below.

**Hydrogen Production and Delivery Funding by Technology:**



### **Majority of Reviewer Comments and Recommendations:**

In general, the reviewer scores for the production and delivery projects were high to average, with scores of 3.9, 3.1 and 1.9 for the highest, average and lowest scores, respectively. The scores are indicative of the technical progress that has been made over the past year for DOE competitively selected and Congressionally directed projects. Recommendations and major concerns for each project category are summarized below.

**Bio-Derived Liquids Reforming:** New technology being developed for distributed reforming from bio-derived liquids (e.g. ethanol, sugars) will build on distributed reforming from natural gas technology while helping to solve outstanding issues with on-site hydrogen production to reach the bio-derived liquids cost goal of \$3.00/gge by 2017. Two primary recommendations emerged from the reviews. First, the catalyst development tasks must move forward and be successful if the reforming of bio-derived liquids is to meet the DOE production cost targets. Second, all projects need to utilize H<sub>2</sub>A production modeling to provide consistent cost estimates.

**Electrolysis: In general projects in this area were scored favorably.** Two projects ended in FY08, one continued, and 2 were new starts. Most of the projects were regarded as well-aligned with current program goals and objectives. The projects focused on increasing stack efficiency and decreasing capital cost. Innovative new membranes presented were able to increase the efficiency to above that of the 2012 DOE targets and advanced manufacturing techniques along with new designs were presented that are projected to significantly reduce capital costs. The reviewers noted: 1) long term durability of the membranes must be tested, 2) the advanced membranes being developed need to be integrated into stacks and tested and 3) balance-of-plant development is needed to increase system reliability while reducing system cost. The newly started projects will be addressing these important issues.

**Biomass Gasification:** Three projects in this area were reviewed; two projects evaluated the potential for central high temperature biomass gasification; the other researching the potential of central plant, low temperature, single step, aqueous phase reforming of hydrolyzed biomass. The project scores ranged from 2.5 to 3.7. Projects scoring higher were noted to have significant technical advancements since last year and to have a focused project plan, which was followed closely.

**Solar-Driven High Temperature Thermochemical:** Two presentations and two posters were reviewed in this topic area. The projects were favorably rated for their collaborative efforts and technical skills and abilities of the researchers. Recommendations for improvement included to ensure that the calculation of overall system efficiency is consistent for each cycle, to complete all material balances, and to identify and resolve waste disposal issues. Finally, the reviewers responded favorably to the centralized H<sub>2</sub>A analysis that TIAX is coordinating.

**Photoelectrochemical Hydrogen Production:** The reviewers noted that the teaming approach that was used in some of the projects in this area was effective and necessary to achieve the DOE targets. Several of the projects received high ratings from the reviewers. Nearly all the projects were viewed to be aligned with the program's long-term goals. The projects have achieved good scientific progress in materials research and have established effective collaborations. The addition of theoretical activities to this area was seen by the reviewers as necessary.

**Biological Hydrogen Production:** The projects in this area were highly rated and the general conclusion from the reviewers was that the researchers are moving toward the DOE goals in this long-term renewable hydrogen production area. The scientific methods used in the majority of the projects are seen as cutting edge and the collaborations are effective and productive.

**Separations:** Reviewers commented, similar to prior year reviews, that there is a great need for investigators to test their hydrogen separation and purification membranes using realistic, mixed gas streams and to complete cost analyses. The potential for membrane technology to reduce the on-site hydrogen production footprint (by eliminating the PSA unit) and to reduce capital costs were frequent comments. Overlap with DOE Office of Fossil Energy membrane separations work was noted.

**Hydrogen from Coal:** The projects reviewed in this area received mostly favorable ratings from the reviewers. Reviewers observed that the projects were in alignment with the DOE Hydrogen Fuel Initiative and Hydrogen from Coal Program goals and objectives. The reviewers suggested that the projects need to advance the technology to the point where experiments using actual or close to actual gas streams are being performed. Specifically, the reviewers noted that the membranes need to be tested in the presence of impurities. The membranes also need to go through temperature cycling to assess mechanical stability. Finally, the reviewers noted that free standing membranes may be difficult to implement in a real world system.

**Hydrogen Production Using Nuclear Energy:** In general, the projects reviewed in this area were scored favorably. Reviewers approved of the breadth of collaboration for some projects and the well-focused approach of other projects. The projects were judged to be well-aligned with the program's goals. As in 2007, reviewers recommended that research be driven by materials and cost. Specific recommendations were made to understand durability and degradation of the high temperature electrolytic cells.

**Hydrogen Delivery:** The reviews recognized significant and very relevant progress in the pipeline research. The reviews also complimented the broad spectrum of collaboration across industry, national labs and universities as well as a good mix of theory, modeling and experimental work. The reviewers suggested benchmarking results achieved in this program with Technology Validation results or with field installations, e.g. hydrogen embrittlement of existing pipelines. Reviewers also suggested measuring the effect of hydrogen impurities on pipeline and storage system performance and on the cost for purification.

**Project # PD-01: Low-Cost Hydrogen Distributed Production System Development**

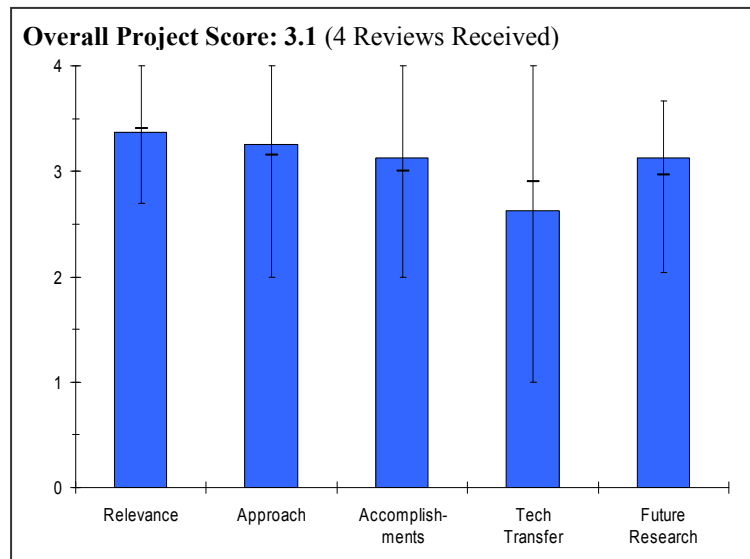
*Frank Lomax; H2Gen Inno. Inc.*

**Brief Summary of Project**

The objectives for this project are to 1) design, build and test a 565 kg/day hydrogen plant for 99.999% pure hydrogen to meet the Department of Energy hydrogen \$3/kg cost target for steam methane reforming and pressure swing adsorption; and 2) develop a catalyst suite based on our current technology suitable for use with fuel grade ethanol to facilitate renewable hydrogen production.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.4** for its relevance to DOE objectives.



- This project is highly relevant toward meeting Department of Energy's short term objectives.
- Project supports achievement of Department of Energy cost targets for distributed natural gas reforming hydrogen production.
- It is not clear that the project is working toward the Department of Energy efficiency goals.
- The development of low cost sources of larger quantities of hydrogen is highly relevant.
- Development of small, distributed reforming technologies will be necessary for Department of Energy to meet Hydrogen Fuel Initiative Goals.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- The approach was sound and ended up proving to be successful.
- The PI is knowledgeable about the market requirements for the hydrogen generation plant (for current hydrogen markets such as metal processing and chemical manufacturing) and appears to be focused on meeting these requirements.
- It is not clear that H2Gen is focused on meeting the requirements of the vehicle refueling market.
- H2Gen has identified the bottlenecks in the original product and has implemented improvements in the second generation product to overcome the bottlenecks of the first.
- The presentation did not include discussion of all the barriers identified; thus, it is not possible to evaluate the contribution of this project in terms of overcoming fuel processing manufacturing barriers, O&M barriers, feedstock issues, or control and safety.
- It was difficult to evaluate the approach taken, since little information was provided in the presentation on the details of the hydrogen production system.
- The approach seems very good.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- H2Gen made substantial progress toward meeting Department of Energy goals with its first design plant.
- The improvements that were identified and implemented should close the gap but additional data is needed to validate this conclusion.

- Production is at 565 kg/day rather than 1,500 kg/day; thus, some work is required to translate the efficiency and costs to those appropriate for a 1,500 kg/day plant that would be directly comparable to the Department of Energy targets. This translation was not shown in the presentation. During Q&A, the PI indicated that the H<sub>2</sub>A cost of hydrogen is about \$2.90/kg hydrogen, which is close to the Department of Energy goal.
- The hydrogen output and efficiency of the prototype plant are good, albeit the hydrogen output capacity is a little short of the target.
- The cost of the plant is not given (proprietary). Hopefully, it is less than the cost of present hydrogen reforming facilities.
- The cost per kilogram of hydrogen is not given.
- Good progress. Very quick identification of heat transfer problem and redesign of plant to correct. Comparison between the performance of the General Motors 5001 and General Motors 5002 will be valuable.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.6** for technology transfer and collaboration.

- The collaboration with catalyst provider and host site were both effective, resulting in a successful project.
- Working with Sud Chemie is appropriate.
- Partnership with a national lab or one of Department of Energy's analysis contractors could be considered. Such a partner could use H<sub>2</sub>A to help H<sub>2</sub>Gen translate this project's results to the correct scale and units to compare with Department of Energy's targets.
- It appears that there is essentially no technology transfer or collaborations on this project.
- Sud Chemie's role is not clear.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- The future plans are to enter full commercialization, while taking orders now.
- Under timeline, it is indicated that the project is complete.
- Future work does not, but should, include additional efficiency improvements to the process to meet the Department of Energy targets.
- It is appropriate for the commercialization of the product to take place without Department of Energy funding.
- Future work related to ethanol is appropriate.
- The PI expressed difficulty with measuring hydrogen purity at the levels that are currently assumed to be required. While probably not an appropriate direction for this project, work on hydrogen quality/impurity measurement instruments should be considered by Department of Energy.
- Future work is stated, but the project is indicated to be complete.
- Focus on additional fuels is a good direction for future research.

**Strengths and weaknesses**

Strengths

- The project demonstrated successful implementation of advanced, more expensive catalysts in such a way that supports lowering overall costs of the production while at the same time improving reliability and longevity of the system relative to other commercially available reformers.
- Project has seemingly strong commercialization potential.
- PI is focused on requirements for current hydrogen markets.
- Team has identified bottlenecks in the project and corrected for them in a second generation product.
- Development and demonstration of a low-cost hydrogen production facility.
- Project focus on identifying and correcting engineering issues.

Weaknesses

- It is not apparent that the Department of Energy cost and efficiency targets have been met.

## **PRODUCTION AND DELIVERY**

- It is not clear that the project intends to continue to improve cost and efficiency of the process.
- It is not clear that the team is focused on meeting the requirements of the vehicle refueling market.
- Little technology transfer from the Department of Energy support. Only benefit to the company.
- Very little cost information was presented. It is not clear whether the Department of Energy cost target was met.
- Very little information was presented on operating costs.

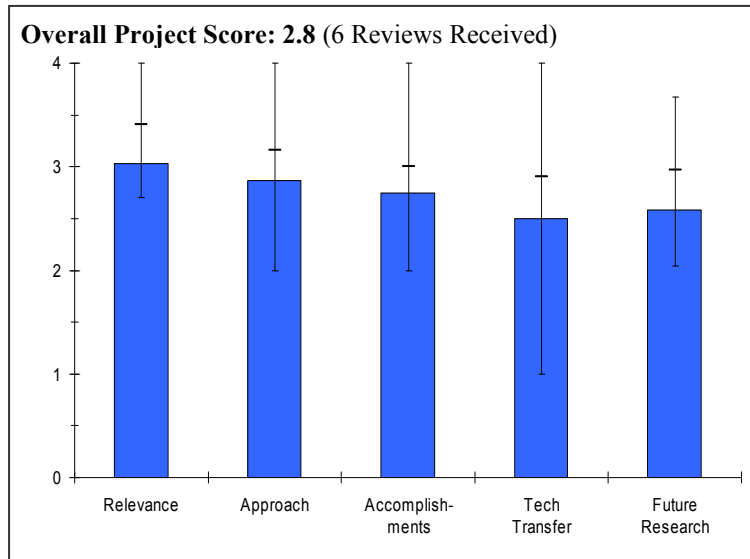
### **Specific recommendations and additions or deletions to the work scope**

- Consider partnering with a National Laboratory or Department of Energy contractor to do H2A cost and scaling analysis.

**Project # PD-02: Bio-derived Liquids Reforming**  
*Yong Wang; Pacific Northwest National Laboratory*

**Brief Summary of Project**

The overall objective of this project is to evaluate and develop bio-derived liquid reforming technologies for hydrogen production that can meet the Department of Energy 2017 cost target of <\$3.00/gge. The specific objectives for this project are to 1) identify at least one catalyst having the necessary activity, selectivity, and life at moderate temperatures to justify scale-up; 2) provide input for H2A analysis to determine potential economic viability and provide guidance to the research and development; 3) identify and control the reaction pathways to enhance hydrogen selectivity and productivity as well as catalyst; and 4) provide preliminary data for H2A analysis.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.0** for its relevance to DOE objectives.

- How does this technology differ from other advancing ethanol reforming technologies with Virent, National Renewable Energy Laboratory, and Ohio State University?
- Project is within Department of Energy bio-derived liquids to hydrogen mission.
- With cost of ethanol production rising, does this approach still have relevance?
- There is no sense of connection to overall outcomes.
- Excellent, clear and steady presentation style.
- Solid review of reaction pathways and kinetic controls.
- Very clear explanations of the chemistries.
- Relevance is clear; but I'm not up to speed on why the comparisons to (and exploration of) the aqueous phase processes are necessary!
- The availability of inexpensive bio-derived liquid feedstocks is rather questionable (barring advances in conversion of ligno-cellulosic matter); however, given the existence of such a feedstock, the proposed work is reasonable.
- The project studies hydrogen production from bio-derived liquids, especially ethanol. Hydrogen today is made from natural gas, a fuel in short supply and whose price is rapidly increasing. Developing other sources seems "relevant".
- Biofuels are an important part of mix of fuels from which hydrogen can be produced for use in fuel cells. Pacific Northwest National Laboratory provided test results from Rh/CeO<sub>2</sub>-ZrO<sub>2</sub> catalyst to H2A analysis.
- Work reveals hydrogen can be produced from ethanol for \$3/kg consistent with Department of Energy targets.
- In helping to elucidate the reaction mechanism for sugar and alcohol reforming with select catalysts the project supports the goal of reduction in fossil fuel dependency.

**Question 2: Approach to performing the research and development**

This project was rated **2.9** on its approach.

- H2A cost analysis with \$1.07 cost may not be relevant at this time.



## PRODUCTION AND DELIVERY

- It would be appropriate at this stage in development, now that many variables have been identified, to see a full cost analysis presented with several market contingencies.
- The idea of fuel produced in situ is appropriate, however can enough feedstocks be made available to provide the ethanol?
- Very methodical (almost pedestrian) approach regarding temperature assessments of catalytic activity.
- Need to explore other supports (beyond ZnO).
- Need to explore other metals (beyond Co species).
- What about porosity effects of support structures?
- What next? Need more details on catalyst down-select and other process.
- Approach is ok, but why not study two inexpensive readily available catalyst materials rather than rhodium? (Co-based is fine.)
- Assumptions in H2A analysis are rather questionable.
- The project focuses on two reforming catalysts, one rhodium-based and the other cobalt-based, very conventional formulations.
- Researcher is leader in reforming.
- Researcher has theoretical and analytical and experimental tools to conduct reformer research.
- Pacific Northwest National Laboratory understands role of variables such as space velocity, catalyst and steam/carbon ratio in reforming and their role in achieving project goals.
- I think the project could benefit significantly from collaboration with Ohio State University. Also I am unclear how much of this work is being leveraged by Virent. This likely came out during the Virent presentation which I missed.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- Perhaps the goal can be more clearly stated to find a low cost catalyst with optimal performance.
- Definitely a solid paper with clear process understanding and progress.
- Need to explore more broadly, e.g., effects of different steam/C ratios; does the short-lived methane plan provide insights?
- Need to better understand why the aqueous processes matter in this paper/project.
- The PIs should comment on how reproducible the data are (conversion, stability, etc.).
- Good progress on stability front, but longer durations must be targeted.
- Rather conventional experiments were described, with nothing surprising. Catalysts were synthesized, and reduced in Pacific Northwest National Laboratory laboratories.
- Improved ethanol catalyst by factor of 4. Improved catalyst life through modification of catalyst support.
- Gained further insights into role of side-reactions leading to concepts to further improve hydrogen selectivity.
- Identified dehydration pathway—methane and ethylene production—as the undesirable dead-end of ethanol reforming.
- Reaction either dies or cokes up. Substantial progress made on increasing lifetime of rhodium-CeO<sub>2</sub>-MO<sub>2</sub> catalyst.
- Generated good understanding of strengths and weaknesses of Co/ZnO catalyst system and proposed approaches for catalyst improvement..
- The project seems to be on track for meeting the cost targets. The 4x improvement in rhodium life for vapor phase ethanol reforming and the improvements in conversion and selectivity for the APR rhodium with base system are significant steps forward towards achieving the research objectives. However a lot of work still needs to be done to improve catalyst activity and to define optimum reaction conditions to obtain the right balance of selectivity, conversion and reactivation.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.5** for technology transfer and collaboration.

- Collaboration is noted in the presentation, however the identification of individual technology development is also highlighted and it is unclear how the collaboration is working. Virent has their own technology with stated results for aqueous phase reforming.
- Mentioned collaboration (or data-exchange) with DTI and Virent; but what about other learnings (from Ohio State University work? From other parties?).
- How have feedback from DTI, Virent, etc. affected this project?
- Could be better outlined, but on the whole, ok. Good, strong team.
- There were no useful collaborations with catalyst suppliers.
- Collaborating effectively enough with Virent. Ohio State University is working on Co-Rhodium with other supports than ZrO. May need to collaborate more with Ohio State University.
- As stated earlier I think more can be done with Ohio State University and I missed the Virent presentation to better understand how they will use the mechanistic information.

**Question 5: Approach to and relevance of proposed future research**

This project was rated 2.6 for proposed future work.

- Future plans must consider the effect on the economy of using food based feedstocks for fuel consumption.
- Success in cost reduction highly dependant on ethanol price volatility and catalyst costs.
- Unclear from presentation how the benefits will unfold or when.
- In comparison to other groups' developments and progress, unclear on the benefit of this approach.
- Go/No go decision should be made at this time.
- Not very clear re: major thematic conclusions?
- Would new pressure experiments affect overall process costs?
- Where would the PM versus NPM comparisons lead to?
- What about effects of impurities?
- More detail would have been welcome.
- Perhaps better to focus on less expensive materials.
- Revisit (if possible) H2A analysis assumptions.
- Needs to continue to update and include cost of precious metals in planned work.
- Plans to downselect ethanol catalyst which should be done.
- How does space velocity effect ethanol catalyst life?
- More rigor could be adopted in characterizing changes in surface active sites under varying synthesis and reaction conditions. For instance it would have been helpful to see Raman, x-ray diffraction and TEM studies for pre- and post-reactions.

**Strengths and weaknesses**

Strengths

- Developing an understanding of catalyst research under certain moderate to low temperature conditions.
- Excellent presentation of process chemistries and understanding of temperature/pressure effects that have been studied.
- Strong team.
- Appear to be hitting targets (perhaps should set more challenging targets).
- Future focus on fundamentals is a step in the correct direction.
- The collaboration with Virent and completion of preliminary H2A analysis demonstrates pre-commercial viability.

Weaknesses

- Lack of clarity of met targets, hard to understand benefit.
- Progress seems slow, but it's possible all efforts were not conveyed in presentation.
- Not clear about why certain alternative catalysts were chosen, e.g., why not Ni-based systems? Why not other catalyst alloys?
- Questionable assumptions in financial analysis (revisit if possible).

## PRODUCTION AND DELIVERY

- Need to show reproducible data - why no error bars?
- Need to expand efforts in characterizing the reaction mechanisms.

### **Specific recommendations and additions or deletions to the work scope**

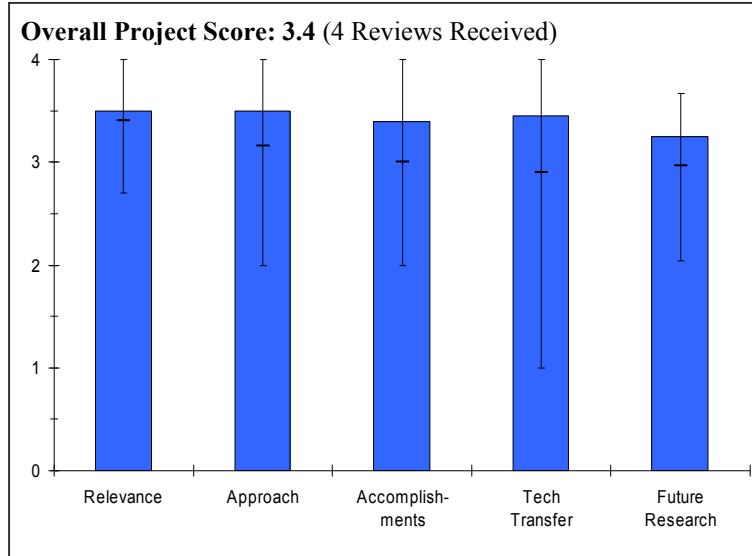
- More clarity and milestones with detailed explanation of how this differs from other advancements in this area.
- Tie together performance milestones with progress in the lab. Explain relevance more clearly.
- May want to consider removing the rhodium component if cobalt-based catalysts are more effective.
- Catalyst fabrication is a complicated but well understood technology. There is a vast literature on Fischer Tropsch (FT) Co-based catalysts and a good set of suppliers for these materials. It is critical that well-characterized catalysts are used for a study of this sort, and that data are taken that show reproducibility and catalyst performance degradation. Reduction is essential for activation; however passivation is also essential. The so-called egg shell catalysts would be highly appropriate and work well. Pressured processing will result in chain growth on Co, and those FT-like products should be looked for. It would be good for the Department of Energy to establish codes and standards for all projects pertaining to catalyst preparation, reduction, storage and measurement. If "home brew" catalysts are used, results need to be compared to results obtained using well characterized, commercial materials. Results should also be shown for several preparations of the same catalyst to demonstrate reproducibility. Although reforming ethanol is understood, bioethanol may contain impurities and learning about fuel processing of contaminated ethanol could reward. The reforming reactions are highly energetic, and modeling should include reacting CFD that includes descriptions of 3D temperature profiles. Even small samples can "hot spot".

**Project # PD-03: Analysis of Ethanol Reforming System Configurations**

Brian James; DTI

**Brief Summary of Project**

The objectives for this project are to 1) assess cost of hydrogen from bio-derived liquids (emphasis on ethanol); and 2) reflect recent research. This includes interacting with Department of Energy laboratories and contractors. The researchers will supply catalysts composition, performance and potential configurations. The output of this work is 1) system/configuration definition; 2) performance specifications and optimization; 3) capital cost estimation; and 4) projected hydrogen \$/kg.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- Assess cost of hydrogen production from bio-derived liquids.
- Ethanol reforming work done at H2Gen, Pacific Northwest National Laboratory, Ohio State University, and other Department of Energy-contractor institutions are considered in this work.
- This project supports hydrogen production R&D by evaluating the cost of distributed production of hydrogen using steam methane reforming of ethanol and recommending R&D pathways that are most likely to meet the Department of Energy goals.
- Distributed reforming of bio-derived liquids is seen as a potentially very important pathway for the transition to the use of hydrogen for fuel cell vehicles and other energy applications. It avoids the need for a large hydrogen delivery infrastructure while providing hydrogen produced from domestic resources with near-zero net greenhouse gas emissions.
- The analysis effort provided by this project is very important to help guide the direction of the distributed reforming research within the Department of Energy Production Program. It provides clear insight as to the cost leverages of the various options being investigated.

**Question 2: Approach to performing the research and development**

This project was rated **3.5** on its approach.

- Reformer capital costs and reformer manufacturing costs are addressed in this project.
- Department of Energy cost targets are analyzed using experimental data obtained in a number of Department of Energy-funded projects.
- Multiple configurations are examined.
- The approach is effective.
- The assumptions appear to be appropriate.
- The analysis approach being taken is excellent. The project has defined and characterized the distributed ethanol reforming technologies that are being investigated for hydrogen production. DTI is working with all the distributed ethanol reforming projects funded by Department of Energy to gather the information needed for the proper configuration and performance of these technologies. It is using sound analysis and cost estimating tools including HYSYS, DFMA, and H2A.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.4** based on accomplishments.

- Six different configurations were analyzed.
- A critical system level evaluation was carried out.
- The impact of integrated membrane on overall catalyst bed size was evaluated.
- Pros & cons of tubular and annular heat exchange reactor were examined.
- Key assumptions and observations were very well explained.
- Various process configurations have been identified, described, and compared.
- It appears that the project is on schedule and is producing the intended results.
- Excellent progress has been made on this project. The various distributed ethanol reforming technologies and process configurations have been defined and fully analyzed for cost and energy efficiencies, identifying all the key cost leverages. This information will enable the Production Program to properly guide research efforts in this area of hydrogen production.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.5** for technology transfer and collaboration.

- Collaborated and transferred data from Pacific Northwest National Laboratory, Ohio State University, and multiple Department of Energy-contractors (H2Gen, Pall, and Virent).
- DTI appears to be collaborating with most or all of the ethanol reforming projects sponsored by the Department of Energy Hydrogen Program, giving them access to current data on the technology and research.
- DTI is clearly collaborating with all the Department of Energy funded distributed ethanol reforming projects.
- DTI is reporting out on this project through the Department of Energy Distributed Bio-Derived Liquids Reforming Working Group.
- The information being generated by this project is very important to those researching distributed hydrogen production technologies and other hydrogen stakeholders. It is important for the results to reach the full hydrogen community through future meetings and/or through publication.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.3** for proposed future work.

- Since this project is going to end in September 2008, not much was presented for future work, except completing the system comparisons and examining aqueous reforming system.
- This work should be continued in FY 2009 and other options listed on slide #5 should be looked into.
- The system comparisons will allow Department of Energy to prioritize ethanol reforming R&D pathways with the most potential to achieve the targets.
- The proposed future directions appear to be appropriate.
- Future work should include some examination of non-ethanol bio-derived liquids for comparison.
- Emphasis was on wrapping up this project, and little was described beyond tasks to do that.

### **Strengths and weaknesses**

#### Strengths

- Good background in H2A analysis program.
- Good knowledge of ethanol reforming hierarchy.
- Good collaboration with multiple Department of Energy contractors.
- Collaborations with Department of Energy ethanol reforming projects provide access to the best available data on ethanol reforming processes including membrane reactors, which is very positive since the value of the analysis depends on the accuracy and appropriateness of the parameters and assumptions.

- The process comparisons presented allow objective assessment of potential ethanol reforming pathways and are a valuable tool for decision-makers to identify research priorities.
- Distributed reforming of bio-derived liquids is seen as a potentially very important pathway for the transition to the use of hydrogen for fuel cell vehicles and other energy applications. It avoids the need of large hydrogen delivery infrastructure while providing hydrogen produced from domestic resources with near-zero net greenhouse gas emissions. The analysis effort provided by this project is very important to help guide the direction of the distributed reforming research within the Department of Energy Production Program. It provides clear insight as to the cost leverages of the various options being investigated.
- The analysis approach being taken is excellent. The project has defined and characterized the distributed ethanol reforming technologies that are being investigated for hydrogen production. DTI is working with all the distributed ethanol reforming projects funded by Department of Energy to gather the information needed for the proper configuration and performance of these technologies. It is using sound analysis and cost estimating tools including HYSYS, DFMA, and H2A.
- The PI knows H2A very well and also knows how to use that code very well. Moreover, his presentation and slides were exceptional.

Weaknesses

- Partial oxidation and oxygen transport membrane were not presented; there may be other pathways that should be studied and compared.
- Much of the analysis turns out numbers in the units of dollars. Unfortunately the value of the dollar is rapidly changing, and thus the value of studies that utilize dollars is fuzzy. It might be better to invent some "basket of currencies" that would compensate for this. This is especially important for any project that uses global commodities, steel, copper, etc., and consumes fuels that are traded globally. One could also just invent a "current dollar" unit, and provide a formula to change modify result to "today's" dollars. Better yet, the calculations could be done in Joules or other engineering units, leaving the currency markets for MBA types.

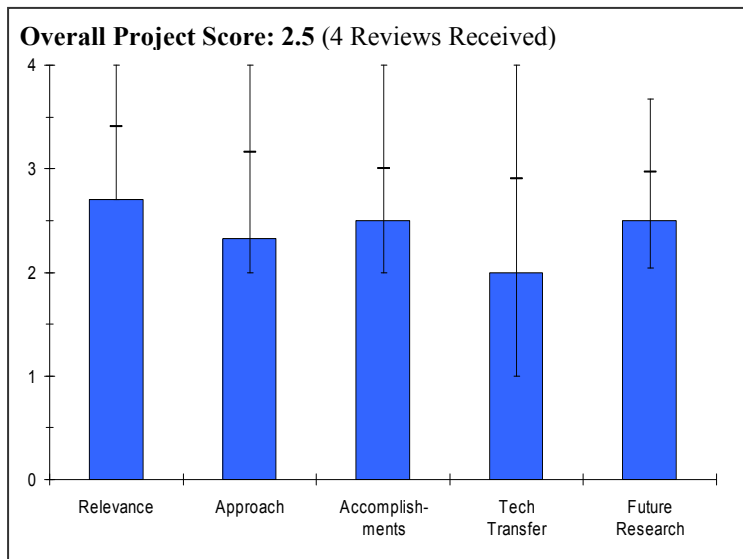
**Specific recommendations and additions or deletions to the work scope**

- Perform H2A analysis for other options listed on slide #5.
- It is surprising to see the cost numbers very close to each other for most of the options analyzed in this study. Please check for accuracy.
- Include some analysis of other bio-derived liquids besides ethanol for comparison.
- This project should be extended to cover all distributed reforming technologies for all possible bio-derived liquids. This would include; partial oxidation/fast catalysis of bio-oils, mixed alcohols and FT liquids from biomass gasification, and other bio-derived liquids; oxygen transport membrane/water splitting assisted reforming; and any other technologies or bio-derived feedstocks of interest.

**Project # PD-04: Pressurized Steam Reforming of Bio-Derived Liquids for Distributed Hydrogen Production**  
*Shabbir Ahmed; Argonne National Laboratory*

**Brief Summary of Project**

The objective for this project is to develop a distributed hydrogen production process 1) from hydrated ethanol and other bio-derived liquids; 2) using a pressurized steam reforming reactor; 3) to develop an efficient hydrogen production/purification process by reducing the hydrogen compression penalty. The rationale for this project is that steam reforming of liquid fuels at high pressure can reduce hydrogen compression costs. In addition, high pressure reforming is advantageous for subsequent separations and hydrogen purification.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.7** for its relevance to DOE objectives.

- Distributed production scale of hydrogen from ethanol and other bio-liquids (feedstock flexibility).
- Lower capital - liquid compression to obtain high pressure reforming without costs of gas compression.
- Lower capital - production and separation/purification combined in one vessel.
- Higher Yield - removal of hydrogen from reaction vessel provides more hydrogen favorable reaction kinetics.
- The work is attempting to produce hydrogen from ethanol, which is a goal of the Hydrogen Production Program. However, the results do not show much promise for this approach.
- Supports Hydrogen Initiative and Department of Energy RD&D. Rational for the project is that successful results will reduce hydrogen compression costs therefore the cost of hydrogen production. Project did not provide specific target for the cost reduction.
- Reforming ethanol makes little sense. Ethanol is too valuable in fuels to be destroyed to make hydrogen. It would make more sense for the Program to focus more on other bio-derived liquids that cannot be used in motor fuels.

**Question 2: Approach to performing the research and development**

This project was rated **2.3** on its approach.

- Very early in the development phase of a combined unit operation approach to reforming and separation/purification. The PI has correctly identified the major technical barriers in the pursuit of an advanced reactor/separator single unit operation.
- The project is attempting to conduct ethanol reforming at high pressure – which tends to increase methane production and decreases the hydrogen production. In addition, this increases cost, steam requirements and increases the potential for coke production. Overall, the approach does not appear to have much benefit, and the work does not appear to show any advantages over a lower pressure process.
- The use of high pressure to produce a high pressure product stream does not appear to be reasonable. If membrane separation is used – a low pressure hydrogen stream will be produced. Even if PSA is used – the hydrogen will be produced at a lower pressure than in the reformer and still require additional compression.
- Project approach is focused on the reduction of hydrogen compression cost.
- Technical and economical feasibility of high pressure reforming of bio-derived liquids are main focus areas to achieve the above.

- Project plans to incorporate membrane technology for the removal of oxygen, carbon dioxide and hydrogen toward achieving technical feasibility. This approach may lead to new critical research targets and new collaborations.
- Project at present is not technically feasible unless new membrane technology to remove carbon dioxide is available and will facilitate reaching the technical and economical targets of this project.
- Chose simplest of feeds. Ethanol reforming easier than for other heavier bio feedstocks. Pros/Cons of reforming at high pressure well known. High pressure only has value if easier membrane separator or less costly compression. No work balancing these factors. Should have started with simple studies to choose best pressure.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.5** based on accomplishments.

- Lab run shows >4 mol H<sub>2</sub> /mol EtOH which approaches the 70% energy efficiency goal (according to PI).
- Up to approx 5.6 mol H<sub>2</sub> /mol EtOH predicted with thinner membrane.
- Up to approx 4.5 mol H<sub>2</sub> /mol EtOH predicted with lower GHSV (gas hour space volume).
- Initial indicators are positive in terms of overall energy balance.
- Work appears to have been ongoing for two years (with a one year break). There appear to be relatively few results from the work. Some high pressure work has been conducted, and all the results indicate that the proposed approach has little benefit over a lower pressure process.
- In general it appears that most of the conversion is occurring from the pre-thermal reactions. There is some additional conversion over the catalyst - but this appears to be very limited. Some improvement may result from the added membrane separation - but again, only very limited improvement.
- The project does not appear to be achieving any of the Department of Energy targets.
- The work does not appear to address the cost of constructing a larger scale unit. However, with all the potential problems, it is likely that cost will be well above the Department of Energy cost targets.
- Project is at technical feasibility research phase, and it also seems to be at a Go/No-Go decision point. Experimental data from high pressure steam reforming of bio-derived liquids provided key results for the combined effect of temperature, pressure and space velocity on the hydrogen yield.
- Research results provided key discoveries toward objectives. Results suggest new membrane is needed to remove carbon dioxide to improve methane conversion and to yield high purity hydrogen.
- Proving methane yield up at higher pressure, hydrogen yield lower. Good technical work but not surprising. Program is generating good data but the results are not surprising. Using rhodium, palladium in process. No appreciation that these materials are outlandishly expensive and makes the approach expensive. No analysis of costs. Using expensive feed (ethanol) with expensive materials little step out potential.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.0** for technology transfer and collaboration.

- The project does not have strong collaboration outside the lab.
- Technology transfer appears very limited. No peer reviewed publications are identified. There are some limited presentations. Membranes were obtained from REB – but these appear to be low performance membranes with limited hydrogen flux (less than 10 cm<sup>3</sup>/cm<sup>2</sup>/min).
- Based on project progress status and results, there is a close coordination between PI, other Argonne divisions and REB research & Consulting.
- No evidence of collaboration.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.5** for proposed future work.

- Better performance data with the existing system (repeatability and experience) should be developed before evaluating the impacts of oxygen or carbon dioxide membranes. The PI indicates up to 5.6 mol H<sub>2</sub> /mol EtOH with palladium membrane



## PRODUCTION AND DELIVERY

- The future work is still focusing on the initial objectives from the start of the project. Little progress has been made.
- The presenter is suggesting alternate approaches such as carbon dioxide separation and oxygen membranes. It is not clear that there would be any benefit of employing these new approaches.
- The PI has planned good future work, based on the critical technical results obtained. Technically and economically feasible transport membranes are critical for this project to reach successful conclusion.
- Need to do more work on analysis. These are well known chemistry and membrane separators. Little to no work looking at costs/effectiveness.

### Strengths and weaknesses

#### Strengths

- Conceptually this is a very economic and efficient approach to bio-based reforming.
- This is a needed engineering project as it is not developing new catalyst or membranes but is building knowledge and experience in the development, design, and operation requirements of systems to produce hydrogen.
- PI demonstrates a very good understanding of the fundamentals.
- Technical feasibility research plan, execution of the technical plan.
- Critical analysis of variables affecting hydrogen yields.
- Identification of critical hurdles, i.e. carbon dioxide and oxygen transport membranes' inclusion in the future research.
- Good experimental data.

#### Weaknesses

- Scale is very small (0.07 gm/min).
- Need more (repeatability) and longer duration (degradation) runs.
- All of the results presented indicate that the use of high pressure has no benefit and in fact has a deleterious effect.
- High steam concentrations will likely be necessary, which will further increase the cost of this approach.
- Economic targets for the key processes, i.e. high temperature and pressure, transport membranes, catalyst types and quantity.
- Key Go/No-Go decision points.
- Economic feasibility target for the project is missing.
- No appreciation that costs are high due to metals. No analysis of Pressure optimization. Little step out here. Old chemistry, expensive catalysts and separators.

### Specific recommendations and additions or deletions to the work scope

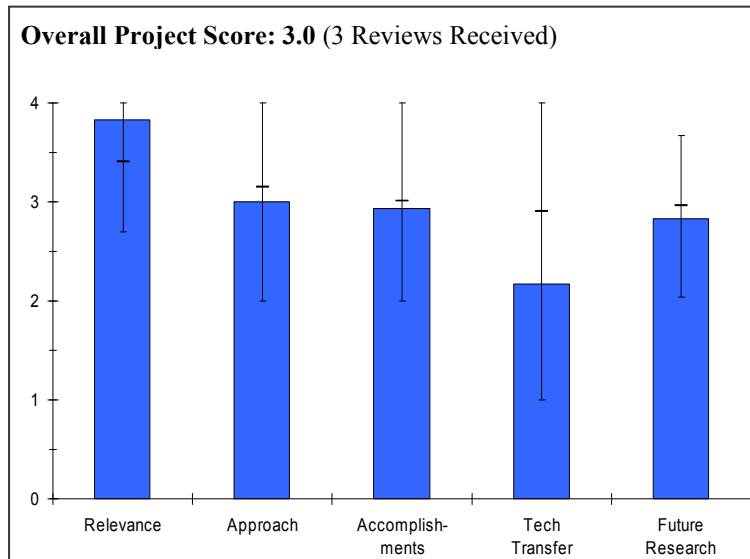
- This work needs to be published as it provides barrier indicators to others contemplating or pursuing the combined membrane reactor concept. It also provides design conditions/performance metrics for the membrane system that would be incorporated in such a system.
- Project should include studies with elevated permeate pressure in order to minimize pure hydrogen compression energy requirements.
- Investigate and measure possible ethanol decomposition in the vaporizer section. Develop controls if this is occurring.
- The work does not appear to be making any significant advancement. Department of Energy should consider terminating funding for this effort.
- Cost related key Go/No-Go milestones need to be added.
- Cost dependent technical targets need to be identified and built in to Go/No-Go decision points.
- Go/No-Go analysis for the technical feasibility.
- To be novel and add value it must step out away from ethanol and away from platinum group metals.

**Project # PD-05: Investigation of Reaction Networks and Active Sites in Bio-Ethanol Steam Reforming Over Cobalt-Based Catalysts**

Umit Ozkan; Ohio State University

**Brief Summary of Project**

The objective for this project is to acquire a fundamental understanding of the reaction networks and active sites in bio-ethanol steam reforming over Co-based catalysts that would lead to 1) development of a precious metal-free catalytic system which would enable low temperature operation (350-550°C), high ethanol conversion, high selectivity and yield of hydrogen, high catalyst stability and minimal byproducts such as acetaldehyde, methane, ethylene and acetone; and 2) enabling hydrogen production from renewable sources at low cost. Ohio State has identified the active sites and reaction mechanism and characterized the deactivation mechanism.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.8** for its relevance to DOE objectives.

- Non-precious metal catalyst development is necessary for long-term matching of Department of Energy cost targets.
- Renewable ethanol reforming is definitely part of the Department of Energy hydrogen goals.
- Developing a renewable pathway to cost effectively produce hydrogen is critical to the Hydrogen Initiative.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- Iterative approach allows feedback. What is the strategy for long-term selection of material? Inclusion of Doctor Hadad is commendable.
- Use of cobalt catalyst is good.
- Mechanistic degradation studies are very useful.
- Use of molecular simulation may provide interesting information and direction for future development.
- Need to concentrate on operating reforming conditions under more realistic case (lower H<sub>2</sub>/EtOH ratio and no diluent addition).
- Need to investigate effects of impurities on realistic H<sub>2</sub>/EtOH ratio. Would the effects be magnified with lower H<sub>2</sub>/EtOH ratio?
- Using a PSA recovery of 85% is not realistic due to limitation/requirement on impurity levels in product hydrogen stream.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.9** based on accomplishments.

- Catalyst characteristics work is impressive. Acidity has been correlated to coking (this confirms expectation).
- Reporting conversion of ethanol is not useful. Suggest mol/mol EtOH.
- Investigating lactic acid impurity effects distracts from catalyst development. Stick to one fuel (neat or impure).

## PRODUCTION AND DELIVERY

- Have made good progress in understanding failure mechanisms.
- Longer life studies need to be done- 100 hours is short, 1,000 hours would be more useful.
- They need to increase the weight hourly space velocity.
- They need to run experiments without diluents.
- Good progress in catalyst formulation and testing work and the application of H2A model to obtain preliminary cost data. Need to consider testing the catalyst for more extended period of time (more than 100 hours).

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.2** for technology transfer and collaboration.

- Still early in the development process, okay to wait for tech transfer.
- Collaboration with other academics is a positive.
- They have made many presentations and published many papers.
- Collaborations with partners outside of the university are not apparent.
- This project is in its early research stage which does not allow for tech transfer at this point. However, more collaborations with other universities/national labs might be needed to share lessons learned.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- Strength: Doctor Hadad simulation.
- Weakness: Engineering test on catalysts that is far from acceptance.
- Catalyst testing under more realistic conditions is needed and planned.
- Proposed research addresses important issues of catalyst life.
- Further testing of impurity effects under realistic H<sub>2</sub>O/EtOH ratio is warranted.
- The future work proposed is in line to address the key barriers.

### **Strengths and weaknesses**

#### Strengths

- Material characterizations.
- They are using a step-wise approach.
- Trying to understand the failure mechanisms is very important.

#### Weaknesses

- Reporting of reaction results.
- Scope is getting too broad — systems, cost, realistic conditions, time on stream...
- Research has focused on unrealistic conditions.
- They need to increase the weight hourly space velocity.
- They need to operate without any gas diluents and at higher ethanol concentration.
- Increased lifetime studies are needed, or increasing the weight hourly space velocity to do an "accelerated" test.
- Lacks realistic operating conditions so far.

### **Specific recommendations and additions or deletions to the work scope**

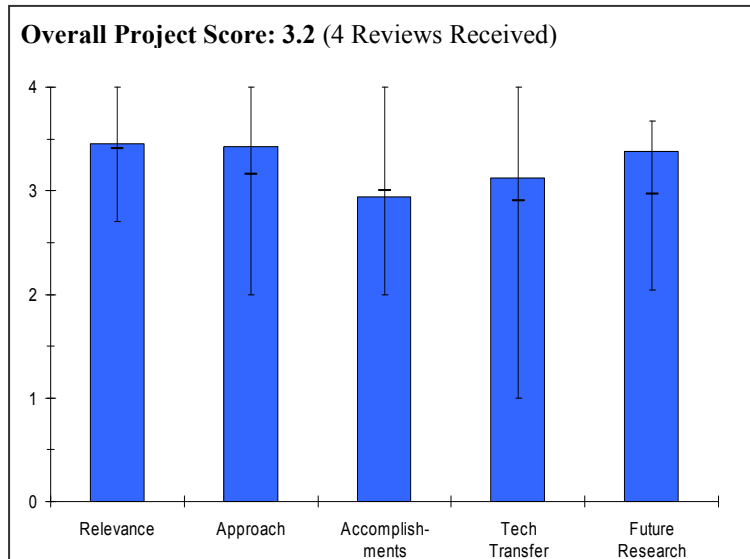
- They should de-emphasize system analysis for a catalyst development project.
- Maintain focus on catalyst formulations.

**Project # PD-07: Integrated Hydrogen Production, Purification & Compression System**

Satish Tamhankar; Linde

**Brief Summary of Project**

The overall objective of this project is to develop an integrated system that directly produces high pressure, high-purity hydrogen from a single integrated unit. The specific project objectives are to 1) verify feasibility of the concept, perform a detailed techno-economic analysis and develop a test plan; 2) build and experimentally test a proof of concept (POC) integrated membrane reformer/metal hydride compressor system; 3) build an advanced prototype system with modification based on the POC learning and demonstrate at a commercial site; and 4) complete final product design capable of achieving the Department of Energy 2010 hydrogen cost and performance targets.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- Project aligns with needs of Department of Energy Production Program.
- Hydrogen from natural gas or liquefied petroleum gas using a membrane reactor and thermal compression.
- Lower capital – combined unit operations.
- Lower energy – thermal compression with reformer heat.
- Higher Yield – removal of hydrogen from reaction vessel provides more hydrogen favorable reaction kinetics.
- The feedstock flexibility, reduction in parts counts, high hydrogen purity and elimination of compression steps all help to move the Program Multi Year Plan forward for achieving the cost and efficiency targets for hydrogen production and moves us closer to reducing dependence on foreign oil.
- Very relevant in the area of low cost hydrogen production, process intensification and flexible feedstock capable reformer.

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- Approach is very good.
- The approach combines good engineering and pilot scale testing to the complex integration of two systems membrane reactor and thermal compressor.
- The project has done well to incorporate Design For Manufacturing and Assembly (DFMA) concepts even in the current POC stage.
- The approach to minimize system components and process intensification is well in line to address the key cost barriers.
- It appears the operational issues the PI has faced so far might be contributed by an integrated approach which might not have allowed for much flexibility and controllability.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.9** based on accomplishments.

- Consider third party economic modeling of systems costs and comparing with other technologies.
- The heat exchanger shown is very novel and should be looked at for synergies in other parts of the Hydrogen Program. Also recent work with neutron analysis (analyzing fluid flow during operation) can be used to optimize design.
- Consider long-term verification testing to demonstrate robustness of system.
- Achieved conversions that were 55-60% lower than target, however system modifications (optimizing membrane to change reaction equilibrium) theoretically brings this up.
- Manufactured multi-stage, dual-line hydride heat exchanger fabricated for continuous operation.
- The fabricated equipment and pilot scale of this project provide valuable data and operational experience.
- The reduction in part counts, the ease in which the fluidized bed membrane can be modified or repaired, the leveraging of heat and mass balance all will hopefully contribute to the fully integrated system meeting the efficiency and cost goals. Further, the use of multiple feedstocks with varying levels of impurities needs validation.
- Comparing the updates of last year to this year, the PI has faced with various operational issues to get the integrated system up and running. The PI so far does not have a great deal of operational data to report.
- The issues with membrane stability, startups/shutdowns, and the ability to recover hydrogen from permeate and retentate streams to allow for 100 bar pure hydrogen remain.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- Linde is a commercial developer. I do not know if Linde plans to create a business unit to supply the technology (a plus) to the market or use it internally for their own hydrogen business development (a minus - since this would slow the market adoption).
- Linde is working closely with the membrane developer.
- Linde is working closely with the thermal compressor developer.
- Collaboration includes MRT and Ergenics Corp.; would have been helpful to partner with a university as well.
- Good collaborations with membrane and hydride compressor partners.
- Might need to have independent third party look at the hydrogen cost.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.4** for proposed future work.

- Future plans and Go/No Go decision points clearly delineated.
- Testing of the hydride compressor in-situ will provide valuable, practical data and experience.
- A previous goal was to reduce the membrane thickness but tests have shown that pinholing was a problem so settled on 25 microns. Also the modularization of the fluidized bed membrane demonstrates systematic progression.
- Go/no go decision on next phase should also consider a run hour target that the system must achieve (without performance loss) and a full analysis of the impurities in the product hydrogen stream to confirm that it meets fuel cell grade (current 50 ppm on some impurities might be too high).

### **Strengths and weaknesses**

#### Strengths

- The system is built from off the shelf components.
- Novel heat exchanger.
- The scale of this project provides a very good basis for testing and collecting performance design data and building economic models (particularly compared to the many lab / table top projects).
- Good run times (>100 hrs), good experience gained.
- This is really two projects in one: membrane reactor combinations and the integrated hydride compressor.

- The collaboration appears to be a mutually beneficial partnership.
- A good pathway/approach to reducing capital cost.

Weaknesses

- Limited testing for 100 hours.
- System sensitivity to impurities not addressed.
- The project depends on good membrane performance, tolerance to coking and life. Longer runs are needed.
- Still have not validated integrated system.
- The unintended consequences of the integrated approach might be increased control complexity; durability/lifetime issues (increased operating costs).

**Specific recommendations and additions or deletions to the work scope**

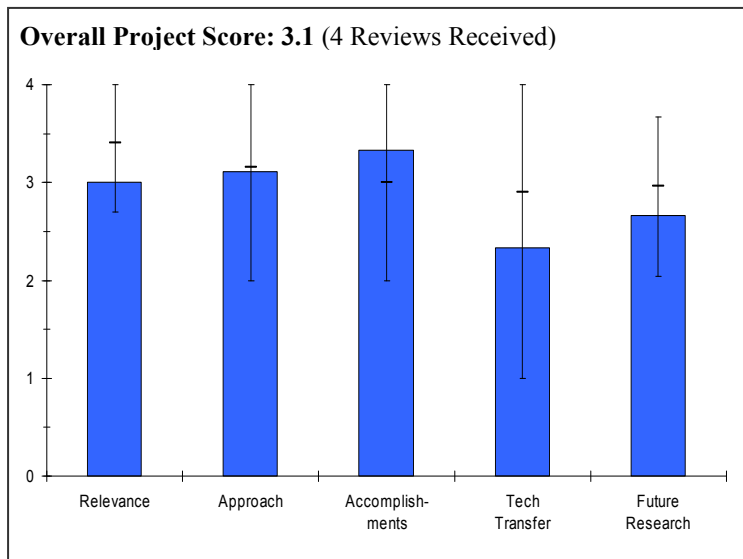
- Consider adding economic analysis and energy balance for process under development.
- Complete integrated installation (i.e., installation of the hydride compressor) and obtain run times >100 hours.
- Need to set a run hour target that the system must achieve (without performance loss) before moving to next step.
- Conduct a full analysis of the impurities in the product hydrogen stream to confirm that it does meet fuel cell grade (current 50 ppm on some impurities might be too high).

**Project # PD-08: Zeolite Membrane Reactor for Water-Gas-Shift Reaction for Hydrogen Production**

*Jerry Y.S. Lin; Arizona State University*

**Brief Summary of Project**

The overall objective of this project is a fundamental study for the development of a chemically and thermally stable zeolite membrane reactor for water-gas shift reaction for hydrogen production. The specific project objectives are the 1) synthesis and characterization of chemically and thermally stable silicalite membranes; 2) experimental and theoretical study of gas permeation and separation properties of the silicalite membranes; 3) hydrothermal synthesis of tubular silicalite membranes and gas separation study; and 4) experimental and modeling study of membrane reactor for water-gas shift reaction.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.0** for its relevance to DOE objectives.

- The objective was to increase yield & lower capital costs. This could be done by removal of hydrogen via membrane from reaction vessel provides more hydrogen favorable reaction kinetics.
- The work was on developing a membrane for separations.
- The work is focusing on the development of a hydrogen separation membrane for use with the water-gas-shift reaction. This is a need for hydrogen production and addresses both hydrogen separation and process intensification. The work supports the Department of Energy Hydrogen Program objectives.
- Unfortunately, the approach will not produce a high purity hydrogen stream (or a high purity carbon dioxide stream). The best H<sub>2</sub> separation factor appears to be around 65 (with reasonable permeance - although below the target level). It is highly likely that a subsequent polishing step will be required and this may have a large impact on the overall cost.
- If other impurities are present in the stream (for example - sulfur), this will also diffuse through the membrane to some extent and additional clean up steps may be necessary for both the hydrogen and carbon dioxide streams.
- Project supports critical cost reduction goal of distributed hydrogen production from natural gas and renewable liquids.
- Project qualitatively anticipates that successful results will achieve Department of Energy hydrogen production cost targets.
- Specific project targets need to be provided toward achieving hydrogen production cost targets i.e., \$1.60/gge at the plant gate by 2012.
- Material development in the photoelectrochemical arena is clearly relevant, especially if such materials could improve over photovoltaics/electrolyzer systems (not sure why funding by Department of Energy is inconsistent).
- Use of iron oxide alloys is a good start, but not particularly innovative and mixed oxides may not have been considered early enough.

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- Approach is to modify zeolites. Researchers keep working with zeolite which is 25 + years old. What are needed are new materials and structures.
- The microwave synthesis and CVD for membranes may be applicable to hydrogen production from other materials.
- This is a fundamental university/academic effort that will provide a moderate purity hydrogen product. This is a reasonable project for a university and the work appears to be obtaining some good data and results.
- The hydrogen purity will be somewhat low. Department of Energy was probably aware of this when the project was selected.
- It is highly unlikely that the work will provide significant data to evaluate scale-up.
- Good technical project plan.
- Technology seems to be technically feasible. Cost analyses needs to follow to validate that the successful technical results yield significant reduction in hydrogen production toward achieving Department of Energy cost target.
- Solid, systematic approach and selection criteria.
- It is not clear how the materials selection process leads to practicable large-scale reactions.
- It is not clear how the different morphologies lead to different properties, except for area and path length effects.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- The experimental zeolite selectivities (hydrogen separation factor -  $H_2/CO_2$ ) are 50, compared to 20,000 for palladium. This low separation factor will require multi-stages or other equipment (both adding costs) for down stream hydrogen purification.
- The work has led to some advancement in membrane preparation (CVD and microwave techniques). The performers have prepared tubular membranes and have conducted a number of tests with the prepared membranes. Thin active layers - 3 micron - have been prepared on supports.
- Testing has been conducted with gas mixtures and has shown the ability to achieve separation. Including water in the feed was also an important factor.
- The work has been flexible enough to change the membrane composition when the original materials performed lower than expected.
- Tests have indicated that the membranes are resistant to sulfur compounds and this is an important factor for membrane lifetime.
- The work has identified some new water-gas-shift catalysts with about the same performance as commercial materials.
- The work has demonstrated separation above Knudsen separation levels, which demonstrates that some form of selective adsorption is in effect.
- Project accomplished majority of its Phase 1 milestones.
- Project reported good results and accomplishments towards technical milestones.
- Progress report on Department of Energy barrier for the hydrogen cost reduction as a result of the technical accomplishments needs to be clearly discussed.
- Targeted hydrogen selectivity of 50 will potentially provide significant reduction in hydrogen production cost. Project objectives should include resulting economic accomplishments.
- High throughput screening achieved.
- Somewhat Edisonian approaches to processing and synthesis methods which led to different hematite phases but similar to XRD's - why?
- Not clear why the different surface treatments lead to different IPCE's (and whether such structural variations are metastable).

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.3** for technology transfer and collaboration.



## PRODUCTION AND DELIVERY

- The researchers need some industrial partners, currently it is composed of only university partnerships.
- The performers have been very active in publishing the results of their work and indicate 36 publications - many in peer reviewed journals.
- The project lacks any input from industry. All of the participants are academic. It would be a major benefit to collaborate with an industry partner to get a commercial perspective. It is unlikely that any commercial product will result without this type of collaboration.
- Project progress report suggests that there is some coordination between collaborators.
- Although a member of the photoelectrochemical working group, the paper does not show clear collaborations with theoreticians for Density Functional Theory (DFT) modeling, nor with the other teams.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.7** for proposed future work.

- The project needs to directly address the overall production of hydrogen using the membrane/reactor system.
- The project needs to show membrane performance targets that directly relate to economic hydrogen production and purification.
- The work is following the original work plan and appears to be on schedule. The future work will evaluate the membrane separation under water gas shift conditions - which was the objective of the project.
- The near-term work should consider testing at higher pressures. Pressure could have a significant impact on the separation factor.
- Plans are exclusively for the technical improvements of the proposed technology.
- Economic feasibility and addressing Department of Energy hydrogen production-related cost reduction targets need to be included in project's future milestones.
- Recognition that hematite modifications may not be fruitful?
- Move to other mixed oxides appropriate.
- Need for continued post-processing modifications; but there must be attempts to correlate performance to structural changes due to such surface modifications.

### **Strengths and weaknesses**

#### Strengths

- It appears to be a very good academic team, strong fundamentals in zeolite structure and chemistry.
- They have expanded the current vast body of knowledge on zeolite use in membranes and have designed a reactor test unit to hold a tubular membrane.
- This is a good academic scale project that is providing some solid fundamental information.
- Synthesis and modification of silicate membranes for separating hydrogen and carbon dioxide produced by water-gas-shift reaction.
- Research and analysis of technical feasibility of silicalite and DDR Zeolite membranes.
- Production of silicalite membranes with high H<sub>2</sub>/CO<sub>2</sub> perm-selectivity, potentially over 50.
- New water-gas-shift catalyst with improved chemical stability for sulfur dioxide and hydrogen sulfide.
- Solid, systematic piece of work.
- Clear progress on showing changes to surface area, path lengths, and effects of electrocatalyst additions.
- While only conceptual, the project discussed reaction design process.

#### Weaknesses

- Membrane hydrogen selectivity is low at 50.
- They need to envision and model the entire system. What equipment and costs will be required to obtain commercial hydrogen purity if this membrane is used?
- Ultimate system scale (area per unit of hydrogen) is likely to be high and costs need to be determined.
- 10 atm operating pressure will limit tube diameter/design and likely increase costs.
- The work needs to address the final potential costs. This should be done with an industry partner.
- There will be a problem with the hydrogen purity if it is to be used with a fuel cell.
- Comparison with other existing and on-going similar technologies in terms of technical and economic advances.

- Economic analysis of the accomplished technical advancements.
- Milestones related to the hydrogen production cost are not included.
- No clear guidance from theoretical calculations (DFT).
- Somewhat singular focus on the hematite systems.
- The project needs new hosts.

**Specific recommendations and additions or deletions to the work scope**

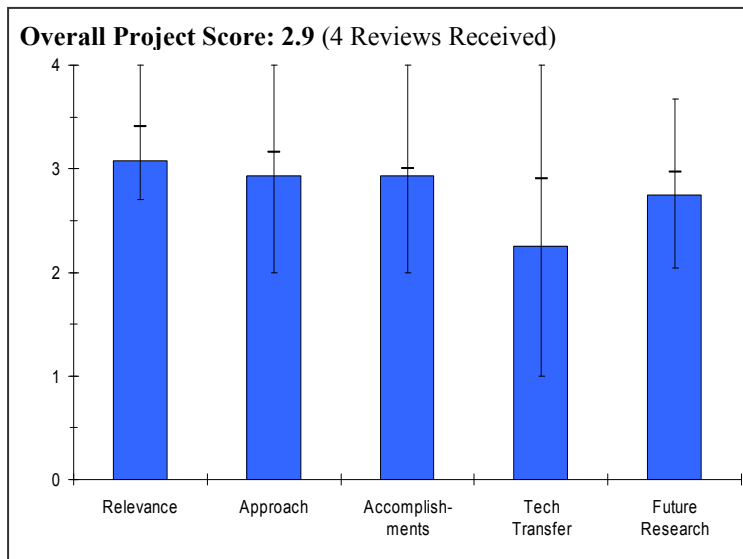
- A back of the envelope calculation of total equipment needed and costs to meet hydrogen purity requirements should be performed. A calculation of the "practical" selectivity and permeability values should be made and the project should address the barriers that must be overcome to reach those practical values.
- Project needs to focus on the membrane reactor system and product purity requirements. Currently the focus seems to be mostly on membrane fabrication.
- Multi-lumen tubes are a geometry that can boost area while lowering costs. This may be an option to bring zeolite membranes into practical/economic operating ranges.
- Include examining the effect of increased pressure as soon as possible.
- Cost reduction-related milestones need to be added.
- Discussion and analysis of project results and targets in reference to other similar technologies in terms of technical and economical advancements.
- The project should include Go/No-Go decision points to address key technical and economical milestones.
- The project should move to mixed oxides (ternary systems).
- The project needs to secure consistent funding support.

**Project # PD-10: Low Cost, High Pressure Hydrogen Generator**

*Monjid Hamdan; Giner Electrochemical Systems LLC*

**Brief Summary of Project**

The overall objective of this project is to develop and demonstrate a low-cost, moderate pressure proton exchange membrane water electrolyzer system that 1) reduces stack capital costs to meet Department of Energy targets; 2) increases electrolyzer stack efficiency; and 3) demonstrates 1,200 psig electrolyzer system. The objective for the past year was to field test the electrolyzer system at the National renewable Energy Laboratory. Further development of a high-strength, high efficiency membrane is recommended. Development of a low-cost, long-life separator is required.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.1** for its relevance to DOE objectives.

- Design & Development of PEM electrolyzers is an important area, not just for water electrolysis, but also for application in thermochemical cycles.
- Clearly a relevant project, but there are already proton exchange membrane-based electrolyzers that are commercial (e.g., the DESC systems-the "old" Proton Energy systems).
- The project needs to clarify why the Giner approach is different from those of Proton and Stuart, and others.
- While the objectives are relevant, the project seems to be limited to bringing Giner Electrochemical Systems, LLC up to cost parity with others in the proton exchange membrane electrolysis community and towards parity with alkaline technology.
- To be significantly relevant, the technology must be economically scalable to hydrogen production rates several orders of magnitude higher than is being addressed.
- Electrolysis is one of the key current hydrogen production methods for decentralized hydrogen (no major hydrogen infrastructure required).
- Decreasing capital cost and improved efficiency (two major barriers) are addressed by this project.
- Cost of electricity is a major issue to economic deployment. The Giner Electrochemical Systems, LLC proton exchange membrane stack electric cost is projected to be 30% less costly.
- Validation of the improved stack performance has been completed at National Renewable Energy Laboratory.
- The 2007 testing has generally achieved the Department of Energy targets for distributed water electrolysis.
- The capability to meet the 2012 and 2017 Department of Energy targets was orally discussed.

**Question 2: Approach to performing the research and development**

This project was rated **2.9** on its approach.

- Nice job. Especially in enhancing efficiency and complexity of components while simultaneously improving components' performance.
- The technical approach provides a good pathway to show the improved performance of the advanced membrane and overall electrolysis cell.
- This is the end of the current program – additional experimentation and required scale-up will be performed under a new contract.

- Reducing complexity of the system through parts-count reduction. Simplified anode/cathode side membrane support structure fabrication by reducing assembly from nine parts to one single piece. Incorporated thermoplastic cell frame - molding process reduces cell cost by 40%. Total cell stack reduction of 40+ parts to sixteen parts.
- Developed lower-cost materials and fabrication methods for cell components, increased operating current density and systems innovations to replace high cost, high maintenance components. National Renewable Energy Laboratory validation testing of cell has not included DSM in last test campaign.
- The approach does not address life, durability or scale-up questions of the membrane/cell.
- The choice of 1200 psig operating pressure seems arbitrary, without a rationale.
- Good breakdown of where the improvement could be made component-wise, but where are the major innovations?
- Titanium separation example is good; but need to explain its limitations.
- Support structure for 2-mil "Nafion" is meaningful only if the system is subject to cyclic testing - steady state tests will not reveal weaknesses such as de-lamination, etc.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.9** based on accomplishments.

- They reported very good progress, one question is why large difference between the Giner Electrochemical Systems, LLC tested cell performance & the stack performance?
- They demonstrated advanced membrane in 160 cm<sup>2</sup> cell and demonstrated 28 cell unit that produced 0.25 kg/hr at 1200 psig at National Renewable Energy Laboratory.
- National Renewable Energy Laboratory validation testing of cell have not included DSM in last test campaign.
- Short term results are better than comparison cell – potential improved performance at lower pressure and lower cost – limited information provided on National Renewable Energy Laboratory tests.
- Additional data is needed, including longer term durability operation.
- Further scale-up is required (possible two cell area scale-ups).
- Use of thermoplastic and molded components has been practiced by other companies already.
- Use of thinner membranes has been done before.
- DSM approach has not been thoroughly checked out, relative to long-term durability.
- The Program seems to have advanced Giner Electrochemical Systems, LLC proton exchange membrane capability, but has not advanced the state of the art.
- Advancements of membrane life and system costs are based on analysis/claims/projections and not demonstrated performance.
- The operating pressure is not significant.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.3** for technology transfer and collaboration.

- It's not clear that the accomplishments indicate a successful team.
- General Motors and Center for Technology Commercialization are partners. General Motors has provided membrane information and expertise on other components. Nothing mentioned about scale-up or mass manufacturing.
- The role of other partners is not clear (General Motors was a cost-share partner and helped with bipolar plates and membranes; but General Motors' interests are in fuel cells, not electrolyzers.) Center for Technology Commercialization role is unclear.
- Not sure if further tech transfer programs are being conducted.
- There is no evidence of outside collaboration other than cost sharing.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

## PRODUCTION AND DELIVERY

- Development of new membranes under the new grant is a step in the right direction.
- This is the end of the current program - additional experimentation and required scale-up will be performed under a new contract.
- The performer identifies that work will be continued to develop the lower cost, high efficiency membrane with emphases on continued reduction of stack capital cost and stack scale-up to a 290 cm<sup>2</sup> active area.
- Giner Electrochemical Systems, LLC acknowledges and identifies areas that need progress, but a significant portion only brings Giner Electrochemical Systems, LLC proton exchange membrane to cost parity with others.
- Longer duration runs will be performed.
- The program details are not discussed.
- Program is complete.
- Need greater clarity as to: Giner productivity more for the market places? Beyond National Renewable Energy Laboratory testing, what next?

### **Strengths and weaknesses**

#### Strengths

- Development of improved components. Meeting major milestones.
- Approach to reducing capital cost of the electrolysis cell membrane system by reducing separate parts is an excellent approach.
- Experimental cell valuations appear to be making good progress.
- Costs are expected to be lower – particularly electricity cost, which is a major concern with distributed electrolysis.
- Based on the progress reported, Giner Electrochemical Systems, LLC appears to have the technical competency required to eventually complete the work.
- Well explained.
- Good component-by-component improvement.

#### Weaknesses

- Stack performances were much lower than cell performances and the differences were not explained?
- Electrolysis requires inexpensive electricity to meet the Department of Energy target goals.
- Need more details on National Renewable Energy Laboratory evaluation and future work.
- Still needs additional experimentation and scale-up to validate 2010 Department of Energy target.
- The project starts out behind the state-of-the-art and behind other technologies and has not yet caught up or advanced.
- The PI needs to develop "system-integrated" improvement plans.
- The PI needs to clarify the roles of partners and how active were the collaborators in this program.

### **Specific recommendations and additions or deletions to the work scope**

- If the project is to be continued, high emphasis needs to be placed on membrane durability and life.
- Operating pressures should either be lowered to 100-400 psi or raised to greater than 5,000 psi.
- Water electrolysis programs (to make sense) must be tied to possible direct DC renewable sources. Otherwise, water-electrolyzers are indeed items in commerce already.

**Project # PD-11: Hydrogen Generation from Electrolysis: 100 kg H<sub>2</sub>/day Trade Study**

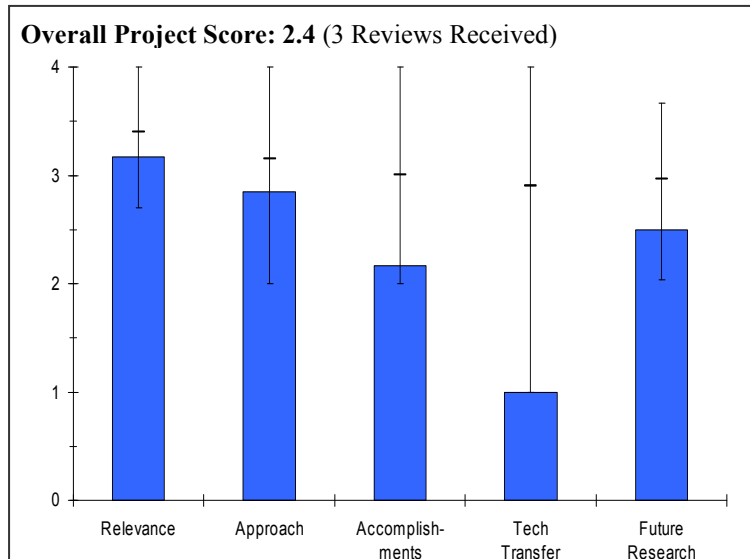
*Stephen Porter; Distributed Energy Systems*

**Brief Summary of Project**

The objectives of this project were to 1) establish a pathway to larger proton exchange membrane systems (100 kgH<sub>2</sub>/day with growth to 500 kgH<sub>2</sub>/day); 2) optimize for capital cost and energy efficiency (emphasis on cell stack and power supply); and 3) refine focus area for future research. Proton Energy Systems performed trade studies and made a conceptual design of a 100 kgH<sub>2</sub>/day electrolyzer.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.



- The work supports the Hydrogen Initiative to a limited extent.
- Economic scale-up, not technology, is a major hurdle for water electrolysis to produce hydrogen. Proton Energy Systems builds and sells commercially 12kg/day hydrogen production units into niche markets. Project addressed scale-up (value-engineering) of their systems for the distributed hydrogen fuel market.
- Proton exchange membrane electrolytes – good topic for R&D; useful for water electrolysis and for thermochemical cycles.

**Question 2: Approach to performing the research and development**

This project was rated **2.9** on its approach.

- Have identified barriers, but the barriers are not new. High capital cost, low system efficiency, difficult integration schemes with renewable electricity generation system are some known barriers.
- Not much suggestion on how to overcome the barriers.
- No suggestion that is new and different from known efforts to overcome the barriers.
- Very linear engineering process approach to scale-up. Would have been nice to pursue some ‘what ifs’, which really go outside the envelope.
- The approach adopted is good.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.2** based on accomplishments.

- The work scope was rather limited.
- The presentation materials are confusing. It appears the electrolyzer capital cost in 2011 is 1,676 \$/kW and the Department of Energy target for a scaled-up unit in 2012 is 400 \$/kW. No discussion or explanation given how the Department of Energy target can be accomplished in one year.
- Identified the integration of optimal power supply and cell stack designs (stack size and operation in series) as the key trade-offs.
- Final results do not meet Department of Energy 2012 targets in terms of energy efficiency, hydrogen cost or capital costs.
- Good accomplishments though efficiency appears to be low.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **1.0** for technology transfer and collaboration.

- This information is not available in the presentation. It is assumed that most work is done at the sponsoring organization.
- Optimization of their own technology, in-house.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.5** for proposed future work.

- This project is complete; future focus areas are relevant.

**Strengths and weaknesses**

Strengths

- Project is COMPLETE.

Weaknesses

- Project is COMPLETE.

**Specific recommendations and additions or deletions to the work scope**

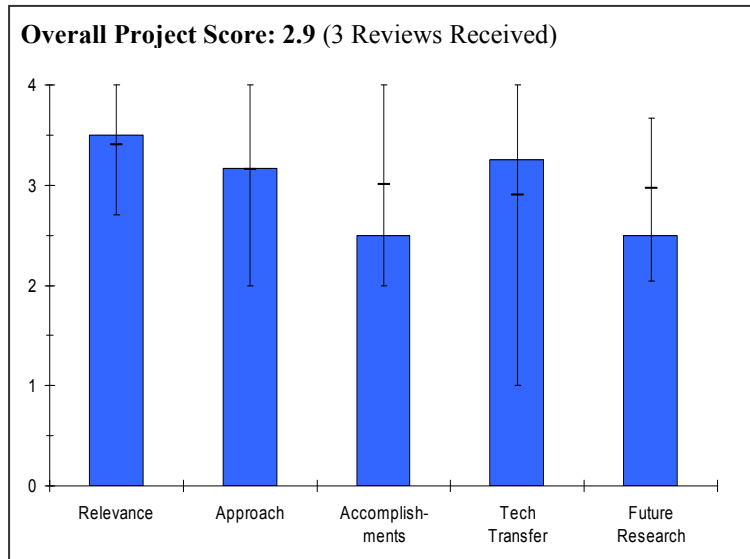
- Project is COMPLETE.
- Future work should also include membrane/catalyst work to enhance efficiency (if possible).

**Project # PD-12: Development of Water Splitting Catalysts Using a Novel Molecular Evolution Approach**

Neal Woodbury; ASU

**Brief Summary of Project**

The objectives of this project are to 1) design and synthesize a peptide based electrocatalyst for water splitting using principles learned from photosystem II; 2) optimize the function and stability of this electrocatalyst through iterative creation and analysis of libraries; and 3) develop efficient water splitting catalysts required for effective electrolysis. Arizona State has designed metal binding peptide to use as starting sequences and has demonstrated the utility of light directed synthesis methods for creating libraries of peptides. Additionally, electrochemically directed synthesis of peptides with a limited number of side chains has been developed.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- The use of biological and biologically inspired materials holds a lot of promise for new materials for water splitting.
- This work uses a novel approach to develop manganese-based water splitting catalyst systems and is in line with Department of Energy objectives.
- The project appears relevant, but the presentation lacked information on why this method is better than existing methods.
- The project aligns well with the President's Hydrogen Fuel Initiative in its effort to develop an efficient catalyst for splitting water into hydrogen and oxygen.
- It is expected that the catalyst coating on an electrode will help drop the required voltage of 2.2 volts of electricity required to produce hydrogen to 1.3 or 1.2 volts, which would be an energy savings of 40 percent.
- This aligns well with the overall Department of Energy goal to produce hydrogen at lower cost.

**Question 2: Approach to performing the research and development**

This project was rated **3.2** on its approach.

- The milestones and technical barriers are clearly laid out for the project.
- They have integrated high throughput methods to address a focused issue of creating and understanding a metal cluster binding environment and associated activity.
- They have abandoned light directed synthesis in favor of chip based combinatorial synthesis which has allowed the project to move forward.
- Approach seems logical. The CombiMatrix approach allows direct synthesis on addressable electrodes.
- The technical approach is logically laid out through six milestones to develop improved catalysts.
- By observing nature where photosynthesis catalysts aid the conversion of carbon dioxide in the air into sugars, the project team is evaluating potential manganese-based catalysts.
- Peptides will be used to develop an array of material combinations as potential catalysts. The best catalysts should be selected and tweaked for further testing and development.



**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.5** based on accomplishments.

- They have made some progress towards addressing their project goals.
- They have not yet shown water splitting and it is not clear just how close they are to achieving this goal.
- They have borrowed and successfully integrated chip-based chemistry with computer aided design to create libraries, which can be used to probe interactions well beyond their initial manganese cluster concept.
- To date, there are not a lot of results.
- Net result: no difference between control and test peptides with no explanation if this is a good or bad result.
- Progress is satisfactory on the establishment of a baseline for evaluation.
- Encountered challenges with chemical deposition methods of catalysts on electrode surfaces.
- Developed an alternate method for deposition based on electrochemical synthesis.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- They have demonstrated collaboration with chip manufacturers and addressable electrode system manufacturers.
- There is one non-governmental partner (CombiMatrix Corporation) and one academic partner. Technology transfer into a commercial venture might occur through CombiMatrix, but it is unclear if this company is large enough to secure private sector financing and implement product development, manufacturing, and sales/marketing.
- Significant R&D may be needed before this concept becomes commercially feasible and attractive for investors.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.5** for proposed future work.

- They have identified an approach for the synthesis, and the future work will focus on resolving some of the teething issues with the new technology (side chain effects, surface preparation, synthesis approaches).
- It's not clear how this will lead to advancements.
- The proposed future research appears sufficient to reach the milestones.
- Given that this work is fundamental, the final end product should be more clearly defined to determine if further research in this area is warranted.

**Strengths and weaknesses**

Strengths

- They have developed a rich platform technology that can be applied to focused combinatorial screening of structure function relationships.
- Good approach to testing large numbers of samples.
- The project PI is aware of current issues facing his research efforts, e.g. the instability of the electrode surfaces to chemical synthesis procedures, and he is developing alternate synthesis methods.
- Teamed up with CombiMatrix and Dr. Bill Armstrong for help and guidance on the use of electrochemically directed synthesis (as opposed to light-directed synthesis in their original plan).

Weaknesses

- It is not clear that this approach and the results achieved so far will allow this team to achieve a viable water splitting device.
- In particular, the new approach shows no difference between control and test peptides +/- manganese.
- There was not enough in the presentation discussing the potential impacts of this work.

- The effort to understand, replicate, and translate a natural process catalyst that facilitates the conversion of carbon dioxide into sugars into a usable coating on an electrode to aid water spitting is somewhat ambitious to be accomplished within the remaining one year timeframe.

**Specific recommendations and additions or deletions to the work scope**

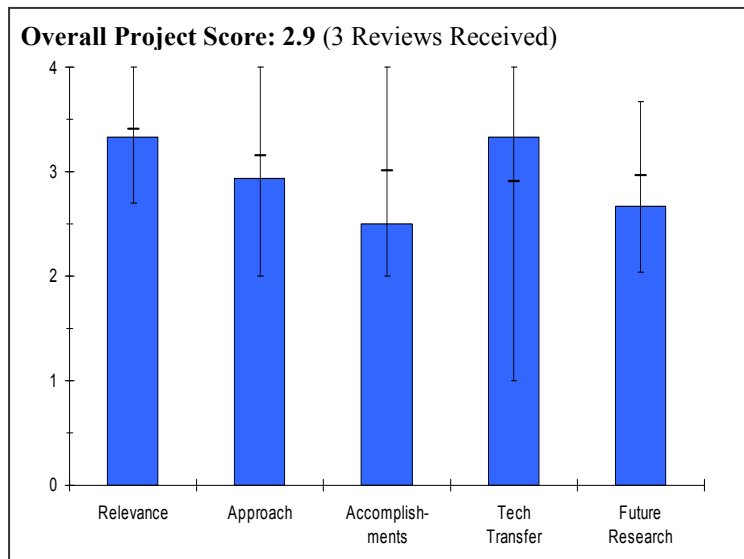
- Some Go/No-go criteria should be established to determine if this concept warrants further investigation. The concept itself appears reasonable, but other competing technologies within the entire spectrum of hydrogen production might render this approach (and hence this research effort) unwanted.

**Project # PD-13: Development of Solar Powered Thermochemical Production of Hydrogen from Water**

*Nate Siegel; STCH Collaboration*

**Brief Summary of Project**

The overall objective of this project is to select one or two cost competitive solar powered hydrogen production cycles for large scale demonstration. The specific objectives of this project are to 1) develop solar receiver concepts; 2) perform experimental validations of the key components of prospective cycles; and 3) produce economic models of all prospective cycle using a common methodology and assumptions. The feasibility studies are progressing and the solid particle receiver has been demonstrated. Other receiver concepts are nearing demonstration and the H2A analysis is underway.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- Thermal chemical water splitting for hydrogen production is within the Department of Energy Hydrogen Program project portfolio.
- The project addresses the application of solar thermal energy to the production of hydrogen.
- It does not appear to be on a critical pathway, even within the production/delivery portfolio.
- Making hydrogen from high temperature heat must be of interest.

**Question 2: Approach to performing the research and development**

This project was rated **2.9** on its approach.

- They developed the different chemical cycles to the point where a techno-economic analysis could be made which was used in the down-selection process.
- The development focused on cycles, materials and reactors, which are the correct areas.
- Consideration should be given to decreasing operation and maintenance requirements.
- More work should be done on long-term stability.
- The project appears to address the barriers, especially U and X.
- The project appears to be doing a good job at integrating work that is being done at several facilities.
- It appears that the selection of possible cycles was made at an earlier date. It would have been helpful to review the criteria used and to discuss how each of these materials meet the criteria. For example, was mechanical strength an issue, or particle density? How about particle size? Thermo?
- What will be the criteria used in the Go/No Go decision on continuing work with any given thermochemical cycle?
- STCH has assembled an excellent collection of collaborators, continuing work on an old, and well-studied problem. The current emphasis is a design-to-cost effort, with some laboratory scale exploration of key unit operations. As before, projected unit operations remain technically challenging.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.5** based on accomplishments.

- Technical progress has been made on developing the different cycles, but after five years, more progress would be expected.
- H2A analysis has been done on several of the cycles; it needs to be done on all of the cycles.
- The H2A analysis should include operation and maintenance and spent material disposal costs.
- Standardized method for calculating efficiency needs to be made.
- Materials development for the reactors and receivers needs to be addressed.
- Material degradation and long-term stability need to be investigated.
- It appears that smaller particles give better performance; what is the limit envisioned in terms of handling fine powders?
- Because so many cycles were being developed, it was difficult to assess progress in any one area or with any specific material. It would have been more helpful to focus on one material as an example and treat in depth, in order to provide the reviewer with a better understanding of the depth of the investigation, criteria used for Go/No Go, etc.
- At this stage of development, it is difficult to assess how seriously to take any H2A analysis unless critical assumptions are also listed.
- Planning and economic projections have gone well. However the technical challenges remain. The plan is to down-select to one (or perhaps two) of the reaction schemes and then pour all efforts into that concept. This could work. However if all the remaining concepts have problems, then that down-selected concept has problems. The team should have concluded they will select zero or one.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- There seems to be strong interaction between the participants with defined roles.
- The degree of collaboration appears to be quite good, involving several partners. It is less clear how technology transfer will be done and what companies are possible collaborators. Perhaps it is too early to assess this latter aspect.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.7** for proposed future work.

- Life time studies on the materials in the extremely aggressive environment need to be done in order to understand the operation and maintenance costs.
- Down-selection is very important to focus the limited resources on the most promising chemistries.
- Thermal management and storage for improved efficiency and 24/7 operation is needed.
- The proposed future research is sufficiently vague and generic to make any meaningful assessment or offer helpful suggestions. Seems basically OK.
- There didn't seem to be a route that accepted the reality of an "unsolved technical barrier".

**Strengths and weaknesses**

Strengths

- Strong team that has begun working together.
- Down-selection to the most promising technologies is in the plan.
- Strength is involvement of many groups, potentially bringing in new ideas and approaches.
- This group has considerable technical horse (people) power.

Weaknesses

- Materials durability is not directly addressed, at least not in this presentation.
- It is unclear if the H2A analysis includes all of the costs for operation and maintenance, thermal storage capital equipment, heliostat maintenance, and materials disposal.

## **PRODUCTION AND DELIVERY**

- Weakness is also involvement of so many groups. It is not clear how decisions will be made and how strong the leadership is to move this project forward and to make tough decisions.

### **Specific recommendations and additions or deletions to the work scope**

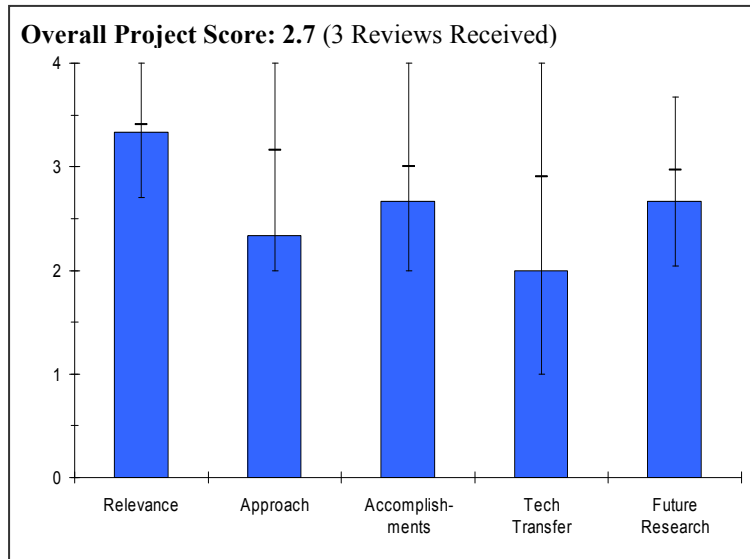
- None

**Project # PD-14: Solar-Driven Photocatalytically-Assisted Water Splitting**

*Ali T-Raissi; UCF/FSEC*

**Brief Summary of Project**

The objectives of this project are to 1) evaluate photo/thermo-chemical water splitting cycles that employ the visible portion of the solar spectrum for production of hydrogen; 2) select a cycle that has the best potential for cost-effective production of hydrogen from water (Department of Energy target of \$3.00/kg H<sub>2</sub>); 3) demonstrate technical feasibility of the selected cycle using solar input in a bench-scale reactor; 4) demonstrate pre-commercial feasibility via a fully-integrated pilot-scale solar hydrogen production system; and 5) perform economic analysis of the selected cycle.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- Solar driven thermochemical water splitting for hydrogen production is within the Department of Energy Hydrogen Program's plans.
- As a process for non fossil fuel hydrogen generation: An interesting combined use of photocatalytic and thermal processes for water splitting.
- This project explores a hydrogen generation technology, an area that is not currently emphasized by the Department of Energy as "relevant", even though conventional fuel supplies are limited.

**Question 2: Approach to performing the research and development**

This project was rated **2.3** on its approach.

- Approach seems reasonable, focusing on the key gaps in a methodical manner.
- Economic analysis is very important.
- While the investigators' approach to water splitting is reasonable, their claim to a 51% efficiency for the process is highly suspect: If visible light in 20% of the spectrum is used to generate hydrogen, the reported kinetically limited step in water splitting, then the efficiency cannot be greater than 20%.
- This project explores a well-explored thermochemical cycle for "water splitting". This cycle uses ammonia and sulfur and a variety of unit operations, including one critical step driven by solar energy. This cycle has been described for several decades and has proven difficult to optimize. The project strives to beat a hydrogen production target of \$3/gge, and thus involves some effort on system design and capital cost estimates.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- The project started Sept. 2007, but they have made solid progress.
- Initial cost analysis is promising.
- The researchers need to increase work on reactor and receiver designs.
- The researchers need to do economic analysis of the current system using current efficiencies.

## PRODUCTION AND DELIVERY

- The project has only recently started and they have done a good job. Their planned methodology for partitioning the sunlight could have been better explained.
- The work was completed on a laboratory scale photochemical experiment but no indication apparent of measuring rate of reaction. Engineering analysis work done using a standard program that indicated that the \$3 target might be addressed. However, the project efficiency numbers for the photochemical step were incorrect; if so the economic analyses are flawed, because the solar collection hardware is too small to provide necessary solar energy to prompt the hydrogen synthesis. The experimental tasks seemed to be in only early phases.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.0** for technology transfer and collaboration.

- They have published many papers.
- SAIC's participation is unclear.
- In cooperation with Solar Concentration System Development – about which little was said.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.7** for proposed future work.

- They need to close the cycle.
- They need to consider scale-up needs.
- Current efficiencies need to be reported as well as the efficiency of model systems.
- Must address and connect their claimed energy efficiency estimates.
- The proposed work will explore two unit operations, generating data to support the system engineering design.

### **Strengths and weaknesses**

#### Strengths

- The cycle is using solar energy directly unlike other cycles which use the solar power as heat.

#### Weaknesses

- Their efficiency analysis should use the entire solar spectrum.
- Discussion on scale-up is needed, especially in using solids and light splitting.

### **Specific recommendations and additions or deletions to the work scope**

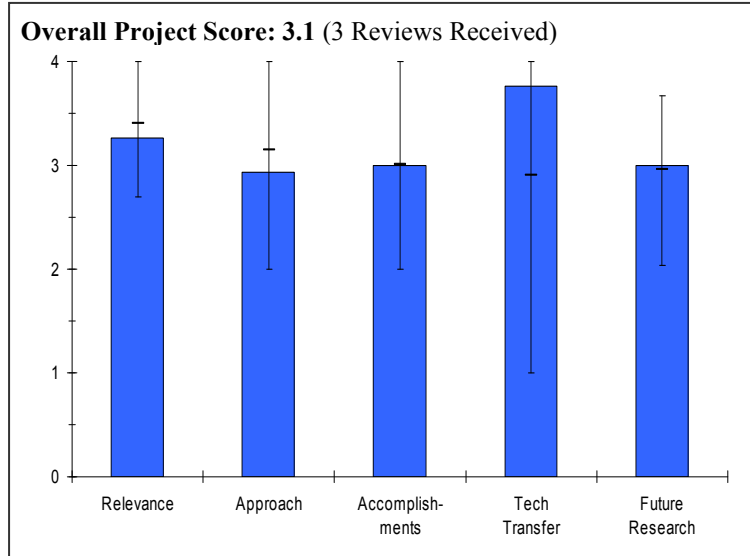
- FSEC should solicit help in the economic modeling effort, and get guidance on sizing the photo reactor and the solar collection hardware.

**Project # PD-16: Hydrogen Delivery Infrastructure Analysis**

*Marriane Mintz; Argonne National Laboratory*

**Brief Summary of Project**

The objectives of this project are to 1) refine technical and cost data in H2A Delivery Models (H2A Hydrogen Delivery Components Model and H2A Hydrogen Delivery Scenario Analysis Model, HDSAM) by incorporating industry inputs and evolving technologies (revised data and analysis, enhanced model capabilities and user options, improved consideration of storage and component sizing, carrier analyses); 2) explore options to reduce hydrogen delivery cost, including storage optimization and novel carriers; and 3) develop enhanced models to assist in program planning and development.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- This will yield an excellent tool for evaluation of various distribution options.
- Department of Energy faces a number of issues and questions regarding hydrogen delivery. However, it is not clear that spending considerable resources on developing a model rather than more thorough, documented, and published studies of delivery costs is the best approach.
- Delivery represents a significant portion of the consumers cost of hydrogen; therefore, it is necessary that we understand the costs associated with the various options.

**Question 2: Approach to performing the research and development**

This project was rated **2.9** on its approach.

- Approach is appropriate but should address integration with the hydrogen production source assumptions such as distributed or centralized, nuclear, natural gas or electrolysis sources or even multiple "central" sites. This is important for accommodating peak demands and outages.
- The layout of HDSAM limits the user to a constrained suite of options, and the components model is extremely difficult to use. This approach severely limits the flexibility of the models.
- The delivery model seems to be continually "overtaken by events". The user cannot easily evaluate costs for new technologies. New technologies must be added by the model developers, so they are always behind the latest advances.
- Began with excellent models and refined from there.
- Refinements are extremely credible due to the high level of industry interaction.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Excellent progress is indicated but obviously cannot yet evaluate future advances.
- Too much emphasis on liquid hydrogen.
- The users' guide should have been published with the model.



## PRODUCTION AND DELIVERY

- In light of the level of funding, the process of vetting the draft version should have gone more quickly.
- Assuming Nexant's funding was linearly distributed over their performance period, the accomplishments for the past year are very good.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.8** for technology transfer and collaboration.

- The report indicates excellent coordination with others.
- The project makes good use of collaborations and appears to obtain needed input from industry and researchers.
- Great industry/consulting/national lab team.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- The inclusion of production and usage considerations should provide more focus for future cases.
- It is not clear that continued refinement of this model is necessary.
- Project is being wrapped up, but as new delivery technologies and scenarios are developed, they need to be added to the model.

### **Strengths and weaknesses**

#### Strengths

- Excellent modeling capabilities and excellent coordination capabilities.
- The project makes good use of collaborations and the team is well coordinated.
- Broad range of delivery options being covered.

#### Weaknesses

- Seems to be limited to existing scenarios without projecting future capabilities/technologies.
- It only considers one, totally isolated centralized system and does not consider a widespread grid-type system, which could reduce storage requirements for outages.
- The model is not flexible and is very difficult to use.
- Could use more interaction with companies that deliver gases.

### **Specific recommendations and additions or deletions to the work scope**

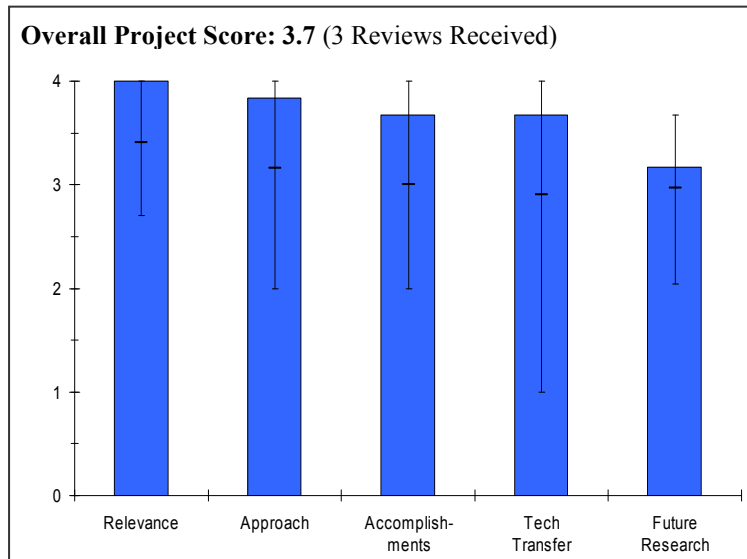
- More emphasis on compressed gas trucking, especially with new higher pressure capabilities.
- Consider adding on-site generation capabilities to model for comparison purposes, i.e. electrolysis or small steam reformers.
- The costs versus benefits of further enhancements to this model should be evaluated.
- As delivery scenarios are developed, they need to be added to the model.

**Project # PD-17: A Combined Materials Science/Mechanics Approach to the Study of Hydrogen Embrittlement of Pipeline Steels**

*Sofronis Petros; U of Illinois*

**Brief Summary of Project**

The objectives of this project are to 1) come up with a mechanistic understanding of hydrogen embrittlement in pipeline steels in order to devise fracture criteria for safe and reliable pipeline operation under hydrogen pressures of at least 15 MPa and loading conditions both static and cyclic (due to in-line compressors); 2) study existing natural gas network of pipeline steels or hydrogen pipelines; and 3) propose new steel microstructures. It is emphasized that such fracture criteria are lacking and there are no codes and standards for reliable and safe operation in the presence of hydrogen.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **4.0** for its relevance to DOE objectives.

- Project is critical to hydrogen initiatives and supports hydrogen delivery technology RD&D.
- Embrittlement is a serious failure mode of steel pipelines for hydrogen infrastructure; this study aims at a science-based approach to obtain mechanistic insights into why failures occur and the R&D products are useful to design/fabricate pipelines less prone to such failure modes. The study may lead to technical know-how development for mitigating hydrogen embrittlement issues with steel pipelines.
- This contribution is based on experimental tests and theoretical analyses, significantly contributing to addressing the issues and achieving the Department of Energy hydrogen energy technology deployment goals.
- Understanding hydrogen embrittlement is essential to mass distribution and storage of hydrogen.

**Question 2: Approach to performing the research and development**

This project was rated **3.8** on its approach.

- Sharply focused on the analyses of failure modes of steel pipelines for hydrogen transport infrastructure.
- Experimental and theoretical approaches are combined to clarify influence of hydrogen to materials for hydrogen pipeline.
- Approach seems to be right on target.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.7** based on accomplishments.

- The results thus far are impressive.
- The study has generated considerable insights on the mechanism of steel pipeline failures due to hydrogen transport; the researcher used pipeline samples supplied by manufacturers (air Products, Air Liquide, OSM steels).
- Identification of the fracture criteria could lead to improved pipeline designs, specifications, coating materials and processes.
- Ultimately, this could impact the cost of pipelines and M&O costs.

## PRODUCTION AND DELIVERY

- Good progress has been made in the basic understanding of embrittlement but more is needed before methods of overcoming the barriers can be suggested.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.7** for technology transfer and collaboration.

- Air Products and Air Liquide, two largest hydrogen manufacturers and suppliers, are only providing pipeline specimens.
- Considering the outstanding results thus far, these manufacturers should be made interested in cost sharing and data interpretation and analysis
- Sandia National Laboratories and Oak Ridge National Laboratory are research and experiment participants.
- Experimental and theoretical approaches are combined to clarify influence of hydrogen to materials for hydrogen pipeline.
- The participants of this project have good contact with standard development organizations.
- The list of collaborators is impressive and indications are that they are being actively consulted.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- Plans to build on evolving knowledge and technical know-how base.
- Appears to be a good continuation of the project.

### **Strengths and weaknesses**

#### Strengths

- Solid unfolding of knowledge based on experiments and analyses of theoretical foundations.
- Project shows strong potential to progress towards a meaningful outcome.
- This project is conducted under collaboration with both experimental and theoretical groups.
- Good coordination with others.
- Solid technical capabilities.

#### Weaknesses

- The chemical reactions, which perhaps initiate the failure modes to then propagating to actual failures have not been studied at levels required for a complete understanding of the reliability issues.
- Comparison with other, novel materials pipelines for hydrogen transport has not been included. At least a literature study is needed.
- There is some recognition that steel pipeline is a no-go for hydrogen transport because of intrinsic chemical reactions of hydrogen with steel components, carbon, iron, etc.; a comparison with other materials of construction may shed some insights on this issue.
- Very theoretical.

### **Specific recommendations and additions or deletions to the work scope**

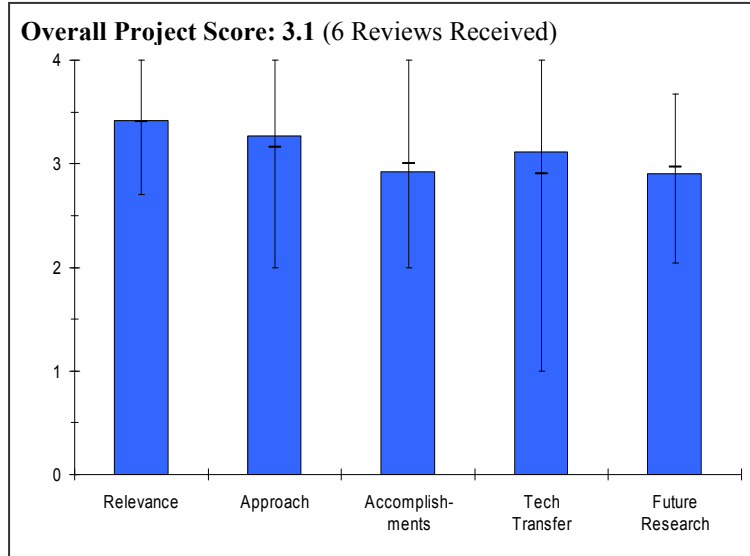
- Study the chemical reactions and kinetics of hydrogen with iron, carbon, etc., and how the reactions cause initial defects to further propagate the failures.
- In depth study of chemical mechanisms, electro-mechanical mechanisms and relating to the physical (e.g., hydrogen diffusion) failure modes ultimately causing mechanical fractures.
- Coordinate this with the similar task by Sandia National Laboratories for practical applications.

**Project # PD-18: Materials Solutions for Hydrogen Delivery in Steel Pipeline**

*Doug Stalheim; Secat/ORNL*

**Brief Summary of Project**

The objective of this project is to develop materials technologies to minimize embrittlement of steels used for high-pressure transport of hydrogen. The deliverables are to 1) identify steel compositions/microstructures suitable for construction of new pipeline infrastructure; 2) develop barrier coating for minimizing hydrogen permeation in pipeline and associated processes (on hold per the Department of Energy); and 3) understand the economics of implementing new technologies.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.4** for its relevance to DOE objectives.

- Very relevant to establishing next steps regarding current infrastructure or new infrastructure.
- Pipelines are important but can steel pipelines contribute to meeting Department of Energy targets. I thought the problem was welding and this program does not appear to address this. Not clear that their team understands the big picture. Comment was made that maybe existing pipeline could be use connected to hydrogen—massive picture that natural gas pipelines will be needed for natural gas.
- This project is relevant to Department of Energy's goals.
- As this project explores the potential to use existing, commercially available steel materials, and includes a task to study the economics, it contributes to addressing the barrier of high capital cost.
- Additionally, the study of the effects of hydrogen relative to the material composition and microstructure addresses the barrier of materials issues with hydrogen embrittlement.
- Pipelines are the most cost effective shipment method; however, barriers to hydrogen shipment must be addressed before long distance pipelines can be used.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- Methodical, clear and forward looking.
- Clear explanation of where they are and where they are going.
- Approach to this problem appears to be good. Have had to defer some work due to funding issue.
- The project is too narrowly focused on microstructures. Other aspects of steel composition could be important.
- Too few analyses have been conducted to assess the effects of variability in microstructures.
- Project contributes to the determination in the feasibility of using certain grades of commercially available steel and alloys for hydrogen pipeline delivery.
- Logical approach and testing being conducted within a limited, focused group of materials (limited manufacturers and materials grades).
- Extensive team partnering is a strength.
- Communication with other projects needs to be established to maximize the benefits of the experiment and calculation/theoretical activities (of other delivery projects).
- Low risk for technical feasibility in testing the commercial steel and alloy materials.

## PRODUCTION AND DELIVERY

- It is not clear how applicable the test results of the subject materials will be towards other materials fabricated by other manufacturers, nor whether manufacturers can accommodate the microstructure improvements needed. Understanding the mechanisms appears to be critical to extrapolate the focused studies to be helpful in the broader sense.
- The four tasks outlined are appropriate for advancement of the technology.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.9** based on accomplishments.

- Progress is proportional to funding.
- The project is only 25% complete, while being 75% of the way through the time. Very little progress has been made.
- Multiple commercial pipeline materials have been tested from one manufacturer, including microstructure imaging, the effect of hydrogen on the mechanical properties of steel (ex-situ testing), and studies of hydrogen-induced cracking.
- Studies in pure hydrogen provide a baseline.
- Testing apparatus is complete for in-situ high pressure hydrogen testing.
- Extensive amount of work in selecting and characterizing candidate materials.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- Impressive list of collaborators, definitely necessary for this type of analysis.
- Cannot tell the time each partner participated.
- In-situ test in hydrogen atmosphere is important in cooperation in SECAT consortium.
- Fairly good collaboration with laboratories.
- The project includes many team members including private companies, national laboratories and universities.
- It is not clear that the extensive collaboration is being fully utilized except for the testing capabilities provided by Oak Ridge National Laboratory.
- Three Project team is an excellent vertical alignment from R&D entities to a pipeline owner, but could be improved with the inclusion of a hydrogen pipeline owner.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- Very focused program, Object is achievable.
- Evaluation of in-situ fatigue testing is highly expected.
- Task 3 activities and the codes and standards integration in Task 4 do not appear in the presented future plans.
- The presentation did not include milestones or stage gates/decision points (i.e. define a clear decision point at which the material compositions and microstructures are either feasible or not, and alternatives need to be explored).
- Future activity includes an economic evaluation.
- The project needs to more clearly define test criteria.
- In-situ high pressure hydrogen testing will be conducted.
- Future work does not seem to go all the way to revising codes and standards.

### **Strengths and weaknesses**

#### Strengths

- Businesslike approach, results focused.
- Focused program testing steels in hydrogen environment.

- Project addresses the barriers of cost and material challenges.
- Technically feasible and focused approach.
- Strongest point is the vertically integrated team.

Weaknesses

- This is a focused "development/communization" program and not propane, which will have any ability to dramatically lower the cost of steel pipelines. Department of Energy programs should lead to step-outs, not the materials.
- Major conclusions are based on a very small number of samples.
- In determining whether existing pipelines and commercially available baseline and alloy materials are feasible for a hydrogen economy, then accelerating testing/aging of steel, hydrogen with impurities, an understanding of the mechanisms for degradation, and safety thresholds would appear to be a high priority. Criteria for continuing with existing steel chemistry/microstructure should be defined (versus at what point alternatives should be pursued).

**Specific recommendations and additions or deletions to the work scope**

- Asses how "impure" hydrogen affects these results.
- Add oxygen to hydrogen, see how this travels, purify at end of pipe.
- Add impurities to allow pipelines to "work" with hydrogen, purify at end of pipe.
- Hydrogen pipelines currently exist. The project should include evaluation of the aging of existing pipeline if feasible.
- Agree with Department of Energy's decision to put coating work on hold, at least until a favorable cost/benefit analysis has been prepared and adequately reviewed.

**Project # PD-19: Composite Technology for Hydrogen Pipelines**

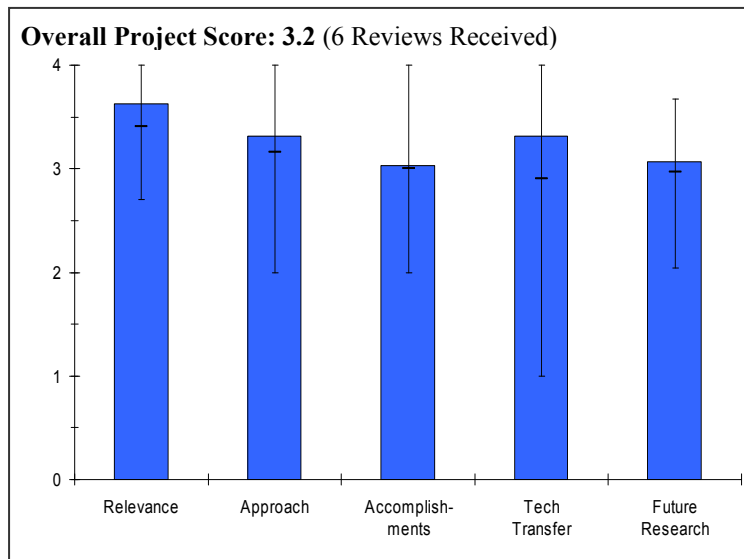
*Barton Smith; ORNL*

**Brief Summary of Project**

Oak Ridge National Laboratory will investigate the applicability of composite pipelines in use in oil and gas gathering operations and develop a path forward for hydrogen delivery. The cost scenario shows composite pipeline will meet the Department of Energy 2012 goals and are close to the 2017 goals. The hydrogen compatibility of pipeline materials is acceptable. The pipeline leakage rates are better than predicted.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.6** for its relevance to DOE objectives.



- It is not clear what specs the Program is trying to achieve. Department of Transportation rules for pipeline? American Society of Mechanical Engineers?
- If so, is there any interaction?
- Composite pipelines may offer a low cost, no hydrogen embrittlement option to metal.
- The objectives are critical but success of composite pipe materials obviously depends upon competing technologies.
- Project is focused on reducing the cost of hydrogen pipelines by using fiber-reinforced polymers to manufacture the pipelines.
- Project appears to have significant potential to reduce the cost of hydrogen pipelines to meet the Department of Energy targets.
- Clearly relevant to the goals of the RD&D plan, regardless of whether or not the end-use will specifically address hydrogen-fuel-cell-powered vehicle infrastructure.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- The Program should be given access to the current technology validation program for hydrogen stations to retrieve materials for testing. Already many of the existing stations have 2-5 years of high pressure hydrogen exposure in cyclical stressed conditions. Of course the PIs have limited access to the other program (and also influence) and this should be coordinated through Department of Energy program managers.
- Immersion test may not be the best way of testing without a pressure differential across the tube wall.
- What are the technical specifications that need to be met (beyond cost)?
- Composites experience in natural gas industry provides a good basis for this work. Barriers are mostly known. Project approach is logical and straight forward.
- Investigation of commercially available materials is an approach to low cost pipeline.
- The approach is satisfactory although it should include other alternative composite pipes, not just Fiberspar.
- Testing of HDPE, PA, and PPS pipelines for hydrogen permeability, tensile strength, and materials compatibility is appropriate and necessary.
- Pressure and temperature effects are appropriately considered.
- Surface treatments and associated testing will yield valuable data on the ability to improve the permeability of polymer pipelines.

- Overall approach is effective.
- Project is addressing pipeline capital costs and hydrogen embrittlement.
- Approach does not yet include thermal fatigue effects on composite pipe assembly. Will such effects be implemented along with future mechanical fatigue experiments?

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Accelerated aging tests would have been more meaningful had a pressure differential been maintained across the pipe. This could have provided both permeation and strength data on a hydraulically loaded pipe. The aging test performed (immersing the entire pipe in a static 1000 psi hydrogen environment at 60 degrees Celsius) is only an indicator of the effect of hydrogen on the materials, not pipe performance.
- I would suspect that hydrogen permeation may decrease over time as the liner surface is fouled with other constituents.
- Acceptable pipeline materials compatible with hydrogen are proposed. This result supports activity to evaluate the practicality of pipeline transportation of hydrogen.
- Accomplishments appear good but it has taken two and a half years to reach an understanding of one material.
- Good progress is being made in testing HDPE, PA, and PPS pipelines for hydrogen permeability, tensile strength, and materials compatibility. Permeation coefficients, tensile properties, and hydrogen leakage results from the tests were presented.
- Surface treatments and associated testing appear to be underway.
- Project appears to be progressing toward achieving technical millstones within the anticipated timeframe.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- The two major composite pipe manufacturers and major liner materials companies are on the team.
- Collaborations appear satisfactory but should be expanded to include other material suppliers.
- Collaborations are appropriate.
- Partners appear to be working closely with the PI.
- Manufacturers of additional polymer types should be considered for inclusion in the project to include additional polymers.
- Potential customers (pipeline purchasers/installers/maintenance) should be consulted to enable transfer of the technology to industry at the appropriate time.
- Strong collaboration with pipe, liner, and coupling manufacturers is evident.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Beginning code work early is essential.
- Plan is limited in terms of pipe lengths (i.e. sample size) and number of joints.
- Needs to focus more on overcoming barriers.
- Proposed research is appropriate and should be funded.
- The cost and pipeline performance impacts of variations in pipeline manufacturing process conditions should be studied to understand potential issues of onsite pipeline manufacturing.
- Brittle fracture in fiber-reinforced polymer materials is always a concern even for buried pipe structures due to environmental acids. In particular, crevice corrosion around couplings may be a concern. Future plans should include experiments aimed at assessing whether crevice corrosion around couplings will lead to brittle failure of fiber-reinforced polymer.



### Strengths and weaknesses

#### Strengths

- Builds on natural gas experience and includes commercial fiber-reinforced polymer fabricators.
- Good depth of technical understanding.
- Good coordination with material supplier.
- Good test and analytical technical abilities.
- Composite pipeline testing is elucidating the performance and properties of polymer pipelines.
- Project is contributing to development of necessary codes and standards for composite pipelines.
- Approach has potential to meet Department of Energy pipeline cost targets.
- The project is globally relevant to hydrogen infrastructure.
- Project is likely to generate useful reference data and standard protocols for hydrogen pipeline testing.

#### Weaknesses

- The immersion test may not accurately reflect the embrittlement effects or diffusion issues.
- Project presentation did not address installed costs, only states that scenarios meet 2012 Department of Energy goals.
- Project is concentrating on 4' nominal pipe. This may have limited application. Large diameter (>6") fiber-reinforced polymer composite pipe may have inherent cost and installation disadvantages.
- Does not give data to support cost effectiveness of pipe material.
- Is not able to generalize to other alternative materials.
- Given the 20% deviation in the results of testing 3 samples, a larger sample size is needed.
- A limited number of coupling, pipe, and liner structures have been selected.

### Specific recommendations and additions or deletions to the work scope

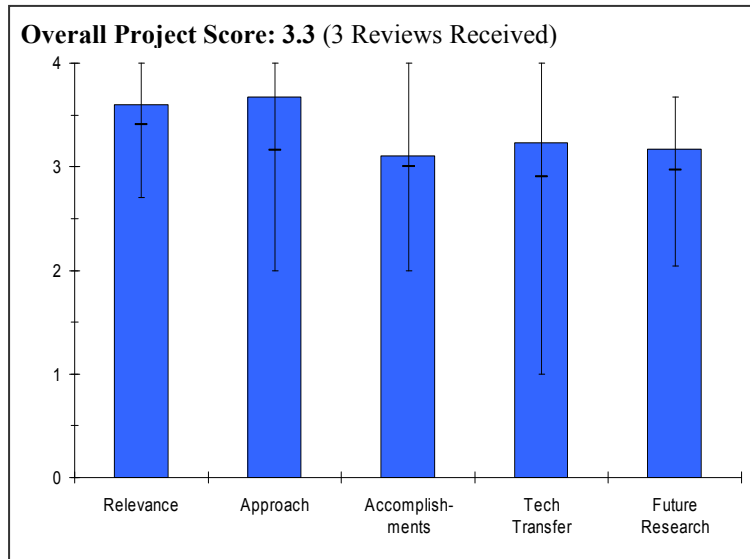
- This is for Department of Energy Program management: coordinate the access to materials aged in Technology Validation Program (hydrogen stations), be it storage cylinders or reformers or other materials exposed to high pressure and/or high temperature hydrogen.
- Calculate if the costs of fluorination offset the amount of hydrogen saved.
- Calculate pressure drop - standard fiber-reinforced polymer pipe plus 0.5 cm liner may have much smaller ID than nominal steel pipes that will result in higher pressure losses per linear foot of pipe. This pressure loss may be offset somewhat (but not completely) by surface smoothness.
- Theorize the differences between hydrogen service and natural gas (is there a hydrogen induced cracking mechanism in fiber-reinforced polymer?). This exercise may strongly support fiber-reinforced polymer use in hydrogen.
- Determine any special requirements for pipe line inspection "pigs".
- Determine corrosion protection requirements for buried joint fittings.
- Include some type of bench-mark for alternative materials such as existing pipe material.
- Include other composite materials and pipes for evaluation.
- Consider the cost and pipeline performance impacts of variations in pipeline manufacturing process conditions.
- Increase the sample size used in the testing effort to account for the large deviation (20%) in the results.

**Project # PD-20: Hydrogen Permeability and Pipeline Integrity/Fiber Reinforced Composite Pipeline**

*Thad Adams; SRNL*

**Brief Summary of Project**

The objectives of this project are to 1) investigate the influence of weld fabrication microstructure (especially weld heat affected zones [HAZ]) on hydrogen compatibility; 2) measure hydrogen transport (diffusivity) in HAZ materials; 3) determine HAZ material susceptibility to hydrogen embrittlement; 4) focus evaluation of fiber reinforced composite (FRP) piping for hydrogen service applications; and 5) assess the structural integrity of the FRP piping and leakage of existing commercial available FRP joint designs and joint components.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.6** for its relevance to DOE objectives.

- Two projects were presented in this talk. One was on hydrogen pipeline integrity and the other is on fiber-reinforced composite pipeline (fiber-reinforced polymer). Both projects are important to address issues involved in transmission/distribution of hydrogen.
- Both projects in this presentation are relevant to the Department of Energy Hydrogen Program.
- The hydrogen permeability and pipeline integrity project ended in March 2008. The fiber-reinforced polymer project should be combined with PD-19. I don't see any justification to having PD-19 & PD-20. PD-20 involves collaboration with Oak Ridge National Laboratory and PD-19 is an Oak Ridge National Laboratory-led project. Good synergy to combine these two projects.
- Fiber-reinforced polymer is the only Pipeline program that can possibly meet Department of Energy targets. Welding in steel P/L's is also a key element of the cost of P/L's.

**Question 2: Approach to performing the research and development**

This project was rated **3.7** on its approach.

- The hydrogen permeation and integrity part of this project is finished. Test samples from actual weldment was prepared and tested for hydrogen solubility, diffusivity, & permeability at sub-atmospheric pressure and moderate temperatures.
- The approach for the fiber-reinforced polymer part of the project is to investigate fiber-reinforced polymer joint types & determine hydrogen leakage rates. This seems to be a good approach for this task.
- Well focused programs. Clearly focused on milestones and deliverables. Refocusing correctly on fiber-reinforced polymer work with Oak Ridge National Laboratory.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- Determined that effect of microstructure on diffusivity of hydrogen in pipeline steels is critical to aiding understanding of hydrogen embrittlement. It is well-known in materials science that microstructures influence the materials property. It is not clear what this work has accomplished other than stating that structure-property-

processing is important. One could open any book on materials science and find the statement that structure-property-processing are interlinked. It is good to see that this part of work is terminated in March 2008.

- Higher hydrogen leakage rates were measured in fiber-reinforced polymer and the reason for this is not known at this time. Oak Ridge National Laboratory and Savannah River National Laboratory are going to get together to analyze the results. It is not possible to measure the progress towards objectives.
- Good progress. Helping Oak Ridge National Laboratory. Little money, getting data. Focus has been too much on weld materials permeability. Should work more on fiber-reinforced polymer.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.2** for technology transfer and collaboration.

- Good collaboration between Savannah River National Laboratory and Oak Ridge National Laboratory.
- Praxair provided the welded samples for analysis.
- Role of Edison Welding Institute is not clear.
- Collaborations with Oak Ridge National Laboratory. No others apparent.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- Plans to determine the cause for higher leakage rates is not included in the future plan. It is important to determine the reason for the higher leakage before proceeding with the other planned activities.
- The rest of the future plans are reasonable.
- It is good that the weld work stopped and work redirected to fiber-reinforced polymer. Do more.
- Test planning of fiber-reinforced polymer materials, joints, and fiber-reinforced polymer pipeline system are expected to be extensively carried out based on their experience on pipeline testing.

### **Strengths and weaknesses**

#### Strengths

- Collaboration between Oak Ridge National Laboratory and Savannah River National Laboratory.
- Good strategy to measure the diffusivity, solubility, and permeability.
- Courage to end the hydrogen permeability and integrity portion of the project back in March 2008.
- Experience of material testing for hydrogen pipeline

#### Weaknesses

- Not following up on analyzing the reasons for higher leakage rates.
- Needs to be more work with manufacturers focusing on mp processes, consistency, on site mp etc and how that affects leak rate.
- Lack of experience of plastic materials and fiber-reinforced polymer.

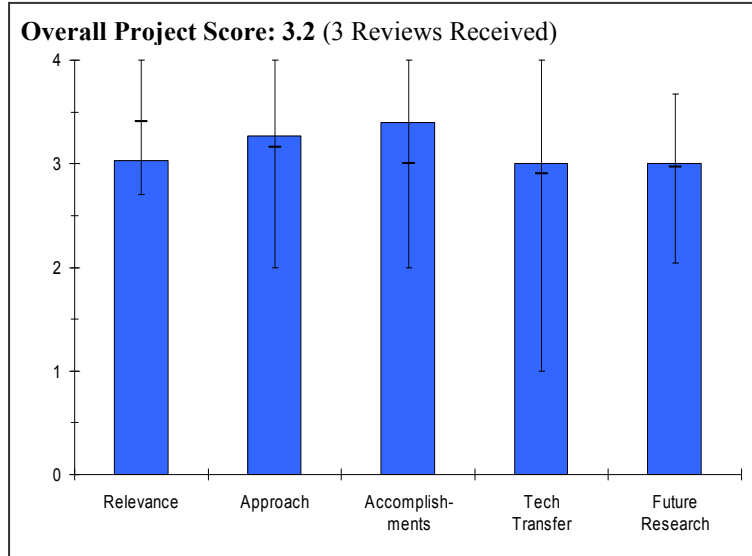
### **Specific recommendations and additions or deletions to the work scope**

- Combine the fiber-reinforced polymer task with PD-19. No need to keep two different projects.
- Determine the cause for higher leakage rate and fix this problem before proceeding with rest of the future plans.
- Need to decrease steel effort and P/L working group and increase efforts and collaborations in fiber-reinforced polymer work.

**Project # PD-21: Innovative Hydrogen Liquefaction Cycle**  
*Martin Shimko; Gas Equipment Engineering Corporation*

**Brief Summary of Project**

The objectives of this project are to 1) design a practical hydrogen liquefaction cycle that significantly increase efficiencies over existing technologies; 2) produce a small-scale (100-500 kg/day) hardware demonstration of a hydrogen liquefaction plant; 3) use low/no risk development components that scale to 50,000 kg/day plant size; and 4) document a significant reduction in the total cost of hydrogen liquefaction at the 50,000 kg/day production level.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.0** for its relevance to DOE objectives.

- Goal of reducing energy losses associated with hydrogen liquefaction is important and should make use of liquid hydrogen delivery system significantly more attractive.
- Increasing cycle efficiency from Linde volume of 30/35% to 45% is a worthy goal, but there remains the question of whether one can more clearly approach Quack "practical limit" of 60%. Author claimed this cycle would be too costly, but did not prove it.
- If efficiencies of liquefaction could be significantly increased, this project would be more relevant but this does not seem to be realistic.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- Approach good, particularly in use of low/no risk development components. Intermediate step of producing a small-scale hardware demonstration is good. Massachusetts Institute of Technology experience is a plus.
- The approach is good regarding the technology but it concludes that liquefaction efficiencies cannot be increased enough to be critical to overcoming barriers to the extensive use of liquid hydrogen.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.4** based on accomplishments.

- Use of para/ortho equations of state good, as is development of "simple" cycle simulation program leading to examination of several cycle options and optimizations
- Good progress is made toward improving the technology but it doesn't appear to be enough to overcome barriers.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.0** for technology transfer and collaboration.

## PRODUCTION AND DELIVERY

- Not clear how much technology transfer is applied.
- Good collaborations appear to have occurred with indicated partners but expansion to others in the industry should be taken.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- The investigators appear to have adequately defined possible limiting problems and have done a reasonable job of estimating cost. Future efforts are well-defined. Doing catalyst heat exchange development incoming year is appropriate.
- Development of the catalytic heat exchanger may be of interest.
- Demonstration of a pilot plant does not seem warranted regarding the achievement of Department of Energy Hydrogen Plan goals.

### **Strengths and weaknesses**

#### Strengths

- Excellent approach to significantly reducing process efficiency losses and thus reducing cost associated with conversion of hydrogen to liquid state (which appears to be an attractive delivery and storage option).
- The project does advance hydrogen liquefaction technology.

#### Weaknesses

- Necessity of liquid nitrogen.
- The improvements identified do not appear to overcome barriers.

### **Specific recommendations and additions or deletions to the work scope**

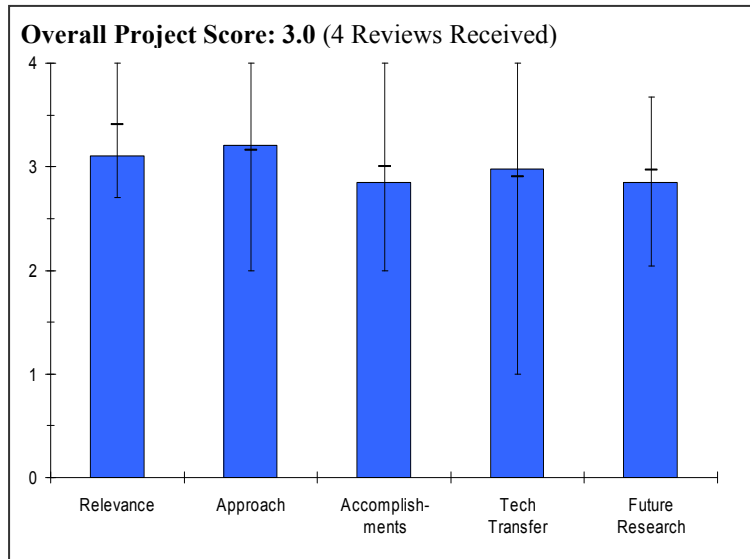
- Combine the objective to lower the hydrogen temperature rather than the just liquefactions.
- Use this technology for hydrogen storage such as cryo-absorption.
- Continue the work on catalytic heat exchangers.
- Refine the cost/efficiency study work.
- Do not build a pilot plant.

**Project # PD-22: High Pressure, Low Temperature Hydrogen Tube Trailers**

Salvador Aceves; LLNL

**Brief Summary of Project**

The objective of this project is to demonstrate inexpensive hydrogen delivery through synergy between low temperature (200 K) hydrogen densification and glass fiber strengthening. Colder temperatures (200 K) increase density ~35% with small increases in theoretical storage energy requirements. Low temperature are synergistic with glass fiber composites. Glass composites (~\$1.50/kg) minimize material cost. Increased pressure (7,000 psi) minimize delivery costs. Dispensing of cold hydrogen reduced vehicle vessel cost ~25%.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.1** for its relevance to DOE objectives.

- High pressure tanks are certainly one alternative to storing hydrogen in the future.
- Unless there is a huge breakthrough in hydrogen storage, future hydrogen fuel cell vehicles will probably use at least a combination of hydrogen storage materials and high pressure tanks.
- A lot of work has already been done on high pressure tanks and the current technology is already being readily used, so this work is a little more long-term, focused on lowering the cost of the composite tanks.
- If the hydrogen storage subprogram achieves their targets, the value added of this project to the Hydrogen Program is significantly lower.
- There are significant issues related to cold hydrogen storage such as slow hydrogen release over time if a vehicle is parked for extended periods.
- This method provides superior strength at lower temperatures, but this assumes that the tank temperature remains low over long periods of time. If the tank weakens over time as it heats up, this could be a significant issue.
- Obviously low temperature will increase gas density which will lead to reduced tank volume per unit mass of hydrogen.
- Indications are that glass fiber strength increases at low temperature (good), but not clear that overall tank strength increase with low temperature.
- Cost of cold glass fiber and the cost of carbon fiber truck systems approach each other at high volumes. Glass meets the target at lower delivery volume, but question whether Department of Transportation would accept design.

**Question 2: Approach to performing the research and development**

This project was rated **3.2** on its approach.

- The project is investigating glass fiber composites, which is an interesting potential substitute for carbon fiber that would provide added strength and potentially lower the delivery cost to less than \$1/gge.
- The project seems a little disjointed with work on composite tanks, cold hydrogen storage, and large tube trailers.

## PRODUCTION AND DELIVERY

- The tensile testing of the glass fibers is not working. There are too many variables surrounding the glass fibers (humidity, temperature, time at temperature) that must be addressed to make any sense of the data. In addition, the fibers are breaking very randomly and close to the holder.
- The tensile data is confusing and hard to discern. Since several individual fibers are being tested at once, the stress strain curves are stepped and this makes it hard to determine anything from them.
- The issue of water weakening the fibers is a concern since it will be nearly impossible to keep water out as there may always be a little water in the hydrogen. It would be vital to know if the tank had been exposed to water, and this would not be something easily measured over time at very low levels.
- Clearly laid out goals and deliverables.
- Concurrent engineering a plus.
- Testing samples consisting of multiple fibers imbedded in resin matrix is the right way to go (critical).
- Novel approach to reducing the cost of storage tanks.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.9** based on accomplishments.

- The progress was slower than expected and most of the work presented was based on concept rather than actual data.
- It was hard to determine the results of the project over the last year versus the results of the project overall. Presenting the status of the project at the time of the Annual Program Review last year and then specifically stating the accomplishments over the last year would have helped.
- Given the amount of time spent they have made great progress in this development.
- Myth busting of glass fiber reliability refreshing.
- Progress appears to be somewhat slow – need to get to testing of full samples (fibers in matrix) as soon as possible.
- Accomplishments are limited, but funding was very limited.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.0** for technology transfer and collaboration.

- Three separate collaborators who all have significant experience in the area of composite tanks.
- Little evidence was given about how the collaborations are specifically benefiting or contributing to this project.
- Team assembled makes sense; they seem to be working well together.
- Having Quantum on board is very important since they have been a real leader in fiber-wound tanks for high pressure operation.
- Industrial partners are significant.
- Adding Department of Transportation as a partner/advisor would be beneficial.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- Very little offered as far as their proposed future work beyond the cryogenic tensile testing and the work with Department of Transportation to make their tube trailer viable.
- Potential weaknesses already identified, plans for remediation already discussed - great!
- What needs to be done is fairly obvious and it looks like they are headed that way, except that there is no mention of pressurization/depressurization cycling tests or temperature cycling tests.
- Proposed research appears to be hampered by funding limitations.

**Strengths and weaknesses****Strengths**

- The proposed concept does have the potential to lower the vessel cost by 25%.
- Very applicable knowledge regardless of hydrogen production pathway.
- Good team.
- Out of the box thinking to reduce cost.

**Weaknesses**

- The concept has several potential issues that could prevent it from being a viable option.
- The tensile testing at cryogenic temperatures has resulted in very little usable data.
- Nothing spelled out for cumulative damage analysis.
- Considering the controls that must be implemented to maintain dry, cold fibers in practice, appears to be adding considerable risk to the application.

**Specific recommendations and additions or deletions to the work scope**

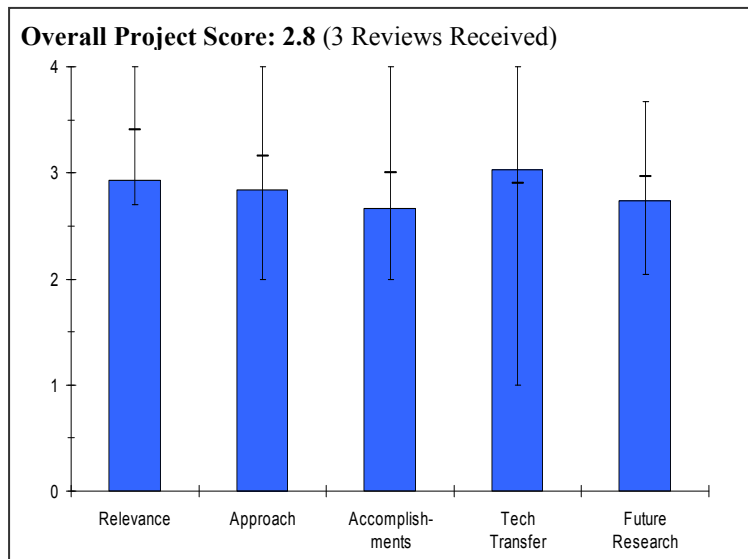
- The group should try to develop alternative ways to measure the strength of the glass fibers rather than the current tensile tests. Similar to tensile testing ceramics, the data will probably never show consistent results.
- The cryogenic tensile testing should be deemphasized.
- Complete cost analysis of construction for scale.
- Revise costing analysis with current parameters in H2A.
- Explore real world scenario for how this would be used in real world conditions, I think this idea is promising, let's see what real world conditions would be necessary to pursue to full fruition.
- Continue and add funding to explore real world.
- Find another group, vendor or lab to build one of these trucks – even a scaled down model to invite private sector development.
- Ultimate failure tests for tanks at purposed operating temperatures. Cumulative damage analysis for multiple cycles of pressure, temperature.
- Recommend an independent risk/benefit analysis of the technology and the application.



**Project # PD-23: Reversible Liquid Carriers for an Integrated Production, Storage and Delivery of Hydrogen**  
*Bernard Toseland; APCI*

**Brief Summary of Project**

The objective of this project is to enable a liquid carrier concept. This includes a economic study to determine the concept's viability. This project supports the liquid carrier by developing a dehydrogenation reactor system for hydrogen delivery. The packed bed reactor works well, but design limitations limit the reactor efficiency. Thin-film catalysts (useful for monoliths and microchannel reactor) can be made with high catalyst efficiency. Monolith reactors are useable, but flow instabilities will cause design limitations. Micochannel reactors still look like the most viable alternative.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.9** for its relevance to Department of Energy objectives.

- Carriers could reduce distribution cost but need to consider total well to wheel cost
- While a hydrogenated fluid could be relevant in theory, no data is supplied to explain this. Thus the relevance of this project is questionable.
- The indicated distribution costs appear to be far from other alternatives.
- Project addresses hydrogen carriers for both onboard and offboard hydrogen regeneration.
- Potential to meet hydrogen production, delivery, and storage targets is not clear.

**Question 2: Approach to performing the research and development**

This project was rated **2.8** on its approach.

- Prototype reactor tested in lab.
- Large gas flow and variable flow challenges identified.
- N-ethylcarbazole carrier system is six weight percent hydrogen.
- The approach seems reasonable within hydrogenated fluid technology but it is not indicated that it will significantly overcome barriers.
- It is unknown if the fluid, N-Ethycarazde is appropriate other than for academic purposes.
- Consideration of multiple reactor configurations was appropriate.
- The results presented provide sufficient data to downselect to the microchannel reactor design for the prototype.
- A system-level analysis is needed to determine whether onboard dehydrogenation in general is likely to be an effective and consumer-acceptable approach.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- Packed bed reactor mass transfer limits identified.
- Effectiveness factor in packed bed.
- Microchannel reactor allows modular design and turndown for variable hydrogen production.
- Evaluation of dehydrogenation reactors appears competent and thorough.

- How this progress will overcome barriers is not indicated.
- Data obtained thus far supports a Go/No Go decision on the reactor designs.
- Progress against the Department of Energy delivery targets for carrier hydrogen content and carrier system energy efficiency was not presented.
- The cost estimates for this project are significantly (~2x) higher than the Department of Energy targets, and it is not clear that all of the relevant costs are included in the PI's cost estimate.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.0** for technology transfer and collaboration.

- Mix of industry and national laboratories.
- Coordination with partners to date has not been indicated.
- Future coordination regarding the source of hydrogen and end use is indicated.
- No collaboration with component suppliers such as for thin film or micro-channel components is indicated.
- Pacific Northwest National Laboratory is an effective partner for microchannel reactor work.
- A fuel cell partner and an original equipment manufacturer partner (unknown at this time) are included in the project. More collaboration with these partners in the early stages of the project is needed to assess potential system issues and show-stoppers related to both technology transfer capability and consumer acceptance.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.7** for proposed future work.

- Reactor selection and test facilities.
- It is not clear how the proposed future tasks will overcome barriers.
- Future plans are appropriate.
- Conduct a system-level analysis of the viability and consumer acceptance potential of an onboard dehydrogenation system. Include an onboard Go/No Go decision in future plans.

**Strengths and weaknesses**

Strengths

- Economic analysis completed using Aspen and H2A models.
- Good understanding of the overall liquid fluid dehydrogenation technology.
- Project has considered multiple reactor configurations.
- Project addresses hydrogen carriers for hydrogen production, storage, and delivery and is relevant to the Department of Energy goals.

Weaknesses

- Original equipment manufacturer partner not yet identified.
- Microchannel reactor cost not yet identified.
- Required solutions/advancements are not identified and quantified.
- Analysis costs are very high.
- Assessment of this project's reactors' performance against the Department of Energy goals was not shown.

**Specific recommendations and additions or deletions to the work scope**

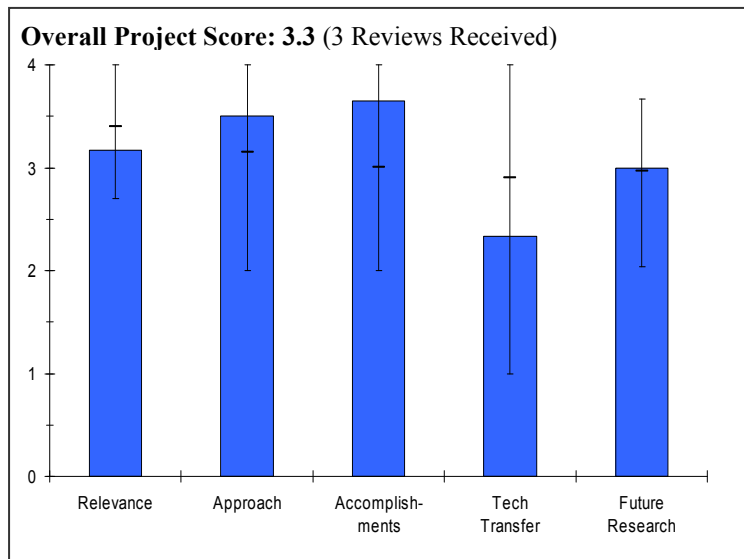
- Review toxicity data for carrier liquid.
- Define specifically what cost/technological improvements are required for liquid fluid hydrogen carriers to overcome Department of Energy distribution barriers and relate the barriers to hydrogenated fluid parameters.
- In terms of these improvements, define the technological improvement required.
- Assess the potential of the systems considered in this project against Department of Energy's goals for carrier content and carrier system energy efficiency.
- Conduct a system-level evaluation of the ability of onboard carrier system to meet market demands.

**Project # PD-24: Coatings for Centrifugal Compression**

*George Fenske; ANL*

**Brief Summary of Project**

The objective of this project is to identify and develop as required, advanced materials and coating that can achieve the friction, wear and reliability requirements for dynamically loaded components (seal and bearing) in high-temperature, high-pressure hydrogen environments prototypical of pipeline and forecourt compressor systems. The reliability and efficiency of hydrogen compressors will depend on the tribological performance of critical bearings and seals. Knowledge of the tribological performance of materials and coatings in hydrogen environments is currently insufficient to design reliable, efficient hydrogen compressors. The rule of thumb/target is friction <0.1.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.

- Good relevance to improving pipeline and forecourt compressors.
- Appears to be very important if high pressure gaseous hydrogen is selected as delivery method of choice.
- There certainly could be benefits coming from this activity, but it is not clear that this is high priority.

**Question 2: Approach to performing the research and development**

This project was rated **3.5** on its approach.

- Good approach. Very logically identified, evaluated, characterized, developed and engineered.
- Could consider some kind feedback upon final testing.
- Program assumes being right the first time.
- Excellent systematic approach.
- Good approach; although, hydrogen impurities could have a significant impact on materials selected.
- Focused on critically loaded components.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.7** based on accomplishments.

- Slow progress due to funding constraints. Not their fault.
- Screening of types of coating excellent: homing in on Argonne National Laboratory DLC6 appears appropriate.
- Establishment of test facilities and initial research accomplishments are appropriate.
- Results for DLCs very impressive.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.3** for technology transfer and collaboration.

- Working with MITT (compressor company). Could they work with more relevant compressor manufacturers?
- Doesn't appear to be a lot of coordination with others (notable VTT Tech Research Centre of Finland).
- Project benefits from the inclusion of a bearing manufacturer performing parallel research.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- Long list of materials to be tested.
- Good approach regarding microscopic studies for wear mechanism definition and studying embrittlement and crack behavior.
- Needs to address thermal loads for various scenarios-how much and how fast will heat build up.
- Good plan for continuation of this project and identification of a suitable coating material.

**Strengths and weaknesses**

Strengths

- Well thought out technical approach.
- Appears to have identified a promising coating approach.
- The PI understands the issues and approaches to a solution.

Weaknesses

- Choose more commercial partners not just someone who is funded by Department of Energy.
- Lack of integrated analysis of thermal loads.
- Lack of a broad team and a compelling reason for the work to be done.

**Specific recommendations and additions or deletions to the work scope**

- Continue at current level as long as project priority keeps it above the funding limit line.

**Project # PD-25: Sulfur-Iodine Thermochemical Cycle**

*Paul Pickard; SNL/GA/CEA*

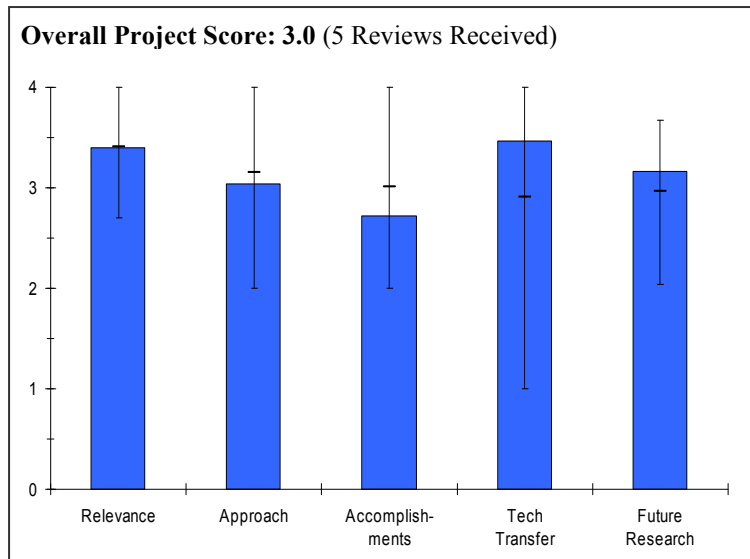
**Brief Summary of Project**

The objective of this project is to evaluate the potential of the sulfur-iodine cycle for hydrogen production using nuclear energy. Sulfur cycles have the potential for high efficiency. The approach of the project is to construct and operate an Integrated Lab Scale experiment to investigate the key technical issues. This will provide a basis for nuclear hydrogen technology decisions.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.4** for its relevance to DOE objectives.

- Perhaps the front-runner cycle for turning heat into hydrogen is some question about whether you want to connect this process to a nuclear reactor.
- The fact that the work will be providing a baseline for Nuclear Hydrogen Program decisions is valuable.
- The production of hydrogen driven by nuclear energy through the sulfur iodide thermochemical cycle has the potential to produce immense amounts of hydrogen without any emissions using only domestic resources.
- Removing hydrogen from the water-gas-shift reactor favors the conversion of carbon monoxide to hydrogen.



**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- Project divided nicely between three groups, some key interface areas seem to be left out. One worry I had was discovering that only ceramic materials worked for the high temperature contactor between the nuclear-heated fluids and the decomposing sulfuric acid. I was also concerned that the hydrogen may not be free enough of iodine for use.
- Integrated lab scale approach with the three modules and interface skid should facilitate testing and performance improvements.
- It is not clear how much hydrogen would be produced for various future system sizes.
- It is reasonable to use the extractive distillation process at this point; however, there should be more work on moving towards a reactive distillation technology.
- Catalyst and materials durability is a significant issue.
- There seems to be a lot of steps in this cycle, which will result in higher costs for capital, operations and maintenance, and controls.
- This is a large, well funded collaborative effort utilizing state of the art science and being performed by excellent scientists and engineers.
- The overall approach that has been taken of initial lab work, and scaling up to the fully Integrated Laboratory System is excellent. The Integrated Laboratory System can provide the information needed for scale-up to a pilot plant operation.
- Three separate excellent research groups (GA, Sandia National Laboratories, and CEA) are each responsible for one of the three steps but also collaborate with each other well. This is a very sound way to approach this complex project.
- An effective stable catalyst for the sulfuric acid decomposition is critical to success. It is good that there is separate focused effort on this issue.
- The research needed on materials of construction for the Bunsen reaction and HI decomposition areas will be done in FY09. It might be appropriate to increase the funding in this important area to ensure it is successfully completed on time vs. the Nuclear Hydrogen Initiative schedule.

- The Nuclear Hydrogen Initiative Program call for pilot plant operations at a 1 MW scale (~240 kg of H<sub>2</sub>/day) and an engineering scale operation linked to a natural gas NP reactor in 2019 at a 50 MW scale (~12,000 kg of H<sub>2</sub>/day). This engineering scale operation will be very expensive. Smaller scale pilot plant and engineering scale operations (perhaps .5 MW and 5 MW) should be adequate prior to commercial scale.
- Initial work on membrane reactor development followed by fabrication and testing seems reasonable.
- Low cost ceramic membranes are preferable over palladium membranes.
- Weakness: Mole sieve membrane sensitivity to water and hydrogen sulfide is not addressed.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- Built pilot scale reactor-separators. Some materials and separation issues left for later – to some extent this is legitimate, to some extent, not. Expect more for this "mature" technology. I do not believe the hydrogen cost numbers presented.
- The price tag for this work is high but good progress has been made and partners are providing some funding.
- It is not apparent how much in kind cost share is being provided.
- The graph of hydrogen price versus electricity costs is good information, however more information on the assumptions for the economic analysis should have been provided, such as projected system size and catalyst costs.
- For the resources made available for the project, progress seems modest.
- Materials is a significant focus of the project, but materials development was minimally discussed.
- It seems a major cost for this technology would be operation and maintenance. It is not clear how this was addressed in the H2A.
- Excellent progress has been made. The three Integrated Laboratory System units have been constructed and put in place to be run in an integrated manner at GA. Each unit has been started up and operated separately.
- It appears the project in general is right on the original schedule that was set except the Bunsen unit is a little behind.
- More progress (and therefore effort?) is needed on the sulfuric acid decomposition catalyst. It is critical to the success of this process.
- It is early in terms of data from the Integrated Laboratory System but there was no attempt at comparing Integrated Laboratory System or lab data performance with the assumptions used in the process cost estimate. This would be very helpful to understand how close the proven process performance is to the projected performance and cost estimate.
- Process simulation has been completed to show 84% efficiency. The researchers have not addressed if coke formation is thermodynamically predicted at these conditions, especially considering such a large amount of hydrogen is being removed from the raffinate stream.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.5** for technology transfer and collaboration.

- Excellent group. Excellent collaboration.
- Involvement by their industry and international partners is significant and provides value to the research.
- There seems to be strong collaboration and well defined roles between participants.
- There is excellent collaboration across the research groups working on this project at GA, Sandia National Laboratories, CEA, and INL.
- The project has published papers and presented at most of the key conferences so that people interested in this project and technology can follow its progress.
- Having one or more private sector nuclear energy companies as a member of the project could add additional value and insight.
- Collaborating with USC, Chevron, and Johnson Matthey. Not clear on the distribution of effort.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

## PRODUCTION AND DELIVERY

- Key issues are recognized. Not so clear how they will be addressed.
- The proposed future work on catalyst durability, materials issues at high temperature, and optimizing the hydrogen output will be important to the success of the technology and should be completed.
- Planned work should include more catalyst development.
- They need to operate the complete integrated system.
- Increased life time tests need to be done.
- The future work plan is very good and fits well with the overall Nuclear Hydrogen Initiative program.
- It would be helpful if the Future Work Plan extended out to 2011 which is when the Department of Energy Nuclear Hydrogen Initiative Program will make its decision on what process will be used for the Nuclear Hydrogen Initiative Pilot Unit.
- Proceeding towards scale-up.
- No indication of decision points.

### **Strengths and weaknesses**

#### Strengths

- Separation and materials issues; catalyst degradation issues are unresolved and appear hard to resolve. I don't believe the hydrogen cost numbers based on the materials cost + complexity of the process.
- There is a strong team that is well funded.
- The cycle they are developing is strong candidate for use in thermochemical water splitting.
- The production of hydrogen driven by nuclear energy through the sulfur iodide thermochemical cycle has the potential to produce immense amounts of hydrogen without any emissions using only domestic resources.
- This is a large, well funded collaborative effort utilizing state of the art science and being performed by excellent scientists and engineers.
- The overall approach that has been taken of initial lab work, and scaling up to the fully Integrated Laboratory System is excellent. The Integrated Laboratory System can provide the information needed for the Pilot Plant unit.
- Membrane reactor will favor water-gas-shift conversion.

#### Weaknesses

- Separation & materials issues; catalyst degradation issues are unresolved and appear hard to resolve. I don't believe the hydrogen cost numbers based on the materials cost + complexity of the process. Safety worries about alumina reactor in close integration with a nuclear reactor - I would like to see a less brittle, less permeable material at this location.
- They need to increase the focus on material durability and lifetime tests.
- For the H2A analysis, they need to make sure to understand the operation and maintenance costs.
- The process has many steps and is relatively complex.
- More effort and progress is needed on the sulfuric acid catalyst.
- More effort and progress is needed on materials of construction for the Bunsen reaction and HU decomposition areas.
- It would be very helpful to compare the data from the lab and Integrated Laboratory System unit to the assumptions used in the cost estimate and to discuss how to close the gaps if there are any.
- Sensitivity of membrane to hydrogen sulfide, water is not addressed.

### **Specific recommendations and additions or deletions to the work scope**

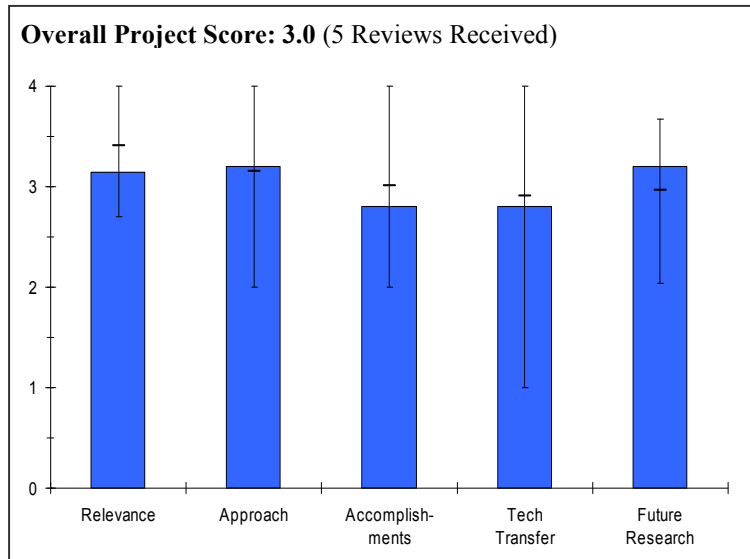
- More emphasis on materials and separation issues. Also address how this system might affect nuclear reactor if, for example, a leak appeared at the high temperature reactor - how do you clean up the helium loop? What are the likely capital and energy costs from cleaning up the various streams?
- Increase the effort on the sulfur dioxide decomposition catalyst.
- Increase the effort on materials of construction for the Bunsen reaction and HI decomposition areas.
- Confirm that coking is not thermodynamically predicted at water-gas-shift with 90% hydrogen removal.
- Review component / plant efficiency, cost, durability with respect to the assumed process conditions (S/C, temperature, pressure, hydrogen permeated through membrane, etc.).

**Project # PD-26: Hybrid Sulfur Thermochemical Process Development**

*Bill Summers; SRNL*

**Brief Summary of Project**

The overall objective of this project is to develop and demonstrate the hybrid sulfur thermochemical process as a viable option for large-scale hydrogen production using nuclear energy. The goal for fiscal year 2008 is the development and testing of an SO<sub>2</sub> depolarized electrolyzer (SDE) using a proton exchange membrane-type cell design. That includes to 1) optimize the HyS process design, update the flowsheet and perform cost analysis in conjunction with an industry partner; 2) continue to identify and develop improved cell components to reduce sulfur crossover and increase cell efficiency; 3) conduct single cell SDE testes at elevated temperature and pressure; and 4) install and test a multi-cell SDE with 100 lph hydrogen capacity.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.1** for its relevance to DOE objectives.

- A nice version of the heat to hydrogen cycle.
- The research is relevant to the program; however, without any cost analysis it is impossible to tell if it might meet program targets.
- Thermochemical water splitting supports the Department of Energy Hydrogen Fuel Initiative objectives.
- The production of hydrogen driven by nuclear energy through the hybrid sulfur cycle has the potential to produce immense amounts of hydrogen without any emissions using only domestic resources.
- The hybrid sulfur cycle is a far less complex cycle than the sulfur iodide cycle and thus would seem likely to be more robust in its commercial operation.
- This project involves proposed technology to manufacture hydrogen from high temperature heat.

**Question 2: Approach to performing the research and development**

This project was rated **3.2** on its approach.

- Concentrating on the electrolysis part - doing a fine job. Assumes the sulfuric acid decomposition & separation step is well developed; announces heat exchange and materials problems are solved. Too much effort on scale-up, not enough on development.
- Leveraging work on the acid decomposition step being performed by the Sandia National Laboratories team is a good approach and ensures the project is integrated with other research in progress.
- They are focusing on the key components.
- They need to identify and focus their development on the critical path (electrolyzer catalyst and membrane component development).
- The efficiency of the electrolyzer needs to be improved, even if they achieve their targets, the efficiency will be less than 40%.
- In the reviewer's opinion, they should focus on high temperature membranes which require less or no water, not a proton exchange membrane fuel cell.



## PRODUCTION AND DELIVERY

- They may want to consider operating at a higher pressure, which may enable them to increase their operating temperature.
- Savannah River National Laboratory has teamed up with other organizations (Westinghouse, Giner, University of South Carolina, and Sandia National Laboratories) with particular expertise germane to the hybrid sulfur cycle resulting in a very good team to tackle the challenges involved with this effort.
- The project has identified the key challenges and is focused on research to overcome them. They include sulfur crossover through the membrane, a membrane with improved ion conductivity, a better and longer lasting catalyst, and good flow field/diffusion media for sulfur dioxide transport.
- Good laboratory apparatus have been and are being developed to do the needed research.
- The activity explores one unit operation in one of the more promising chemical schemes for high temperature water splitting. The activities are well focused.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- Good progress. Still over voltage is quite high – S generation in electrolyzer is problematic.
- Project funding is at a reasonable level for the work being accomplished.
- Project has accomplished important milestones; however these milestones are based on completion of tasks and not achieving quantitative results with the work.
- No information was provided on projected costs even though their plant cost analysis task is nearly complete.
- Their progress seems modest for the time and resources available for the project.
- They need to improve their electrolyzer. They may be able to increase their efficiency and possibly their durability by using a high temperature stack.
- Significant progress is being made and the effort remains on schedule.
- Significantly improved membranes that reduce sulfur crossover and enable higher temperature operations have been identified and tested.
- Catalyst work is progressing.
- A multiple cell unit has been designed, built and operated.
- An integrated plant design has been further optimized for efficient use of heat and power coupling a natural gas NP reactor to the hybrid sulfur operations to reduce hydrogen costs.
- Considerable progress, but challenges remain.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.8** for technology transfer and collaboration.

- Excellent collaboration
- Collaboration with partners to leverage proton exchange membrane R&D and process design work is apparent.
- The roles of some partners (universities, Westinghouse) are not clear.
- There seems to be a strong team, but interactions are not apparent at least in the presentation.
- There is good collaboration between the organizations working together on this project.
- They project has issued several publications and given talks at several meetings but it has not gotten the results of this effort to a broad enough audience of potential stakeholders and other scientists who might have ideas that could help the project. Presenting at conferences such as those of the American Chemical Society, National Hydrogen Association and Fuel Cell Conference could be very helpful.
- Collaborations appear internal and with vendors.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- Seems prepared to address key issues.
- Multiple approaches have been identified to address the sulfur deposition problem. It will be important to solve this problem while still increasing cell efficiency.
- Focus on the electrolyzer development is appropriate for the future work.
- Improved H<sub>2</sub>A analysis needs to be done.
- The future work plan covers the key research areas and needs of this effort.
- The project has identified the key challenges and is focused on research to overcome them.
- The described activities were those to complete testing of their electrochemical reactor. However that small scale device could solve one part of the cycle they are working on, the sulfuric acid--to-sulfur dioxide problem persists. It is necessary but not sufficient.

### **Strengths and weaknesses**

#### Strengths

- Good project - some progress.
- The simplicity of the process compared to other nuclear hydrogen work is a plus.
- They have a strong team.
- They are working on the critical issues.
- The production of hydrogen driven by nuclear energy through the Hybrid Sulfur cycle has the potential to produce immense amounts of hydrogen without any emissions using only domestic resources.
- The Hybrid Sulfur cycle is a far less complex cycle than the sulfur iodide cycle and thus would seem likely to be more robust in its commercial operation.
- Savannah River National Laboratory has teamed up with other organizations (Westinghouse, Giner, University of South Carolina, and Sandia National Laboratories) with particular expertise germane to the hybrid sulfur cycle resulting in a very good team to tackle the challenges involved with this effort.
- Significant progress is being made and the effort remains on schedule.
- Their electrochemical concept is sound, and could work. The team is solid.

#### Weaknesses

- No discussion of projected cost of hydrogen production. Even having a rough estimate of this is very important.
- The project does not seem well organized.
- Sulfur crossover will not be solved by a physical barrier as described in the presentation. Since a proton exchange membrane fuel cell uses water as the electrolyte and sulfur is miscible in water, they will always have significant sulfur crossover. They need to select a membrane that does not use water in order to decrease the crossover. The second reason that the fuel cells experience crossover is low kinetics, therefore increasing kinetics will significantly decrease their crossover.
- The key challenges of this effort may be difficult to overcome in time for the 2011 Nuclear Hydrogen Initiative planned decision on the process to scale-up to the Pilot Plant operation. Given the potential of the hybrid sulfur process, it may be appropriate to increase funding to this effort vs. the S-I process effort.

### **Specific recommendations and additions or deletions to the work scope**

- A Go/No Go decision point based on hydrogen cost/system durability (specifically requiring a solution to the sulfur crossover issue) should be required by the Program.
- This is a very promising cycle for hydrogen production driven by nuclear or concentrated solar energy. The funding for this project should be increased. And the effort expanded to try to make more progress at a quicker pace.
- Savannah River National Laboratory is working with a proton exchange membrane fuel cell concept. The electrolysis cell design can be far simpler than the hydrogen-oxygen fuel cell. Some thought needs to be given to electrode design.

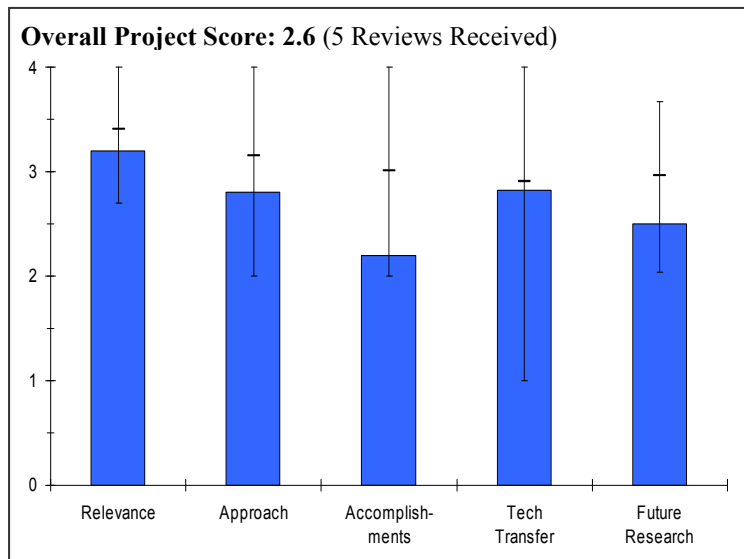
**Project # PD-27: Laboratory-Scale High Temperature Electrolysis System**

*Steve Herring; INL/ANL/Ceramatec*

**Brief Summary of Project**

The objectives of this project are to 1) develop efficient solid oxide electrolysis cells building on solid oxide fuel cell research; 2) decrease cost, increase durability; 3) determine reasons for long-term cell degradation; 4) optimize plant designs; 5) co-electrolyze CO<sub>2</sub> and steam to CO and hydrogen; 6) develop designs to apply nuclear heat and hydrogen to heavy petroleum and oil sand upgrading; and 7) integrate nuclear energy sources and fossil/biomass carbon sources for hydrocarbon synthesis.

**Question 1: Relevance to overall DOE objectives**



This project earned a score of **3.2** for its relevance to DOE objectives.

- Project aligns with needs of Department of Energy hydrogen production program.
- This project is developing high-temperature electrolysis for hydrogen production and therefore supports the President's Hydrogen Fuel Initiative.
- Addresses few cross-cutting barriers.
- High temperature electrolysis pertains to the Department of Energy Hydrogen Program.
- Hydrogen is produced at 1.3V at a nuclear reactor site in thermal contact with the nuclear reactor. Although this represents a modest increase in efficiency in the power used to make hydrogen, it is not clear that this increase makes up for the great increase in capital cost, and the great decrease in generator siting flexibility of putting the electrolysis unit next to a nuclear reactor.

**Question 2: Approach to performing the research and development**

This project was rated **2.8** on its approach.

- Approach is very good.
- Approach depends on availability of high temperature nuclear heat. It is a very long range goal.
- It appears cell degradation studies are going on since 2003 - what else can be done? No new ideas are presented to investigate the cell degradation behavior.
- This project should integrate with activities going on in SECA program.
- They have identified the critical issues and are working them in parallel.
- It would have been nice to have more discussion on the electrolyzer development.
- Carbon dioxide processing seems to be a diversion from the hydrogen production goal of this project.
- Mostly electrode potential was addressed, not durability and this was the largest show stopper. Too much emphasis on scale-up, not enough on development.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.2** based on accomplishments.

- FY08 technical objectives were clearly presented; however, there was no presentation on stack performance or degradation, and no assessment of alternative interconnect materials. In fact there has been not degradation testing initiated to date in FY08. This project is falling short of its listed objectives.
- A technical issue arising from steam corrosion in the balance of plant leading to chromia formation and contamination of the electrolyzer stack has not been addressed from last year. This problem was been solved by the fossil energy industry and a solution should be easily found by working with suppliers to the boiler industry.
- No new information on cell degradation was presented.
- Half-Integrated Laboratory System module was tested.
- Performed initial Integrated Laboratory System-single module test series (240 cells).
- Completed economic analysis for high temperature electrolysis using H2A methodology.
- Completed CFD analysis of multiple-cell stack geometry.
- Too high area-specific resistance; The hydrogen production rate decayed very fast within first 100 hours.
- Corrosion was a big issue last year, but nothing was mentioned about it in today's presentation.
- Total voltage for electrolysis was 1.3V, only about 0.2V better than for room temperature, conventional electrolysis. Durability improvements, if any, were not presented. Economic assessment details were not presented, and overall price of hydrogen projected did not look like the researchers had correctly accounted for the cost of electricity or safety or high temperature materials. It was not clear that the cost of hydrogen made this way won't be higher than for conventional electrolysis at room temperature. Corrosion problems noted last year had not been addressed.
- Lab scale tests are important to the project development.
- The SOEC stack lifetime needs to be improved. Discussion on the work in this area is necessary.
- They should consider engaging SECA for additional insights on the solid oxide electrode materials they are using.
- The H2A cost seems higher than expect, it is recommended that they engage Tiax, DTI, or others intimately familiar with H2A to review their analysis.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.8** for technology transfer and collaboration.

- Massachusetts Institute of Technology and University of Nevada Las Vegas were listed as collaborators but their roles were never explained.
- This team needs more industrial partners to execute the work plan and less academic involvement.
- Collaborating with Ceramtec, Argonne National Laboratory, Massachusetts Institute of Technology, and University of Nevada Las Vegas.
- Good to see they have evaluated a cell made by another fuel cell manufacturer.
- There seems to be adequate communication between the partners.
- Good collaboration group. Information did not seem to flow well between members.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.5** for proposed future work.

- Proposed future work is meaningless if team cannot execute planned FY08 work plan.
- This team should not be allowed to scale-up this technology and it should be transferred to an industrial partner as soon as possible.
- The project end date is FY 2015. Slide #18 gives plans for 2008 but nothing for 2009-2011 periods. Plans jump from 2008 to 2012.
- Use quantitative rather than qualitative terms for future plans. Just saying "we will continue to investigate cell degradation" is not enough. Need to be more specific about what exactly will be done.
- No plans presented to address the high area-specific resistance that is seen in the results presented today. It is important to reduce the area-specific resistance.
- Why is the corrosion issue dropped from the future plan?
- Parallel approach seems reasonable.

## PRODUCTION AND DELIVERY

- Since the stack is the critical component, its development should receive more attention and resources.
- Vague - generally sounds like going in right direction regarding durability, but would prefer to see plans for scale-up shelved until durability problems solved. Ideally, would prefer to see a better economic assessment at this stage, plus plans for accelerated aging tests to show 5000 hours of electrolyzer operation with minimal degradation at a temperature that would be at least 100 degrees Celsius higher than the target operation temperature.

### Strengths and weaknesses

#### Strengths

- Good team with solid oxide fuel cell experience.
- They are pursuing a technology that has the highest potential efficiency of all of the high temperature thermochemical water splitting technologies.
- The team seems adequate.
- They are well funded.
- Good group of researchers. Product made more hydrogen than any of the other thermal cycles presented today.

#### Weaknesses

- Team lacks leadership and cohesion. FY08 is 75% over and most of the key FY08 R&D issues have not been initiated.
- Lack of coordination of results. Lessons learned from prior work are not used/implemented in the on-going work.
- For example, what was learned in the assessment of degradation in long-duration test cells that was completed in 2006? How is that result used in the work going on since 2007? It is not clear to this reviewer how the results are being analyzed and used for future research.
- I think this project is going tangentially into other areas — why integrate nuclear energy and fossil/biomass sources for hydrocarbon synthesis. Focus should be on hydrogen production.
- Stack component development needs increased resources. It is the critical path.
- Durability seems like a show-stopper, economic value seemed unclear. General sense that this is not something you would want attached to a nuclear reactor.

### Specific recommendations and additions or deletions to the work scope

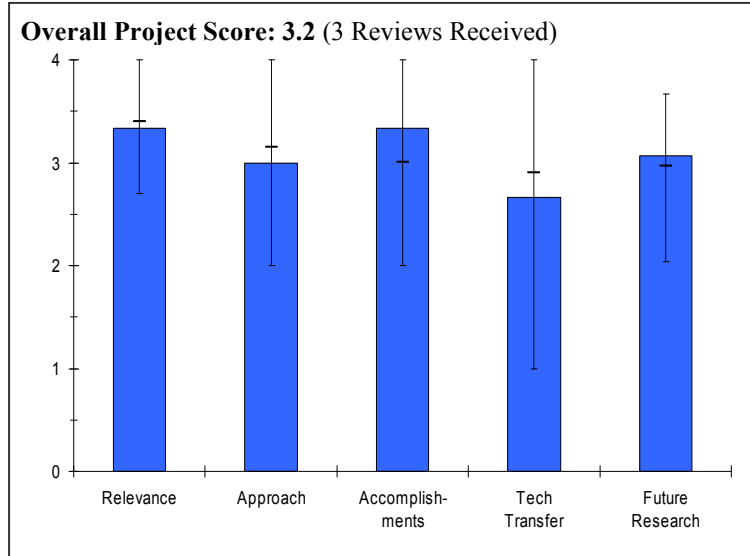
- PI should come up with a detailed research plan for 2009 and 2010.
- Delete the co-electrolysis of carbon dioxide and steam to carbon monoxide and hydrogen. Focus on steam electrolysis for hydrogen production.
- Is there a timeline to end the research on understanding the cell degradation phenomena?
- Carbon dioxide processing will only divert attention from the hydrogen production goals of the process and should be removed.
- They should have an outside company help them with their H2A analysis.
- Concentrate on improved durability and less effort on scale-up. Would prefer to see durability addressed at this scale before scaling up. Would prefer accelerated aging test that shows 5000 hours with minimal degradation at higher temperature.

**Project # PD-28: Alternative Thermochemical Cycles**

*Michelle Lewis; ANL*

**Brief Summary of Project**

The objectives of this project are to 1) develop a commercially viable process for producing hydrogen based on a thermochemical cycle that meets the Department of Energy cost and efficiency targets; and 2) coordinate university evaluation of alternative cycles considered in the literature as promising and down select to the most promising cycle. Selection criteria were chemical viability, engineering feasibility, projected efficiency and hydrogen production cost, and the Department of Energy-NE's timeline for an integrated laboratory-scale demonstration.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- Thermochemical water splitting for hydrogen production supports the Hydrogen Fuel Initiative.
- Work on interesting previously little studied confined thermochemical/ electrochemical cycle.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- Approach seems reasonable.
- The cycle is low temperature which enables it to integrate with solar or nuclear.
- Electrolyzer efficiency will be a critical component.
- For this "Copper-Chlorine" cycle the focus has been on improving the  $\text{CuCl}_2$  to  $\text{Cu}_2\text{OCl}_2$  and electrolysis process.
- While the relatively low temperature for oxygen generation (530 degrees Celsius) has process advantages, it is limiting the energy efficiency in terms of a carrot(?) cycle analysis - need to understand this better.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- It appears that progress has been made on understanding the chemistry for all the reactions other than the electrochemical ones.
- Progress on the electrolysis is difficult to assess since only sparse data was reported.
- Overall very good work toward the development of this "Copper-Chlorine" cycle. It's not clear what the yields and selectivities were for the engineering lab scale hydrolysis reactor.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.7** for technology transfer and collaboration.

## PRODUCTION AND DELIVERY

- The AEC member does not seem to be a "team player".
- Other than the electrolyzer work, there seems to be appropriate levels of interaction between the team members.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- More details on the electrolysis reactor need to be reported before review on that critical component can be made.
- This project is in the early stages and significant development in each of the components and in understanding the chemistry is needed.
- Performing the proposed continuing process development research would be assisted from a better understanding of fundamentals of the underlying chemistries, particularly the operative thermodynamics.

### **Strengths and weaknesses**

#### Strengths

- The cycle selected operates at relatively low temperatures making it acceptable for use in nuclear as well as solar driven systems.
- There appears to be the needed expertise on the team to address the critical issues.
- The apparently clean oxygen release at 530 is quite remarkable - a process asset.

#### Weaknesses

- It is not clear when this method compares with normal electrolysis with the use of excess heat use.
- Further understanding is needed on the electrolyzer operation and performance.
- Significant work will be needed on developing a durable system.
- Breaking the azeotrope and maintaining an efficient system will be difficult.
- Use of inert carrier gases will increase the operating costs significantly.

### **Specific recommendations and additions or deletions to the work scope**

- None.

**Project # PD-29: Indirectly Heated Biomass Gasification**

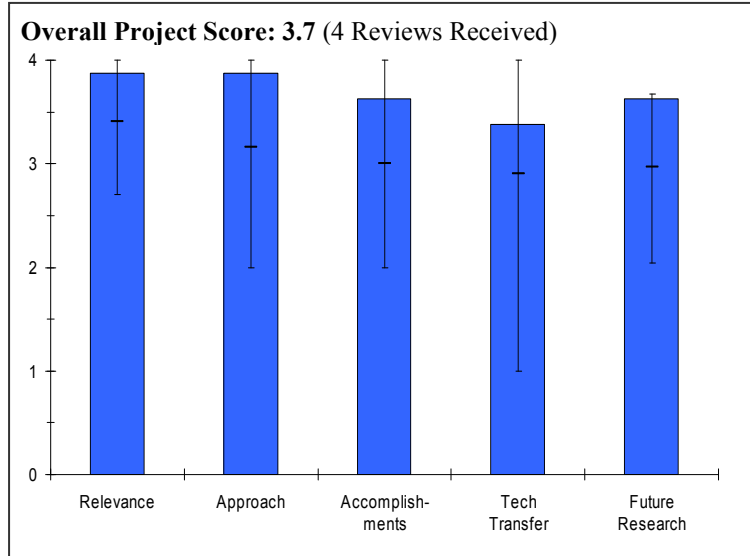
*Richard Bain; NREL*

**Brief Summary of Project**

The objective of this project is to experimentally update the technical and economic performance of an integrated biomass gasification-based hydrogen production process based on steam gasification. The expected key outcomes are 1) production of clean syngas; 2) production of high purity hydrogen; 3) development of updated yield and gas quality correlations; and 4) development of updated technoeconomic model.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.9** for its relevance to DOE objectives.



- They have addressed issue associated with 2012 and 2017 targets of gge for hydrogen production from biomass gasification.
- The project is evaluating the production of hydrogen from biomass-steam gasification. This is a key goal of the Hydrogen Program and the work is directly supporting this objective. The work is being conducted at a scale that will provide solid data to extrapolate the costs of a larger scale system. The results will be used to determine if the Department of Energy cost target can be obtained - and based on information provided at the presentation - preliminary analysis indicates that this process can achieve the Department of Energy cost targets.
- Project milestones and targets fully supports Department of Energy RD&D objectives.
- \$1.60/gge hydrogen in 2012 and \$1.10 gge hydrogen in 2017 both at the plant gate are identified as the achievable project targets.
- This approach to renewable hydrogen is one of the least-costly and most ready-to-use.

**Question 2: Approach to performing the research and development**

This project was rated **3.9** on its approach.

- They have utilized an integrated approach for analysis that incorporated technical data, process modeling, and economic modeling which is both thorough and fundamental.
- Identified and correlated new sets of variables for analysis of gasification and reforming data.
- The work consists of a comprehensive test program at a reasonable scale (20 g/hr biomass feed).The work is evaluating all aspects of the process including gasification, hydrocarbon reforming, clean up and hydrogen separation. In addition, the work is considering process intensification - combining methane reforming and heavy hydrocarbon reforming at the same time (which is typically not done together).The work is using an existing facility that is capable of generating a large amount of useful data. The work is providing large amounts of information on all the system components.
- Objectives and milestones clearly addressed technical barriers for biomass gasification for hydrogen production to achieve Department of Energy cost targets.
- Approach is well focused on obtaining data needed to understand the barriers.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.6** based on accomplishments.



## PRODUCTION AND DELIVERY

- They have completed an evaluation of gasification and tar reforming.
- They have identified and correlated new sets of variables for analysis of gasification and reforming data.
- The work is about 1/3 complete and has already generated a significant amount of data - in particular detailed composition of the syngas stream from hardwood biomass - including the higher hydrocarbons. This is valuable information for future work on biomass gasification.
- National Renewable Energy Laboratory has tested their reforming catalyst and provided extremely encouraging results. The reactor is operated as a fluid bed and can be recycled numerous times with little decrease in activity. This is a novel approach, in that the reforming is typically carried out in a fixed bed reactor.
- The work is using steam rather than oxygen gasification. This reduces the cost and helps to reach the Department of Energy cost target.
- The results are demonstrating good conversions and overall hydrogen yield.
- Completed one gasifier/reformer campaign and initial update of gasifier correlation.
- On target with 2008 milestones timeline.
- Very good approach along plan... but how far it has come to address the barriers will not be clear until the system level modeling is completed.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.4** for technology transfer and collaboration.

- The technical application of the work is clear and will benefit the refinement of this as a viable industrial process. Not clear how the PI will institute this.
- The results of the work will be published as have the results obtained previously. The work is producing detailed data that will be valuable to future research.
- National Renewable Energy Laboratory should consider involving an industrial partner - mainly just to validate the results being obtained and to get some independent input for the direction of the project.
- Project update suggests that there is good coordination with Department of Energy Biomass Program-sponsored research at National Renewable Energy Laboratory related to Gasification and tar reforming work.
- Not evident in presentation, but technology transfer axis could be very important if/when industry is ready to commercialize.
- Coordination around development of reforming catalyst might be increased.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.6** for proposed future work.

- The PI will move forward to complete gasification, reformers, and shift reactor testing.
- Evaluation of technical models and H2A economic evaluation will be completed.
- They will include an additional parameter not included in their initial parameterization - the role of the catalyst.
- The work is on schedule and the future plans are appropriate. The work will evaluate a biomass softwood feed that will provide a good comparison between two different biomass feedstocks.
- The data will allow for a good cost analysis using H2A.
- Plans include critical tasks to complete the technical work and modeling work.
- Future work includes economic analysis using H2A model and making Go/No-Go decision.
- Plans are excellent but very short term (not a criticism, I understand this is a short term program).

### **Strengths and weaknesses**

#### Strengths

- This project has a strong integration of technical evaluation, process modeling, and economic modeling.
- Excellent and comprehensive project to develop detailed data and information on several important processes in the production of hydrogen from biomass feedstocks.
- Good project plan with technical and economic targets clearly identified.

- Good execution of the project plan.
- Well executed short term program to obtain data about gasification of biomass.

Weaknesses

- As it stands, the project has not dealt with the role of catalyst in product distribution (which must surely affect the downstream modeling). It seems though that this aspect will be incorporated in future work.
- None identified.

**Specific recommendations and additions or deletions to the work scope**

- No changes are required in the project work scope.
- It is a well organized, planned and executed project.
- This could be an important user facility if/when industry is ready to commercialize.
- Continued or occasional operation might be warranted to further improve reforming catalyst as well as processes ancillary to the gasifier, such as the separations and shift, etc.

**Project # PD-30: One Step Biomass Gas Reforming-Shift Separation Membrane Reactor**

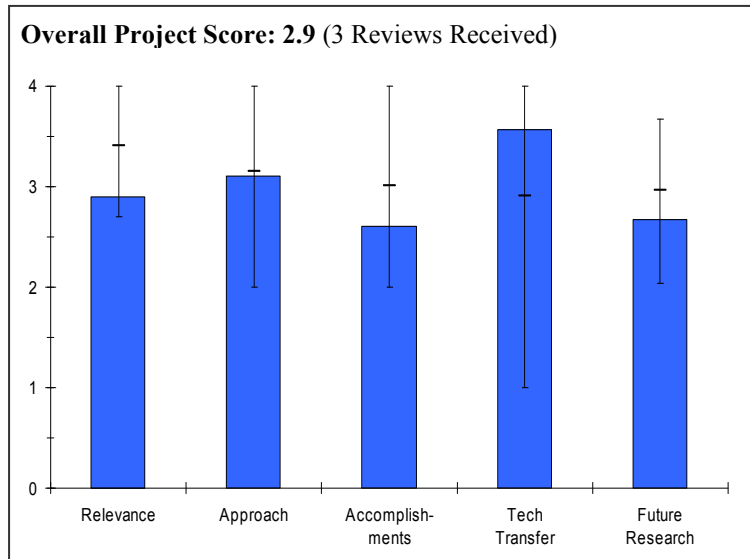
*Michael Roberts; GTI*

**Brief Summary of Project**

The long-term objective of this project is to determine the technical and economic feasibility of using the gasification membrane reactor to produce hydrogen from biomass. The first year goal was to select an initial candidate membrane material that can be fabricated into a module for testing with the bench scale gasifier by evaluating ceramic, metallic, composite and glass ceramic membranes.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.9** for its relevance to DOE objectives.



- Removal of hydrogen in the gasifier should favor hydrocarbon and carbon monoxide conversion after initial gasification reactions.
- Potential for fouling of membrane by ash, tars, and/or carbon deposition. The latter becomes more likely with hydrogen removal.
- If the membrane is in the cyclone at 1500°F where there is no heat source, only the water-gas-shift conversion will be benefited. The bulk of the hydrogen will still remain with the hydrocarbons.
- They have addressed issues associated with 2012 targets of gge for hydrogen production from biomass gasification.
- They have taken on a challenging problem for which the benefits appear to be great and are in line with stated Department of Energy goals.
- Goal is to facilitate hydrogen production from biomass gasification, which is nominally aligned with Department of Energy RD&D objectives.
- The approach - of adding to the gasifier a membrane for hydrogen removal - does not clearly improve gasification. It could easily increase cost (due to added components) or decrease yield of hydrogen (because hydrogen and carbon monoxide that does not go through the membrane are downgraded to local fuel), or both.
- This can only really help with gasifier yield if it is actually deployed inside the gasifier, where the exotherm of shift can be used to supplement gasifier energy. Deploying right after the cyclone may enable use of a high temperature membrane, but that does nothing, in itself, to address gasification barriers.

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- Membrane material development will be key.
- Will the membrane be tested in gasification / pre-gas clean up environment, in the presence of tars and solids (char, ash)?
- Location of membrane will be an important factor, i.e., exposure to constituents.
- Not clear if the oxygen membrane will have sufficient flux to make a reasonably compact gasifier.
- They have adopted a challenge to incorporate membranes directly into gasifier and the benefits of this approach appear to be great (calculated at 40% improvement in hydrogen production with this approach).
- Since this technology must be inside the gasifier to add value, there should be more analysis of critical barriers related to membrane survival in the gasifier environment... i.e. what materials issues are raised by exposure to ash, sulfur, etc.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.6** based on accomplishments.

- A hydrogen-membrane has been selected. Not clear if its flux is sufficient to meet their reactor size targets.
- Good sulfur tolerance at 850 °C.
- Permeation tested with syngas. Use of sweep gas improves flux – they expect to use steam as a sweep gas in their final design. How will this additional steam affect the process efficiency?
- 50% flux loss in twenty hours. What is the degradation mechanism?
- They have identified a lead candidate membrane (copper-palladium) material with which to proceed.
- They have demonstrated failure mechanisms (grain boundaries) in existing materials and developed palladium incorporation at grain boundaries in CMAS. The connection between these aspects was not clear from the presentation or whether the high palladium incorporation resulted in increased hydrogen permeability.
- Nice work exploring new approaches to hydrogen membranes, new approaches are needed to reduce or eliminate the unaffordable levels of palladium in current membranes.
- Real barriers will be exposure to gasifier environment, and there has been little progress here.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.6** for technology transfer and collaboration.

- Good team of collaborators.
- The integration of academic research with national lab and industry partners is a powerful combination.
- Good coordination among subcontractors.
- Not clear (not discussed) how much program draws best membrane ideas from broader institutions.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.7** for proposed future work.

- Membrane material development is planned. Flux goals are not mentioned.
- It is not clear why they are making thin membranes before confirming a material with high permeance and durability.
- They will continue to evaluate new materials with enhanced properties for hydrogen permeability and catalysis.
- They will expand the palladium-glass materials synthesis on larger scale.
- They will fabricate parts for hydrogen permeation studies.
- Plans are well designed to incrementally improve palladium membrane, and provide proof of concept for ceramic and glass membranes.
- It is not clear that any membrane success, applied as proposed, would address the gasifier barriers described, how actual membrane barriers will relate to exposure to gasifier environment, and the plans get to proof of concept on that feature proceed much too slowly.

**Strengths and weaknesses**

Strengths

- Initial focus on membrane material development is good.
- They have identified a lead candidate membrane material with which to proceed with the project while at the same time continuing to evaluate new materials for enhanced performance.
- Multiple (3) membrane approaches.

Weaknesses

- Locating membrane in cyclone where there is no catalyst or heat source is not very promising.
- Data interpretation is difficult when all experimental information is not provided.

## PRODUCTION AND DELIVERY

- While hydrogen in this scheme is potentially recovered through the membrane with great benefits, there is the potential that not all the hydrogen will be recovered this way. In that case the PSA will presumably have to be re-introduced thus diminishing the overall cost-benefit.
- Lack of materials exposure to gasifier environment (does not need to be a functioning membrane, even coupon exposure would allow evaluation of impact of exposure).
- The reviewer thinks this concept will really struggle to be economically advantageous. A techno-economic analysis is needed.

### **Specific recommendations and additions or deletions to the work scope**

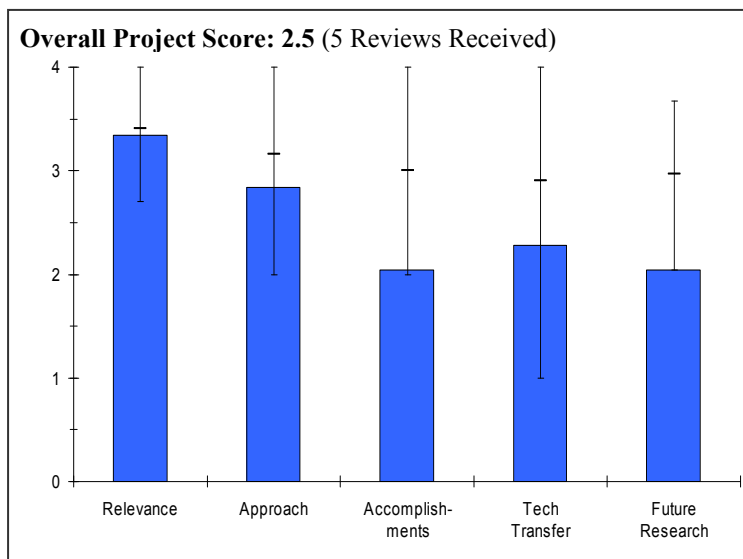
- Membrane testing should be conducted at conditions closer to anticipated environment - presence of tar, high hydrogen removal across membrane, etc.
- Define criterion for selecting membrane material to proceed to testing in biomass reactor.
- Better quantify the potential advantages.
- Find some way to "coupon test" prospective materials in a gasifier.

**Project # PD-31: A Novel Slurry Based Biomass Reforming Process**

*Thomas Vanderspurt; UTRC*

**Brief Summary of Project**

The objectives of this project are to 1) illustrate through an initial feasibility analysis on a 2000 ton/day (dry) biomass plant design that there is a viable techno-economical path towards the Department of Energy's (DOE's) 2012 efficiency target (43% lower heating value) and assess the requirements for meeting the DOE's cost target (\$1.60/kg hydrogen); 2) demonstrate through preliminary results that an acid tolerant model sugar solution reforming catalyst with acceptable kinetics has been synthesized and that a viable technical path for scale up (mass production) of this catalyst in a cost-effective way exists; 3) identify hydrolysis conditions for a simulated biomass system and viable techno-economic path towards the achievement of the hydrolysis of the real biomass system; and 4) demonstrate through extensive test results an acid tolerant, long life, cost-effective biomass hydrolysis product reforming catalyst.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- They have addressed Department of Energy target goals for hydrogen production costs and lower heating value.
- Their model systems are both relevant and feasible and as such, are in line with the Department of Energy objectives.
- The work, as originally proposed, directly supports Department of Energy's objective of producing hydrogen from biomass.
- Project with its overall objectives supports the hydrogen vision and Department of Energy RD&D objectives.
- Key features outlined in the Project Progress Report propose steps toward 54.2% lower heating value energy efficiency.
- Project targets hydrogen production cost of \$1.60/Kg hydrogen when biomass is obtained at \$25/Ton
- Novel slurry based biomass reforming is a great concept.
- The project addresses an important aspect of the Department of Energy Program involving production of hydrogen from biomass.

**Question 2: Approach to performing the research and development**

This project was rated **2.8** on its approach.

- Good process concept.
- They have utilized an integrated approach for analysis that incorporated both technical and economic feasibility of using a gasification membrane for hydrogen production from biomass.
- They have tackled an important problem, and developed a nice conceptual design-synthesis-modeling approach to catalyst design.
- The original approach was to utilize molecular modeling and basic chemical principles to design and prepare effective catalysts for the proposed conversion. This is a reasonable approach, and United Technologies Research Center (UTRC) has had success with this approach in the past.

- However, based on the current technical results - this approach does not appear to be working in this project. This may be due to the fact that conversion is extremely complicated - but UTRC is having little success even with one model compound (glycerol). Conversion rates and hydrogen yields are extremely low and tend to indicate that continuing with the current approach will not lead to success.
- Project plan is addressing biomass gasification efficiency barrier.
- Project, at the present, is not addressing feedstock cost and availability barrier.
- Technical work is focused on catalyst selection and testing to improve hydrogen production in the reformer.
- Project uses mainly sugar and sugar alcohols for test cases and planning for simulated biomass system for future work.
- Good analysis of the catalyst work was provided.
- The project is well aligned with addressing the barriers listed. A "one pot" method to produce hydrogen from raw biomass is a noble goal.
- This is a very difficult project given all that must be accomplished. It is not clear that at the end of the day it would not be better to separate some of the key unit operations.
- Some important details were not clearly presented. For example, how would one separate out the lignin, ash, and protein at the end of the process?
- It is not clear that the quantum mechanical approach used by UTRC to design the water-gas-shift catalyst could simply be extended to this much more complex catalyst system with such a complex feed, especially in the absence of any mechanistic information to determine what is needed. At the end of the day, a previously developed catalyst was used.
- The HYSYS simulation demonstrating possible 54% efficiency is not helpful unless many of the assumptions that went into that model are spelled out.
- Might it be better to neutralize the acid function and then proceed?

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.0** based on accomplishments.

- Systematic progress, nicely reported. Unfortunately, results are discouraging.
- What is the hydrogen productivity expressed as mol of hydrogen produced compared to maximum achievable in the Annual Program Review? At what level do they need to be for the \$1.60 target?
- Addition of  $\text{KHSO}_4$  shuts down hydrogen production.
- They have achieved 50% lower heating value and production costs of \$1.60/kg (although the data showing this was from last year and not presented here - it would have been nice to see).
- They have solved their problems of reproducibility by switching to stirred Zirconium autoclave reactor.
- They have solved catalyst issues by switching to a platinum/CeZrO system which has stable performance below 190°.
- To date - the project has limited technical accomplishments and progress.
- Reaction rates and hydrogen production, even with the model reactions (glycerol) is minimal. The actual feedstock will be considerable more complex. Moreover, UTRC was unable to provide any suggestions on the actual reaction mechanism for the conversion.
- Tests conducted in the autoclave indicate some hydrogen production, but UTRC could not provide any quantitative information. These tests were evidently conducted with actual biomass (sawdust) samples.
- It is not clear that UTRC was able to produce the identified catalyst structures. During the presentation, UTRC could not provide any technical or analytical information to indicate that the proposed structures were actually prepared.
- With the project approximately 50% complete, UTRC has obtained minimal (to none) positive technical results.
- Based on the current results – it is unlikely that any of the current catalysts could meet the Department of Energy cost target for hydrogen production.
- The progress report summarizes catalyst test results for several bio-based liquids, primarily glycerol. They also tested one wood sample.
- Project was started in May 2005 and three years later reported accomplishments suggest that progress has been slow. PI stated that this is partly due to funding interruptions.
- Work to date so far provided some key directional results for further future catalyst tests.

- Addition of milestones with Go/No-Go decision point for the success of catalyst in terms of both technical and economic performance will be critically important for the project.
- It is unclear why glycerol was selected as the model compound for the complex sugar solutions.
- The poisoning effect of sulfur, both by computation and by experiments with NaHSO<sub>4</sub> raised questions how this problem would be addressed.
- A statement of measured vs. required rates of hydrogen production would have been helpful to know how much greater activity must be achieved.
- Was the addition of KHSO<sub>4</sub> meant to simulate the possible effect of acid on catalyst performance? Or was it sulfur stability, or both? It was not clear how the possible negative effect of the acid function used for the hydrolysis was addressed in the test protocol.
- What level of feed conversion was achieved in Slide 15?

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.3** for technology transfer and collaboration.

- Collaborating with UND. What is their role?
- Their catalyst systems have been outsourced for synthesis, which is a good indication of the maturity and 'transferability' of that aspect of the technology.
- Tech transfer and external collaboration appears to be minimal.
- Other than the Annual EERE Hydrogen Review, only one other presentation at an American Chemical Society meeting is identified. No publications or other means of tech transfer are identified.
- The summary slide indicates some collaboration with UNDEERC - but it is not clear what this collaboration involves.
- Project report suggests that some coordination exists. It is not clear what part of the project is conducted by University Of North Dakota
- The extent of collaboration with North Dakota was not apparent.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.0** for proposed future work.

- No new catalyst strategies were discussed.
- They will show cost effectiveness of the catalyst system and identify hydrolysis conditions to optimize biomass reforming.
- They will scale-up to a 2-L autoclave to build on current successes and the planned scale-up of reaction to a 1kW demonstration scale will be an excellent validation of the technology
- There have been few technical accomplishments in this project. UTRC and Department of Energy need to come to a mutual agreement on the future work scope and redefine the future research direction.
- Project management will be more effective with inclusion of key milestones for technical and economic feasibility with Go/No-Go decision points.
- Future work suggests more catalyst testing.
- Future plans need to focus on overcoming barriers, feedstock availability and cost and efficiency of gasification.
- The future work was rather broadly defined with no specific detail. Greater discussion of the vision of the entire process would be helpful to the reviewer, and which specific tasks would be taken on in what order.
- The term "viable path" appears to be rather loosely used.

**Strengths and weaknesses**

Strengths

- Good process strategy to convert biomass to hydrogen.
- They have tackled an important problem, and developed a nice conceptual design-synthesis-modeling approach to catalyst design.



## PRODUCTION AND DELIVERY

- The work attempts to develop active catalytic materials based on basic molecular principles. This is a reasonable approach for catalyst development (however, the current results are not supporting initial assumptions).
- Catalyst design and catalyst testing.
- Good technical team, smart people.

### Weaknesses

- Result to date is not great. New catalyst approaches may be needed.
- It is not clear what the final catalyst will be in the final scale-up demonstration of the technology and whether or not they will continue the effort to develop new catalyst systems (it is not part of future plans).
- According to the summary slide - this project is approximately 50% complete and there are no solid results to suggest that UTRC should continue with the current approach.
- At the current time, this project appears to lack any clear sense of technical direction. During the presentation, UTRC indicated that they would continue to produce more catalyst materials with different metals and compositions - but there does not appear to be any clear plan for what these compositions will be.
- Based on the presentation, it is not clear that UTRC has a clear plan to separate the reaction products and the remaining unreacted solids (which could be a complex mixture).
- Milestones and Go/No-Go decisions addressing both technical and economical feasibility.
- Cost analysis.
- Lack of more specifics in terms of how the many challenges involved in this project will be addressed and handled, and in what order.

### Specific recommendations and additions or deletions to the work scope

- Concentrate on the catalyst and aqueous phase reforming until breakthrough. Proceeding with water-gas-shift can at best be a distraction.
- UTRC needs to provide Department of Energy with a detailed revised work plan to complete the work.
- The work plan needs to contain specific targets, goals and objectives to ensure that the project is making adequate advancements.
- The specific milestones should be based on a semi-annual basis – and mutually reviewed (on the determined completion dates) by Department of Energy and UTRC to ensure they are being met.
- Due to the lack of technical success – Department of Energy should consider a complete revision of the current work scope.
- Addition of milestones with Go/No-Go decision point for the success of catalyst in terms of both technical and economic performance will be important for the project.
- Experimental Tasks to address economic targets in reference to Department of Energy goals.
- Inclusion of feedstock cost and availability.
- Consider some simplifications by perhaps increasing the number of unit operations to reduce problems of reactor type, acid handling, solids removal, etc.

**Project # PD-32: Hydrogen From Water in a Recombinant Oxygen-Tolerant Cyanobacteria System**

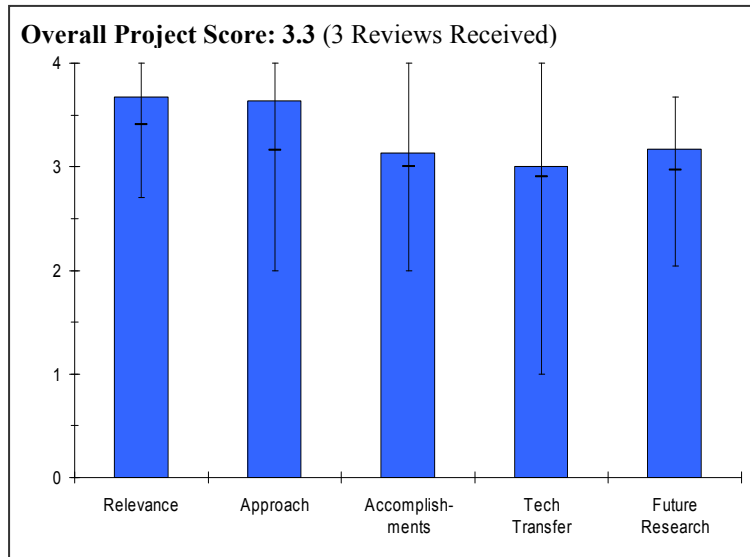
*Qing Xu; J Craig Venter Institute*

**Brief Summary of Project**

The objective of this project is to develop an oxygen tolerant cyanobacterial system for continuous light-driven hydrogen production from water. The approach is to transfer oxygen tolerant hydrogenases into cyanobacteria to overcome the hydrogenase oxygen sensitivity issue. Environmental DNA encoding hydrogenase was converted into a functional hydrogenase with both hydrogen evolution and uptake activities.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.7** for its relevance to DOE objectives.



- The project goals are well-aligned with Department of Energy program targets for novel biologically-derived catalysts for hydrogen production.
- The focus on identification of novel hydrogenases is good.
- The focus on increasing the level of hydrogen production from the heterologous system is good.
- Obtaining oxygen sensitive hydrogenase and developing molecular biology-based techniques to manipulate the enzyme is absolutely critical to the initiative.
- It seems relevant. However, explanation was very complex, making it difficult to assess relevance.

**Question 2: Approach to performing the research and development**

This project was rated **3.6** on its approach.

- The metagenomic approach for identification of novel hydrogenase-related sequences is logical, and builds upon progress in the investigators' lab.
- The focus on construction of new molecular biology toolkits for introducing hydrogenase-related gene cassettes into heterologous host strains is appropriate.
- The control experiments have been carefully designed to increase confidence in the experimental results with the heterologous expression studies.
- The use of retrogenomes as sources of hydrogen genes is very exciting. The approaches are appropriate, although it is not clear why they choose the genes that they did.
- Approach seems reasonable, however hard to assess in given presentation.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- The progress towards goals was excellent, with reconstruction and identification of a novel environmental nickel-iron hydrogenase and stable expression in a heterologous host.
- Demonstration of hydrogen production from the novel nickel-iron hydrogenase was good.
- There was good progress in demonstrating the correct maturation and targeting to membrane fraction of the Thiocapsa hydrogenase in the heterologous Synechococcus host.
- There was good progress towards introducing other hydrogenase genes into different heterologous cyanobacterial hosts (e.g. Synechocystis 6803).

## PRODUCTION AND DELIVERY

- It is important that catalytically active enzymes were not obtained but it is clear that the PIs are very close to achieving their goal

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.0** for technology transfer and collaboration.

- Good evidence was presented for coordination with other university investigators, including some not formally listed as co-investigators on the project (Michigan State University).
- Good partnerships/MTA with international entities for global ocean survey genome mining project.
- The J. Craig Venter Institute and National Renewable Energy Laboratory components seem quite distinct and parallel, displaying little synergy.
- The two institutions bring enormous expertise in molecular biology and the growth and physiology of anaerobes and hydrogenase biochemistry. However, the interactions between the PIs need to be developed further to obtain the achieved enzyme.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- Future goals of stable hydrogenase subunit expression in industrial "workhorse" E. coli strains are good.
- Introduction of different environmental hydrogenases into various heterologous expression host strains is logical and appropriate.
- This was not as usefully described as it might have been. The resources of the PI and JVICI in bringing high throughput assays to this project should be a priority.

### **Strengths and weaknesses**

#### Strengths

- The investigators' knowledge of canonical hydrogenases and structure-function relationships is very robust.
- The investigators' track record of novel gene identification and development of synthetic biology toolkits is very strong.
- The multi-pronged use of different combinations of known hydrogenases, novel hydrogenases, different maturation cassettes, and different heterologous hosts ensures casting a wide net for knowledge of optimizing hydrogenase activity.
- The experiences of the PIs and their inhibitors, the unlimited "molecular" resources in terms of the metagenomes and the overall project goals.

#### Weaknesses

- The project has not identified contingencies for identification of novel, noncanonical hydrogenases. Although screening experiments have been proposed, it is not clear how the screens will be designed to discriminate between low level of protein expression or stability but extremely high activity vs. high level of protein expression or stability with modest hydrogenase activity. Some more defined metrics would have been preferred.
- The project has not demonstrated hydrogenase activity in the catalytic subunit expressed in the heterologous E. coli host
- The project has not identified contingencies for co-evolution of novel hydrogenases; perhaps targeting the catalytic subunit is not the target with the highest return—what if testing accessory genes from environmental samples will provide a new way to protect the existing hydrogenases from destruction?
- It is a pity that the active enzymes were not obtained but this is only a matter of time.
- All of the pieces are in place for the PIs to be successful.

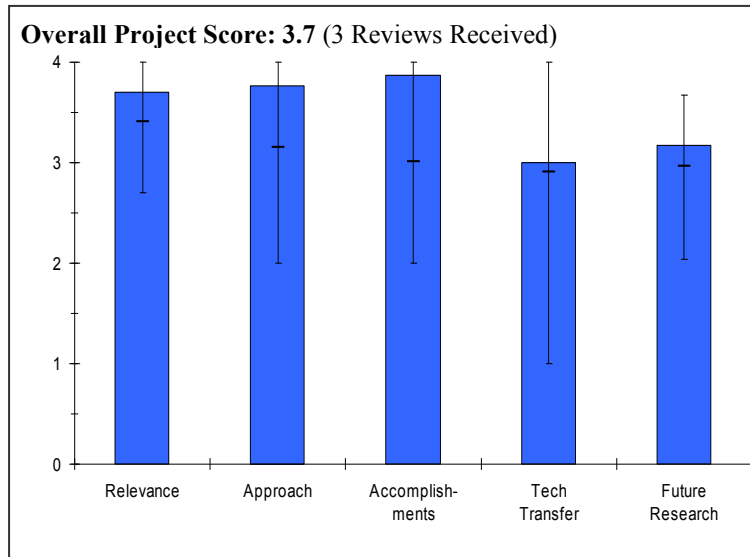
### **Specific recommendations and additions or deletions to the work scope**

- None.

**Project # PD-33: Maximizing Light Utilization Efficiency and Hydrogen Production in Microalgal Cultures**  
*Tasios Melis; UC Berkeley*

**Brief Summary of Project**

The objectives of this project are to 1) minimize the chlorophyll antenna size of photosynthesis to maximize solar conversion efficiency in green algae; 2) identify and characterize genes that regulate the Chl antenna size in the model green alga *Chlamydomonas reinhardtii*; and 3) apply these genes to other green algae as needed. The approach is to 1) interfere with the molecular mechanism for the regulation of the chlorophyll antenna size; and 2) employ DNA insertional mutagenesis and high-throughput screening to isolate tagged green algae with a smaller Chl antenna size.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.7** for its relevance to DOE objectives.

- The project goals are well-aligned with Department of Energy program targets for maximizing efficiency of biologically-derived hydrogen production.
- The focus on construction of a minimal photosynthetic antenna complex is good.
- Increasing solar conversion efficiency in algae is a fundamental priority.
- Very relevant for biological production.

**Question 2: Approach to performing the research and development**

This project was rated **3.8** on its approach.

- The discovery-driven approach for screening of efficient hydrogen production from reduced antenna is appropriately conducted.
- The focus on usage of molecular biology toolkits for introducing altered hydrogenase-related gene cassettes into heterologous or homologous host strains is appropriate.
- Not well described but the results speak for themselves.
- Strong emphasis on outcome - good!
- Good explanation of how this is working and how it will work.
- Clear representation of complex issues.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.9** based on accomplishments.

- The progress towards goals was excellent, with efficiency targets achieved ahead of schedule.
- Dramatic improvement over the last four years. Excellent progress.
- Have already completed 2010 milestones.
- Fascinating correlation of Tla1 gene in other species.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.0** for technology transfer and collaboration.

- Specific transfer of technology via licensing to a start-up algal biofuels company is excellent
- This is a weakness of the project. The PI need to collaborate with groups involved in engineering hydrogen production. This area needs to put 2+2 together to make 4.
- This is a sole source project.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- Future goals of quantification of photosynthetic yields in tla mutants are well-defined.
- Advanced biophysical analyses of tlaX and tlaNew mutant seem unnecessary in view of the achievement of target volumetric goals.
- With great success this project need to move to the next level and involve hydrogen production.
- Clear track on tlaX and tlaNew research.

### **Strengths and weaknesses**

#### Strengths

- The investigators' knowledge of photosynthetic systems is very robust.
- The investigators have demonstrated superior progress towards defined goals.
- The identification of a novel gene regulating antenna size is interesting and unique.
- Accomplishments to date are impressive.
- The main researcher gives much strength to this project.

#### Weaknesses

- The project has not completed comparative genomic analyses to determine biological function of tla1 (and its alleles). If this gene is present in a variety of organisms ranging from microbes to humans, there ought to be more information known about its role in those other organisms, perhaps relevant to what it is doing in algae.
- Are tlaX and tlaNew alleles of tla1? Do they represent different genes with redundant functions? Do they represent members of a gene family?
- Are there synergistic or pleiotropic effects of tla that might shed light on its role in antenna size?
- The investigators have not demonstrated hydrogen production, merely vigorous gas production.
- It is unclear how full-scale molecular genetic, biochemical, physiological characterization of tlaX and tlaNew strains will be conducted and thus actually shed knowledge on potentially pleiotropic effects on antenna size. A systems biology approach might be fruitful to decipher regulatory effects.
- Lack of collaborations to involve hydrogen aspect.

### **Specific recommendations and additions or deletions to the work scope**

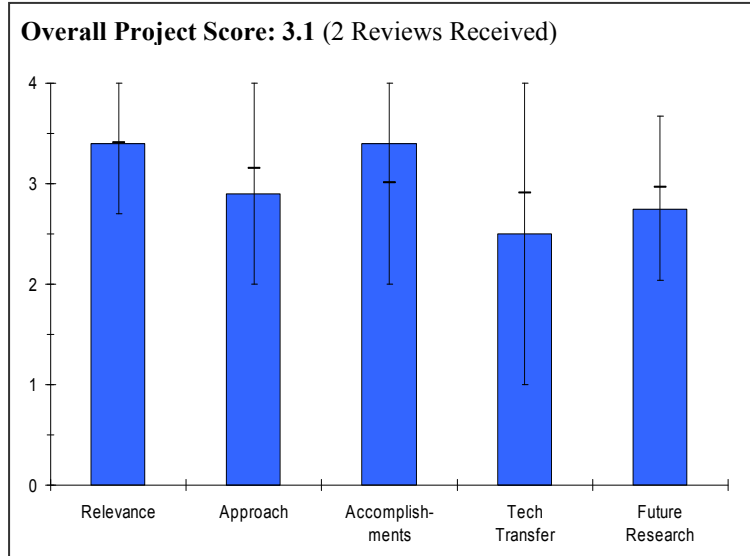
- Keep going!

**Project # PD-34: Use of Biological Materials and Biologically Inspired Materials for Hydrogen Catalysts**

*Trevor Douglas; Montana State University*

**Brief Summary of Project**

The objectives of this project are to 1) optimize the hydrogenase stability and electron transfer; 2) optimize the semiconductor nano-particle photocatalysis, oxygen scavenging and electron transfer properties of protein nano-cages; 3) perform gel/matrix immobilization and composite formulation of nano-materials and hydrogenase; and 4) perform device fabrication for hydrogen production. Montana State will incorporate hydrogenase and mimetics into stabilizing matrices as well as into electroactive poly (viologen matrices).



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.4** for its relevance to DOE objectives.

- The project goals are well-aligned with Department of Energy program targets for novel biologically-derived catalysts for hydrogen production.
- The focus on improvement of hydrogenase stability is good.
- The focus on improvements of enzymes and catalyst supports is good.
- Obtaining stable catalyst and comparing the biological and inorganic versions side by side is very worthy.

**Question 2: Approach to performing the research and development**

This project was rated **2.9** on its approach.

- The approach for targeting the nickel-iron hydrogenase is logical, and builds upon progress in the investigators' lab.
- The focus on encapsulation of purified hydrogenase within the sol-gel is interesting, and has demonstrated success in increased stability at room temperatures.
- The platinum cluster encapsulated within protein cages is clever and represents a good target for achieving improved catalyst activity with corresponding palladium encapsulated nanoparticles.
- The approach demonstrates a good synergism between enzymology and protein structure-function with materials composite synthesis and design.
- Overall theme was appealing but the goals were not specific.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.4** based on accomplishments.

- The progress towards goals was difficult to ascertain, and had to be specifically drawn out of the oral presentation. The target goal of improved fold stability (80% as stated) was not easily related to the information presented on protection from external protease action vs. activity enhancement due to sustained protection from oxygen inactivation.
- Encapsulation of active hydrogenase and recovery of activity encapsulated in Sol-Gel showed very good progress.

## PRODUCTION AND DELIVERY

- There was good progress in demonstrating the linear relationship between activity and platinum cluster size.
- Unfocused presentation. It was not clear just what has been achieved, how the different aspects related to each other, and where each would go in the future.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.5** for technology transfer and collaboration.

- Effective collaboration with industrial partners was demonstrated, with the use of specialized photochromic and thermochromic films.
- Does not appear to be at the stage to take to the next level.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- Future goals of incorporation of stable and active catalysts into polyviologen matrices were good.
- Full implementation and testing of the prototype device is a logical and feasible goal.
- Only very general plans with specific milestone.

### **Strengths and weaknesses**

#### Strengths

- Project strengths are the investigators' knowledge of nickel-iron hydrogenases and structure-function relationships.
- Strong biological experiences and background of the PIs.

#### Weaknesses

- The project did not clearly define its benchmarks for hydrogen production, with respect to improvements in enzyme stability, enzyme activity, or metrics for sol-gel encapsulants or supported/caged matrices.
- Underdefined and unfocused research plan.

### **Specific recommendations and additions or deletions to the work scope**

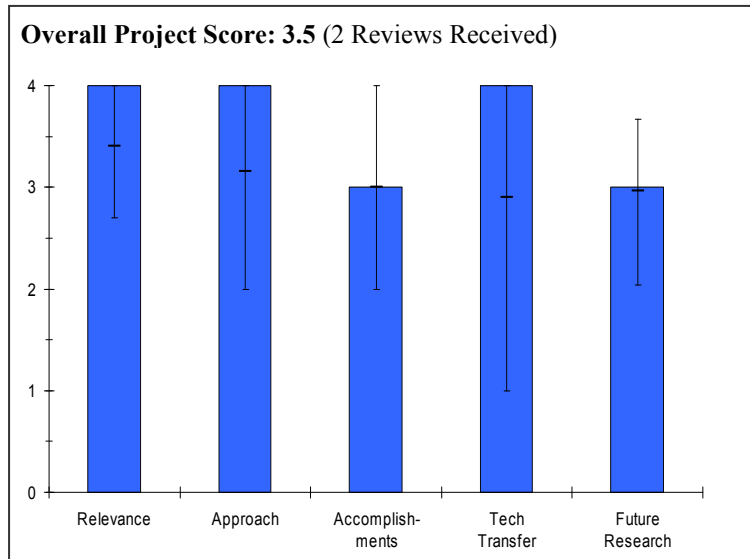
- None.

**Project # PD-35: Photoelectrochemical Hydrogen Production: UNLV-SHGR Program Subtask**

*Eric Miller; MV Systems*

**Brief Summary of Project**

The primary objective of the Department of Energy (DOE) Photoelectrochemical (PEC) Working Group is to develop practical solar hydrogen-producing technology using innovative semiconductor materials and devices research and development to foster the needed scientific breakthroughs. The objectives of the DOE-SHGR PEC are to 1) identify and develop PEC thin-film materials systems compatible with high-efficiency, low cost hydrogen production devices; 2) demonstrate a functional multi-junction device incorporating best-available PEC film materials; 3) develop collaborative avenues (national and international) integrating the best theoretical, synthesis and analytical techniques, for optimizing future PEC materials and devices; and 4) explore avenues toward manufacture-scaled devices and systems.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **4.0** for its relevance to DOE objectives.

- Focused on key issues of solar to hydrogen using photoelectrochemical.
- Concern about cost issues.
- Set goal to out-perform photovoltaics + electrolysis.
- Realistic understanding of the barriers to practical success.
- The photoelectrochemical working group is an important effort aimed at coordinating research from a dozen institutions. The University of Nevada, Las Vegas-SHGP program is an effort to discover new photoelectrochemical hydrogen materials using theory, synthesis and analysis.
- There was almost no original science in this presentation.

**Question 2: Approach to performing the research and development**

This project was rated **4.0** on its approach.

- Good integration of theory, synthesis, surface science, and electrochemistry.
- Program takes advantage of knowledge base available in solid-state electronics/physics.
- State of the art materials characterization.
- The concept for this project, the development of the photoelectrochemical "tool chest" is sound.
- WO<sub>3</sub> has too large a band gap to be useful in a practical system. N incorporation, as admitted, cannot improve the material.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Interesting new materials have been identified that demonstrate the power of the integrated approach.
- State of the art (and in-house developed) characterization.



## PRODUCTION AND DELIVERY

- Elegant next generation materials have been produced.
- So far, most of the effort in this project has been directed towards assembling "tools". Comparatively little has been accomplished in terms of discovering new materials with improved properties.
- Almost no time in the talk was devoted to any specific technical accomplishments.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **4.0** for technology transfer and collaboration.

- Exceptionally strong collaborations that have leveraged unique abilities.
- Coordination with other institutions is a very strong focus for this project.
- This is almost a subcontract to transfer some program administration to University of Hawaii?!

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- The Program outlined is on-track.
- New materials should continue to be generated and characterized.
- Development of community-wide standardized protocols is critical.
- While interaction with other researchers is fine, this group needs to focus on discovering and characterizing some new classes of photoelectrochemical materials rather than just extending the findings from other groups.
- I didn't see any specific or original research ideas.

### **Strengths and weaknesses**

#### Strengths

- Important collaborations.
- Important development of a community resource for characterization.
- Access to instrumentation and interactions.
- They seem to be good at networking and facilitation, but not clear on science.

#### Weaknesses

- None.
- Lack of new ideas about classes of materials to explore.

### **Specific recommendations and additions or deletions to the work scope**

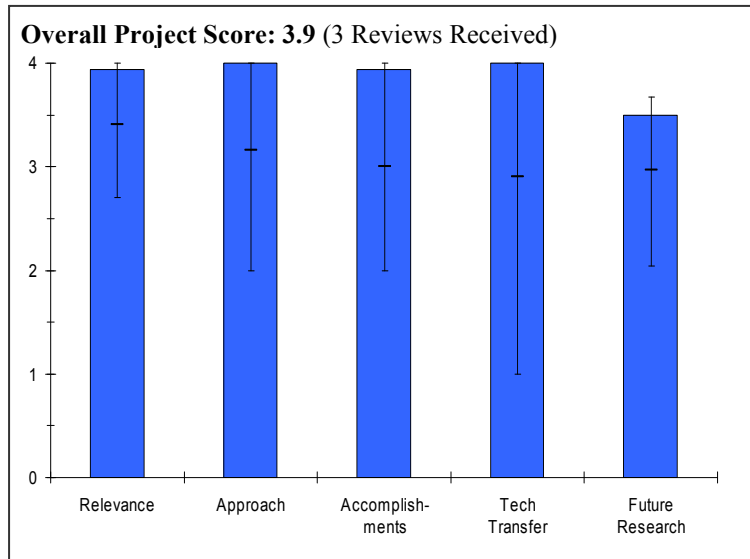
- Continue as is.
- Make finding new materials the major focus of research rather than developing tools.

**Project # PD-36: Photoelectrochemical Water Splitting**

*John Turner; NREL*

**Brief Summary of Project**

The objective of this project is to discover and characterize a semiconductor material set or device configuration that 1) splits water into hydrogen and oxygen spontaneously upon illumination; 2) has solar-to-hydrogen efficiency of at least 5% with a clear pathway to a 10% water splitting system; 3) exhibits the possibility of 10 years stability under solar conditions; and 4) can be adapted to volume-manufacturing techniques. The main objective for the past year has been to develop and optimize state-of-the-art materials that we have identified as promising for meeting the Department of Energy’s near-term efficiency and durability targets and to develop PEC modeling and analysis efforts.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.9** for its relevance to DOE objectives.

- Development of new materials that will allow pragmatic solar to hydrogen production.
- Realistic goals for conversion efficiency.
- Understanding that photoelectrochemical must compete on all levels with photovoltaics + electrolyzer.
- Turner's group at National Renewable Energy Laboratory has been a consistent bright spot in the photoelectrochemical hydrogen field since 1991. His research program is critical for progress towards Department of Energy goals and objectives.
- Very clear articulation of objectives and relevance.
- Very direct presentation of simultaneous need for efficiency, durability, and energetics.
- Graphic description of max current density/ %IPCE/ eV.
- Good basic science to understand the limitations of various classes of materials.

**Question 2: Approach to performing the research and development**

This project was rated **4.0** on its approach.

- Use of knowledge base to generate new multi-element materials (alloys?).
- Excellent electrochemical characterization.
- Amazing solid-state synthesis capability.
- Good mix of theory and wet chemistry (important approach – start with a known material, use theory to suggest improvements, make theoretically suggested materials and see what happens).
- Due to his deep understanding of photoelectrochemistry, the PI is able to choose materials that have high potential. His willingness to utilize breakthroughs from the photovoltaics community and to engage theorists have led to technological and conceptual breakthroughs.
- John's oral presentation was direct, clear, and concise.
- Assertion that photon-to-electron conversion efficiency must equal or exceed photovoltaics systems was clear.
- Similarly, the color correlations for the InN/GaN alloys made his correlations to eV transitions very clear.
- Good connection to DFT calculations.

## PRODUCTION AND DELIVERY

- The PI has knowledge and experience with most all techniques needed to characterize photoelectrochemical materials.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.9** based on accomplishments.

- New GaN+InN= GaInN system (very interesting).
- New low temp synthesis of  $\text{Cu}_x\text{Se}_y$  thin films.
- New SiN systems.
- New ZnO+N (nice interaction of theory and experiment).
- Despite recent budgetary issues, this group had produced many new results on photoelectrochemical materials. Experimental and theoretical results on InGaN, CuGaSe<sub>2</sub>, SiN, CoFeAl oxide were all new and interesting.
- Systematic presentation of key points by examples: mixed metal oxides, GaN/InN alloys (band gaps and transitions correlations), CuGaSe<sub>2</sub> thin film studies.
- Connections to theory.
- The nitrides are interesting but are still very inefficient.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **4.0** for technology transfer and collaboration.

- A historical record (which continues) of collaboration with universities and industry.
- Virtually all of the other photoelectrochemical hydrogen presenters acknowledged significant interactions with the Turner/National Renewable Energy Laboratory project.
- Well-documented collaborations with: DFT group, other National Renewable Energy Laboratory teams (photovoltaics), CSM.
- Good interaction between experiments and theory.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.5** for proposed future work.

- Program is ending since it is not a Department of Energy funding priority.
- I was VERY disappointed to learn that Department of Energy is not planning to continue funding for this program. What a ridiculous decision.
- Builds on the GaN/InN materials and extrapolates to other III-V nitrides.
- Continues photoelectrochemical WG collaborations.
- Turner knows enough and has enough experience to make good decisions about projects and paths.

### **Strengths and weaknesses**

#### Strengths

- This program has powered the hydrogen Program photoelectrochemical work since its beginning.
- Excellent science.
- Excellent collaboration.
- Innovative ideas, solid results on a variety of new materials, expertise of PI and other National Renewable Energy Laboratory researchers associated with the project.
- Well-presented and systematic articulation of key principles.
- Well defended series of exploratory work with correlation to theory.
- PI has a vast experience in photoelectrochemistry. Many students are getting exposure to and trained in photoelectrochemical techniques at NREL.

Weaknesses

- None.
- None, other than lack of adequate Department of Energy funding.
- Needs more computing power to calculate more band structures to identify materials trends.

**Specific recommendations and additions or deletions to the work scope**

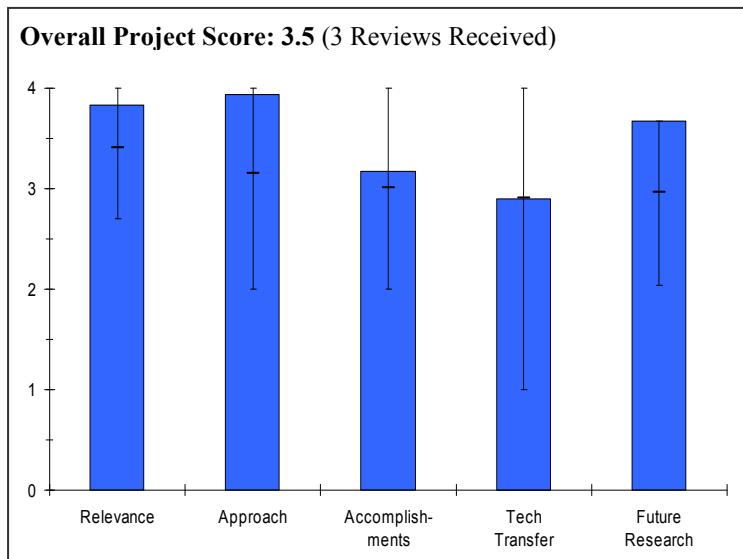
- Although money is limited and hard decisions have to be made, I believe discontinuation of this program represents a critical path error.
- Provide adequate funding so that work in this important area, and by this group, can continue.
- Keep up the good work and the collaborations (and the strong summary of findings).
- Provide more computation resources.

**Project # PD-37: Critical Research for Cost-Effective Photoelectrochemical Production of Hydrogen**

*Liwei Xu; Midwest Optoelectronics*

**Brief Summary of Project**

The objectives of this project are to 1) develop critical technologies, including transparent, conducting, and corrosion resistant coatings and photoactive semiconductor materials, required for cost-effective production of hydrogen from sunlight and water using thin film-Si based photoelectrodes; and 2) develop and demonstrate at the end of the three-year project, tf-Si based photoelectrochemical photoelectrodes and device designs with the potential to achieve systems with 8% solar-to-hydrogen efficiency with a durability of 1,000 hours by 2013.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.8** for its relevance to DOE objectives.

- Follows Department of Energy proposed standards for photoelectrochemical solar to hydrogen.
- Silicon-based systems.
- Aimed at real world stability.
- This project provides a good balance with respect to other material - discovery oriented projects. The project addressed a number of important applied issues associated with development of photoelectrochemical-hydrogen technology.
- While not clearly a photoelectrochemical project, this "almost" commercial system shows a functional, practical approach to hydrogen production with sunlight.
- Two approaches - immersion cell and substrate cell also illustrates two practical time-lines (mid-term and long-term) toward commercialization. The Department of Energy needs more such "market transformational" projects.
- This project is largely engineering, but as engineering projects in this area go, this one shows some promise of producing an actual prototype.

**Question 2: Approach to performing the research and development**

This project was rated **3.9** on its approach.

- Two viable approaches.
- In situ photoelectrochemical.
- Integrated photovoltaics-cell.
- New corrosion resistant front surface junction materials (alloyed ZnO).
- Tunable multijunction photovoltaics to match water splitting energetic needs.
- Philosophy: use materials that have low technology barriers.
- The project leverages Midwest's expertise in manufacture of multi-junction thin film photovoltaics devices. Two distinct approaches are being developed for photoelectrochemical water-splitting cells (immersion-type and substrate type). Both approaches are worth exploring.
- It is good to have "practical" projects than just the traditional "support the labs-type" basic research.
- The approaches here recognize practical engineering challenges and the focus on TCCR materials is methodical with clear Go/No-go decision points - Bravo!

- The concept is just a solar cell immersed in an electrolyte. The advantages of this over an external solar cell and an electrolyzer are not clear. An advantage is the adjustable band gap and perhaps cheaper than the separate systems.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.2** based on accomplishments.

- Develop triple junction photoelectrode.
- Develop corrosion resistant oxide layers.
- Large scale electrodes are now available (1x3 feet) but not protected at this time.
- High quality ZnO layers have been made and characterized.
- Demonstrate defect shunting.
- Test large area photoelectrodes 12x12 (some degradation observed with time in outdoor testing - 3% conversion is observed).
- Considerable progress has been made towards the goals of this project; however, most of the results were for existing photovoltaics materials. Despite its importance to the immersion type approach, little information was presented on the TCCR films.
- No earth-shaking basic discoveries, but very solid engineering progress.
- The need for improved TCCR's (for the immersion systems) and for the semi-con/electrolyte junction layer (for the substrate systems) is well articulated.
- The technology for large area  $\alpha$ Si cells is being developed independently from this project.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.9** for technology transfer and collaboration.

- Good collaborations on underlying science.
- Strongest interactions are with University of Toledo.
- National Renewable Energy Laboratory collaborations well explained; so was the connection to the University of Toledo.
- Not sure about the role of Xunlight.
- Definitely a technology transfer from the lab to a developmental company.
- This project has the possibility of producing a commercial system to "test the water" for photoelectrolysis.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.7** for proposed future work.

- Good materials and chemical strategies.
- Good engineering approaches.
- If this project can be successfully completed, it will constitute an important, practical benchmark for an integrated photoelectrochemical hydrogen system.
- Again, solid engineering considerations for both types of systems.
- No clear exposition of what the next generation oxides or classes of materials are being considered.
- Good direct coupling of solar capture and electrolysis in the substrate-type system.

**Strengths and weaknesses**

Strengths

- Good engineering.
- Good manufacturing capability already in place.
- Good approach (and collaborations) on materials science.
- Low technology barrier approach is a plus.

## PRODUCTION AND DELIVERY

- Existing fabrication expertise at Midwest and commitment to developing systems for solar hydrogen generation.
- Practical demonstration of near-commercial system.
- Very clear presentation of project background and approaches.
- Very solid understanding of engineering design and challenges.
- Will be a good demonstration of photoelectrolysis in an integrated system. There may be some advantages to local hydrogen generation rather than separate electrolyzers other than simply cost.

### Weaknesses

- Cells have net efficiency now of 3% even though the photovoltaics works at 12%.
- Work on electrocatalysts is needed.
- Maybe a shortage of publications and presentations, but understandable for a project in a company.
- No indication of economics (capital, operations and management, etc.).
- No attempt to estimate life-times of systems/components, etc.
- I have a feeling that this is a small side interest for the company rather than their major thrust which is to produce  $\alpha$ Si solar cells.

### Specific recommendations and additions or deletions to the work scope

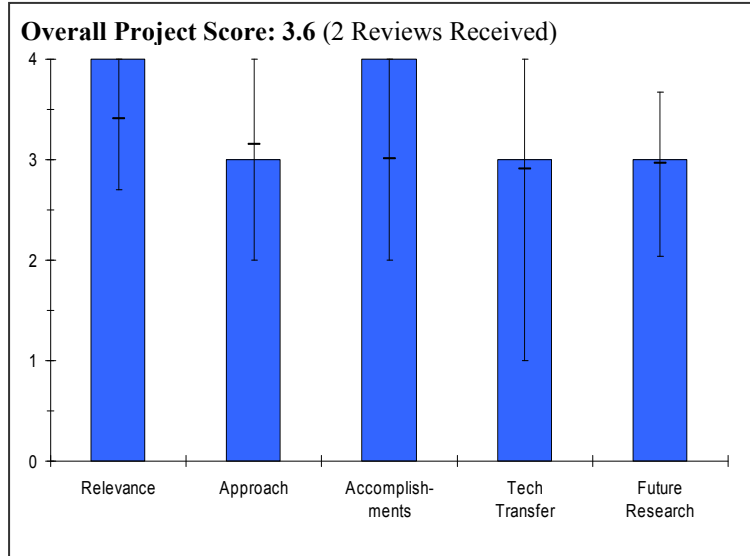
- Wonderful program, continue it.
- Plans for future are sound.
- Keep up support of such "near-term commercialization" projects to balance out the multitude of basic, fundamental research.
- Need more support of "engineering" projects, which explore engineering challenges.

**Project # PD-38: Development and Optimization of Cost Effective Materials for PEC Hydrogen Production**

*Eric McFarland; U. of CA Santa Barbara*

**Brief Summary of Project**

The overall project objective is to discover and optimize an efficient, practical and economically sustainable material system for photoelectrochemical (PEC) production of bulk hydrogen using solar light energy as the primary energy input making use of novel syntheses and high throughput experimentation methods. The task objectives of this project are to 1) identify improved materials for solar photon absorption using high throughput methods and exploratory design and synthesis of new mixed metal-oxides; and 2) optimize the morphology of the PEC material system for maximum efficiency.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **4.0** for its relevance to DOE objectives.

- Addresses key programmatic issues related to solar to hydrogen via photoelectrochemical production.
- Addresses solar optical response limitations.
- Attempts to incorporate cost issues up front.
- Uses a 10% conversion Go/No Go decision screen.
- This project is advancing many areas of understanding and technology in the area of photoelectrochemical hydrogen production.
- Materials development is important to the goal of efficient photoelectrochemical water splitting.  $\alpha\text{Fe}_2\text{O}_3$  is not a material that can be efficient, but it is a useful prototype system for understanding lower band gap metal oxide photoelectrodes.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- Project has identified key limitations in materials synthesis.
- There is very little understanding developed of the chemical mechanisms that are limiting control over the material.
- Program uses (in combination) many well-known materials approaches.
- Results, while useful, are empirical and thus not producing strong guiding principles. The suggestion that glucose or glycol be used as the oxidant makes no sense (thermodynamics are downhill, i.e. no optical conversion.)
- The PIs tasks #1-5 represent a nice combination of combinational and directed science that is likely to achieve many of the project's objectives. Pursuing tasks #6-9 at this point in time is premature.
- McFarland is an experienced and creative materials scientist. My opinion, however, is that the homogenous (slurry) systems will not be viable.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **4.0** based on accomplishments.



## PRODUCTION AND DELIVERY

- Synthetically strong program.
- Improved optical response and ICPE of native  $\text{Fe}_2\text{O}_3$ .
- No progress to date on an actual reactor or reactor design.
- Water splitting has been observed at short circuit (very important).
- Some system stability has been observed, but not tested to the extent needed to draw pragmatic conclusions
- Despite some interruptions in funding, the PI and his group have made good progress in improving the ability of  $\text{Fe}_2\text{O}_3$  and related materials to split water.
- Has made progress in understanding  $\alpha\text{Fe}_2\text{O}_3$  that may be useful when developing other low gap oxide materials or for using  $\alpha\text{Fe}_2\text{O}_3$  in a tandem system.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.0** for technology transfer and collaboration.

- Number of publications and presentations are moderate, but PI does interact in significant way with photoelectrochemical community.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- Program is on-track. It should continue as is with a focus on issues of stability and conversion efficiency.
- For the most part, future plans are sound. As indicated in tasks #6-9, PI seems determined to develop a photoelectrochemical structure that mimics a cell, despite the obvious problems with such systems.

### **Strengths and weaknesses**

#### Strengths

- Strong materials synthesis approach.
- Good real-world evaluation of systems.
- High level of expertise in material synthesis and characterization.

#### Weaknesses

- Perceived weaknesses may be a result of zero funding last year.
- Issues are: materials stability testing, the use of glucose etc. in place of water oxidation which dramatically decreases solar conversion efficiency (one is adding in an effective combustion component).
- Inclination to "engineer" a complete system before finding an adequate photoelectrochemical material.

### **Specific recommendations and additions or deletions to the work scope**

- Continue with everything except alternate oxidation reactions.
- Less emphasis on tasks #6-9.

**Project # PD-39: Scale-up of Hydrogen Transport Membranes for IGCC and FutureGen Plants**

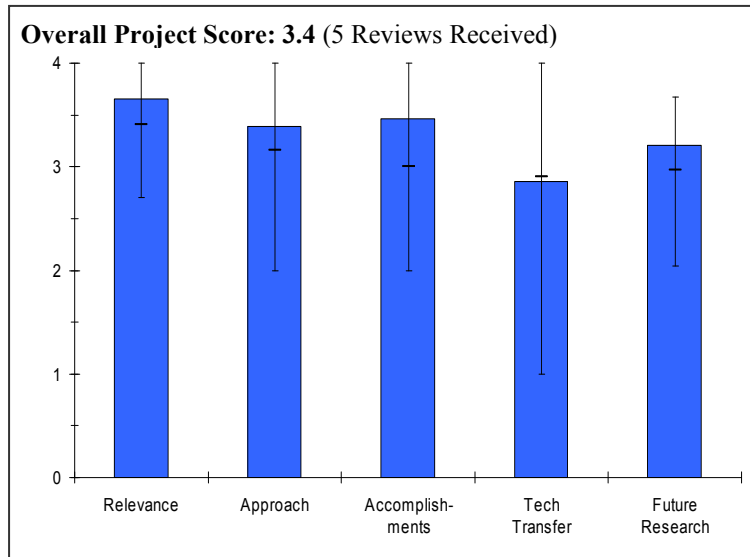
*Doug Jack; Eltron Research Inc.*

**Brief Summary of Project**

The overall project objective is to develop a H<sub>2</sub>/CO<sub>2</sub> separation system that 1) retains CO<sub>2</sub> at coal gasifier pressures; 2) operates near water-gas shift conditions; 3) tolerates reasonable achievable levels of coal-derived impurities; 4) delivers pure H<sub>2</sub> for use in fuel cells, gas turbines and hydrocarbon processing; and 5) is cost effective compared to alternative technologies for carbon capture.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.7** for its relevance to DOE objectives.



- Economic and practical hydrogen separation/purification is essential to the industry.
- Hydrogen production from coal is one of the goals of the President's Hydrogen Fuel Initiative.
- This project is clearly important to hydrogen production from coal and contributes to achievement of Department of Energy's hydrogen separation goals and the goals of the Fossil Energy office.
- The project may help to enable coal gasification as a hydrogen production option in a carbon-constrained environment.
- Matches well with carbon dioxide sequestration - no pressure drop. However, re-pressurization for hydrogen is required.
- Thermodynamic advantages are favorable.
- Small and large units are possible.

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- Good approach, as it is focused beyond just membrane material and how to make a working membrane module.
- Comprehensive approach to scale-up/demonstration and incorporating test and evaluation results.
- It seems they could test the membrane separator on a slip stream or simulated feed rather than a H<sub>2</sub>/N<sub>2</sub> mix.
- Durability tests should include tolerance to contaminants such as sulfur, trace metals, etc. Understanding the impact of sulfur is a key to success.
- Longer term life tests and / or accelerated life tests are needed.
- The approach appropriately incorporates gradual increases in the scale of hydrogen production to address the technical challenges associated with each scale.
- The stage gate approach is appropriate but Go/No Go decision points with clear criteria should be incorporated to guide direction of the project at the various production scales proposed.
- Self-supporting membrane is very ambitious considering the need for high efficiency (thick membrane).

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.5** based on accomplishments.

- Hydrogen transport resistance model is a good tool.
- Early phase work shows that membrane material performance will meet Department of Energy goals.

## PRODUCTION AND DELIVERY

- Good progress and a great value for the budget. Strong characterization work.
- Researchers have begun lifecycle tests, but longer tests or accelerated lifecycle tests are required.
- The PI has made significant progress – initial hydrogen flux results are encouraging – toward developing membranes that meet the Department of Energy goals and targets.
- Model development is supported by experimental data.
- Milestones were explained in detail.
- Results explained in a qualitative fashion. Difficult to evaluate progress made-due to the lack of quantitative data.
- No discussion on membrane material impact on performance.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.9** for technology transfer and collaboration.

- Partners have dropped out and technology transfer plans are unclear. Team needs to acquire test site partners and should work with industrial gas companies to gain industrial insights into practical operational challenges. Inclusion of Praxair (an industrial gas supplier) should ensure ease of technology transfer beyond the host site that is now being sought.
- Collaborations with test and evaluation systems and sites important-need more specifics.
- They have a solid team, but team responsibilities and interactions were not clearly identified, so it is difficult to assess their collaboration.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- Membrane thickness and configuration (tube vs. disc) are critical to reaching Department of Energy goals. Project should concentrate on techniques for producing and testing long 500 micron wall, catalyst coated tubes and incorporating these tubes into modules (tube sheets) for testing.
- The costs of life cycle use were not clearly addressed.
- Future work seems appropriate.
- They need to add tests on real syngas streams to assess contaminant tolerance. Tests should also be conducted at higher temperatures and lower partial pressures to assess hydrogen flux at these levels.
- Future plans are appropriate and adequate and focused on the barriers.
- Manufacturing costs reductions should be included.

### **Strengths and weaknesses**

#### Strengths

- Good membrane development based on projected performance and costs.
- Very frank and open presentation.
- They are well funded and have a solid team.
- Good progress (flux, etc.) is being made toward meeting the Department of Energy separations membrane targets.
- Non-palladium based membranes are cheaper.

#### Weaknesses

- 500 micron just meets the Department of Energy goal when lab tested. "Real" gas streams are likely to significantly lower this rate (impact the catalyst layer). Team needs to show understanding and plan to compensate/control membrane module performance.
- Tube manufacturing, catalyst coating, tube sheet system will all impact performance and more importantly costs. The degree of impact needs to be accessed.
- Testing on real gas streams is needed.

- They should consider operation at higher temperatures (up to 600 degrees Celsius) and lower partial pressure.
- Life of membrane is less than one year. Needs to be improved.

**Specific recommendations and additions or deletions to the work scope**

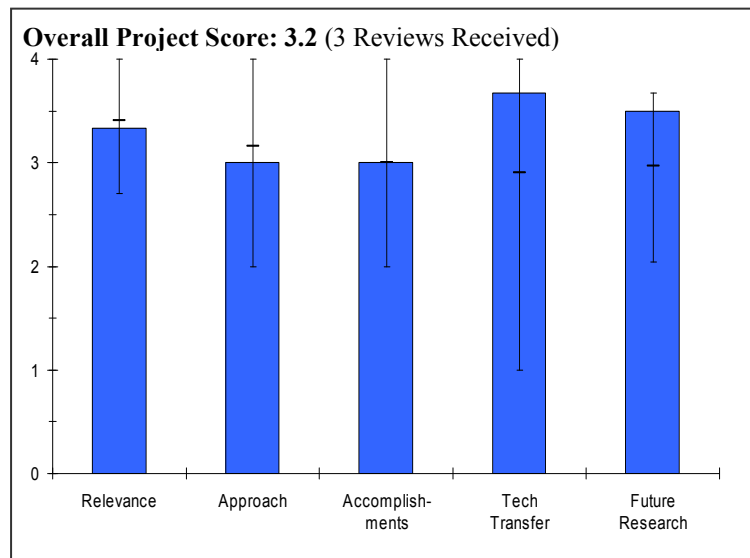
- The very thin tube wall combined with the economic need for long tubes dictates that knowledge about tube strength/stresses under pressure (including quick ramp-up and ramp-down) and pressure cycling: plus double sided catalyst surface adherence/wear (will tubes flex against each other); plus tube sheet connections... all be evaluated in detail.
- Suggest accelerating and expanding the project.
- Include Go/No Go decisions with clear criteria to guide future research.
- Tests that include all contaminants and measure the rates/cumulative effects.

**Project # PD-40: Cost-Effective Method for Producing Self-Supporting Pd Alloy Membrane for Use in the Efficient Production of Coal-Derived Hydrogen**

*Kent Coulter; Southwest Research Institute*

**Brief Summary of Project**

The overall project objective is to develop technologies that effectively and economically separate hydrogen from mixed gas streams that would be produced by coal gasification. The objectives of this project are to 1) develop a process methodology for the cost-effective manufacturing of thin, dense, self-supporting palladium alloy membranes for hydrogen separation from the mixed gas streams of coal gasification processes; and 2) reduce Pd membrane thickness >50% over current state-of-art and show potential to meet the Department of Energy 2010 technical targets.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- Project fully supports Department of Energy RD&D goals.
- Department of Energy hydrogen flux targets are surpassed.
- Membranes are essential to hydrogen process flows/purity.
- The use of palladium-based membranes may find limited use because of cost and scale-up, although the use of thin membranes appears to be the right way to go with such an expensive metal.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- Project providing innovative technology and product development for thin film (3-10 Micron) membrane with high hydrogen flux (more than Department of Energy levels are achievable).
- Generated depth in production of membranes using variety of binary and ternary palladium alloys.
- Membrane is not self supporting and they have challenges to overcome in construction of membrane modules.
- The experimental approach is adequate but suggest that the PI conduct additional background literature research on palladium alloy behavior to avoid duplication of previous efforts.
- The first part of the talk described work that was completed. An effective way to produce thin unsupported membrane films appears to have been demonstrated. Implementing these films in an operating device appears to be difficult. The second portion of the presentation focused on a new project examining ternary compositions, starting first with computational work and then followed up by experiment. This is a reasonable approach assuming that the density functional theory (DFT) computations give reliable results that can be validated with experiment.
- It is likely that it will prove difficult to produce materials that are as well formed as designed theoretically. Phase segregation or surface enrichment could occur that would not be predicted by modeling.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Successful results with hydrogen flux surpassing program goals.
- Team plans for more work with membrane assembly. Issues are identified and they plan to fine tune annealing process to eliminate surface defects.
- Pinholes at the edges of foil on the supporting material occur. Steps to overcome the issues with modularization are in progress.
- The testing conducted on prototype membranes seems logical but some concern that the research activity duplicated previous efforts by past DOE projects.
- Technical accomplishments from the previous program seem reasonable.
- The recent work using the DFT calculations shows promise and the fact that the work has been submitted for publication (if accepted) speaks well of the work.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.7** for technology transfer and collaboration.

- Excellent cooperation and teamwork between collaborators.
- The project appears to have done well in seeking collaborations with others. Each has a specific role to play. It does not appear that potential collaborations have been well defined with possible commercialization partners. IdaTech is a possible commercial partner, but the relationship appears to be less strong based on recently described issues. This project appears to be mostly in the research stage.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.5** for proposed future work.

- Clearly identified steps to eliminate issues related to membrane fabrication and to carry out modularization work.
- Future plan includes the cost estimate work for production of membranes.
- Suggest as part of future work that the PI perform a literature review of past DOE projects on behavior of palladium alloys for hydrogen sensors to help guide future research.
- The proposed forward plan is reasonable and appears to be on track.
- With the proposed future fabrication of several new membrane compositions, it would be good to see that the plan would include some science into the analysis of the materials, either as produced or following testing. Detailed surface and bulk analysis of some of the best materials might be in order. Otherwise the Program sound like a fairly simple make and test without a lot of insights gained.

**Strengths and weaknesses**

Strengths

- Well-defined, timely and successful execution of the project plan and alignment with targets.
- Successful teamwork and partnerships.
- Good progress made on creative membrane technology and membrane production. Estimates look promising for low-cost production of thin film membranes.

Weaknesses

- Did not address the broad knowledge base on palladium embrittlement for hydrogen sensors as it applies to this project. Concern that the PI is re-discovering existing knowledge.
- The difficulties of the actual implementation of the free-standing membranes are left somewhat unresolved. Understand that other partners will be approached, but it is not clear whether the problem is with IdaTech or with the membrane materials themselves.

**Specific recommendations and additions or deletions to the work scope**

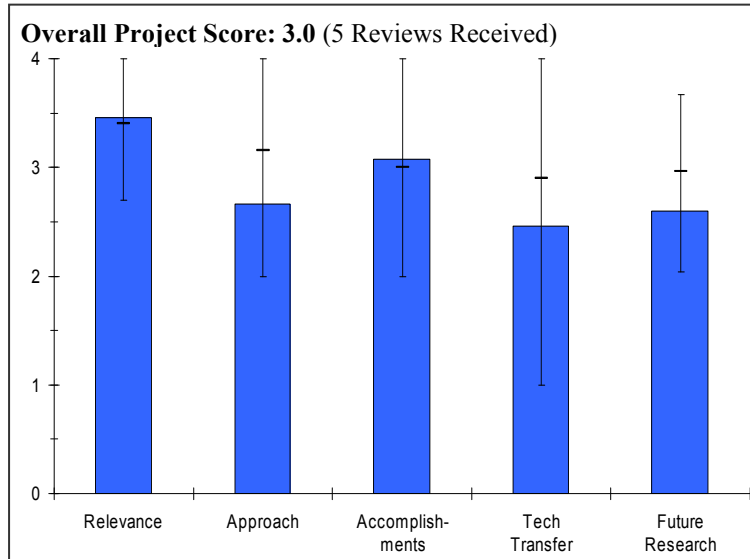
- Very good project. Film technology and thin film membrane might have other key application areas.
- Suggest a comparison of the knowledge gained in this project to past DOE efforts on palladium alloy work for hydrogen sensors.
- Add more science and characterizations to the materials, and seek to understand the strengths and limitations of the DFT computational method applied to this problem.

**Project # PD-41: Experimental Demonstration of Advanced Palladium Membrane Separators for Central High-Purity Hydrogen Production**

*Sean Emerson; United Technologies*

**Brief Summary of Project**

The objectives of this project are to 1) confirm the high stability and resistance of a PdCu trimetallic alloy to carbon and carbide formation and, in addition, resistance to sulfur, halides and ammonia; 2) develop a sulfur, halide and ammonia resistant alloy membrane with a projected hydrogen permeance of  $25 \text{ m}^3 \text{ m}^{-2} \text{ atm}^{-0.5} \text{ h}^{-1}$  at  $400^\circ\text{C}$  and capable of operating at pressures of 12.1 MPa; and 3) construct and experimentally validate the performance of 0.1 kg/day  $\text{H}_2$  PdCu trimetallic alloy membrane separators at feed pressures of 2 MPa in the presence of  $\text{H}_2\text{S}$ ,  $\text{NH}_3$  and  $\text{HCl}$ .



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- Membranes are essential for hydrogen separation/purification for both central and distributed hydrogen production.
- The project helps with development of hydrogen infrastructure.
- Power+Energy (P+E) and United Technologies Research Center (UTRC) alloy separators can meet or exceed DOE targets.

**Question 2: Approach to performing the research and development**

This project was rated **2.7** on its approach.

- Did not clearly address the engineering issues associated with heated membranes. The technical plan is narrow but well-equipped. Combination of low pressure screening, high pressure with poisons, and modeling is good. Standardized testing approach is good for reproducibility and reliable screening.
- UTRC has good capability for membrane material and tube development.
- The strategy for making membranes tolerant to the three poisons needs to be more clearly defined.
- Materials alloy construction should incorporate the information learned from the extensive characterization being done. Little information presented on how material alloys are being defined.
- Use of thermodynamic solubility data and modeling tool is a good approach, but project researchers should use existing data to make better decisions in the modeling approach.
- Fundamental understanding of the issues of membrane durability, impurities, hydrogen selectivity, and flux.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- Conducted a logical experimental program and made significant progress in its first year.
- UTRC and P+E possess capability to make state of the art Pd membranes.
- Constructed and tested 10 membrane materials and quantified effect of  $\text{CO}$ ,  $\text{CO}_2$ ,  $\text{N}_2$ , and  $\text{H}_2\text{O}$  on hydrogen permeability. None of the membrane materials have been tested with any of the poisons yet ( $\text{H}_2\text{S}$ , etc.).



## PRODUCTION AND DELIVERY

- High degree of characterization (XRD, XPS, EBSD) helps fundamental understanding of material properties and changes.
- Modeling projections estimate that the flux target will be met at 500+°C.
- Model calibration data good.
- Not enough data on membrane configuration for performance estimates.
- Evaluated performance of first fcc-PdCu separator.
- Produced five separators with UTRC ternary composition.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.5** for technology transfer and collaboration.

- Collaboration between membrane fabricator, characterization, and system integrator is good.
- Partners are well qualified and roles defined: (P+E for membrane separator fabrication and Metal Hydride Technologies for hydrogen solubility measurements).
- No technology transfer plan included.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.6** for proposed future work.

- There is a narrow test program planned that should be completed under current project.
- Suggest as part of future work that the PI perform a literature review of past DOE projects on behavior of palladium alloys for hydrogen sensors to help guide future research.
- Testing with poisons is planned.
- Future work seems limited to testing next set of approximately five materials.
- Test plan is well organized and consistent with objectives.
- Contaminant tolerance improvement details are not adequate.

### **Strengths and weaknesses**

#### Strengths

- UTRC's experimental and research capabilities are very good. Project strength appears to be testing capability and modeling of test results.
- The team has a very good history of producing Pd membranes.

#### Weaknesses

- Did not address the broad knowledge base on palladium embrittlement for hydrogen sensors as it applies to this project. Concern that the PI is re-discovering existing knowledge.
- None of the membranes have been tested with any of the poisons.
- Materials testing is limited due to length of time required to test materials.
- Ag addition is considered beneficial, but not pursued here.

### **Specific recommendations and additions or deletions to the work scope**

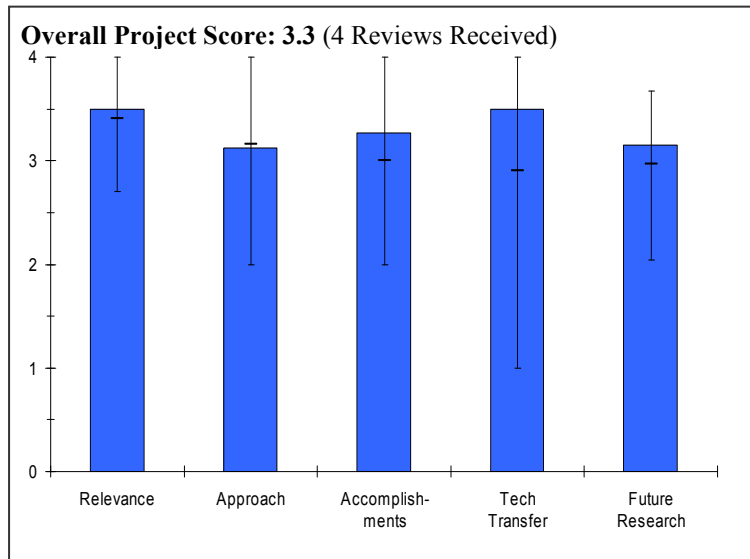
- Suggest a comparison of the knowledge gained in this project to past DOE efforts on palladium alloy work for hydrogen sensors.
- Deal with materials that can tolerate the poisons before refining them to meet the flux targets. Effect of sulfur on carbon-deposition as hydrogen is removed should be considered.
- Need to develop an accelerated stress test to speed the testing portion of the Program.
- Need to incorporate thermal cycling stability tests.
- Need a more detailed cost estimation and relate to the DOE hydrogen production targets.
- Materials alloy construction should incorporate the information learned from the extensive characterization being done.

**Project # PD-42: Integration of a Structural Water Gas Shift Catalyst with a Vanadium Alloy Hydrogen Transport Device**

*Thomas Barton; Western Res. Ins. & U of Wyoming Res. Corp.*

**Brief Summary of Project**

The 2007 objective of this project is to integrate the water-gas shift (WGS) catalyst and metallic membranes into a device and test under gasifier conditions. The 2008 objective of this project is to build a modular WGS/membrane integrated device capable of producing 10,000 L/day hydrogen from coal-derived syngas. The ceramic catalysts developed are superior to commercially available WGS materials with respect to survival in a pressurized device. Two different viable integrated device designs using vanadium membranes are under fabrication that should meet scalability issues and performance criteria.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- Combination of water-gas shift (WGS) and hydrogen membrane separation is an attractive option. The project appears to be well focused on addressing the two tasks of reducing WGS costs capital costs and membrane costs by integrating the two unit operations together.
- Development of a non-Pd membrane is a necessary technology need for lowering cost.
- Water gas shift (WGS) catalyst does not contain precious metals. WGS catalyst monolith will help enable low-cost high-efficiency integrated gasification combined cycle (IGCC) designs.

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- Focus on non-precious metal WGS catalyst is good.
- The approach described is clear but fairly minimalist. There is no indication of where challenges might exist and how specific focus might be put to address these challenges.
- Vanadium-based membrane has been very good potential.
- WGS catalyst-based on aluminum-ceria monolith is a logical support.
- Fundamental understanding of the barriers for hydrogen separation and purification, namely WGS capital costs and hydrogen transport membrane costs.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- Effects of catalyst formulations and synthesis techniques on performance have been investigated.
- Significant progress is being made. Fe-Al-Cr-Cu-Ce system catalysts have been tested by impregnation into porous mullite substrates. Highest activity and stability has been shown for 75Fe-15Al-8Cr-2Cu. Small additions of CeO<sub>2</sub> look promising.

## PRODUCTION AND DELIVERY

- Reaction rate has diminished by 50 percent within 100 hours which leads to several questions. Is there an acceptable rate that must be maintained? What is the deactivation mechanism? Does the activity correlate with surface area or is there something special about the catalyst compositions? Understanding why the catalyst has deactivated could be very important in scaleup work or predicting long term behavior of the system.
- The water gas shift work appears to be mostly a make it and test it approach. From a catalyst perspective there may have been interesting materials and properties, but there is no characterization of the materials.
- Although it is outside of the apparent scope, some measurement of the kinetics of the system would be helpful on scale-up and predicting performance as a function of temperature, pressure, and feed composition away from the specifically tested parameters.
- It was not clear why one would operate the membrane in series rather than parallel. It was claimed that either option appears possible.
- Good activity; however, stability improvement are needed.
- Multi-pass HEX design is quite scalable.
- Does ceramic adhere well to the vanadium? They may not have to be physically connected.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.5** for technology transfer and collaboration.

- Good, experienced collaborative team of University of Wyoming, Chart Energy and Chemicals, REB Research and Consulting, DOE Ames Laboratory.
- The interaction with Chart and REB is a very good one. The microchannel-type device is attractive if it can avoid excessive weight issues, and a reasonably low cost method to fabricate can be identified.
- WGS catalyst commercialization is a good idea.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Catalyst will be supported on honeycombs within a heat exchange reactor.
- The reactor should be modeled to show expected temperature and concentration profiles, with outlet compositions matching design point.
- The future plan is clear and scale-up design is well planned. Tests under gasifier conditions will be useful.
- Commercialization of the water gas shift catalyst monolith will be pursued with the assistance of a catalyst manufacturer.
- Successful testing of the two scaled integrated devices will be followed by design of a 10x assembly based on the economic and performance data for testing under coal gasification conditions. Ceria is expensive and use has to be limited.

### **Strengths and weaknesses**

#### Strengths

- Focus is on non-precious metal materials.
- Good progress, plan, collaborators, path toward possible commercialization.
- Integrated WGS-membrane reactor is an attractive option.
- Presence of gasifier facility is very good.

#### Weaknesses

- Catalyst is still deactivating rapidly after 100 hours.
- Better understanding of the WGS aspect of the device would seem appropriate, in order to interpret future results and troubleshoot as necessary.
- Effect of high humidity and low hydrogen in presence of sulfur and the exit of the reactor needs to be understood (ceria stability and poisoning). Appears as if future testing will help address these issues.

**Specific recommendations and additions or deletions to the work scope**

- Need to establish the rate at which the catalyst can be expected to maintain reaction rate, before proceeding to reactor scale-up.
- Need to understand vanadium membrane fabrication issues at large scale.

**Project # PD-43: High Flux Metallic Membranes for Hydrogen Recovery and Membrane Reactors**

*Robert Buxbaum; REB Research & Consulting*

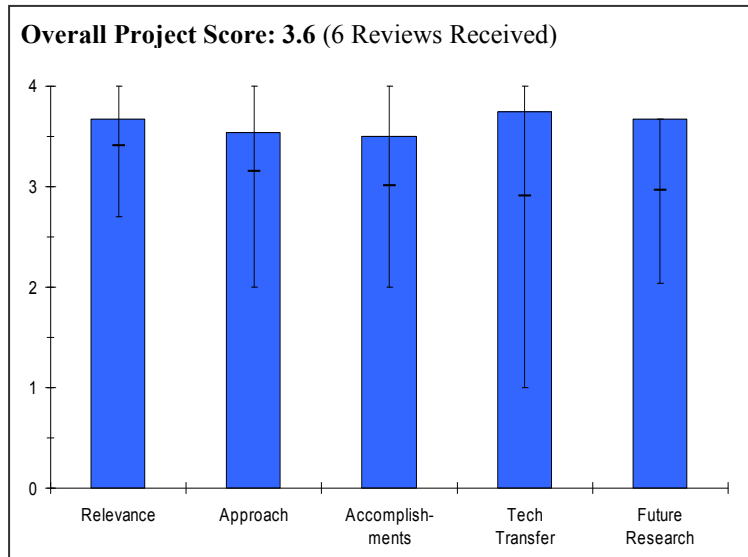
**Brief Summary of Project**

The objective of this project is to find a base metal replacement for palladium (\$470/oz) and for REB's own sandwich membranes for use in hydrogen purifiers and membrane reactors. The 2008 milestones are 1) good manufacturing capabilities; 2) to repeat the demonstration of long life tests; and 3) to manufacture reactor purifier discs.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.7** for its relevance to DOE objectives.

- Project attempts to lower the hydrogen production cost by significantly lowering the cost of hydrogen permeation membranes through reduction/replacement of Pd with base metal alloys.
- Successful project will fully support DOE research, development and deployment objectives and meet DOE targets.
- Project is targeting lowering the hydrogen production cost by significantly lowering the cost of hydrogen permeation membranes.
- The project appears to have a single task to reduce membrane cost. The project seems to be well focused on this.
- Low cost hydrogen using cheaper membranes with 15 years life is focused in the right direction.



**Question 2: Approach to performing the research and development**

This project was rated **3.5** on its approach.

- Producing hydrogen from coal gas would be good. Cleaning of the coal gas can raise the cost significantly. Since zero impurities would be difficult to achieve, the membranes should be tested/demonstrated for impurity tolerance.
- PI has fundamental understanding of the goal and provided good discussion of technical approach to select new membrane material.
- Initial results are achieving significant cost reduction in hydrogen production.
- Creative membrane design using B<sub>2</sub> intermetallic structure sandwiched between very thin Pd layers to reduce cost and extend life. Achieving 100 percent selectivity like Pd using cheap B<sub>2</sub> metal.
- Lower pressure drop is required.
- This approach is logical and seems to be based on many years work and experience by PI in this field. PI provides the competency base for producing the unique membrane with high flux.
- It seems that implementation of these materials is finally coming to fruition. The basic concepts for the potential attractiveness of non-Pd membranes have been known for some time.
- Well organized team member with assigned tasks.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.5** based on accomplishments.

- Project investigators achieved majority of their targets. Based on the technical accomplishments slides, good progress has been made on achieving flux targets and cost.
- The principal investigator reports that technical accomplishments are at a level that they are ready for market study.
- Concepts appear ready for manufacturing.
- Some of their alloys produced were brittle. They researched about 260 alloys and narrow down to a few which work properly.
- There is the potential for much scientific understanding to be gained through the synthesis and testing of several different alloy membranes. One hopes that some of the scientific information gained will make it into the published literature at some point.
- There is room for some type of combinatorial/high throughput testing of candidate membranes. The one-at-a-time approach appears to have been reasonably effective but there may be better ways to synthesize and characterize materials using the new developments in high throughput capabilities, including data management.
- It is not clear what maximum size of membranes can be produced. How the membrane assemblies are envisioned (flux per unit and # units) would be helpful.
- B<sub>2</sub> alloys are promising however need to improve fabricability; may affect overall cost advantages.
- Significant progress. Lowered the cost/flux hydrogen permeation membranes to lower the cost of hydrogen. Replaced palladium with base metals having \$100/ft<sup>2</sup> vs. \$3000/ft<sup>2</sup> – 100 percent selectivity like Pd – 50 scfh/ft<sup>2</sup> UHP H<sub>2</sub> at ΔP=200psi – 15+year life projected – low embrittlement. Alloys not identified.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.8** for technology transfer and collaboration.

- Good collaboration and distribution of tasks. Iowa State University helps pick alloys, x-rays; Ames Laboratory makes alloy samples; LANL coats, welds alloys, some tests; NETL conducts permeation and life tests; G&S Titanium Co. fabricates membranes; and REB Research manages and assembles.
- Close well-coordinated collaboration between all of the team members. Team members’ responsibilities and their work and part in the team clearly described.
- The project appears to have a good set of collaborators, and a path to commercialization through REB.
- Good team, excellent work scope assignment.
- Already got a side-benefit for nuclear material applications.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.7** for proposed future work.

- Impurity tolerance should be conducted early during material selection. Evaluate trade-off between flux and impurity tolerance.
- Economic analysis to show DOE hydrogen production target costs are addressed.
- The proposed plan appears to be a reasonable continuation of work done thus far.
- Excellent comparison with previous year’s future work.
- Willingness to make corrective action on a timely basis is very good.
- Logical and straightforward planned work. Make larger non-porous membranes (Great Western, REB). Higher pressure tests, sulfur tests with current, tweaked alloy (NETL). Test membranes, purifier w/coal gas (REB, WRI). Continue life tests with new tweaked alloy (LANL). Make disc-membrane membrane reactor with new alloy membranes (REB). Confirm that behavior matches flux, cost, and durability goals (REB, ISU).

**Strengths and weaknesses**

Strengths

- Good collaborative team and technical approach.
- Capability in making commercial membrane reactors.
- Building high performing cost effective hydrogen permeation membranes.

## PRODUCTION AND DELIVERY

- Good work plan with specific targets with specific timelines.
- Excellent team work.
- A lot of experience and familiarity with this area of research and materials. A good collaborating team.

### Weaknesses

- Membranes appear to be limited to sulfur-free fuels. Need to expand on this area further.
- This project might benefit from some computational work, not just in gaining new insights or possible leads, but also in providing information in the other direction to assist the computational projects dealing with such materials. Where do the models fail or what important aspects are not included in the models? There appears to have been a lot of data generated, additions to the science-based are to be encouraged.
- Test with WRI gasifier may be beneficial.

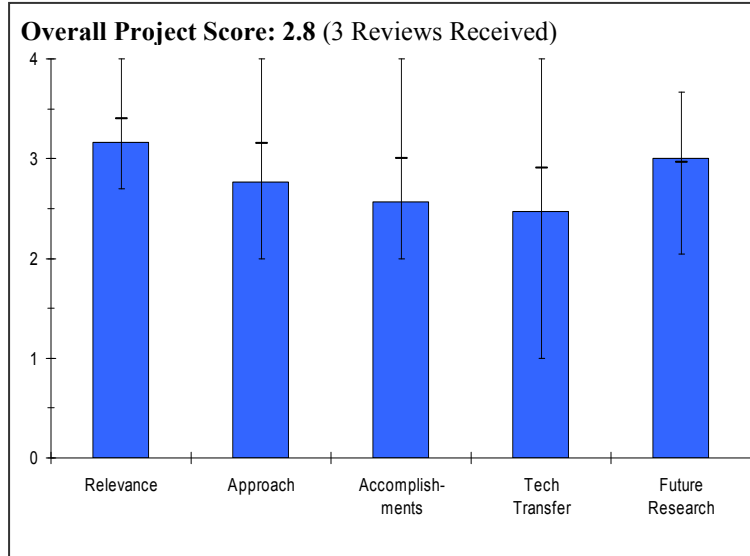
### Specific recommendations and additions or deletions to the work scope

- Place high priority on impurity tolerance.
- Inclusion of discussion how project cost targets specifically contributing to achieve DOE hydrogen production cost targets.

**Project # PDP-01: Fundamentals of a Solar-Thermal Mn<sub>2</sub>O<sub>3</sub>/MnO Thermochemical Cycle to Split Water**  
*Al Weimer; CU*

**Brief Summary of Project**

The objective of this project is to research and develop a cost effective Mn<sub>2</sub>O<sub>3</sub>/MnO solar-thermal thermochemical cycle through theoretical and experimental investigation. Additionally, based on the previous, the University of Colorado will develop a process flow diagram and carry out an economic analysis of the best process option. A reaction mechanism has been hypothesized for Mn<sub>2</sub>O<sub>3</sub> dissociation. Mixed manganese oxides have been shown to improve the product recovery steps. Experimental investigation using a mixed manganese oxide is ongoing.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.

- Project aligns with needs of DOE Production Subprogram.
- This project's objective is to research and develop a cost effective solar-thermal thermochemical cycle through theoretical and experimental investigation.
- Based on the above study, a process flow diagram and economic model will be developed.
- Project objective is solar powered hydrogen generator on a large scale.

**Question 2: Approach to performing the research and development**

This project was rated **2.8** on its approach.

- Approach is very good; however, efficiency and energy balance should be the initial part of any cycle analysis and should be described on a poster presentation.
- Thermodynamic assessment of Mn<sub>2</sub>O<sub>3</sub>/MnO cycle will be carried out.
- Mn<sub>2</sub>O<sub>3</sub> dissociation will be experimentally investigated.
- NaOH recovery is an important step for this cycle to work and this project is investigating this issue.
- It is not clear why this cycle should be better than so many other cycles that are investigated for a very long time.
- It is not clear that this is a closed cycle - it may be an irreversible process. The values of [ $\Delta H$ ,  $\Delta S$ ,  $Q + \Delta G$ ] have not been calculated for most steps, nor have the value of rate constants for key steps. No way to ascertain likely equipment designs or efficiencies.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.6** based on accomplishments.

- ZnMn<sub>2</sub>O<sub>3</sub> needs to be evaluated in an effusions cell to determine Zn vapor pressure. Zn tends to show high vapor pressure as low as 1,000°C and could lead to short term materials degradation and cycle inefficiencies.
- Found a probable mechanism for decomposition of manganese oxide (using TGA & Aerosol flow reactor).
- Used mixed manganese oxide to study NaOH recovery & hydrogen production. NaOH is a critical step in the production of hydrogen by this cycle. Good to see progress made in this area.



## PRODUCTION AND DELIVERY

- Initial PFD work has been done.
- Mixed manganese oxide has been prepared and the synthesis route is scalable for manufacturing large quantities.
- Conversion ranged from 50 to 75 percent and conversion increased with temperature and gas flow rates.
- More than half the money has been spent without clear results in any area. Design seems to presume a spray system with solid manganese oxides whose oxygen leaves instantaneously at 1,500°C but where zinc remains trapped in the manganese and the manganese-zinc-sodium undergoes no destructive reactions.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.5** for technology transfer and collaboration.

- Collaborations could be strengthened to greatly improve this project and to identify issues with the cycle.
- Collaborating with University of Nevada, Las Vegas and Swiss Federal Institute of Technology.
- It would be good to establish collaboration with other groups working on thermochemical cycles for hydrogen production (General Atomics, SRNL, INL, etc.).
- Many groups were involved, but not a sign of clear integration of their work.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- Good research plan. NaOH recovery is important step in this process. The principal investigator has identified that mixed manganese oxide is better than manganese oxide and have synthesized the mixed oxide. The next step is to investigate its dissociation mechanism.
- Should Evaluate hydrogen production rate using mixed manganese oxides and compare it with the conventional manganese oxide cycle.
- Update the process flow chart using the mixed manganese oxide cycle and re-evaluate the economics of hydrogen production.
- Researchers' main objective at this time seems to be to show that the cycles close, when, in fact, it is likely that they do not.

### **Strengths and weaknesses**

#### Strengths

- Strong background/knowledge in chemistry.
- Lot of results obtained with small amount of funding. This is possible only in an university — definitely not possible in any of the DOE laboratories.
- Good international collaboration with the Swiss institute.
- Innovative and politically useful cycle.

#### Weaknesses

- Overall process efficiency is low at 32 percent while heat required is exceptionally high (1,500°C) and may present materials development issues.
- Initial reaction of  $Mn_2O_4$  to MnO will not proceed to 100 percent completion and no results were shown on if the initial reaction of the mixed metal systems have higher conversions than the pure  $Mn_2O_3$  base case.
- Recycling of the mixed oxide might be a problem. The temperatures are very high and therefore I suspect Zn will be lost.
- Any reason why Zn-mixed oxide is better than Fe-mixed oxide?
- High temperature materials are an issue for this thermochemical cycle to work.
- The researchers seem unaware of all the project weaknesses, and seem to have no systematic way of addressing those they do recognize. Then again, it may be only poor presentation.

**Specific recommendations and additions or deletions to the work scope**

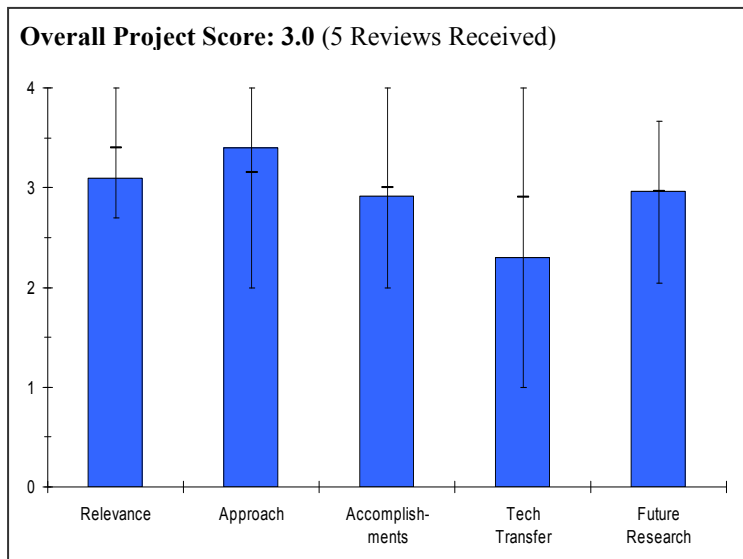
- Perform H2A analysis for this process.
- Work should be focused on mixed manganese oxide cycle only. No more work on straight manganese oxide system.
- Perform research to understand why Zn-mixed oxides are better than Fe-mixed oxides. Determine what will be the ultimate mixed-oxide system.
- Need thermodynamic analysis of cycle, and estimate of parasitic loss at pumps, sprays, heat-exchangers
- Need cost analysis of cycle, temperatures, materials, vessel size.
- Need a plan that moves project forward to go/no-go decision points.

**Project # PDP-02: Novel Low-Temperature Proton Transport Membranes**

*Andrew Payzant; ORNL*

**Brief Summary of Project**

The objective of this project is to develop a novel ceramic proton conductor based on  $\text{La}_2\text{Mo}_2\text{O}_9$  for use as a hydrogen separation membrane. The objective will be achieved through 1) compositional development; 2) characterization of the electrical properties, chemical stability, hydrogen flux and thermo-mechanical properties; 3) neutron diffraction analysis of selected materials to better understand the hydrogen transport properties; and 4) evaluation of surface exchange catalysts. The goal will be to synthesize this asymmetric membrane from candidate materials with and without exchange catalysts for additional flux testing to determine the range of flux possible in these materials.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.1** for its relevance to DOE objectives.

- Development of non-Pd based hydrogen membrane is a good option/pathway for hydrogen production.
- $\text{CO}_2$ ,  $\text{H}_2\text{O}$  tolerant-separation membrane for 300 to 500°C operation. It is likely to be hydrogen tolerant as well. Quite relevant.
- Energy efficient and economic hydrogen separations provide not only separation/purification opportunities, but also can be used to advantageously alter reactor kinetics.
- This project explores a unique crystal structure that is apparently permeable to hydrogen, and might have utility for the separation of hydrogen from other gaseous species. If successful, this research could provide an improved method for hydrogen purification, and subsequent utilization as a fuel or chemical reactant.
- The project is evaluating a high risk alternative for hydrogen separation. The technique utilizes a solid oxide membrane that will selectively separate hydrogen from any gas mixture. This is a fundamental, long term research effort that will not meet any of the near term DOE targets (2015), but may provide information for future hydrogen separation membrane techniques.

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- Tasks 3 and 4 are good strategies for improving material formulations.
- Task 1 contributes toward fabrication methods. This work (making thinner membranes) can also be done when the project moves toward commercialization.
- Task 2 can be avoided since the flux that is to be reported under this research and development activity is supposed to be normalized with respect to pressure differential (20 psi?) anyway.
- Innovative proton-conducting ceramic, low cost.
- The project is based on a material whose beta phase was identified as an oxygen ion conductor in 1999/2000 and in 2003/2004 identified as a proton conductor when in the alpha phase. The material structure and chemistry appear to be very stable in  $\text{H}_2$  and  $\text{CO}_2$ .

- The project team is in the very initial stages of taking a material and producing a useful membrane. Initial flux measurements are very low on thick 3-mm samples. The project team has identified the barriers to increasing flux greater than four orders of magnitude and is working towards that goal.
- The approach is to prepare a series of lanthanum molybdenate compounds and then test these materials hydrogen transport. Such transport might be permeation along grain boundaries and other micro fissures, or it could be dissociative absorption and then dissolution of atomic hydrogen. One goal is to determine the transport mechanism. Another goal is to maximize the rate of hydrogen transfer, and another goal is to evaluate the system to determine poisons that might interfere with the transport step.
- The work is examining a technique that has been researched in the past - solid oxide proton membrane separation. However, the unique aspect of this work is the attempt to develop materials that will operate at low temperatures (200 - 500°C), rather than approximately 850°C. This could be a big advancement for these materials; however, achieving high flux levels will be a major barrier.
- This is a fundamental research effort to identify and test new transport materials. No commercial materials will be developed in the near future. This is an appropriate long term fundamental research project for a National Laboratory as long as funding is maintained at the current levels (approximately \$200K per year).
- The work is considering a different family of compounds (non-perovskite) that have not been examined in the past.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.9** based on accomplishments.

- Good material characterization work, includes flux, conductivity, XRD, expansion.
- Pr doping does not seem promising, but the researchers should not lose heart. This is the nature of such research and development.
- Weakness: Some plots do not have the y-axes!
- Flux is still low and mechanism still not understood, but they've made thinner membrane, done basic experiments, made key measurements.
- They have solved membranes-sealing problem
- Thin (10-20 micron) supported membranes have been made. Team has a good match between the membrane thermal expansion and potential substrate material. Full membrane density is required, but not yet achieved.
- High Temperature tests completed indicate very stable material in H<sub>2</sub> and CO<sub>2</sub>
- This activity was initially funded by the Department of Energy's Fossil Energy, and then transferred to the Office of Energy Efficiency and Renewable Energy. The work had just begun when funding was withdrawn and just now new funding is available to restart the project. There is no significant progress to date, but a well thought through technical plan was developed.
- Hydrogen flux levels are extremely poor at this time - well below 1 cm<sup>3</sup>/cm<sup>2</sup>/min. This is barely at detectable levels. If increases are not obtained within the next year - DOE should consider ending this work.
- Leaks do not appear to be a significant problem with these membranes, which is probably due to the lower temperatures being used for this separation. However, current tests are being conducted with thick membrane disks (3 mm) which may be easier to seal.
- The project has had some success with materials development. The work has been able to produce defect free, thin layers (10 micron) of the membranes on a zirconia support. Thin membranes will be required to achieve high flux levels – probably on the order of 3 - 5 microns.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.3** for technology transfer and collaboration.

- Some collaboration with the University of Cincinnati.
- Suggest the principal investigator also consider collaboration with organization with similar material expertise.
- Oak Ridge National Laboratory and the University of Cincinnati will want broader collaboration on the project progress if there is to be any commercial product.
- One university partner is involved in membrane characterization.

## PRODUCTION AND DELIVERY

- This is very early stage work (and wider coordination probably has IP concerns). Industrial partners, (experienced with commercial production of the substrate and potential end users) however, could accelerate this development.
- Technology transfer is minimal and there does not appear to be any external collaboration. The work is being conducted 100 % at ORNL. No publications have been produced from this work. This work has been ongoing since 2004 and there should have been some technical publications by this time.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- See comments in Approach.
- Weakness: Incorporating Pd goes back to precious metals again.
- Trying to understand mechanisms. Adding pressure and catalyst.
- Production and flux testing of numerous thin fully dense supported membranes is needed to demonstrate the practicality of producing and using this membrane. Demonstrate that the approaches to improving flux are doable and practical.
- The proposed research will evaluate the feasibility of using this material for hydrogen purification.
- Future work will just continue materials development to reduce membrane thickness and increase flux. This is an acceptable approach for this stage of the research.
- The project needs to meet some pre-determined yearly targets and goals - in particular a reasonable flux rate.

### **Strengths and weaknesses**

#### Strengths

- It investigates hydrogen transport in non-PM membranes.
- They have a good approach.
- It is a well run and worthwhile project.
- New/novel dense film separation materials are being developed that opens up new opportunities.
- Alpha phase should permeate very high purity hydrogen.
- Material shows H<sub>2</sub> and CO<sub>2</sub> stability.
- The PI is highly competent and knowledgeable in solid state transport.

#### Weaknesses

- Results to date are not great, but the problem is challenging.
- Hydrogen flux is very low.
- Many performance metrics are unknown. This is a result of hydrogen permeation being a very new use for this material and limited work has been done or reported. However, structure and chemistry suggest performance could be similar to other dense ceramic/cermet membranes
- Limited flux testing has been done.

### **Specific recommendations and additions or deletions to the work scope**

- This project can be categorized as a high risk/reward activity. The researchers should be encouraged to continue the focus on non-PM materials.
- Incorporate sensitivity to H<sub>2</sub>S, CO<sub>x</sub> in material characterizations.
- Modify substrate so that can use thinner membrane coats or so that membrane can be used as solid oxide fuel cell.
- Focus on the production of fully-dense very-thin supported membranes before exploring surface treatments to promote hydrogen dissociation.
- Develop back of the envelope projections for metrics.
- DOE needs to define some yearly technical targets/milestones for this project. The work is simply continuing with no clear goals or direction. The targets should be mutually determined by DOE and the Oak Ridge National Laboratory; and if the yearly targets are not met, the work should be discontinued. DOE should support these fundamental, high risk research efforts – but needs to be able to terminate these projects when no technical achievements are being produced.

**Project # PDP-03: Ultra-Thin Proton Conduction Membranes for H<sub>2</sub> Stream Purification with Protective Getter Coatings**

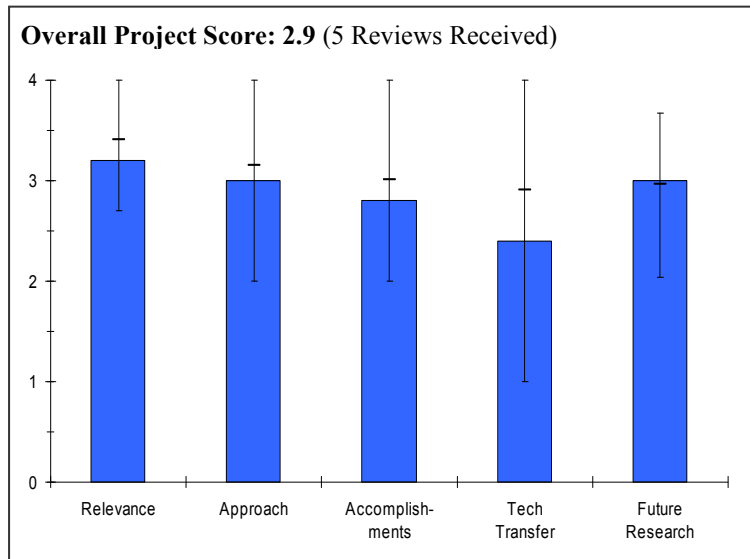
Margaret Welk; SNL

**Brief Summary of Project**

The objectives of this project are to 1) provide a functional support that will protect membranes from corrosive species in reformat gas stream; and 2) synthesize an “ultra-thin” dense ceramic proton conducting membrane to increase hydrogen flux over existing membranes. Dense membranes, whether metallic or ceramic, are especially vulnerable to sulfur attack. Sandia was successful in the deposition of titania and recently SrO. The deposition of ZnO was also successful.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.



- Sulfur tolerant membrane for hydrogen extraction.
- Project objectives deal with hydrogen stream purification through innovative membrane production.
- Project needs to address its targets in terms of DOE cost targets for hydrogen production.
- Overall project objectives and technical plan are provided; however it seems to be quite appropriate for potentially significant cost reduction for hydrogen production toward achieving DOE's cost goal.
- Dense membranes, whether metallic or ceramic especially are vulnerable to sulfur attack. The functional support will protect membranes from corrosive species in reformat gas stream.
- The PI will synthesize an “ultra-thin” dense ceramic proton conducting membrane to increase hydrogen flux over existing membranes.
- Project is responsive to DOE’s 2012 Target.
- System Cost \$/kg H<sub>2</sub> \$0.70 (\$400/kW).
- Electricity Cost \$/kg H<sub>2</sub> \$2.00.
- O&M Cost \$/kg H<sub>2</sub> \$0.60.
- Excellent understanding of markets and cost.
- Developing a membrane that could lead to cost, operability and footprint advantages over PSA is in line with DOE’s goal.
- Removal of sulfur post water gas shift is perhaps not as critical since sulfur must be removed before shift and in some cases before SMR catalyst due to negative effect of sulfur on the catalysts.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- Project is only 25 percent done. Some basic technologies are complete-on schedule. Their approach is reasonable.
- Project approach addresses several technical barriers for Hydrogen Production identified under Hydrogen Separations.
- Researching for functional support to protect against corrosive species such as sulfur.
- Investigating synthesis of an ultra thin dense ceramic proton conducting membrane to increase hydrogen flux.

## PRODUCTION AND DELIVERY

- Formation of ultra thin membranes (atomic scale) SrTiO<sub>2</sub> could improve flux. Coating of supports with ZnO could getter materials.
- Not clear whether alumina or silicate will be used as the support or both.
- Approach is sound and logical to complete objectives. They will: 1) Define market and requirements. 2) Conduct an industrial users survey. 3) Design and build pressurized electrolyzer stack. 4) Develop plastic stack technology demonstrate electrolyzer performance and capital costs, perform testing.
- Coming up with a membrane that can handle real life, post shift, reformat conditions is the right approach. Especially if the membrane can show clear advantages over well-proven PSA system.
- Again, removal of sulfur post water gas shift is perhaps not as necessary since sulfur must be removed before shift and in some cases before SMR catalyst due to negative effect of sulfur on the catalysts. The sulfur getter might have to be a separate part of the membrane to allow for installing in the feed stream to reforming system to trap out sulfur species.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- Project is only 25 percent done. Some basic tech complete. On schedule. It would be nice if the membrane were gas tight.
- Successful results reported for the deposition of TiO<sub>2</sub> toward synthesizing an ultra thin proton conducting membrane.
- Work on SrO deposition has just been completed. Thus they are able to successfully deposit SrTiO<sub>3</sub> on the ceramic surface. Following tightly deposited SrTiO<sub>3</sub> thin film they plan to start conducting hydrogen flux experiments.
- They reported success for building support with fine pore structure to enable synthesis of ultra thin proton conducting membrane. They are successful in adjusting the pore size to desired levels.
- They reported successful ZnO deposition within the pore structure of Al<sub>2</sub>O<sub>3</sub> mesoporous disc support. They showed good results in sulfur scavenging and regenerating ZnO.
- Regeneration of ZnO will enable this technology to achieve continuous operation when two alternating units are used.
- Only limited progress has been made.
- Good progress has been made. A stack has been completed. 1 kg H<sub>2</sub> / hr production rate is currently being upgraded to 15 bar pressure capability.
- Would like to see data of membrane performance on either simulated reformat stream (with steam) or real reformat from a reformer system.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.4** for technology transfer and collaboration.

- Plan is okay. It is too early in project to expect much.
- No partners at the present. The principal investigator is considering appropriate potential partners since they are now successful with building the ultra-thin proton conduction membrane.
- Although a score of 1.0 is given according to the criteria, this score in reality should be N/A and should not affect the overall score.
- The principal investigator is looking at ultra-thin SrTiO<sub>3</sub> deposition work to be successfully accomplished before bringing in new collaborators to the project. Successful results gave a “go” for this milestone.
- Collaboration is planned with Eltron and Pall.
- Collaboration is strong and effective with General Electric and the National Renewable Energy Laboratory.
- Perhaps too early at this stage partly due the progress of the project, but the membrane will need to be tested under real life or close to real life conditions (to be accomplished by working with projects working on reforming).

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- Main future research is making membranes gas tight and measuring flux.
- They addressed critical steps to overcome technical hurdles faced in the first year.
- Technical future work plan seems to be sound.
- Inclusion of cost analysis in their fiscal year 2008 work plan will be valuable. The technical targets may be addressed in terms of hydrogen production cost targets toward achieving DOE goal of reducing the cost of hydrogen to \$2.00 - \$3.00/gge delivered.
- The project needs to continue work to get the SrTiO<sub>3</sub> on the support.
- System testing at ambient and 15 bar pressure is planned.
- Operation and management cost assessment will be completed. System design will be done. This will complete project objectives.
- Perhaps need to establish some near term intermediate goals to better evaluate progress and future funding decision.

**Strengths and weaknesses**

Strengths

- It is a reasonable project.
- Technical objectives are planned appropriately and they successfully executed the planned work in the first year.
- Technical progress seems to be in line with their proposed timeline.
- Future technical work plan outlines tasks appropriately to achieve targeted technical results.
- Technical work plan and successful execution within the planned timeline are strengths for the project.

Weaknesses

- Concentration polarization or seals may doom project.
- Economic feasibility study will strengthen the project.
- Critical go/no-go decision points are needed.
- Plasma assisted atomic layer deposition (ALD) while one can control fine control thickness, depth of penetration, stoichiometry, etc. may not be an economical process. This needs to be investigated.

**Specific recommendations and additions or deletions to the work scope**

- Keep on going.
- Build go/no-go decision points into the work plan with regard to both technical and economic targets.
- Economic feasibility study with critical cost analyses to validate that the technical success will result in cost reduction for Hydrogen production to meet DOE goals.
- Do not need to look at removing sulfur post water gas shift. Might need to decouple the getter from the membrane and have it put in front of the system to remove sulfur in feed stream prior to SR reactor.

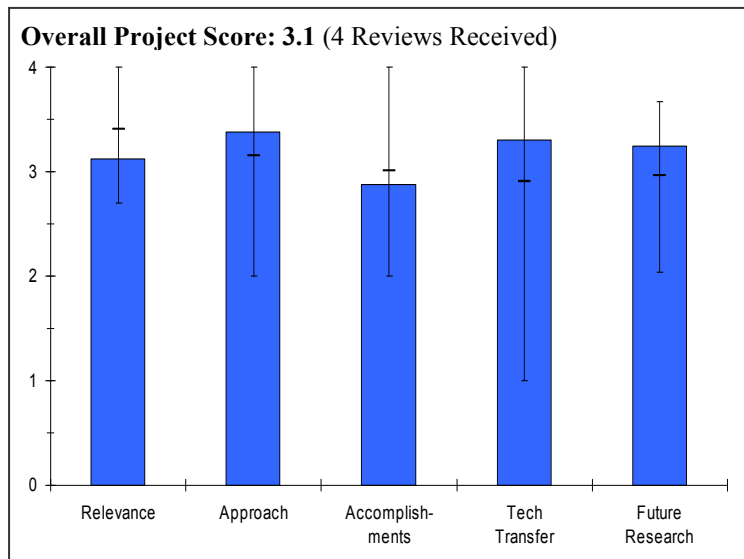


**Project # PDP-04: Renewable Electrolysis Integrated System Development and Testing**

*Kevin Harrison; NREL*

**Brief Summary of Project**

The objectives of this project are to 1) characterize electrolyzer performance with variable input power; 2) design, build and test shared power electronics; 3) identify opportunities for system cost reduction and optimization; and 4) test, evaluate and model the renewable electrolysis system. The National Renewable Energy Laboratory (NREL) has increased energy capture of the second generation wind to stack power electronics. And verified stack voltage efficiency to help meet the Department of Energy milestone. NREL has also integrated grid, wind and photovoltaic functionality into single power electronics module to reduce capital cost.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.1** for its relevance to DOE objectives.

- The project supports the hydrogen vision and research, development and deployment objectives to an extent. The principal investigator did complete the contractual tasks successfully. Although theoretically possible, the key technology challenges to practical deployment of distributed small-scale PEM electrolyzers integrated with renewable electricity generation is not addressed to the comprehension of the reader or reviewer.
- Very good. Clear and distinct objective which matches up well with the DOE program.
- For electrolyzers to be a cost effective pathway, capital cost must be reduced and efficiency boosted.
- Project directly addresses these two required developments.
- Performance evaluation is essential to the Program.
- Effective use of renewable energy is a key component of an energy transition to carbon-free energy.
- Electrolyzer performance is essential to renewable electrical energy utilization for a hydrogen economy.

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- The identified, listed barriers are not new or unknown. (Most presenters on the subject listed the same three, common-sense barriers.)
- Difficult to figure out what new info the project has unfolded; seemed more like routine data collection rather than research and development.
- Presentation of the activity description and conceptual integration schemes by the principal investigator was impressive, but this does not develop a commercially viable, workable system; what new and different approach the principal investigator plans to take to overcome the known barriers should be addressed in the presentations. The stability of sulfonated tetrafluorethylene copolymer for long-term use, the use, recyclability, cost of noble metal or any other material electrodes, overall efficiency including compressor parasitic load, etc., issues the presenter should be prepared to discuss.
- Very good. Would have hoped that this section would have been more detailed.
- Project shows technical feasibility by actually constructing and testing devices.
- Approach is sound: analytical modeling alone would not conclusively prove feasibility.
- Methodical approach is a strength.

- Broad choice of energy sources is a strength.
- Good analytics.
- Using a standard performance protocol is a good approach - based on published international drafts of related work.
- Broad choice of electrolyzer types and manufacturers is a strength.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.9** based on accomplishments.

- Phased approach to overcoming barriers and accomplishing DOE cost and performance targets.
- However, since the key technology challenges are not unknown, and difficult, the PI did not clarify what new approach the PI will take to achieve the DOE targets.
- Very good - project appears to be where it should be at this point in the schedule.
- Gen 2 energy capture improvement is substantial.
- Project is still in progress, with continuing work and future work to follow.
- Operation of such a system is complicated and challenging. The project is to be commended for accomplishing this effort and keeping this complicated system operating.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- Several partner's names are listed; but the roles and responsibilities of each or any of the partners are not discussed.
- Outstanding for collaboration.
- While it is hard to gauge the quality of the interactions, there are a large number of partner companies and even larger number of companies providing feedback. Overall, I judge the level of interaction to be much above average.
- Manufacturer feedback is included, as strength.
- Publication of the protocol, as an international standard, is encouraged.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.3** for proposed future work.

- Rational follow-on work scope.
- Very good - sound engineering approach.
- Funding may stop and this work is too important to allow this to happen.
- Continuing work to evaluate new electrolyzer designs would be a strength.
- Publication of the testing protocol would be valuable to the entire industry.

**Strengths and weaknesses**

Strengths

- Strengths are the collaboration followed by the verification with what appears to be actual, commercially available hardware.
- Good to have actual test data.
- Excellent number of electrolyzer companies involved in project.
- Broad and suitable choice of electrolyzers with manufacturer feedback.
- Broad and suitable choice of energy sources.
- Broad and suitable choice of power conditioning.

### Weaknesses

- How does the distributed generation cost become lower than the central generation cost (not including shipment)? This infers that small electrolyzers are more efficient than larger units.
- It is not clear why efficiency drops off with current density. Electrolyzer efficiency should be higher at part load.
- Graphical representation of Gen 2 energy capture is good but I'd also like to see a numerical evaluation ( e.g., X percent of energy captured at speeds under 30mph).
- Power electronics capital cost reductions by combining functionality and eliminating redundant components seems logical and feasible but question is "by how much?" I don't see any quantification of cost reduction or description of a costing methodology.
- Presentation showed results of optimization, but did not include description of how exactly improvements were made.
- Possible lack of future funding.
- Performance protocol has not been published as a standard.

### Specific recommendations and additions or deletions to the work scope

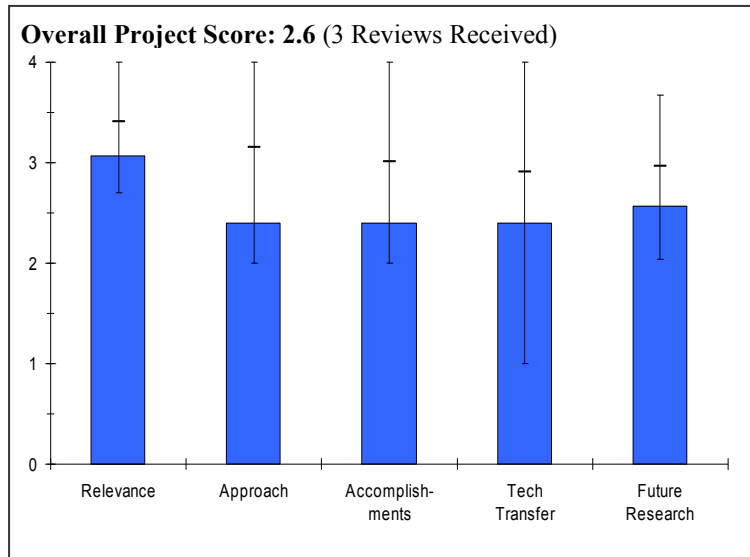
- Continue the good work.
- Publication of the testing protocol as an international standard would add credibility to the project, support the international efforts on the same topic and give credit to the laboratory.

**Project # PDP-07: Photobiological Hydrogen Research**

*George Philippidis; Florida International University*

**Brief Summary of Project**

The overall objective of this project is to identify which structural and active site maturation genes of the O<sub>2</sub>-tolerant NiFe-hydrogenase from the photosynthetic bacterium *Rubrivivax gelatinosus* CBS are critical to optimal expression of the enzyme in *E. coli*. Expression in *E. coli* will facilitate eventual expression of the hydrogenase in cyanobacteria at the National Renewable Energy Laboratory. The 2007-2008 objectives of this project are to 1) clone the largest structural gene *cooM* of the hydrogenase into duet expression vectors under the T7 promoter; and 2) detect and purify the fully efficient (recombinant) hydrogenase in *E. coli*.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.1** for its relevance to DOE objectives.

- Although still somewhat in its infancy, this work has great potential for numerous applications.
- This is an essential but very difficult problem that several other projects also seem to be involved with.
- The project goal of constructing molecular biology cassettes of hydrogenase genes is well-aligned with the Program goal of understanding and optimizing biological hydrogen production.

**Question 2: Approach to performing the research and development**

This project was rated **2.4** on its approach.

- Standard non-innovative approach.
- The cloning strategy for construction of hydrogenase cassettes seems straightforward.
- The "top-down" approach of reconstructing a functional hydrogen-producing gene cassette in a heterologous host is not particularly innovative but seems feasible.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.4** based on accomplishments.

- Clear methodology and roadmap activities accomplished.
- Not yet achieved the goal of obtaining an active enzyme and it isn't clear why.
- The progress towards goals was good, with some specific milestones achieved in a timely fashion.
- The progress on several tasks (3.0 and 4.0) is weak and behind schedule.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.4** for technology transfer and collaboration.

- Working with the National Renewable Energy Laboratory, the pathways overlap, appears to be good communication.

## PRODUCTION AND DELIVERY

- It was not clear what would be done once the main enzyme was obtained by the collaborator.
- The partnership between a university and national lab is good.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.6** for proposed future work.

- The future work proposed is in line with DOE mission.
- Plan and direction completed for future work, sounds like funding is the unknown.
- What will be done if this product is successful?
- Future tasks are well defined.
- Future plans to finish cassette construction and optimize hydrogenase expression levels are logical.

### **Strengths and weaknesses**

#### Strengths

- Molecular experience of PI and overall goal of obtaining an active enzyme.
- The investigators' prior record of collaboration is very strong.
- The investigators have demonstrated good progress towards defined goals.

#### Weaknesses

- Overall goal. What is the next step?
- The project plan is "brute-force" construction of known components. It is unclear that reconstruction of a functional hydrogenase cassette will necessarily lead to determination of the "minimum number" of hydrogenase genes required for fully efficient hydrogenase expression. There may be nonlinearity in terms of specific maturation elements that are not reflected in stoichiometric combinations of gene cassettes.
- The need to purify back the recombinant hydrogenase enzyme from the heterologous host is not clearly articulated.
- The techniques for testing successful transformation are somewhat old-fashioned and laborious. Why can't the investigators use PCR to look for co-transformation rather than having to grow up mini-preps and run out gels?
- There is no contingency plan for modification of co-expression if induction results in little or no activity (likely due to formation of insoluble or inactive inclusion bodies, etc.).

### **Specific recommendations and additions or deletions to the work scope**

- None.

**Project # PDP-11: Enabling Hydrogen Embrittlement Modeling of Structural Steels**

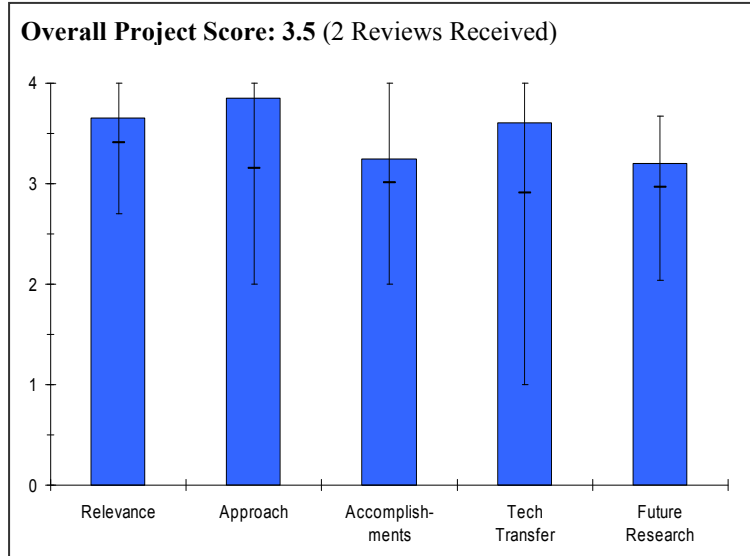
Brian Somerday; SNL

**Brief Summary of Project**

The objectives of this project are to 1) enable application of structural integrity models to steel hydrogen pipelines; and 2) enable development of micromechanics models of hydrogen embrittlement in pipeline steels. Models can demonstrate that hydrogen embrittlement can be accommodated and pipeline safety margins can be quantified. Micromechanics model are essential for understanding the fundamentals of hydrogen transport and embrittlement in steels.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.7** for its relevance to DOE objectives.



- Understanding hydrogen embrittlement is essential to mass distribution and storage of hydrogen.
- This project promises to improve understanding of failure mechanisms of steel pipelines carrying hydrogen.
- This project supports achievement of DOE's targets for reliability/integrity and hydrogen leakage of hydrogen pipelines.
- It is not clear that this project will lead to capital cost reductions for H<sub>2</sub> pipelines.

**Question 2: Approach to performing the research and development**

This project was rated **3.9** on its approach.

- Approach seems to be right on target.
- The approach is effective and is focused on meeting the needs of ASME code.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- Good progress has been made in the basic understanding of embrittlement but obviously more is needed before methods of overcoming the barriers can be suggested.
- Project is making progress in measuring the properties of pipeline steels in high-pressure hydrogen gas using fracture mechanics methods.
- Barriers to further progress are being appropriately addressed.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.6** for technology transfer and collaboration.

- The list of collaborators and the fact that Sandia is dependant on others for test data and material samples indicates that collaboration is excellent.
- Sandia National Laboratories (SNL) is a member of the Pipeline Working Group, which allows them to share information with a number of other organizations doing pipeline research, as well as stakeholders.

## PRODUCTION AND DELIVERY

- It does not appear that any universities are involved in the working group. University participation should be considered if they offer any capabilities that SNL does not already possess.
- Modeling does not appear to be included in SNL's scope. The anticipated modelers should be collaborators in the project.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- The future indicates a continuation of efforts but should start to propose methods of overcoming the barriers.
- Proposed research is appropriate.

### **Strengths and weaknesses**

#### Strengths

- Good coordination with others.
- Solid technical capabilities.
- This project promises to improve understanding of failure mechanisms of steel pipelines carrying hydrogen.
- Collaborations with the Pipeline Working Group will lead to effective information-sharing.

#### Weaknesses

### **Specific recommendations and additions or deletions to the work scope**

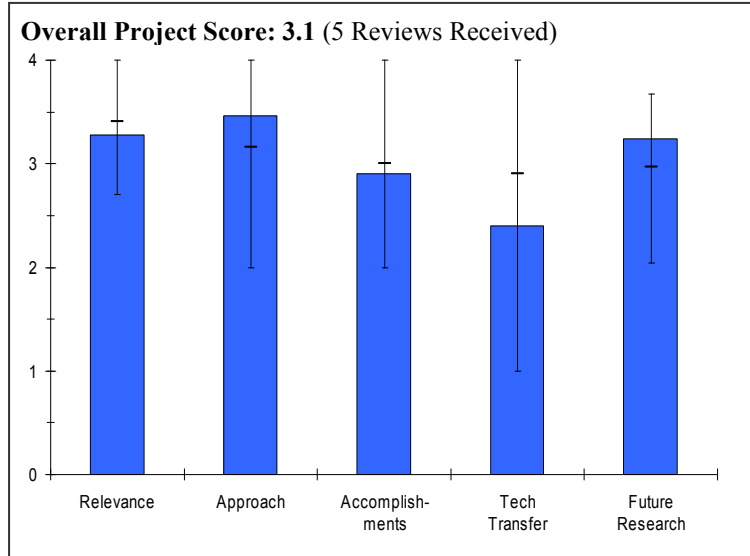
- Start to focus on screening methods for identification for acceptable materials.
- Consider including structural integrity and micromechanics modelers as partners/collaborators.

**Project # PDP-14: Advanced Alkaline Electrolysis**

*Dana Swalla; GE Global Res.*

**Brief Summary of Project**

The objective of this project is to study the feasibility of using alkaline electrolysis technology with current-generation nuclear power for large scale hydrogen production. The approach of the project is to 1) define market and requirements; 2) design and build a pressurized electrolyzer; 3) conduct plastic oxidation life test; 4) demonstrate electrolyzer performance and capital costs; 5) conduct system operation testing; 6) create industrial-scale system conceptual design; and 7) create 1-kg per second demonstration system conceptual design.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- This project has potential to produce hydrogen on site at reasonable costs.
- The project is working toward several DOE goals including lowering hydrogen production costs and increasing efficiency.
- Electrolysis is certainly one of the most viable options for near-term hydrogen production.
- This electrolysis work can be applicable to any electricity generating technology not just nuclear.
- Reducing the capital cost of electrolyzers would be a key step towards overall DOE goals.
- While the objectives are relevant, this is mostly an attempt to bring General Electric up to the state-of-the-art.
- Project is focused on reducing the cost of electrolysis and in deploying a system that can be used for many different applications of value to the hydrogen economy transition as well as to stationary and portable power sources that potentially have more immediate commercial applications.

**Question 2: Approach to performing the research and development**

This project was rated **3.5** on its approach.

- The project has a systematic and methodical approach.
- This project is focused on leveraging viable electrolysis technology with nuclear power and GE's advanced manufacturing to lower both the cost of electricity and capital costs which are two of the major hurdles for hydrogen via electrolysis.
- Good background work to identify existing hydrogen customers to bridge the gap to the eventual transportation sector demand for hydrogen.
- Design of stack for lower cost seems well engineered and thoughtfully conducted.
- The approach tries to bring GE up to the state of the art, but does not appear to be advancing it.
- The costs of current alkaline stack modules seem too high relative to existing commercial products.
- PI is focused on major technical improvements to achieve cost reduction and has followed a well designed plan.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.9** based on accomplishments.



## PRODUCTION AND DELIVERY

- Good progress with electrocatalysis/electrode design.
- Why does the performance curve not show the current density (x-axis)?
- The project has demonstrated increased electrodes performance leading to a lower cost per unit area and higher efficiencies.
- Stacks have been successfully assembled using their plastic stack construction design.
- While these stacks have been constructed, they have yet to be tested.
- More experimental data would be expected at this point in the project especially since it is set to end on September 30, 2008.
- Similar to last year, they have yet to test the potential plastic degradation resulting from the plastic stacks being exposed to an alkaline electrolyte.
- Good concept definition of stack design.
- Electrodeposition seems to yield good performance, but would like to see more detailed performance comparisons with alternative methods.
- Completed market study for distributed hydrogen applications.
- Progress to date does not demonstrate any advancement of the technology or manufacturing techniques to significantly overcome any barriers. The costs of the stacks still seem high.
- All advancements are suggested as promising, but are not demonstrated on a large enough scale to be believable.
- Project is 70 percent complete and the results show significant progress toward the cost target. Technical innovation has resulted in significant improvement in cost on the order of 50 percent reduction.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.4** for technology transfer and collaboration.

- Not explained in the poster.
- The project has obtained useful real-world data from Entergy Nuclear to benchmark the system costs.
- The project has worked with the National Renewable Energy Laboratory to benchmark the cost of hydrogen via electrolysis based on the H2A model.
- Very little outside collaboration on the research and development aspects of the project.
- It is not clear there was much (if any) technology transfer or collaboration. However, it's not clear that any was needed.
- While there seems to be collaborations about market conditions, etc., there is nothing to suggest any collaboration with others in the electrolysis technology community.
- There is little collaboration with external organizations at this point, but the project is being successfully executed by resources and knowledge bases available from within the principal investigator's institution.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- Future work planned is sound.
- The proposed future work to test the system at ambient and 15 bar is good.
- The operation and management cost assessment is important.
- It seems as if the project still has significant barriers to address in a very short time to ensure a successful project.
- Overall, the plan builds on their past progress and it focused on potential barriers.
- System testing at pressure is key.
- The future work suggested seems to be more of the same without indications of advancement.
- Future work to conduct system testing and complete the operation and management cost assessment builds upon the significant progress to date and will bring the project to a successful conclusion.

**Strengths and weaknesses**

Strengths

- The use of plastic components.
- Strong emphasis on materials durability.
- The overall technology has the potential to lower stack costs and provide for large scale hydrogen production.
- A strong research and development/engineering project conducted professionally.
- There is obvious technical capability in the General Electric organization.
- If cost targets are met following the systems testing phase, the technology has potential to be commercialized for various fuel cell applications as well as mid to small industrial hydrogen uses. The inventions made in the course of the work will facilitate differentiating this technology for commercial applications.

Weaknesses

- Stack testing must ramp up to successfully demonstrate the approach and the technology.
- Market projections are important and necessary, but I hope they didn't spend a lot of money on it. Seems like General Electric should have had a pretty good handle on the market from Day 1 of the project.
- Plastic joining method is poorly described.
- No linkage showing how stack costs combine with BOP costs to yield target \$400/kW.
- If market demand study is for distributed generation, why are nuclear plants being considered?
- Bill of materials for system is not provided.
- Would like to see a fuller cost projection and more detailed system level definition.
- There is a lack of practical field experience in the organization.
- They have not addressed scale up, life, or mass production issues.
- There are no project weaknesses thus far; however, the principal investigator must report a final cost that shows the degree to which the target costs have been met.

**Specific recommendations and additions or deletions to the work scope**

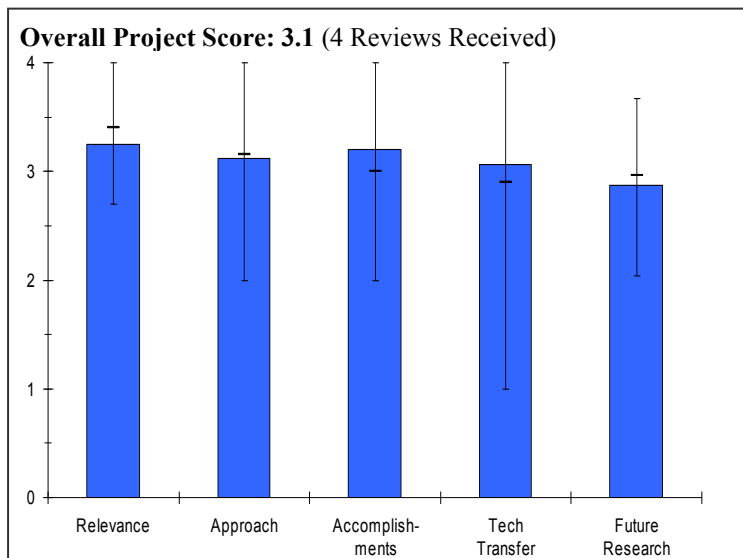
- Would it be possible to use an alkaline exchange membrane?
- Project should be expanded to include existing electrolysis manufacturers or deleted.

**Project # PDP-15: Photoelectrochemical Generation of Hydrogen Using Heterostructural Titania Nanotube Arrays**

*Mano Misra; U of Nev. Reno*

**Brief Summary of Project**

The overall objective of this project is to develop high efficiency hybrid-semiconductor materials for hydrogen generation by water splitting. The 2007-2008 objectives were to 1) develop organic-inorganic hybrid photoanodes; 2) develop combinatorial approach to synthesize hybrid photo-anodes having multiple semiconductors in a single photo-anode; and 3) develop cost-effective cathode materials. The 2008-2009 objectives are to 1) develop mixed metal oxide nanotubular photoanodes; 2) develop multi-junction photoanodes; and 3) design photoelectrochemical systems for on-field testing under real solar irradiation.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- Even optimization of TiO<sub>2</sub> as a hydrogen producing photoelectrode will not result in a useful system since it has too large a band gap to use much of the solar spectrum.
- A well constructed program aimed at building novel metal oxide/ metal sulfide macroscopic structures capable of photoelectrochemical water splitting.
- This program provides a good mix of basic science, system design, and engineering.
- Quite relevant as this research theme has the potential to be a contributing technology in decades to come.
- Long term, high risk research is exactly what should be funded.
- Photoelectrolysis concepts and subsequent funding are well aligned with the long term energy solutions.
- Most aspects of this project are aligned with the important goal of improving the efficiency of direct solar water-splitting.

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- The principal investigators have developed a good level of expertise in the area of synthesizing TiO<sub>2</sub> nanotube arrays and related structures. Unfortunately, the principal investigators are committed to the idea that they can empirically find a way to lower the band gap of TiO<sub>2</sub> through doping or alloying, despite the numerous unsuccessful attempts to do this over the past 30 years. Similarly, their ideas about sensitization of TiO<sub>2</sub> are not novel.
- TiO<sub>2</sub> nanotubes are being produced and studied by at least a dozen groups (and with more success in many groups) and so there is no novelty in this project. CdS will be unstable in a non-sacrificial system and still will not extend the spectral response enough to make this useful. A strong materials science approach is employed coupled with good electrochemical support.
- The project is focused and productive.
- The materials approach is creative and sound.
- Use of nanotubes and variations of titania is pointing in the right direction. The approach is good and will lead to new and other novel materials.

- Approach and execution of the work is good - the key elements of the materials science are being addressed.
- New combinations of nanotubes, titania, and other relevant tunable band gap materials will emerge - leading to other potentially interesting combinations and thereby increasing the stability and efficiency.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.2** based on accomplishments.

- Most of the approaches being explored in this project have been tried before and have little chance of success. Some of the "accomplishments" are trivial or misleading. Shining light on both sides of a porous electrode to achieve a 6 percent solar to hydrogen conversion efficiency with their TiO<sub>2</sub>/CdS system - they are using a sacrificial donor (sulfide) and not splitting water.
- Much of what is being done was well known 20 years ago, so it is difficult to call any of it progress.
- Synthesize high quality anatase rod structures.
- Introduce a carbon component to reduce the band gap.
- Generate TiO<sub>2</sub> rod/CdS particle mixed structures.
- Carried out PEC characterization of indicated materials.
- Demonstration photo-induced hydrogen production from TiO<sub>2</sub> rod/CdS particle mixed structures in the presence of an aqueous sulfide electrolyte. (System stability is uncertain.)
- All research goals are being met.
- The accomplishments with respect to stability are positive yet additional testing needs to be performed to assess if stability is maintained beyond a "few" hours.
- Result is very clear and presentation is very understandable.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- It is a good sign that the principal investigators have been active in publishing and presenting their work. However, some of their ideas about how photoelectrochemical devices work are not physically sound.
- The appropriate collaborative relationships are in place, especially with the National Renewable Energy Laboratory.
- This project seems to be in communication with other projects.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- The proposed future work is not well focused. The basic idea seems to be to keep trying things a hope for a miracle.
- See former comments, but in summary, even perfecting a TiO<sub>2</sub> system will not produce a useful system or device.
- The success of this project rests on understanding the oxidative component. If the semiconductor is being oxidized the system is not viable. Thus, it is appropriate that the researchers are focused on this issue.
- Continued materials development is well defined and appropriately focused.
- The proposed work will attempt to drill down into the mechanisms and materials science. All appropriate for this stage as it is nearing the end of the effort.
- Longer term testing to assess stability under real sunlight conditions will be valuable.
- Newer compositions/configurations should be looked at.
- Please accelerate as much as possible and discuss with engineers to build more realistic design of the reactor.

### **Strengths and weaknesses**

#### Strengths

- A strong track record of materials development.
- Interesting heterostructures mixing metal oxide and metal sulfide functionalities.
- A good mix of materials science, electrochemistry, and photoelectrochemistry.
- Strong technical team and partners.
- Materials science and facilities and capabilities.

#### Weaknesses

- Photoelectrochemistry is not well developed.
- The oxidation process may lead to a major materials instability.
- Weak understanding of photoelectrochemical principles and literature. Willingness to believe that ideas that have been tried and failed in the past will work in this project.
- Not novel and will not produce a useful or stable device and is also not producing any new fundamental information.

### **Specific recommendations and additions or deletions to the work scope**

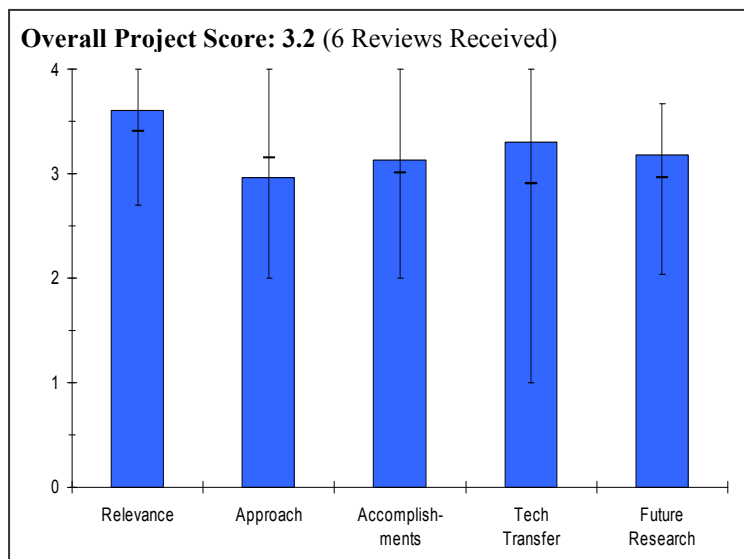
- There are some good aspects of this project. But the idea that this technology is ready for scale-up or commercialization (UNR easy H<sub>2</sub> PEC cell) is absurd.
- Redirect project.
- The work plan is well supported. Continue as is.

**Project # PDP-16: Distributed Bio-Oil Reforming**

*Bob Evans; NREL*

**Brief Summary of Project**

The overall objective of this project is to develop the necessary understanding of the process chemistry, compositional effects, catalyst chemistry, deactivation and regeneration strategy as a basis for process definition for automated distributed reforming. The fiscal year 2008 objectives are to 1) improve bio-oil atomization with less MeOH addition; 2) conduct a study of partial oxidation at 650C; 3) demonstrate catalytic conversion consistent with \$3.80/kg hydrogen; and 4) design, build and operate a bench scale unit capable of long duration runs (8 hours/cycle) with better material balances.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.6** for its relevance to DOE objectives.

- Hydrogen generation from bio-oils has the potential to be a key source of renewable hydrogen in the future.
- This project specifically supports key milestones related to the cost reduction of distributed hydrogen production from renewable liquids.
- The work is evaluating a process to convert biomass derived liquids to hydrogen. This is a goal of the Hydrogen Program and the work directly supports this objective.
- This project is important to the stated goal of hydrogen production from renewable biomass.
- The conversion of whole bio-oil is an important area of investigation because it can serve to minimize unit operations.
- Excellent project of clear relevance because biomass conversion into syn-gas allows for greater flexibility than simply a hydrogen target (e.g., it could go to higher value products, as needed).
- Use of pyrolysis product (bio-oil) is a solid idea.
- Poster was not quite clear; but the presenter's explanations were very helpful!
- Project is responsive to production of reformable fuels for production of hydrogen, etc. Supports 2012 Targets: \$3.80/gallon gasoline equivalent, 72% energy efficiency (bio-oil to hydrogen).
- The object to produce hydrogen from renewable sources is in line with the overall goals and objectives.
- Due to the undesirable properties of bio-oils, it might not be best suited for reforming route.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- Initial energy efficiency estimates have been made with Aspen Modeling and more are planned in the future.
- Good approach addressing the key issues related to biomass pyrolysis including a parallel modeling effort.
- The project is attempting to convert a complex biomass liquid to hydrogen. Instead of simply considering ethanol (for example), the project is considering a pyrolysis derived liquid. The liquid contains a variety of compounds, including high molecular weight aromatics. This is a complex mixture to convert and the approach is unique. The process is relatively simple and, if successful, the cost to scale up the process would be reasonable.

- Although several barriers are identified, it appears that feedstock cost is the primary barrier being addressed; secondarily operation and maintenance. Fuel processor cost may be too early to address or at least it does not appear to be addressed yet.
- The project appears to be appropriately focused on developing methods of producing hydrogen from bio-oil, taking into account the complexity of the fuel, its difficulty in handling, etc.
- The interaction with Lanny Schmidt at the University of Minnesota appears to be a good step toward identifying possible catalytic approaches to processing these complex materials.
- Sound approach to developing "basic" chemical engineering understanding.
- Good understanding of unit ops in an integrated reaction concept.
- Volatilizing approaches could be better researched; but choice of ultrasonic system is "good enough" initially.
- Good use of secondary air flow to control surface reactions at the catalyst bed.
- Approach is sound and logical to complete objectives. High conversion of bio-oil in non-catalytic step leads to significant yield of CO at 650°C.
- Lower methanol levels (less than 30 percent) have yet to be demonstrated due to technical problems with the new system.
- Rhodium catalyst can be used to attain equilibrium levels of hydrogen with and without added steam.
- Feedstock effects are under study.
- Experimental results were used as a guideline for ASPEN simulations.
- Again due to properties of bio-oils, significant fraction of methanol has to be used to break down the bio-oil. This approach might not be ideal due to toxic nature of methanol which can pose safety/storage issue for forecourt application.
- The majority of the focus for this project should be on the elimination or minimization of Rh catalyst. This could be a show stopper should the others barriers are resolved/overcome.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- The new nozzle designed to improve bio-oil volatilization was not utilized due to a component failure. This seems to have set back some of the oxidation, catalyst, and reduced methanol work.
- Initial Aspen mass and energy balance modeling has been completed.
- The project has achieved good conversions of the bio-liquid. Near equilibrium levels of hydrogen are being obtained.
- There is formation of some coke on the water-gas shift (WGS) catalyst, but this is to be expected due to the presence of the high molecular weight compounds. However, the catalyst can be regenerated and activity remains high.
- Some benzene remains in the products and this will have to be addressed.
- The need for large amounts of methanol solvent is the key drawback to the process. At best, it appears that about 30 percent methanol will be necessary. This problem needs to be further addressed. This may be overcome by designing a more effective atomizer.
- The process keeps the water requirement to a minimum.
- It seems that progress has been somewhat slow, driven in part by the need to develop a fuel atomization method.
- There appears to be little other work in this area by others so that it is difficult to assess what is reasonable project progress. DOE might consider funding a second separate project in this area with some alternate ideas.
- A better understanding of the effect of different feedstocks on bio-oil quality and composition is planned and seems to be well-advised. It may be that certain bio crops are better aligned with this technology than others.
- Good collaboration with the Schmidt group regarding catalysts.
- Need to explore other viscosity modifiers (why just CH<sub>3</sub>OH?).
- Need to see feedstock spectra (correlations between spectro and cracking products?).
- Reasonable data on oxidative cracking (micro-reactor results only?).
- Good progress has been made. Fiscal year 2006: Bio-oil volatilization method developed; oxidative cracking to CO with minimal CO<sub>2</sub>.
- Fiscal year 2007: Demonstrated equilibrium catalytic conversion to syngas at low temperature and low H<sub>2</sub>O/C.
- Would have liked to see more results on catalyst performance and effects of impurities in bio-oil.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- This project benefits from a strong team from industry and academia.
- More interactions with the biomass program at the National Renewable Energy Laboratory may be fruitful.
- Publications and presentations of the work appear very limited.
- The project has a number of participating partners, including Chevron, who would be capable of commercializing the process.
- The collaboration with Lanny Schmidt and with Chevron is good. It seems a bit premature to be talking about technology transfer.
- Good work to collaborate with the University of Minnesota group.
- Not very clear about the CSM contributions and the Chevron people.
- Collaboration is strong and effective CSM and NREL.
- Need more interaction with catalyst developers/manufacturers to address catalyst reduction and effectiveness with presence of impurities.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- Additional modeling work with Aspen is underway.
- Plans to lower the percentage of methanol are underway along with long-term testing.
- The future plans are appropriate. In particular, the researchers have recognized the need to reduce the methanol and are working to achieve this objective.
- Additional plans are to scale-up and demonstrate the process at a larger scale.
- The future work aims to reduce methanol concentration but it is unclear how this will be done and whether the use of methanol is a result of the scale of the testing or will be a consideration even at a larger scale.
- Much of the work appears to depend on the proper operation of the atomizer. One needs to ask whether this or some other technology will be applied if and when the process is scaled up. Is the vaporization of the fuel a show stopper at a larger scale, or is it easier?
- Excellent; and I hope you are better funded!
- Need to spell out what you mean by optimization (catalyst search? Or process changes - if so, which variables?)
- Fiscal year 2008 work is proceeding well. PI should: Demonstrate catalyst performance (in progress); design, build, and operate bench scale system (in progress).
- Need to establish clear criteria for go/no-go decision (working with DOE and HPTT).

**Strengths and weaknesses**

Strengths

- The project is aligned with DOE targets and it provides a potential renewable source of hydrogen.
- This is a good project for NREL. This is a high risk research project involving a difficult conversion process. It is unlikely that industry would be willing to conduct any significant research in this area. NREL has had some good success and generated some very useful information and data.
- Experienced team that is well versed in bio-oil after several years of work.
- Well conceived and laid out.
- Good choice of partners (University of Minnesota and Chevron).
- Appropriate "unitized" reactor; but many need more control points.
- Out-year work well conceived.



### Weaknesses

- Little mention about the potential of coke formation and how the project plans to deal with this issue over a long cycle.
- Overall, the project still seems a long way away from being a viable option and the path forward is not obvious especially without an energy cycle analysis.
- The Aspen model is a good step, but it is not obvious that this project has sufficient chemical engineering/reaction engineering help. It seems to be at a research and development stage but perhaps a engineering component could help guide the work, for example what needs to be considered if one were to scale up the process.
- For example, is methanol a requirement at a larger scale, or not? If not, then one needs to revisit how to best carry out the tests to avoid this possible artifact to full scale operation.
- Need greater chemical engineering (process control) inputs.
- Need correlations of bio-oil inputs (spectra) with resulting syn-gas products (any interesting correlations?).

### Specific recommendations and additions or deletions to the work scope

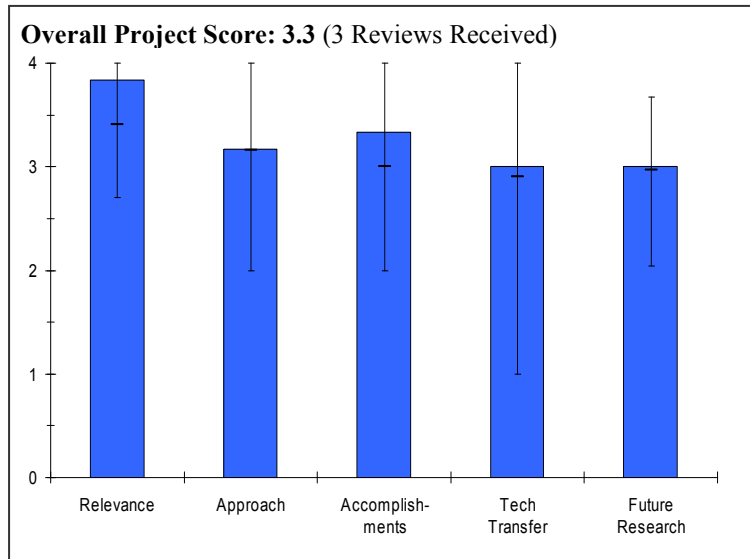
- Specifically examine this process of producing hydrogen (from biomass to bio-oil to hydrogen) from an energy standpoint.
- Fiscal year 2008 funding for this project appears extremely high. Yearly funding should be at the prior year levels - approximately \$300 to \$350K per year.
- Add more capability in reaction engineering and modeling.
- Fund the project more consistently!
- Get more feedstock info (spectra).
- Develop broader steam/C ratios.

**Project # PDP-18: Solar Thermochemical Hydrogen (STCH) Production - H2A Analysis**

*Kurt Roth; TIAX*

**Brief Summary of Project**

The objective of this project is to evaluate which solar-thermochemical hydrogen (STCH) cycles have the potential to meet the Department of Energy central production cost target of \$3.00/kg. The tasks for this project are to 1) support cost analysis of STCH cycles carried out by STCH Development Teams using H2A; 2) identify key cost drivers to guide research efforts to improve STCH economics; and 3) ensure meaningful comparisons of hydrogen production cost estimates among cycles to enable the most effective cycle down-select process.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.8** for its relevance to DOE objectives.

- Solar driven thermochemical water splitting is a renewable way to generate hydrogen and is applicable to the DOE objectives.
- There are many solar thermal hydrogen production options available, economic analysis such as this project is key to focusing efforts on the most promising approaches.
- Provided a well informed review and cont-analysis of thermochemical cycles for hydrogen production.

**Question 2: Approach to performing the research and development**

This project was rated **3.2** on its approach.

- Techno-economic analysis enables DOE to focus their limited resources on the technologies which have the highest probability of meeting their cost targets.
- Providing guidance to the researchers is an important role for Tiax.
- The DOE managers should also be trained so that they can evaluate the H2A spreadsheets on their own after the contract of Tiax is over.
- Approach is sound and logical: use of the H2A cost spreadsheet populated by values suggested by knowledgeable researchers and vetted to assure fair assumptions among the various approaches.
- Close and iterative collaboration with the technology development team.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- They should increase their attention on the operation and maintenance costs which will be significant for this technology.
- The chemicals used are the STCH processes are very toxic, costs should be included for spent chemical disposal.
- They should not include oxygen production credits in their cost analysis. The market is not large enough for the amount of oxygen produced.
- Review and feedback on 11 separate pathways.

## PRODUCTION AND DELIVERY

- Identified specific items for improvising hydrogen analysis, as well as key issues as on cost of thermal versus thermal energy. Comment: In some solar thermal locations there may be a use for long scale oxygen, as in coal gasification processes for the production of liquid panels.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.0** for technology transfer and collaboration.

- They are providing valuable feedback to many different collaborators.
- They need to educate the DOE managers, so when the contract is over, the DOE managers will understand what is in H2A and why.
- Number of cases investigated (11) forces collaboration with multiple groups.
- Extensive collaboration with "customer" partner.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- Collaboration with researchers seems adequate.
- Future plans are obvious: continue analysis to complete full set of cases.
- Continue and refine to present project needs with partners. Said funding for HY 2009 is noted.

### **Strengths and weaknesses**

#### Strengths

- They are providing valuable feedback to the collaborators to make their H2A analysis more realistic.
- Use of H2A spreadsheet is fundamental to this project.
- Use of a single group to examine full set of STCH approaches ensures commonality of assumptions and validity of relative cost comparisons.
- Listing of "lessons learned" is good.

#### Weaknesses

- They need to make sure to capture all of the costs for operation and maintenance, diurnal operation, thermal storage (if used), and spent toxic material disposal.
- They need to work with the DOE managers to help the managers understand how to apply H2A to this area.
- Project scope (11 analyses) makes listing of technical and economic assumptions difficult in a poster format. However, presentation of \$/kg results without description of assumptions is weak.
- There are no descriptions of the various cases (other than their titles).

### **Specific recommendations and additions or deletions to the work scope**

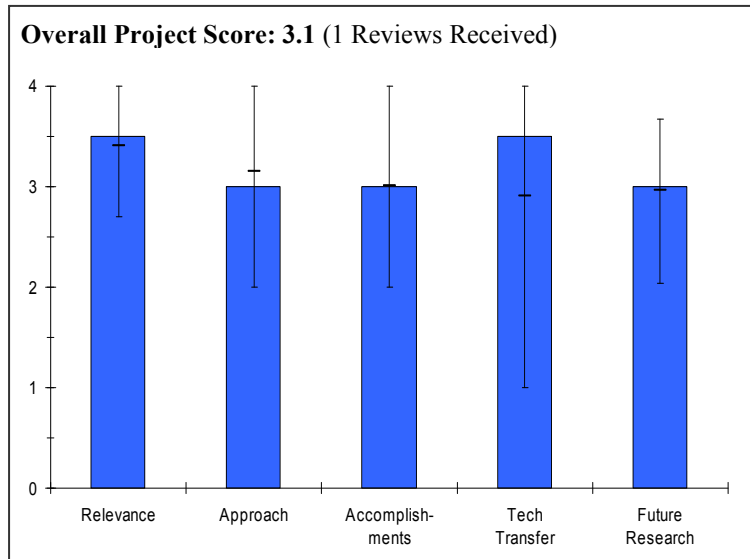
- None.

**Project # PDP-19: Ocean Thermal Plantships for Production of Ammonia as the Hydrogen Carrier**

*Chandrakant Panchal; ANL*

**Brief Summary of Project**

The objectives of this project are to evaluate the technical and economic viability of at-sea ocean thermal plantships for production ammonia as the hydrogen carrier to meet the HFCIT cost goal of \$2 to \$3/gge (delivered, untaxed, 2005\$ by 2015); and 2) evaluate the economic impact of co-production of desalinated water. The cost of ammonia as a fertilizer has been significantly impacted by natural gas prices. Ammonia can be an alternate fuel for distributed power generation (combustion turbine or internal combustion engines). Ocean thermal plantships deployed in the Gulf of Mexico can be a source of hydrogen for refineries in the Gulf of Mexico states.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- Economic analysis assumptions and results were presented clearly.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Project provides analysis of a new technology area for very little funding spent.
- Solid approach that incorporates relevant milestones and go/no-go decision points.
- Go/no-go decision point appeared to be based on funding and not on achieving a quantitative milestone, such as projected hydrogen cost, to show probability of technology success.
- It would have been beneficial to see a summary of comments provided by industrial participants at the September 11<sup>th</sup> workshop.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.5** for technology transfer and collaboration.

- Project is coordinating with multiple partners.
- Based on the presentation materials, the roles of each partner were not fully defined.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

## **PRODUCTION AND DELIVERY**

- Proposed future development and design work could come at a significant cost. It is unclear what the price tag would be for this work.
- Input on the possible technical challenges that would need to be overcome in future work would be helpful in assessing the likelihood of success of the technology.
- Future work is relevant to the proposed technology.

### **Strengths and weaknesses**

Strengths

Weaknesses

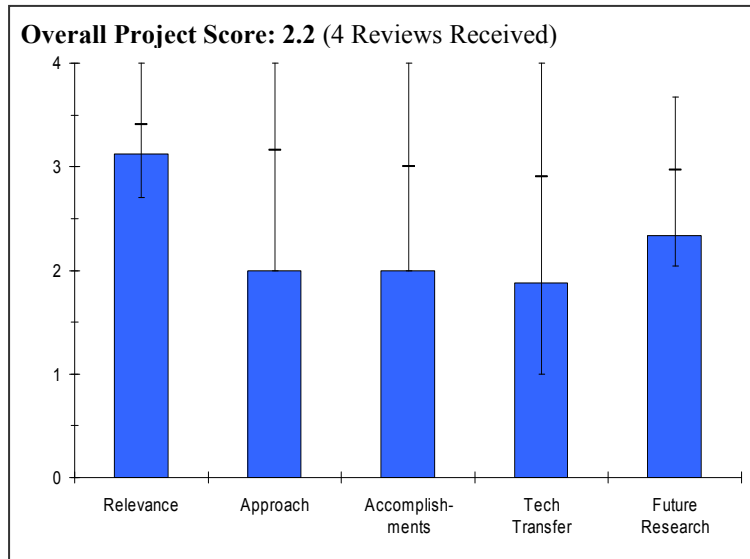
### **Specific recommendations and additions or deletions to the work scope**

**Project # PDP-21: Photoelectrochemical Hydrogen Production**

Malay Mazumber; U. Arkansas Little Rock

**Brief Summary of Project**

The overall objective of this project is to optimize surface properties of anodes for efficient photoelectrochemical (PEC) generation of hydrogen. The objectives of this project are to 1) use plasma surface engineering to control surface states for removing electron traps and improving photo-conversion efficiency; 2) use surface doping for interfacial photo-conversion for hydrogen generation with a minimal change in the bulk for improved durability; 3) correlate surface structures with light absorption and interfacial charge transfer; 4) measure photocurrent density for the test nano-structure TiO<sub>2</sub> electrodes against different bias voltages; and 5) perform comparative efficiency analysis for different photoanodes.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.1** for its relevance to DOE objectives.

- Hydrogen generation by PEC is critical to the presidents Hydrogen Fuel Initiative.
- The object of this project is to use plasma treatments to modify the surface of TiO<sub>2</sub> so that it will absorb more of the visible portion of the solar spectrum and split water. Researchers from around the globe have been working on this system for over 30 years and have achieved very little.
- This project attempts to use plasma treatment of TiO<sub>2</sub> to improve light absorption and photocurrent conversion efficiency.
- Improving semiconductor band gap, conversion process efficiency, and durability is consistent with the DOE goals and objectives.
- Project lacks comparison to DOE goals or system analysis to determine the likelihood that the results of the project will contribute to achievement of the DOE goals for PEC hydrogen production.
- This project supports the long term goal of cost effective renewable production of hydrogen.
- If a useful water photoelectrolysis system is the objective, TiO<sub>2</sub> will not work since its band gap is too large to be efficient. Fundamental science to help understand charge transfer or surface chemistry of oxide semiconductors will be useful but this project is mainly empirical.

**Question 2: Approach to performing the research and development**

This project was rated **2.0** on its approach.

- TiO<sub>2</sub> with little modification not novel.
- The PIs assert that plasma treatments provide a mechanism for creating TiO<sub>2</sub> alloys (e.g. w/ N) at the electrode surface, but there was little direct evidence that this has been accomplished. Also, the plasma is supposed to "remove contaminants" from the electrode surface, but under illumination the TiO<sub>2</sub> surface is self-cleaning.
- It is not clear that successful modification of TiO<sub>2</sub> properties will lead to achievement of the DOE goals.
- The project does not incorporate system design to produce hydrogen.
- Approach is focused on removing electron traps and improving photo-conversion efficiency of TiO<sub>2</sub> and improving durability, which are necessary for achieving DOE goals.

## PRODUCTION AND DELIVERY

- The study utilizes a well thought through systematic study of changes in photocurrent density due to varying anodized Ti samples prepared with and without plasma treatment using several different gases. Good use of XPS to monitor exchange of O<sub>2</sub> for N<sub>2</sub>.
- Adding N to TiO<sub>2</sub> to extend the spectral response will not improve performance since: 1) there is a limited solubility of N in TiO<sub>2</sub>, 2) it does not absorb much light, 3) it can act as a recombination center (not often reduced band gap response), and 4) it will be unstable to oxidation.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.0** based on accomplishments.

- Not clear that this will absorb visible light.
- So far, plasma treatment has had little or no effect on the ability of TiO<sub>2</sub> to absorb visible photons. There are many possible explanations for the observed increase in photocurrent for plasma-treated electrodes. Very little has been done to distinguish between these possibilities.
- The project has apparently not produced any hydrogen to date from the photocells.
- The project appears to have made progress in increasing the photocurrent density of TiO<sub>2</sub> photoanodes.
- The reduction of the band gap for TiO<sub>2</sub> from 3.32 down to 2.80 due to nitrogen doping provides encouragement that further improvements may be possible through further plasma treatment optimization.
- Much of what has been done was already in the literature 20-30 years ago.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **1.9** for technology transfer and collaboration.

- No industrial collaborations.
- While PIs assert that there is an "active partnership" with Univ. of Reno and Ark. Nanotech Center, it is not at all clear what this partnership entails.
- University of Nevada Reno is testing treated samples.
- There are no industry collaborators; thus, technology transfer is a weak point for this project. A systems engineer should be involved in the project to determine the likelihood that plasma treatment of TiO<sub>2</sub> will contribute to achievement of the DOE PEC hydrogen production goals.
- The Program has ongoing collaboration with University of Nevada Reno and Arkansas Nanotechnology Center.
- There appears to be good communication with other "earmark" projects.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.3** for proposed future work.

- So far, the research in this project has been highly empirical. Future work calls for optimizing the plasma treatment. But since the PI's do not know what the plasma actually does, there is little to optimize. Future work also mentions photocatalytic activity. It is unclear what this is about.
- Future research should include systems engineering as well as continued characterization and optimization of photoanodes.
- The next steps which include further optimization of plasma treatment and systematic study of the impacts of varying catalysts on photoconversion efficiency seem reasonable.
- Again, even perfecting a system based on TiO<sub>2</sub> or even "doped" (actually alloyed) with N will not produce a useful photoelectrolysis system.

### **Strengths and weaknesses**

#### Strengths

- The principal investigators have set-up a plasma treatment apparatus and a basic photo electrochemistry experiment.
- This project incorporates a seemingly novel approach to TiO<sub>2</sub> surface modification.

- The project supports achievement of DOE's targets for usable semiconductor band gap, chemical conversion process efficiency, and plant durability.
- Clearly demonstrated that there is a cumulative effect of reduced band gap and removal of contaminants.

Weaknesses

- TiO<sub>2</sub> has been studied for many years by many researchers without much promise as a successful PEC material.
- Many. The rationale for this project is weak and the principal investigators lack the instrumentation and experience to correctly interpret what they are doing.
- The project has not conducted systems engineering and analysis to determine the ultimate likelihood of success with respect to meeting the DOE targets.
- The project does not appear to be focused on improving hydrogen production capability, but only improving materials properties.
- Need to design experiments which will further differentiate the impact of reduced band gap versus removal of contaminants on photocurrent density.
- Not original, no new fundamental knowledge, and will not produce a useful device even if all problems with the system are solved.

Specific recommendations and additions or deletions to the work scope

- There is little reason to recommend continued funding for this project.
- Add an industrial partner to conduct systems engineering and analysis.



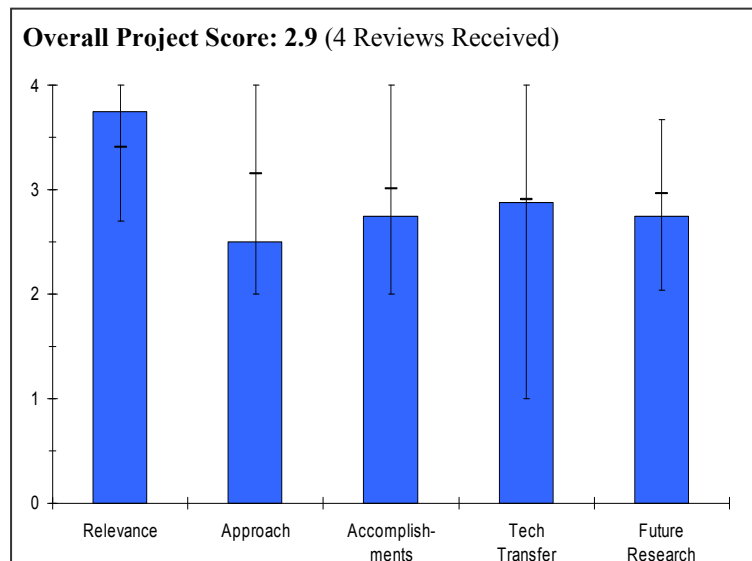
**Project # PDP-22: Distributed Reforming of Renewable Liquids via Water Splitting using Oxygen Transport Membrane (OTM)**

*Balu Balachandran; ANL*

**Brief Summary of Project**

The overall objective of this project is to develop a compact, dense, ceramic membrane reactor that enables efficient and cost-effective production of hydrogen by reforming bio-derived liquid fuels using pure oxygen formed by water splitting and transported by the membrane. The 2008 objective of this project is to optimize the performance of the oxygen transport membrane and demonstrate reforming of ethanol. Membrane technology provides the means to attack barriers to the development of small-scale hydrogen production technology.

**Question 1: Relevance to overall DOE objectives**



This project earned a score of **3.8** for its relevance to DOE objectives.

- Program is aimed at making hydrogen from renewable liquids, which is aligned with DOE's objective.
- Process under investigation is extremely unlikely to be economically competitive for hydrogen production.
- Oxygen transport membrane (OTM) materials are being developed for distributed reforming of renewable liquids via water splitting. Supports 2012 Targets.
- The Program helps to support the DOE objective of using renewable feedstocks (bio-derived liquids) to cost effectively generate hydrogen. Cost reduction goals may be obtained by combining the separation and purification step for oxygen transport to be used to process the bio-liquid. Further the use of one material eliminates concerns about thermal expansion/contraction so likely to add to cost reductions and system reliability. Additionally the  $PO_x$  system is an exothermic reaction so energy efficiencies may also be obtained.
- A potentially cost effective, renewable hydrogen process is very relevant to the overall objectives.

**Question 2: Approach to performing the research and development**

This project was rated **2.5** on its approach.

- I don't believe they have properly identified the barriers.
- Presenter indicated satisfaction with present performance, but cost numbers he provided suggest this performance fall short of capital targets.
- The approach to providing heat for this highly-endothermic reaction (using hot steam) is completely inadequate. A simple heat balance (took me five minutes) indicates that steam/feed ratios over 20 would be needed, and this is simply not competitive.
- Approach is sound and logical to complete objectives. Fuel is reformed using oxygen formed by water splitting and transported by the OTM. Hydrogen is produced on both sides of the OTM. Non-Galvanic. No electrical circuitry or power supply. Single material.
- Given that the project lost funding in 2007 a switch was made from processing natural gas to processing bio-derived liquids the Program is a bit behind but still making significant progress.
- Those working on the project are very experienced in developing transport membranes for other commercial applications and have a very well thought out plan for utilizing existing systems and building on that knowledge to produce more suitable membranes.

- Also initial efforts utilize chemical grade ethanol and builds on those learnings before assessing more challenging fuel grade ethanol.
- Material stability and durability are potential issues due to high temperature operation and presence of reduced and oxidative environments.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- Given the newness of the bio-liquids thrust, team has made good progress on proof of concept experiments.
- However, I don't believe they have a good grasp of the barriers related to flux and heat, and those barriers have been present even in the original configuration of the Program (for CH<sub>4</sub> reforming).
- Good progress has been made despite rapid shifting of work from methane.
- Given that funding was interrupted the progress in membrane fabrication to date is acceptable.
- Lack of actual conditions (no N<sub>2</sub> diluent) testing and extended testing of the OTM.
- Cost data are based on premature process conditions; need refinement/updates.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.9** for technology transfer and collaboration.

- Appears to have some good collaborations on materials.
- Collaboration is strong and effective. Related membrane R&D is sponsored by Fossil Energy-National Energy Technology Laboratory.
- Fossil Energy-National Energy Technology Laboratory is funding related membrane work at ANL; so potential for technology transfer for a variety of uses.
- Would be helpful to progress this to the point where private industry might have an interest.
- Collaborations with membrane developers and industry partners are needed.
- Have a third independent party such as DTI to conduct the cost analysis.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- Plans address certain issues, such as durability and performance at higher conversions and concentrations.
- Plans do not appear to address important barriers of flux and heat management (means to provide heat of reforming).
- Fiscal year 2008 work is proceeding well. The principal investigator is optimizing the performance of the oxygen transport membrane (OTM) and demonstrates reforming of ethanol (EtOH). Suggest Pt/Pd thin surface layer as catalyst be explored.
- More tests on membrane stability/durability will be conducted during fiscal year 2009.
- Longer test time and possibility of coking of membrane need to be addressed.
- The next step approaches are reasonable however a lot needs to be accomplished in 2008 including optimization of the membrane thickness and composition in order to get to the full system integration and demonstration phase of ethanol reforming. For instance there is a need to increase membrane flux while also minimizing membrane thickness, increasing porosity and finding the right reaction conditions.
- Again need to have third party to conduct techno-economic analysis of the process.

**Strengths and weaknesses**

Strengths

- Impressive ability to extrude OTM tubes, nice development of tube morphology to relieve surface limited transport.
- Out-year work well conceived and comprehensive.
- The greatest strength of the project is the experienced scientists who are undertaking the effort.

## PRODUCTION AND DELIVERY

### Weaknesses

- This technology has NO CHANCE of beating simple ethanol steam reforming (ESR).
- It has all the ancillaries of ESR (steam gen, shift, separation), plus a reactor that must be substantially more complex and expensive.
- The overall reaction has stoichiometry (heat and mass balance) that is identical to ethanol steam reforming. There is no justification to splitting the reaction into two parts using the membrane. Splitting the reaction with a membrane adds nothing but complexity and cost, reduces efficiency, and increases the challenge of providing heat of reaction.
- Lack of consistent funding.

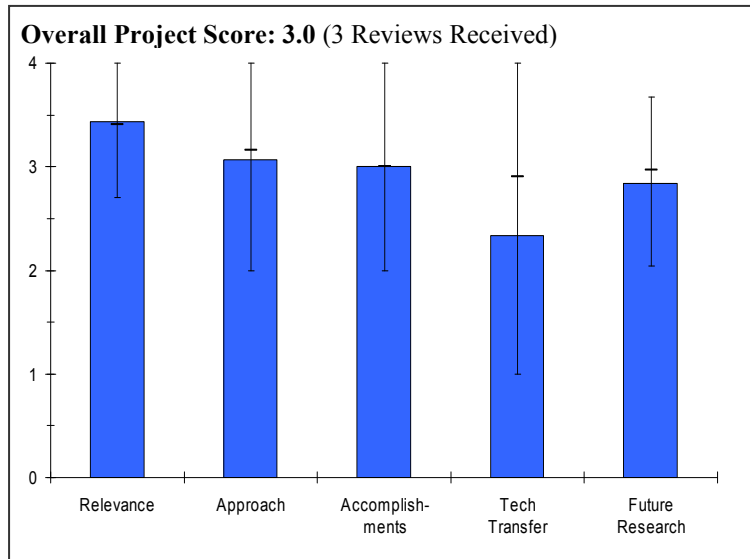
### Specific recommendations and additions or deletions to the work scope

- I am a fan of OTM's but this embodiment makes no sense to me.
- I would delete the entire scope of this project.

**Project # PDP-25: Carbon Molecular Sieve Membrane as Reactor/Separator for Water Gas Shift Reaction**  
*Paul Liu; Media and Process Technology Inc.*

**Brief Summary of Project**

The objectives of this project are to 1) evaluate a membrane reactor system using existing membranes and catalysts via math simulation; 2) validate membrane and membrane reactor performance and economics; 3) prepare membranes, module and housing for pilot-scale testing; 4) perform pilot scale testing and demonstration; 5) perform economic analysis and technical evaluation; 6) prepare field testing; 7) fabricate membranes and membrane reactors and prepare catalysts; 8) prepare site and install reactor; 9) perform field test; 10) conduct system integration study; and 11) finalize economic analysis and refine performance simulation.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.4** for its relevance to DOE objectives.

- This projects uses (what could be) low cost methods to purify hydrogen for direct stationary PEM systems, or potentially distributed hydrogen production.
- The degree of relevance depends upon comparison with existing technologies, such as PSA.
- A low cost combination water-gas shift (WGS) and membrane unit would be a significant step towards research and development objectives.
- The project focuses on meeting the DOE hydrogen production efficiency and cost goals by combining the LTS and HTS reactions into one and by combining hydrogen purification and separation.

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- Project uses LTS, membrane separation, followed by regenerable sorption step to purify hydrogen.
- Approach is fundamentally sound but is made difficult to evaluate due in inadequate description of inner device workings.
- The elimination of the extra WGS step and the reduction in PSA beds through use of the HICON process appears to be an approach that will lead to substantial cost reductions and improved efficiency but we still have to wait for the testing of the complete system to know if this is really the case.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- They modeled hydrogen recovery and hydrogen purity.
- PDU unit was being assembled.
- Preliminary H2A analysis was performed.
- Experimental demonstration of Temperature Swing Adsorption (TSA) is good, but would be improved by demonstration at actual expected operating conditions.

## PRODUCTION AND DELIVERY

- They have analytically shown 90 percent hydrogen recovery at 99 percent purity. Experimental verification is now needed.
- The bench tests of their WGS/MR show that 99.999 percent hydrogen can be produced with 80 percent recovery.
- Elimination of the high temperature shift will help reduce costs and improve efficiency. Still remains to be seen if the efficiency, purity and cost targets can be met once the pilot and field units are assembled and tested.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.3** for technology transfer and collaboration.

- Collaborations with the University of Southern California, Chevron, and Johnson Matthey.
- Unclear what role the partners play and have played (Johnson Matthey is a partner, but stated no catalyst development).
- Little interaction cited.
- Still unclear what the role of Chevron is in this partnership. Do they see this as a viable process?
- What contributions to the project have been made by Johnson Matthey or Chevron?

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- Project formally ended June 2007, with no cost extension.
- Remainder of project completes the on-going work and demonstrates the technical approach.
- Pilot scale testing and verification of entire process, as they have a plan to do, is the key next step.
- Further economic analysis is necessary: current analysis is weak.
- It looks like the Program will come to an end this year; hence, I am not sure if they will be able to build the pilot and field unit and do sufficient testing and incorporate learnings to produce an optimized system.
- The same concern remains for the H2A analysis; will reliable numbers be generated with out a fully optimized system?

### **Strengths and weaknesses**

#### Strengths

- Interesting hydrogen purification train for a fuel processing system.
- WGS via a carbon coated membrane is innovative and appears to achieve excellent WGS conversion.
- Modeling appears to achieve low cost and high efficiency.
- Concept of linking a membrane/WGS with a TSA to achieve high CO conversion and very high net hydrogen recovery is clever and sound.
- While membrane unit only achieves 99.5 percent hydrogen purity and thus requires a second purification device (TSA), their argument that all membrane systems (even metal membranes) will require a secondary "guard bed" purifier has some merit. Thus their system is not truly penalized for having a TSA since other system also will have one.
- Tubes (on a ceramic support) are relatively inexpensive, taking some of the burden out of their required high tube surface area.
- Looks like some good collaborative partners; Johnson Matthey, Chevron, and USC.

#### Weaknesses

- The adsorption 'polishing' step needs careful analysis, especially to understand removal of species such as H<sub>2</sub>S to the low concentrations needed for PEM.
- Adsorption step durability needs to be understood and demonstrated especially for gas constituents such as sulfur.
- Inner workings of their unit are poorly/inadequately described.
- Unit has low hydrogen permeance leading to high-required surface area.

- Process flow diagram and heat integration inadequately described. Not clear that unit has sufficient waste heat for SMR endotherm.
- Since you did not do any catalyst development, I am unclear of the role of Johnson Matthey.
- What is the role of Chevron?

**Specific recommendations and additions or deletions to the work scope**

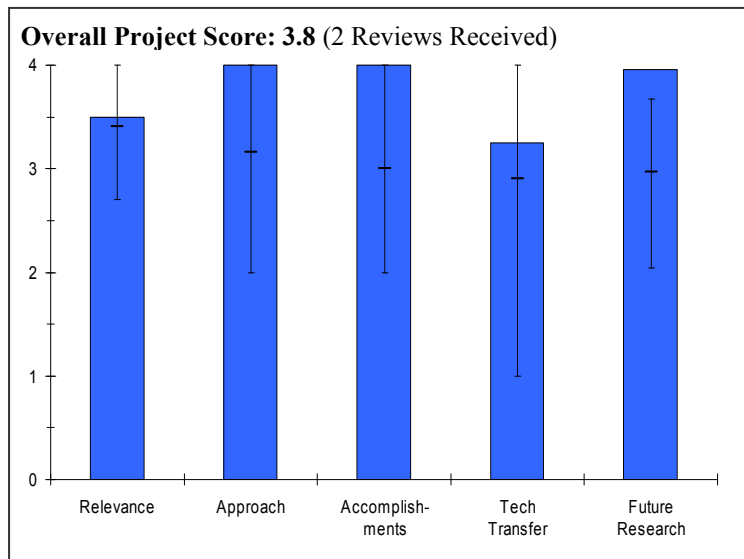
- Hydrogen purity analysis needs to measure low-level impurities (H<sub>2</sub>S).
- Ninety percent hydrogen recovery seems low to have a high overall hydrogen production efficiency.
- They need to experimentally demonstrate the modeled 90 percent hydrogen recovery and 99 percent purity.
- Economic analysis needs to be completed.

**Project # PDP-26: Biological Systems for Hydrogen Photoproduction**

*Maria Ghirardi; NREL*

**Brief Summary of Project**

The overall objective of this project is to generate an algal strain capable of efficiently producing hydrogen gas from water under atmospheric oxygen concentrations. This goal is pursued by 1) molecular engineering of the algal hydrogenase to limit oxygen access to its catalytic site, and 2) development of a system that induces culture anaerobiosis and hydrogen production by means of a physiological switch. In addition, NREL is working with other research organizations to develop a system where several biological hydrogen production are integrated into one efficient system. .



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- High priority for the green algae work.
- Highly innovative to bring in photosynthetic bacteria.
- The project goal of optimizing photosynthetic water-splitting biological hydrogen production is well-aligned with program goals for engineering improved biological hydrogen production systems.
- The project goal of increasing catalyst stability and improving oxygen tolerance is also well-aligned with program goals for engineering improved biological hydrogen production systems.

**Question 2: Approach to performing the research and development**

This project was rated **4.0** on its approach.

- Excellent, cutting edge, molecular and physiological approach.
- The catalyst engineering strategy seems straightforward and feasible, using well-tested site-directed mutagenesis techniques.
- The use of molecular simulations to aid in catalyst re-engineering is appropriate.
- The use of alginate immobilization strategies is a good combination of biological and materials expertise.
- The fermentation and hydrogen production strategies are appropriate.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **4.0** based on accomplishments.

- Virtually all aspects had been taken to the next level. Very impressive.
- The progress towards goals was very good on this project that has only recently secured robust funding.
- The progress on specific milestones is excellent, with most of them on schedule.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- This is truly a team effort with each member bringing unique attributes and experience.
- The partnership between various universities, an international institution, and a national lab is good.
- The specific mechanisms for coordination between all project partners are not clearly described, although the specific tasks are.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **4.0** for proposed future work.

- Well thought out.
- The problem in that there are many avenues to go down, and the principal investigator may need to focus in the next area.
- Future tasks are well-defined.
- Future plans to finish reporter gene construction and optimize heterologous hydrogenase expression levels are logical.
- Future plans to improve and stabilize the alginate films are good.
- Future plans to optimize fermentation and performance of different photosynthetic cultures in the stacked bioreactors are logical and systematic.

**Strengths and weaknesses**

Strengths

- Robust molecular and biological approaches, plenty of strengths on the aspects of enzyme and cellular hydrogen production.
- The investigators' prior record of collaboration is very strong.
- The investigators have demonstrated expertise in the study of hydrogenase enzymes and biophotolytic hydrogen production.
- The project team expertise is balanced and complementary.
- The ability of the investigators to leverage off other federal funding is an advantage.

Weaknesses

- Only that there are perhaps too many aspects and focus may be needed.
- The project plan is somewhat diffuse, and it is difficult to determine the necessary sequence of milestones for individual subtasks against the project whole. For example, how does testing of natural samples link to optimizing hydrogen production in heterologous systems?
- The contingency plan for possible failure of heterologous expression is not well-defined.

**Specific recommendations and additions or deletions to the work scope**

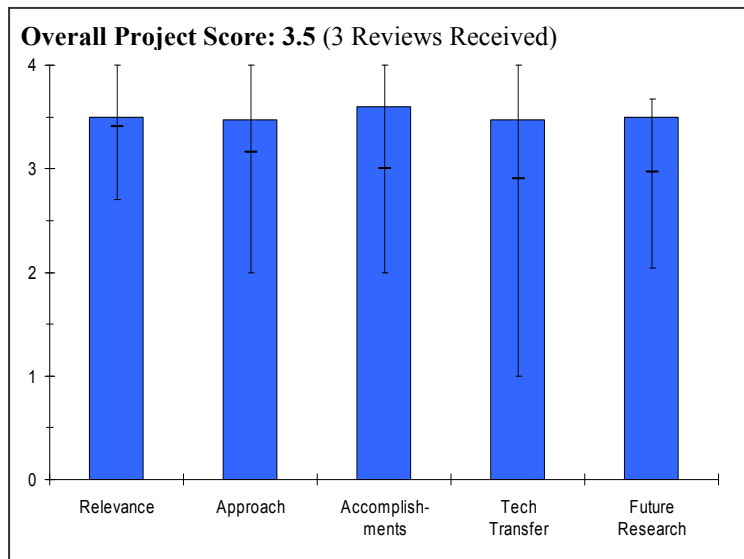


**Project # PDP-27: Fermentative and Electrohydrogenic Approaches to Hydrogen Production**

*Pin-Ching Maness; NREL*

**Brief Summary of Project**

The long-term objective of this project is to develop direct fermentation technologies to convert renewable lignocellulosic biomass resources to hydrogen. The near-term objectives of this project are to 1) optimize bioreactor performance for the cellulose-degrading bacterium *Clostridium thermocellum*; 2) identify key metabolic pathways to guide generic engineering to improve hydrogen molar yield; and 3) integrate microbial electrolysis cell (formerly BEAMR: bio-electrochemically assisted microbial reactor) process to improve hydrogen molar yield.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- The project goals are well-aligned with DOE program targets for maximizing efficiency of biologically-derived hydrogen production via fermentation and electrohydrogenesis.
- The focus on *Clostridium thermocellum* is good.
- The combination of fermentation and electrohydrogenesis is innovative.
- Very relevant to overall hydrogen.
- High relevance along the lines of biological hydrogen.

**Question 2: Approach to performing the research and development**

This project was rated **3.5** on its approach.

- The cell growth optimization approach using bioreactors and defined cellulosic substrates is appropriate.
- The pathway inhibition and flux redirection approach is appropriate.
- The microbial electrolysis cell design using optimized fermentation cultures is good.
- Very good approach, particularly the inhibitors, but the approach needs to be complimented by genomics and genetic-based technique, possibly through collaborations.
- Logical and replicable.
- High applicability, pertinent to current biological /energy issues, easy to adapt to current technologies, without much infrastructure changes.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.6** based on accomplishments.

- The progress towards goals was excellent, with pathway engineering targets achieved ahead of schedule.
- The demonstration of robust hydrogen production from corn stover substrates is good.
- The progress has been excellent given the delay in project start.
- Very good progress, particularly with the collaboration to use the bioreactor to utilize non-hydrogen products.
- The microbial energy cell is a brilliant adaptation.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.5** for technology transfer and collaboration.

- The partnership between a university and national lab is good, although any explicit synergy for tech transfer to Bruce Logan's business venture, Ion Power, is not described.
- The new interactions with the University of Manitoba are excellent and add desired project expertise in microbial physiology and pathway engineering.
- The Logan collaboration is outstanding.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.5** for proposed future work.

- Future tasks for each partner institution are well-defined.
- Future plans to scale up fermentation are logical.
- The goal of testing biomass fermentation waste in the MFC/MEC device is logical.
- The future of this project must include molecular and genetic approaches, possibly as outside collaborations.
- A clear plan has been stated.

**Strengths and weaknesses**

Strengths

- The investigators' expertise in microbial fuel cells is excellent.
- The investigators have demonstrated superior progress towards defined goals.
- The investigators have demonstrated expertise in fermentation testing and quantification.
- The organism is a mainstay of any cellulosic based system and this research will be very valuable.
- Harnessing biological forces will prove themselves in the years to come as overhead costs increase.

Weaknesses

- There is not a well-described, logical plan to test inhibitors in a systematic way to continue optimization of metabolic pathway flow; this is especially apparent in the plan to test combinations of inhibitors.
- The development of genetic methods for pathway engineering is not described, although the inclusion of the expert collaborator from the University of Manitoba adds necessary expertise.
- The workflow for testing of specific components to the MEC device is not clearly laid out.
- The techniques for metabolite determination have not been clearly described, and the investigators have no prior demonstrated expertise with this experimental component.
- Genetics and DNA arrays need to be applied.
- Need a full scale demonstration or early adopter soon.

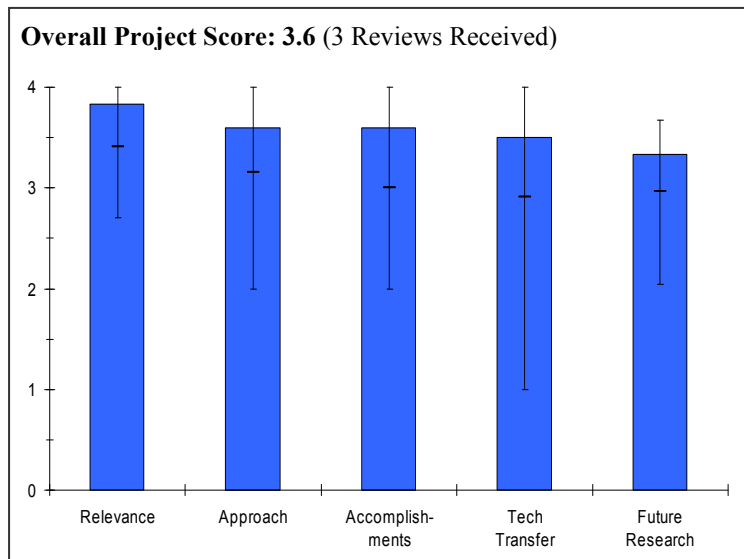
**Specific recommendations and additions or deletions to the work scope**

**Project # PDP-34: Theory of Oxides for Photoelectrochemical Hydrogen Production**

*John Turner; NREL*

**Brief Summary of Project**

The objective of this project is to discover and characterize a semiconductor material set or device configuration that 1) splits water into hydrogen and oxygen spontaneously upon illumination; 2) has solar-to-hydrogen efficiency of at least 5% with a clear pathway to a 10% water splitting system; 3) exhibits the possibility of 10 years stability under solar conditions; and 4) can be adapted to volume-manufacturing techniques. The main objective for the past year has been to develop and optimize state-of-the-art materials that we have identified as promising for meeting the Department of Energy’s near-term efficiency and durability targets and to develop PEC modeling and analysis efforts.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.8** for its relevance to DOE objectives.

- An important demonstration of how a clever mix of theory and experiment can be used to design new multi-element semiconductors that move toward the DOE goals for an effective solar water splitter.
- While the work presented here is a nice proof of concept with regard to the experimental approach, it has not, at this point, provided a next generation semiconductor that advances the DOE specs in the area of photoelectrochemistry.
- Finding new materials with improved properties is critical for photoelectrochemical water splitting. This project examines novel materials, not the same materials (e.g. TiO<sub>2</sub>) that researchers have looked at for decades.
- Very important "background" project because such theoretical approaches will reduce costs and time for experimental work.
- Once such theories are better correlated to experiments., more such number-crunching pre-work will enable resource use in DOE.
- There is an increasing need to apply modern theoretical approaches to materials that are useful for photoelectrolysis of water.

**Question 2: Approach to performing the research and development**

This project was rated **3.6** on its approach.

- This project optimizes the beneficial interactions of quantum theory and laboratory experiment.
- A novel semiconductor material is predicted that would not normally be considered. Synthesis of the theoretically predicted system demonstrates that the theoretical predictions are solid.
- The work clearly demonstrates that the search for improved optical response semiconductors that are thermodynamically able to split water can be dramatically enhanced by using a DFT based materials search.
- The approach is demonstrated to provide an important new avenue to discovery materials that have not been experimentally accessible over the past 30 years of PEC research.
- The attempt to shed theoretical light on the materials discovered by Parkinson's combinatorial approach is especially interesting.

- Very solid and clear explanation by the poster presenter (actually, having the poster presenter is essential to the success of this poster - which actually merits an oral presentation!)
- DFT approaches coupled with combinatorics (e.g., in the ternary oxides) led to very persuasive conclusions - kudos!
- Isovalent substitution in the Zn-O: N case - inspired.
- Uses state of the art computational methods to explain the behavior of existing materials and to provide guidance for new materials to test for photoelectrolysis activity.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.6** based on accomplishments.

- All technical components are in place and demonstrated.
- A new alloy type semiconductor photoelectrode material has been theoretically identified and demonstrated to have the predicted properties.
- All project goals are being met in a timely manner.
- No real breakthroughs yet, but the project provided some valuable insight into several complex materials.
- Clearly excellent; but the proof of the pudding, correlation with experimental data, would be a crowning achievement.
- The examples show value of this theoretical predictive tool!
- However, is there a tool to go beyond the "band engineering"? Is there a tool to hint at current magnitudes?
- Has been very productive since many systems have been calculated and understood.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.5** for technology transfer and collaboration.

- The principal investigators have established useful collaborations with several experimental groups.
- Internal NREL collaborations (theoreticians and experimentalists) are evident; but were there external collaborations?
- Any reach-out to other photo-chemistry interests in other institutions? Purdue? CIT?
- Has worked well with experimentalists providing feedback on known materials and guidance on new materials.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.3** for proposed future work.

- Systems of potential interest have been identified.
- Computational analyses are being initiated.
- All selected targets are interesting systems that should be pursued.
- This is a well-designed study that is correctly focused and effective.
- The PIs did propose some new systems to examine, but these choices appear to be ad-hoc.
- Good, logical, extensions to experimental projects.
- Not clear as to whether the theoretical structures are readily fabricable or economically manufactured.
- What about stability or meta-stability of the predicted structures?
- Will continue to investigate interesting systems and provide insight into other possible systems that may be the "holy grail" of photoelectrolysis.

**Strengths and weaknesses**

Strengths

- Researchers have an excellent track record.
- The present study is well constructed and fruitful.
- New, highly complex materials having optimized photoelectrochemical properties are being identified.

## PRODUCTION AND DELIVERY

- Developing meaningful and ongoing dialog between theoretical and experimental approaches to discovering materials with improved properties.
- Excellent use of the DFT approximations in developing the ternary oxides and the differentiation between the super-lattice structures and the random alloys.
- Good correlations (albeit only a few) between theory and experiment.
- High quality theoretical work and very productive.

### Weaknesses

- NONE.
- None really because this is pioneering work in developing a predictive tool for new studies.
- Not enough computation resources available.

### Specific recommendations and additions or deletions to the work scope

- Continue as is.
- Key to this project is having collaborations with experimental groups that can test the theoretical predictions.
- Fund this work to do more band-engineering work!
- Fund the reduction to practice to quickly decide whether the current obtained from these novel studies could be "practical" for scale-up.
- Provide more computation resources.

## 2008

# Hydrogen Storage

### Summary of Annual Merit Review Hydrogen Storage Subprogram

#### **Summary of Reviewer Comments on Hydrogen Storage Subprogram:**

Reviewers stated that the Hydrogen Storage subprogram was well managed with a robust and diverse R&D portfolio. The storage program is sharply focused on technical targets and milestones. DOE acknowledged that progress towards volumetric capacity targets has lagged progress towards gravimetric capacity. The portfolio has benefitted from the down-selection of different storage technologies. It is recognized that on-board vehicular storage is a technically difficult application and that future strategic revisions and additional down-select points will be required. The reviewers stressed that DOE should continue to direct the researchers to emphasize all material performance attributes and cost and not solely gravimetric capacity. Reviewers recommended that DOE continue to periodically assess the funding allocation of the portfolio based upon the potential to meet on-board vehicle requirements.

Some reviewers rated the DOE storage subprogram as “outstanding.” The materials-based centers of excellence (CoEs) were assessed to be well-managed and organized. For the CoEs, it is important to continue to ensure transparency in the methods of operation and management (e.g. structure, decision process, communication flow and synergy among the sub-program areas, and intellectual property management). It is critical that the CoEs have mechanisms to share experiences and lessons learned particularly on cross-cutting issues across the DOE portfolio. The reviewers encouraged strong interactions among the CoEs and closer collaborations to stress commonalities, avoid duplication of efforts and optimize use of resources. These collaborations among the materials CoEs will also need to be extended to the new Hydrogen Storage Engineering Center of Excellence, which will start in FY 2009.

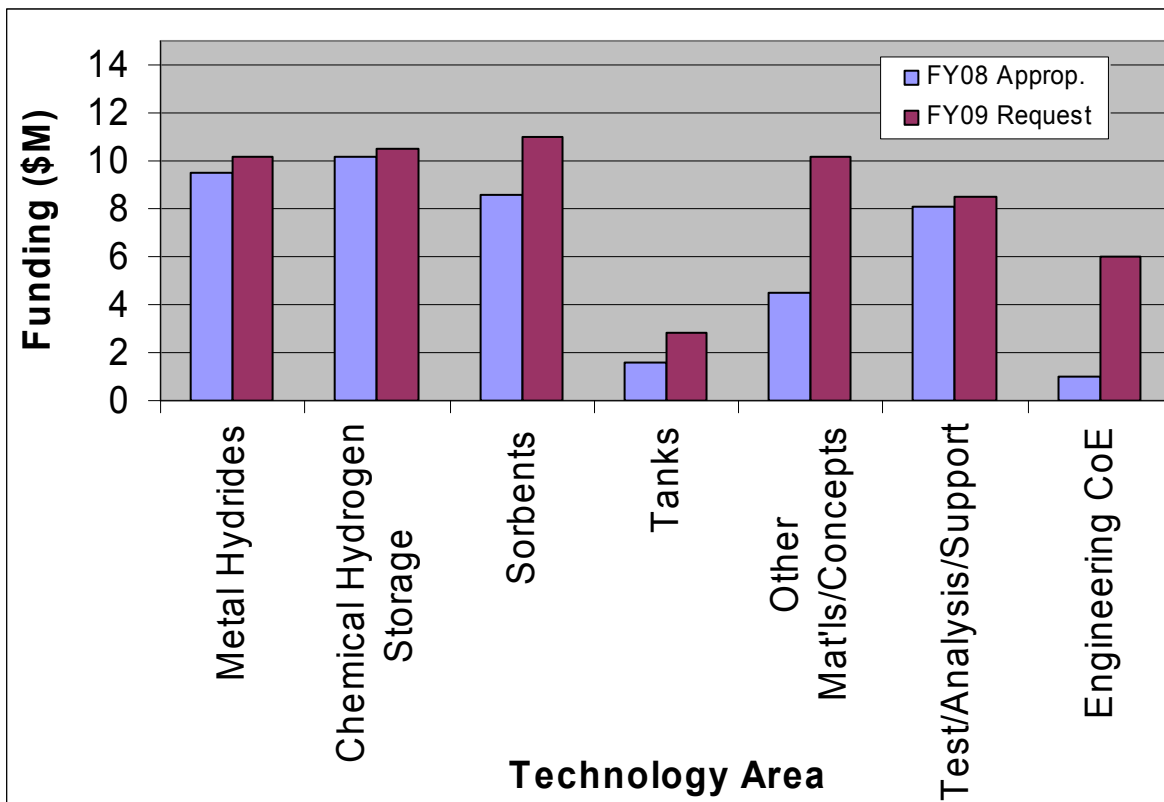
Finally, the reviewers identified hydrogen storage as “part of a long-term national research portfolio.” The program was encouraged to continue its “lessons-learned” efforts, both technical and strategic, to contribute towards a “self-critical analysis of the effectiveness, progress, and the methodology for future program portfolio design.” The reviewers recommended that DOE include in its portfolio strategy, consideration of the impact of scenarios where material(s) solutions are not found to meet the application’s requirements. The reviewers suggested that DOE consider future funding scenarios that increase emphasis of approaches using high-pressure cold hydrogen or cryogenic hydrogen. Changes in the portfolio may be required to close the gaps of performance and cost requirements of using these physical approaches.

#### **Hydrogen Storage Funding by Technology:**

The funding portfolio for hydrogen storage addresses primarily long-term materials based R&D for on-board transportation applications. The EERE applied hydrogen storage program’s goal continues to be developing and demonstrating commercially-viable hydrogen storage technology that enables greater than 300-mile vehicle driving range, while meeting safety, vehicular packaging, cost and performance requirements. The requested EERE FY2009 funding profile, which includes the materials-focused CoEs, the new Hydrogen Storage Engineering CoE and independent projects, continues to address the National Academies’ and FreedomCAR and Fuel Partnership’s recommendations. As mentioned above, plans for FY 2009 (subject to congressional appropriations and direction) include initiating the new Hydrogen Storage Engineering CoE to address on-board engineering R&D needs and system issues, as recommended by reviewers and stakeholders. The storage subprogram also plans to continue its annual solicitation process to allow flexibility in eliciting new concepts and approaches that may not be in the

## HYDROGEN STORAGE

current portfolio. A key milestone for FY2009 will be to conduct a down-select decision on sorbent materials under study in the portfolio. The chart below illustrates the appropriated funding in FY2008 for each major activity along with planned funding in FY2009 based on the Program's budget request.



### **Majority of Reviewer Comments and Recommendations:**

#### **Chemical Hydrogen Storage:**

The chemical hydrogen storage R&D is conducted with a well-balanced approach, considering both material aspects and engineering issues, with good coupling between theoretical modeling and experimental activities. The reviewers suggested that the theory work be refined and validated with input from experimentalists. The chemical hydride R&D has made good progress toward addressing issues related to ammonia borane (AB) by reducing foaming and release temperature, as well as significantly increasing the kinetics for the release of the second equivalent of hydrogen from AB. Continued R&D is required to further improve these AB release parameters as well as addressing heterogeneous catalysis, liquid fuel formulation, and cost effective first fill. Reviewers noted heavy focus on ammonia borane. R&D has diversified to metal-boron-nitrogen materials. Significant progress was made in regenerating ammonia borane from spent fuel. It is recommended that future work incorporate cost analysis to assess AB regeneration schemes. The Chemical Hydrogen Storage Center of Excellence's (CHSCoE) down-select process and criteria were well received and 50% of the materials were discontinued as a result of the down-select process. It was recognized that the CHSCoE is a well coordinated group of quality researchers who understand the challenges related to chemical hydrogen storage materials and are focused on relevant research to the Hydrogen Storage Program.

**Sorbent-based Materials:**

The overall goal of sorbent materials applied research is to develop materials that will store hydrogen at close to ambient temperature and at moderate pressure. Very promising results in near room temperature hydrogen storage were presented that build upon R. Yang's work at the University of Michigan on materials that use a hydrogen spillover mechanism. This technique has expanded within the DOE portfolio and internationally. Issues remain to be explored include synthesis reproducibility, net available capacity, and hydrogen uptake and discharge kinetics. The reviewers recommended that this area of research be expanded to address these issues. The majority of reviewers emphasized the need to understand the system implications of the use of cryogenic (e.g. 77K) sorbents, and to continue to emphasize estimation of "net available" volumetric and gravimetric capacity, hydrogen uptake/discharge kinetics and durability. The reviewers suggested that theory work be refined and validated with input from the experimentalists to establish simulation models that best represent the experimental systems under study. It was recognized that the Hydrogen Sorption Center of Excellence is leveraging its partners' capabilities to expand its focus beyond carbon-only materials. The reviewers recommended that the portfolio be periodically reviewed to ensure that the projects emphasize vehicle application performance issues.

**Advanced Metal Hydrides:**

The overall goal of metal hydride materials applied research is to develop materials that can be charged with hydrogen on-board the vehicle at conditions amenable to the vehicle environment. Key barriers to this goal are the hydrogen charge and discharge kinetics at acceptable temperatures and pressures and the thermodynamics of the reactions which directly impact the net available capacity of the material. Since most of these materials may be embodied in a system as a packed powder, volumetric capacity of the material is also an issue. The Metal Hydride Center of Excellence (MHCoe) was considered by the reviewers to be a well coordinated group of quality researchers focused on relevant research to the Hydrogen Storage Program. The reviewers were in favor of the materials down-selection performed by the MHCoe and the flexibility demonstrated by the MHCoe in rescoping the engineering effort with the upcoming establishment of the Hydrogen Storage Engineering Center of Excellence. The computational modeling effort was also praised for the improvements and advances in methodology made over the past year, however it was recognized that more potential products, such as hydrocarbons, need to be included in the modeling database. It was recommended that the MHCoe and DOE continue to assess the viability of materials being investigated and minimize efforts on those that are not reversible under practical conditions.

**Tanks:**

Tank projects were not reviewed in FY2008. Reviewer comments on the validation of the cryo-compressed hydrogen storage tank project (Lawrence Livermore National Laboratory) are presented in the Technology Validation subprogram of this report.

**Testing, Material Reactivity, Analysis:**

These topics were considered critical to the overall subprogram and will be continued as planned. The new project to document best practices in the measurement of hydrogen storage materials was commended by the majority of reviewers. The area of materials' chemical and environmental reactivity R&D (a project under the International Partnership for the Hydrogen Economy) was also commended and will be strengthened, with increased coordination among the materials CoEs, engineering CoE and independent projects. The two storage systems analysis projects by TIAX and Argonne National Lab were rated highly. Further refinement of assumptions, continued coordination among stakeholders and developers, and validation of models were considered essential.



### Note on Storage Report Structure:

#### **Chemical Hydrogen Storage**

ST-4 to 11 are partners of the Chemical Hydrogen CoE.

STP-5 is an independent project

#### **Sorbent-based Materials**

ST-15 to 25 and STP-6, STP-8 and STP-11 are partners of the Hydrogen Sorption CoE.

ST-13, STP-28 and STP-29 are independent projects

#### **Advanced Metal Hydrides**

ST-29 to 39 and STP-16, STP-18 to 21 are partners of the Metal Hydride CoE.

ST-14 and STP-24 are independent projects

#### **Other New Materials and Concepts**

ST-12, ST-26, ST-27, STP-26 and STP-27

#### **Testing, Safety and Analysis**

ST-1 to 3 and ST-40 to 42

#### **Cross-Cutting**

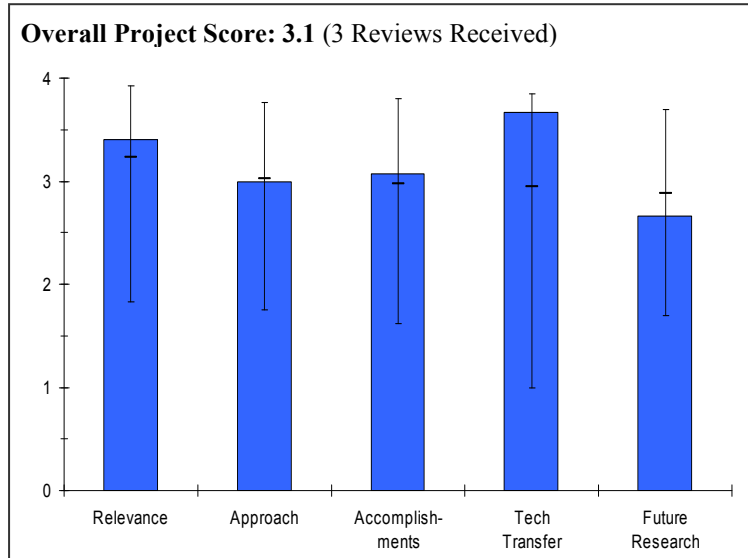
STP-4 and STP 32 to 34

**Project # ST-01: Analyses of Hydrogen Storage Materials and On-Board Systems***Stephen Lasher; TIAX LLC*

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

TIAX is evaluating the projected manufactured cost and performance of several on-board hydrogen storage options: baseline (compressed hydrogen), liquid and cryo-compressed hydrogen, reversible on-board (e.g., metal hydrides, high surface area sorbents/carbon-based materials), and regenerable off-board (e.g., chemical hydrogen storage). System-level conceptual designs, process models, activities-based cost models, and lifecycle performance/cost predictions are being developed for each system based on developers' on-going research, input from DOE and key stakeholders, in-house experience, and input from material and component experts. This is an on-going and iterative process so that DOE and its contractors can increasingly focus their efforts on the most promising technology options.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.4** for its relevance to DOE objectives.

- The project is expected to provide DOE and developers guidance by evaluating the status of various on-board storage options, and is therefore highly relevant to overall DOE RD&D objectives.
- On-board storage technology is well known to be one of the challenging areas that must have breakthrough technology to meet its targets. This project is supplying important cost and performance analyses of the various storage technology approaches being researched. It is imperative to have these analyses to help guide the overall storage program.
- The project is highly relevant to the DOE Hydrogen Program objectives. It is providing an early indication of the cost and efficiency of various hydrogen storage technologies.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- The approach used appears to be adequate.
- The overall approach to this analysis effort is excellent. Careful and state-of-the-art in-depth analysis of the systems is being done resulting in excellent cost and performance information.
- The overall objective of the project includes both on-board and upstream systems. This is very important. Unfortunately only recent on-board results were presented. This can be misleading without discussing the upstream system costs and performance as well.
- The project includes analyzing all the critical cost and performance measures for on-board systems as well as the upstream system needs. It is very important to have complete well-to-tank cost, energy efficiencies, and greenhouse gas emissions for good decision making concerning on-board storage system research directions.
- There appears to be good collaboration between this project and the other relevant projects in the storage and hydrogen delivery program. It is important that this is maintained and possibly further strengthened.
- It is important that all the performance issues of the on-board systems are included in the overall analysis comparisons. For example, standard liquid hydrogen tanks will have boil-off issues and the full hydrogen

charge will not be available for use by the fuel cell. Comparing ~10 kg cryo-compressed and liquid hydrogen systems with ~5 kg high pressure gas or other storage technologies is not really an “apples-to-apples” comparison. Issues such as these were mentioned but only appear as footnotes in the presentation.

- The approach is based on established methods for estimating high rate manufacturing costs. It appears to have been generally accepted by the developers who also have provided input to the assumptions and manufacturing processes assumed in the analysis.
- The methods have been validated for some commercial type products but applying the methods for high rate manufacturing of storage materials and systems that have not been developed into viable systems are more speculative.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- None of the on-board storage systems evaluated in this project meet the 2010 volume target based on their assumptions. However, the project identifies the dominant contributions to the overall costs, which will help developers to concentrate their efforts in these key areas in the initial developing stage.
- Considering the funding that has been made available by DOE, the project has made considerable progress this past year.
- With somewhat better collaboration between this project and some of the other storage and delivery projects, there could have been more accomplished relative to analysis of the other on-board storage systems being researched.
- Progress appears to be reasonable; refining compressed H<sub>2</sub> designs and cost estimates is worthwhile as is the first formalized look at cryo-compressed systems. Not sure what benefit was derived from the sodium borohydride update.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.7** for technology transfer and collaboration.

- The research team attempted to incorporate the latest developments in hydrogen research from various centers.
- This project has made a considerable effort to collaborate with other storage and delivery projects and to present the results of its efforts for the benefit of these other projects. Even more effort to disseminate the results to the broader hydrogen community of stakeholders and to have even more in depth discussions with key projects in the storage and delivery program would be very helpful.
- Collaboration with other organizations is very good. The developers of a particular material/system have provided input to TIAX to enable a model system to be defined and costed. ANL provides a model system analysis and design that accounts for reaction kinetics, thermodynamics, and heat transfer.
- Several other organizations have reviewed the results of the analysis and assumptions.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.7** for proposed future work.

- The planned research is on-course. However, how realistic these analyses are will strongly depend on the overall economy.
- In addition to the liquid hydrocarbon and ammonia borane systems, it is very important to begin the analysis of the promising adsorption based systems such as metal organic frameworks.
- This effort should continue full well-to-tank analyses and include not only cost and performance issues but also energy efficiency and greenhouse gas emissions.
- The presentation materials did not indicate what analyses will be conducted next year.

**Strengths and weaknesses****Strengths**

- On-board storage technology is well known to be one of the challenging areas that must have breakthrough technology to meet its targets. This project is supplying important cost and performance analyses of the various storage technology approaches being researched. It is imperative to have these analyses to help guide the overall storage program.
- The overall approach to this analysis effort is excellent. Careful and state-of-the-art in-depth analysis of the systems is being done resulting in excellent cost and performance information.
- The methods used for cost estimating have been validated with reference to established commercial products.

**Weaknesses**

- Only recent on-board results were presented. This can be misleading without the upstream system costs and performance as well.
- It is important to do these analyses on a well-to-tank basis which is being done. However only system cost and performance is being analyzed. Energy efficiency and greenhouse gas emissions also need to be included. [DOE clarification: The analyses to estimate energy efficiency and greenhouse gas emissions are conducted by ANL. See project ST-02.]
- Because materials-based storage systems are not currently manufactured at high rates, the systems configuration and manufacturing processes are not well defined. Thus the analyses are preliminary.

**Specific recommendations and additions or deletions to the work scope**

- A preliminary analysis of a generic or most promising adsorption system would be very enlightening.
- Well-to-tank costs, energy efficiencies and greenhouse gas emissions all need to be included as well as recognizing any other particular performance issues (i.e. a standard liquid hydrogen system has severe boil-off issues).
- It is important to recognize that these cost estimates are based on assumptions regarding the physical and chemical characteristics of the systems that may not be completely validated. It is probably not worth the effort to refine the estimates much further until a prototype of a viable system that meets DOE targets is demonstrated.

### Project # ST-02: System Level Analysis of Hydrogen Storage Options

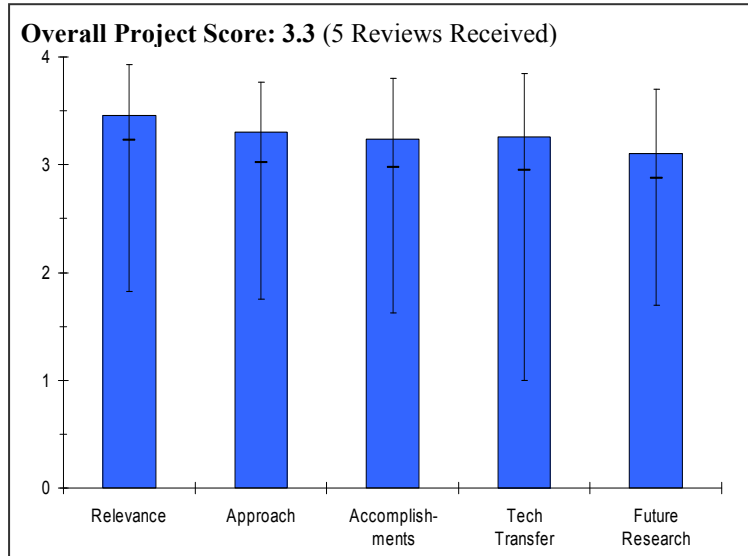
Rajesh Ahluwalia; Argonne National Laboratory

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

#### **Brief Summary of Project**

The objective of this project is to perform independent systems analysis for DOE on all approaches for on-board vehicular hydrogen storage technologies. Specific goals include the following:

- Model and analyze various developmental hydrogen storage systems to determine system performance (e.g. gravimetric and volumetric capacity, operability, etc.).
- Analyze hybrid systems that combine features of more than one concept.
- Develop models that can be used to “reverse-engineer” particular technologies to determine material requirements to meet DOE system targets
- Provide guidance on properties required to meet targets.
- Provide input for go/no-go decisions; and
- Identify interface issues and opportunities and data needs for technology development.



#### **Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- It appears some of these technologies could have been down-selected earlier without a full analysis.
- Provides important system-level analysis of all hydrogen storage approaches.
- The system level analyses covered in this project are extremely important to assess the feasibility of various hydrogen storage options in a future hydrogen economy and set targets for various R&D efforts.
- PI is providing information that should accelerate the process of hydrogen storage technology prioritization.
- Excellent work, which allows a direct comparison of the different storage technologies on a system level.
- Emphasizes “the credo the DOE Hydrogen Storage Team”, that for hydrogen storage materials and systems, gravimetric and volumetric densities are not the only parameters.
- Shows in an educational way the complexity of the overall systems.
- Translates basic material research data into real-world automotive demands.
- Overview gives directions to the different storage technologies, in which fields they can improve their materials and efforts.

#### **Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- The storage performance results of  $\text{AlH}_3$  hydride appear to be biased by the artificially high hydrogen on-board demand assumptions.
- Approach seems to be thorough and comprehensive.
- The approach appears to be adequate.
- Well done!

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.2** based on accomplishments.

- For an analysis project it is hard to tell what the technical accomplishment was.
- Completed analysis of metal hydride storage approach this year.
- Provided important input to and support for go/no-go decision for sodium borohydride storage concept.
- The team analyzed metal hydrides, sodium borohydride and hydrogen storage in liquid carriers, and is on-course to complete analysis of hydrogen storage in amine borane.
- Project seems to be ahead of project ST-01 [TIAX LLC project].
- Inclusion not only of efficiencies, but also start-up energy, time and hydrogen-buffering is highly appreciated.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- Many, many interactions and collaborations.
- The team worked closely with other stakeholders.
- Good inter-DOE-contractor collaboration. It may be time to get some input from the automotive OEMs regarding packaging, interface and other requirements and limits.
- Input from other partners seems to be well-organized and considered in the work.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- It is not clear that the proposed future work, if successful, would yield better candidate storage systems that address the barriers.
- Future plans will extend analysis techniques to the remaining storage approaches and will continue to support scheduled go/no-go decisions.
- The proposed research attempted to refine their analyses for a number of systems to reflect the latest experimental results as well as emerging new systems.
- Future research seems to be very well planned and structured.

**Strengths and weaknesses**Strengths

- A lot of effort put into individual projects.
- Very quantitative, especially on kinetics.
- Good analysis methodology and strong interactions with the centers of excellence.
- Good modeling with the alane slurry.
- Excellent work, which allows a direct comparison of the different storage technologies on a system level.
- Shows in an educational way the complexity of the overall systems.
- Translates basic material research data into real-world automotive demands.
- Overview gives directions to the different storage technologies, in which fields they can improve their materials and efforts.
- Important project to compare different storage technologies amongst each other.
- Calibration and validation of modeling explicitly mentioned and integrated as part of the project's approach.
- Includes and addresses parameters like heat-up energy, time and hydrogen buffering.

Weaknesses

- There is a bias towards being comprehensive when this may not be necessary for down selecting technologies.
- It is unknown whether the shown processes and overall systems are the best and most representative ones.

### Specific recommendations and additions or deletions to the work scope

- Should be more strategic rather than comprehensive. The PI should focus on the critical weaknesses.
- Include single solid phase alane study, at least to learn the kind of innovation needed for material handling for on-board and off-board. Potential in higher weight percent.
- With the collaboration with TIAX, include a multi-parametric model for technical performance and cost.
- Addition of metal organic frameworks and other sorbent materials is recommended.
- Disclosure of values (mass and volume) for the additional system components like burners or hydrogen ballast tanks is recommended.
- Harmonizing and synchronizing of presented results of project ST-01 [TIAX] and ST-02 recommended.

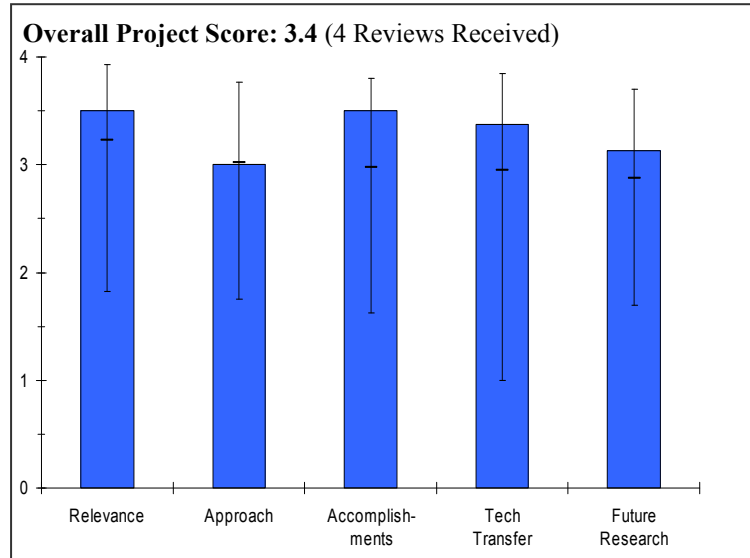
**Project # ST-03: Best Practices for Characterizing Hydrogen Storage Properties of Materials***Karl Gross; H<sub>2</sub> Technology Consulting LLC (formerly of HyEnergy)*

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

The objective of this project is to develop and publish a reference document on best practices and limitations in measuring hydrogen storage properties of materials, including kinetics, capacity, thermodynamics and cycle life. The benefits include:

- Transferring the knowledge and experience in making critical performance measurements from experts in this field to the entire hydrogen storage research community.
- Aiding in the establishment of uniform measurement practices and presentation of uniform performance data.
- Providing a published resource to aid those just entering to this rapidly expanding field.
- Improving international communications on these issues among government, university, and industry entities and enabling the reporting of data using standardized measurement techniques.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- Due to the number of investigators in the program with little or no previous experience in the study of hydrogen storage properties, a compendium of this type has value, provided that this work is made required reading by those who are new to the field. For those in the field and amongst reviewers, it will still make-up valuable reading so that data can be judged in a critical fashion.
- A project of this type probably should have been initiated earlier in the life of the program.
- The project is important to the overall subprogram and clearly of value for its advancement. It will be making a contribution to the development of uniform practices for making measurements and presenting performance data for hydrogen storage candidate materials.
- This program is highly relevant to meeting the program goals.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- Web dissemination is probably the most effective way of getting this information out.
- Most aspects of the work being done by investigators who will need this seem to be addressed.
- There are no actual technical barriers so this weighting for the work should not be used.
- It has a straightforward approach, with go/no-go decision points based on the delivery and quality of produced documents. It addresses important issues for assessing the performance of hydrogen storage materials. Quite useful is the latest restructuring of the project into sections including a background introductory section.
- Its main output will be best practices documents on measurements covering definitions and procedures, which will be made publicly available. Such guideline documents will be useful particularly to newcomers for improving the quality of data obtained and published. The PI gets input and feedback to his drafts from experts in the field ensuring that the end result is accurate and useable.



## HYDROGEN STORAGE

- The approach is well constructed. However, care should be taken to ensure broad applicability rather than too much focus on one technical field (e.g. metal hydrides).

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.5** based on accomplishments.

- Most of the areas covered appear to cover the more relevant areas of technological interest.
- It is definitely useful to have this data in one source rather than having to interpret information that otherwise needs to be gleaned from textbooks or papers.
- During questioning, the subject of the hydrogen equation of state was brought up and the author was able to address this.
- Seems to be on time with its first deliverable – the kinetics section – posted on the web for feedback and a second document on capacity already drafted. The kinetics deliverable released is actually the latest version following edits and recommendations by a number of experts in the field.
- The progress towards the stated objectives appears to be on track.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.4** for technology transfer and collaboration.

- There appears to be good collaboration with those who are involved with subtleties of measurements.
- Exploring strong links established at international level - a number of experts in the field are kindly contributing with their edits, suggestions and improvements to the draft best practices documents.
- The PI has obtained guidance from a broad group of knowledgeable scientists in the field. The program calls for open input from any interested parties.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Unfortunately, it may be necessary to address spillover effects in some way. The kinetics of these systems are extremely poor and looking specifically into issues related to acquiring data over long periods of time would be handy. While this runs counter to the on-board refueling model, there may be some value in addressing measurement instrument stability against pressure or high pressure and temperature.
- Use of excess density: it should be noted that the excess density is not the engineering system's energy density target of the DOE. Although on a materials science basis it makes sense to use it (because of the lesser ambiguity of the definition), it does not represent the end goal of the DOE hydrogen storage program. It should be pointed out that comparing excess densities between, say, physisorption materials and metal hydrides could be construed as questionable when discussing their relative merit, as the weight, volume and nature of the required containment unit and subsystems may differ qualitatively.
- The proposed future work is well defined and it is targeting the deliverables for the various sections.
- It appears that, at the moment, the whole project is focused on experiences from the metal hydrides work and does not accommodate the specificities of the different hydrogen storage materials currently handled by the researchers. No apparent planning has been made to demonstrate how these best practices could translate to other material types.
- The forward plan appears to be appropriate for meeting the project goals.

### **Strengths and weaknesses**

#### Strengths

- The issue of a common and proper definition of the storage capacity, in view of the DOE storage objectives and in the context of a new center of excellence on storage systems, will be an important contribution.
- Valuable contribution. Excellent progress overall and good response to input from reviewers.
- Important attempt at standardizing the terminology and definitions.

- Lots of useful information in one tome.
- Excellent and important contribution to provide a common framework for the materials storage community.
- A solid contribution to the development of testing protocols, harmonization of data acquisition and reporting. Also a valuable step in the right direction for enabling accurate, reliable, critical performance assessment and benchmarking of potential hydrogen stores.
- This project brings relevant learnings from the conventional metal hydride work of the past forward to the present where they can help educate new hydrogen storage researchers.
- This project attempts to define a common terminology and standardize measurements methodology, the write-up of this document constitutes a very valuable contribution.

#### Weaknesses

- The work is a bit metal hydride-centric, efforts should be done in integrating terminology and concepts from physisorption.
- The deliverables are limited to metal hydrides at the moment. No future plans are made for addressing the same issues for non-hydride materials, for instance metal organic frameworks, carbon, chemical hydrides.
- It may prove to be difficult to get wide acceptance and approval of the proposed guidelines, particularly from scientists in whose laboratories such measurements are routinely performed for a number of years.
- This project may be too focused on metal hydrides at the moment. Hopefully the final document will be more balanced and include significant content related to sorption materials and chemical hydrides.

#### Specific recommendations and additions or deletions to the work scope

- This project may be too focused on metal hydrides. The final document should be more balanced and include content related to sorption materials and chemical hydrides.
- In the presentation, a detailed discussion of the feedback (to date) from the community would be valuable to gauge the degree to which this document constitutes a consensus (how many responded of the 50+ participants of IEA HIA Task 22, what were the highlights of the comments etc).
- Gathering feedback from IEA HIA Task 22 and other experts in the field is extremely valuable to bring about a consensus document.
- An explicit recommendation as it pertains to the grade requirements of hydrogen for uptake measurements (particularly adsorptive measurements) would be interesting as part of section 2.6.1.1. Suggestions on which electro-optical system for hydrogen should be minimally acceptable (say in volumetric approaches) would be a valuable contribution for a best practice document.
- At the project's end, some means of project maintenance or updating may be of value as engineering related issues may arise that the present work does not cover.
- A relative discussion on the thermodynamics (and on the proper thermodynamic definitions of response functions and observables) specifically for physisorption would help clarify several concepts which surprisingly remain ill-defined or misused in the literature.
- Consider expanding the scope of the best practices documents to accommodate all forms of hydrogen storage materials, and also account for future, as required, refinements.
- Address also sample handling and preparation conditions - not clear at the moment whether this is accounted for in the introduction or the other sections.
- Any help from the PI on teaching the correct methods for volumetric adsorption measurements is very welcome. This will hopefully assist researchers in the field in making correct measurements and avoiding either "false positives" or "false negatives".

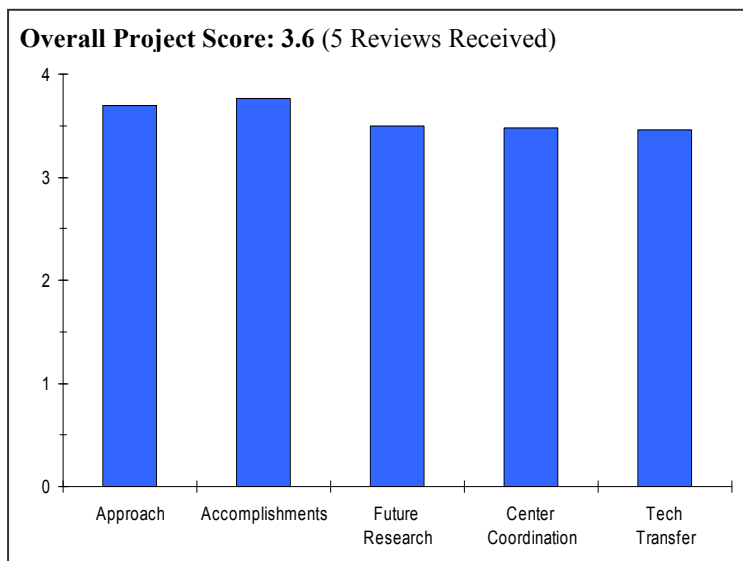
**Project # ST-04: DOE Chemical Hydrogen Storage Center of Excellence Overview**

*Kevin Ott; Los Alamos National Laboratory*

[NOTE: This presentation was to evaluate the entire Chemical Hydrogen Storage Center of Excellence as a whole. A separate review form was used and can be found in Appendix C. LANL’s technical contribution to the center is evaluated in ST-6.]

**Brief Summary of Project**

The overall objective of this project is to identify, research, develop and validate advanced on-board chemical hydrogen storage systems to overcome technical barriers and meet 2010 DOE system goals with the potential to meet 2015 goals. The specific goals are to 1) develop chemistries, materials, catalysts and new concepts to control thermochemistry and reaction pathways for hydrogen release; 2) develop and demonstrate chemical steps leading to efficient off-board regeneration of fuel from spent fuel; 3) assess concepts and systems using engineering analysis and studies using DOE targets as guidance; 4) down select the most promising chemical systems for more detailed work and engineering development; and 5) develop life cycle analysis.



**Question 1: Approach to performing the R&D including Center Management**

This project earned a score of **3.7**.

- The director, coordinating council and DOE are doing a very good job of leading and directing the group.
- The ideal value of well-managed and coordinated center of excellence approach is nicely shown here.
- Outstanding relevance clearly demonstrated. Management is keeping the Chemical Hydrogen Storage Center of Excellence (CHSCoE) focused on virtually all aspects of DOE goals and objectives for hydrogen storage in relation to the Hydrogen Fuel Initiative and Multi-Year RD&D plan.
- Approach is engineering oriented; modeling is an important component.
- The center uses a well-balanced approach, considering fundamental aspects as well as engineering considerations in their materials development. There is good coupling between theoretical modeling and experimental activities. It is very focused on the targets and is effective in keeping individual center projects aimed at overcoming obstacles toward achieving the targets.
- Facing the key challenges, mostly well-designed – only a few weaker programs, uses skills well. Planned downselects are needed and process is pretty good, too.
- Chemical hydride materials have the potential for high hydrogen storage capacities and rapid release rates.
- The center has very effectively reconfigured itself after the no-go decision on sodium borohydride.
- The approach avenues of hydrogen capacity, hydrogen release rate, and spent fuel regeneration are the correct ones.
- The engineering assessment approach to guide downselection is the right one.
- Approach to improving kinetics is not clear.
- Does the superacid regeneration approach have any chance of meeting the 60% efficiency target?

**Question 2: Technical accomplishments and progress toward DOE goals**

This project was rated **3.8**.

- Recent results have been many and impressive. DOE 2010 system weight and volume targets seem close to achievement in this CoE.
- There is a good balance among materials, operational materials properties and spent fuel regeneration work.
- Important progress has been achieved on a number of fronts and significant improvements have been demonstrated in ammonia borane materials in terms of capacity, temperature and kinetics. Regeneration process steps for spent ammonia borane materials have been developed and currently have multiple pathways toward effective reprocessing. Downselection process on materials was completed this fiscal year.
- The downselection criteria are very good and a 50% downselection has recently taken place.
- The go/no-go decision and downselection processes have been finely tuned here. The sodium borohydride no-go decision process was done as a valuable experiment for the future, using expert outside inputs.
- Good catalytic accomplishments on ammonia borane, and antifoaming
- The 2008 heterogeneous catalyst shows good hydrogen capacity, but the release rate still needs to be improved.
- Results for the non-precious metal copper catalyst for ammonia borane look good.
- Good flow rates demonstrated.
- 0.02 g/sec hydrogen release is not easy for these materials since we cannot heat up and shut all the material at once.
- Keeping the fuel liquid is a key, though also good to be sure they also have good regeneration still.
- Given the bottom line for commercial vehicle storage is spent fuel regeneration cost, not strictly energy efficiency, cost calculations seem to be underutilized at this stage. That is the ultimate potential show-stopper.

### **Question 3: Proposed future research approach and relevance**

This project was rated **3.5**.

- The future work proposed is broadly and qualitatively fine.
- Regeneration is correctly listed as the most important task of the future.
- A quantitative go/no-go target on ammonia borane regeneration (efficiency and cost) would have been useful for FY2009.
- Hope for developing on-board regenerable materials is welcome.
- The description of the planned future work was done at a high level, but could have been a little more detailed. There was not much discussion of potential new materials (this may have been done to allow the individual PIs more freedom to present their future plans).
- Continue to concentrate on regeneration for ammonia borane.
- Kinetic improvement must also be promoted.
- Engineering concerns are the key in this area, good choice of future work.
- New materials are important.
- When will the complete recycle of the one gram of actual spent fuel be completed?
- Is a downselect of solid ammonia borane versus liquid ammonia borane planned before the end of the center?
- In the final analysis, the success of chemical hydride materials hinges on the success of regeneration. The overview indicates that 60-70% of the center's activities are on regeneration. This emphasis should be maintained.

### **Question 4: Coordination, collaborations and effectiveness of communications within the CoE**

This project was rated **3.5**.

- The center seems to be working very well. There is a very good synergism and communication among the partners.
- The center has effective methods of communication. Regularly scheduled phone conferences fill in the time gaps between face-to-face meetings. Additional meetings are held on specific topics (e.g., the downselect process).
- Seem well coordinated in general. Some degree of running largely separately, but very little.
- Some of the new materials activities may have relevance to and may benefit from the Metal Hydride Center of Excellence work.
- The level and extent of interactions between the various participants in the center is very good.

### Question 5: Collaborations/Technology Transfer Outside the CoE

This project was rated **3.5**.

- Collaborations and technology transfer seem outstanding, both within the center and between the center and outside organizations.
- International connections (International Partnership for the Hydrogen Economy (IPHE), Japan & others) are unusually good.
- Good collaborations with the other two centers. IPHE project gives the PIs an opportunity to collaborate with international research organizations.
- International collaboration good to very good.
- The IPHE work has yielded excellent results.
- Not clear how theoretical work couples to other centers. But to be fair there is less need for interaction than between the Sorption Center of Excellence and the Metal Hydride Center of Excellence.
- Alane is the logical place and it is not clear that there is as much communication between the Chemical Hydrogen Storage Center of Excellence and the Metal Hydride Center of Excellence on this topic.

### Strengths and weaknesses

#### Strengths

- Excellent, well-working example of a center.
- Many knowledgeable researcher involvements.
- Various methods of approach to generate and regenerate the materials.
- Excellent technical team.
- Proper emphasis on the key issues.
- Excellent integration of the various activities and participants.
- Good organization; recognizes and faces major shortcomings of the chemical area, good team by and large, theory and experiment and engineering.
- Has moved gracefully from NaBH<sub>4</sub> focus to other chemistry.

#### Weaknesses

- Could be a little more effort on economics.
- Theory does get some calibration from experiments but to at least some extent, not incorporating feedback to improve the calculations fundamentally, and that would benefit the center.
- Probably vulnerably dedicated to ammonia borane at this point; deliberate effort to diversify somewhat (not a huge amount) is indicated.
- None.

### Specific recommendations and additions or deletions to the work scope

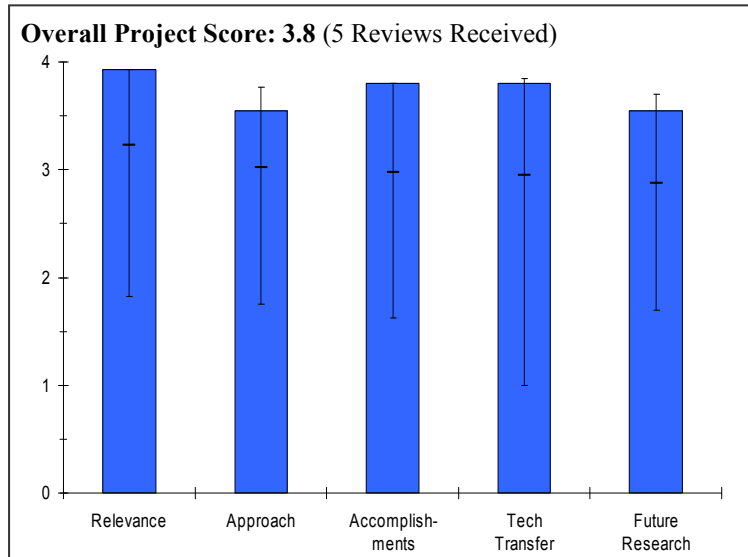
- Increase effort at getting some regeneration cost estimates. In terms of \$/kg hydrogen stored (\$/gge), how will this compare to DOE hydrogen production targets (or ever-changing gasoline price).
- Add some more view of how the material will be used.
- Material characteristics such as thermal conductivities and density will be very important for the real reactor design.

**Project # ST-05: Chemical Hydrogen Storage R&D at Pacific Northwest National Laboratory***Chris Aardahl; Pacific Northwest National Laboratory*

[Member of the Chemical Hydrogen Storage Center of Excellence]

**Brief Summary of Project**

The Center of Excellence's (COE's) objectives for this project are to 1) develop methods for on-demand, low temperature hydrogen release from chemical hydrides that can achieve the Department of Energy targets; and 2) develop high efficiency off-board methods for chemical hydride spent fuel regeneration. Pacific Northwest National Laboratory's goal is to meet the COE objectives through studies and development of high capacity chemical hydrides that increase kinetics while maintaining high capacity.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.9** for its relevance to DOE objectives.

- The project is critical to the Hydrogen Fuel Initiative.
- Project has outstanding, virtually complete relevance to DOE objectives.
- Project fully supports DOE objectives.
- The object to increase kinetics while maintaining high capacity in chemical hydrides is good.
- Regeneration of  $\text{NH}_3\text{BH}_3$  is an important objective.
- Focused on major problems and the methods are appropriate to actually generate relevant results.
- Engineering, science and theory are good mix that is consistent with mandate.
- The materials being investigated are very high hydrogen capacity ones with the potential for high release rates at relatively low temperatures.

**Question 2: Approach to performing the research and development**

This project was rated **3.6** on its approach.

- Logical engineering problems chosen and approached with a good combination of science and engineering approaches - both in house and out of house.
- The project is focused on high hydrogen capacity materials, fast hydrogen release kinetics, and regeneration of the spent product.
- Consideration of engineering issues in materials development is an important attribute of the work.
- Project focuses very largely on ammonia borane ( $\text{NH}_3\text{BH}_3$ ) and its many possible derivatives. This family of compounds has the greatest near-term potential to meet DOE weight, volume and rate goals for vehicle applications.
- The project is a good combination of ammonia borane release and regeneration technology.
- It is obvious that the project activities fit well into the Chemical Hydrogen Storage Center of Excellence and does not significantly overlap other technical approaches to use and regenerate ammonia borane.
- Fully focused on overcoming limitations of ammonia borane material systems for hydrogen storage applications.

## HYDROGEN STORAGE

- Effective use of analytical techniques available at PNNL to help understand material properties. The nuclear magnetic resonance (NMR) work has been shown to be a valuable technique, both for material behavior and for regeneration.
- The approach is focused on technical barriers such as to achieve rate target.
- Would prefer to see feedback to theory which generated the experimental approaches.
- The focus on solid ammonia borane materials, while of high capacities, may not ultimately prove viable for vehicular applications due to the problems with solids handling. To be successful for vehicles, excellent hydrogen capacity and release rate/temperature characteristics must overwhelm the handling issue.
- What is the evidence that "activated hydrogen" actually occurs?
- Using cobalt may not be good to regenerate the hydride. It may be of help to use oxidizing material such as titanium.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.8** based on accomplishments.

- Results obtained during the past year were numerous and progress very well in the direction of the DOE system goals.
- Good progress toward overcoming issues with ammonia borane, e.g., foaming, diborane release, release temperature, kinetics.
- Impressive publication.
- Lithium ammonia borane material studied this year has excellent potential as a storage material.
- Lithium ammonia borane is a VERY promising improvement.
- The lithium ammonia borane results look excellent. Release temperatures are lowered and release rates are increased.
- Very promising results on lithium ammonia borane. Weight, volume and kinetic results suggest the chances are very good, a workable prototype system can soon be built.
- Improved kinetics is valuable in this ammonia borane system. But reduced temperature is probably more valuable.
- Significant progress towards achieving morphology control during hydrogen release in  $\text{NH}_3\text{BH}_3$ .
- Excellent progress on the issue of foaming; identification and synthesis of hydride transfer reagents; and digesting solvent system.
- The anti-foaming results for the ammonia borane look good.
- The idea and implementation of a binder seems to be viable and surely will be valuable if proven out long term.
- The key to the  $\text{NH}_4\text{BH}_4$  materials is improving their stability.
- Excellent progress has been developed on regeneration. Theory and experiment are working in concert. The ultimate answer on regeneration will make or break ammonia borane as a potential vehicular storage medium.
- Good progress toward regeneration process for spent ammonia borane.
- Using "failures" to find success in regeneration.
- Progress on regeneration appears to be slower than progress on new materials and hydrogen release rates.
- On the negative side, worrisome levels of impurities (e.g., 170 ppm  $\text{NH}_3$ ) were shown to be contained in the exit hydrogen from decomposed ammonia boranes. Can they really be trapped in a practical vehicle environment?

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.8** for technology transfer and collaboration.

- Very impressive collaboration with center and other organizations.
- Well-connected via the center and seem to be using those connections.
- Also well connected outside.
- The excellent lithium ammonia borane results were obtained in association with the International Partnership for the Hydrogen Economy (IPHE).
- Interactions with other members of the center are very good.
- Excellent collaborations and coordination within the Chemical Hydrogen Storage Center of Excellence.

- Excellent international collaborations with the IPHE.
- Collaboration with center partners in a number of areas.
- Good coordination with partners on regeneration processes.
- The IPHE project is a good approach to international collaboration.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.6** for proposed future work.

- Plans build on past progress.
- Theory to guide in regeneration schemes will be helpful.
- Suitable.
- Again would prefer to see feedback to theory so that the theory is improved.
- The  $\text{NH}_4\text{BH}_4$  approach is high pay-off, but also high risk because of the instability issue.
- The reduction aspect of the regeneration process is being aggressively addressed.
- The lithium ammonia borane approach looks very promising, provided that regeneration does not become too difficult.
- In general, good and logical list of future work.
- There are many irons in the fire; more downselection may be necessary.
- New work on ammonium borohydride should be very interesting, both on fundamental and practical bases. Many questions remain to be answered.
- Focus on downselected materials good.
- Focus on regeneration of spent ammonia borane materials and important element in achieving storage goals.

#### **Strengths and weaknesses**

##### Strengths

- Impressive group of researchers.
- Good interaction between theory, science, and engineering to keep focused on meritorious approaches, rather than systems with some highlights but also huge weaknesses.
- Team quality.
- Excellent team.
- Excellent international collaborations.
- Excellent technical approaches.
- Pioneering efforts on ammonia borane with excellent thoughts on the paths forward.
- Very close to the DOE targets, perhaps the closest of all activities in the program.
- Very productive in a practical sense.
- Effective use of advanced diagnostic capabilities available at PNNL.

##### Weaknesses

- Fuel cost & fuel cycle energy efficiency were not addressed.
- Cost of work at national labs - might benefit by using lower cost labor where possible and use higher cost lab personnel for analysis and expertise to a greater extent.
- None.

#### **Specific recommendations and additions or deletions to the work scope**

- Strongly suggest regeneration of lithium ammonia borane be looked at directly as it seems your lead candidate from a purity and kinetics of hydrogen point of view, and with good capacity to boot.
- Work on single pot regeneration is laudable but not highly likely, so some effort on minimizing unit operations and then developing those steps is a good practice to consider.
- In view of the fact the regeneration scheme(s) is (are) getting filled out well, the next year should be ripe for some hard cost estimates.
- Consider a slightly increased effort on safety studies.



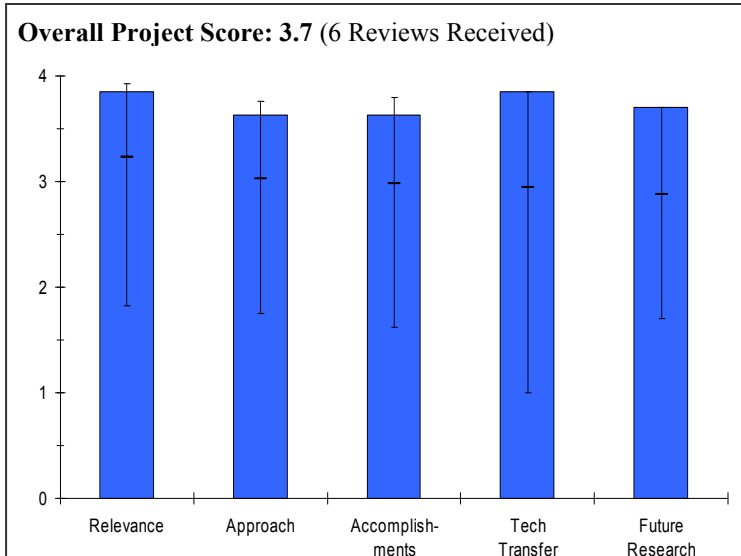
**Project # ST-06: Chemical Hydrogen Storage R&D at Los Alamos National Laboratory**

*Anthony Burrell; Los Alamos National Laboratory*

[NOTE: This review is for LANL's technical contribution to the CHSCoE. Member of the Chemical Hydrogen Storage Center of Excellence]

**Brief Summary of Project**

The objectives for this project are to: 1) develop liquid ammonia-borane (AB) fuels and increase rate and extent of hydrogen release; 2) identify and demonstrate new materials and strategies for near-thermoneutral hydrogen release; 3) demonstrate all chemical steps and conduct engineering assessment for energy efficient AB regeneration process (high yields, rates and energy efficiency, integrate steps when possible); and 4) develop materials and processes to minimize gas phase impurities and demonstrate adequate purity of hydrogen stream.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.9** for its relevance to DOE objectives.

- High hydrogen capacity chemical hydrides in a liquid form and with suitable hydrogen release rates and efficient, cost-effective regeneration would have a very major impact on vehicular hydrogen storage.
- Outstanding relevance to the DOE objectives.
- Project is directly focused on storage system targets and fully supports DOE RD&D objectives.
- Project is directly relevant to DOE objectives for chemical hydrogen storage.
- Identification and synthesis of new ammonia borane-related systems.
- Developing a detailed mechanistic understanding and proof of hydrogen release catalysis.
- Develop and optimize a spent fuel regeneration system.
- Initiate testing of impurity impact on a PEM fuel cell.
- Initiate evaluation of a heterogeneous catalyst system for hydrogen release.
- Ammonia borane has the potential of meeting DOE 2010 targets.
- Catalysis is a problem of merit.
- Liquid would be a useful state for off-board regeneration.
- Energy is a major concern in spent fuel recycling - but it is not clear this is well-designed.
- Demonstration is critical.

**Question 2: Approach to performing the research and development**

This project was rated **3.6** on its approach.

- Theory, experiment and engineering work are very well integrated.
- Good mix of theory, synthesis and characterization.
- Good feedback strategy between above activities.
- Good balance between ammonia borane liquid forms, regeneration and exploration for new materials.
- Good effort on catalyst development that should fill the gap.
- Good coupling between materials development and engineering properties (e.g., gas purity).
- Engineering-guided research is an excellent approach to guide downselection of materials and processes.

- Seems good overall.
- Downselects are key.
- Important emphasis on mechanism and kinetic studies.
- New ammonia borane liquid fuels can avoid many engineering issues associated with solid fuel.
- Well-planned approach to maximize storage capacity and hydrogen release rate.
- The search for thermoneutrality is important.
- Interesting new ammonia borane derivative materials are being investigated.
- Catalyst work is excellent. Improved release rates and non-precious metal catalysts.
- Looking at catalyzed ammonia borane for increasing rates and liquid ammonia boranes for handling convenience.
- The liquid ammonia borane-based route has engineering advantages over the solid ammonia borane-based route.
- Looking at purity is a key item that is not really looked at to date in as definitive of a way.
- The use of a fuel cell element as an ultimate test for impurities (borazine) in the output hydrogen is a very nice, practical twist.
- Initiation of PEM fuel cell testing is excellent, but the data presented does not address key poisoning issues.
- The regeneration issue is being aggressively addressed.
- Approach generally complementary to PNNL activities.
- I compliment LANL for their very timely action to investigate alternative ammonia borane regeneration pathways that do not require formic acid.
- Organometallic, transition metal hydride digestion and reduction is different approach for regeneration.
- The regeneration flow diagrams look rather complex. Will costs of regeneration be as low as the relatively high estimated efficiencies suggest?
- A good case is not made for the interest and emphasis on a neat liquid system. This should be a very low priority.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.6** based on accomplishments.

- Very good progress has been made, both for understanding the catalyzed and liquid ammonia borane variants studied and the necessary engineering integration of same.
- Accomplishments this year move the project forward in a major manner.
- Project is moving close to the DOE system goals.
- Demonstrated new heterogeneous catalysts that increase hydrogen release rate at lower temperature than previously achieved.
- New experimental capabilities developed.
- Good progress in experimental work for new heterogeneous catalyst screening.
- Catalyst work is promising.
- Identified effective heterogeneous catalysts.
- Non-precious metal catalysts are being identified.
- Promising results have been shown with a copper-based catalyst.
- New hydrogen storage materials are being discovered.
- Low melting point liquids are being studied.
- New liquid fuels developed.
- Liquid fuels that are liquid down to  $-30^{\circ}\text{C}$  have many advantages over solid fuel.
- Maintaining liquid is great at  $-30^{\circ}\text{C}$  – please be sure they are also ones that can be recycled efficiently while maintaining capacity.
- The successful demonstration of an in-line borazine removal cartridge was very interesting. It would have been nice to see more details on this presented, e.g., what an actual on-board purification device would look like.
- Low-level impurities are being evaluated via a fuel cell system.
- Test of hydrogen is not exotic, but is valuable, glad they are doing that because it is another key concern. What is missing is how they will deal with the problem.
- Impressive progress that demonstrates the necessary steps in ammonia borane regeneration.
- Regeneration with only 25% overhead energy is impressive if it actually works and actually is that low in a real system.

## HYDROGEN STORAGE

- Progress toward completing this particular regeneration scheme is good. Reviewer looks forward to a complete lab-scale demonstration and cost estimate.
- A carbon dioxide-free regeneration process is being developed.
- The possibility for an onboard regeneration (direct rehydrogenation) scheme is exciting.
- I would have liked to hear some preliminary concepts for an on-board storage system.
- Good progress though also high cost.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.9** for technology transfer and collaboration.

- Extensive interaction with collaborators.
- Excellent interaction between labs on the identification and synthesis of hydride donors.
- Excellent interaction on interface with a PEM fuel cell.
- Good interplay of science and engineering concerns.
- Extensive collaboration across the board with center partners.
- Good relations with center partners and using them well.
- The International Partnership for the Hydrogen Economy (IPHE) collaboration is producing very valuable results.
- Excellent collaboration and integration of the activities of the other participants.
- Good collaborations within and integration with the Chemical Hydrogen Storage Center of Excellence. Obviously there is good coordination.
- Good international activities via IPHE.
- Industry involved.
- Good coupling with partners on ammonia borane regeneration routes and processes.
- IPHE project affords an opportunity for international collaborations.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.7** for proposed future work.

- The continued emphasis on new materials, high release rates via non-precious metal catalysts, and liquid ammonia borane-type systems is very good.
- Good plans based on this year's findings.
- Excellent strategic approach.
- New engineering-guided research in ammonia borane regeneration will help to improve overall energy efficiency.
- Further work to identify non-precious metal heterogeneous catalysts is on track.
- Appropriate and suitable work planned.
- Attack the problem on several fronts.
- Seems to learn from current work.
- Going to look at regenerated fuel to see how well it works. This is very good.
- Regeneration appears to be the only potential show-stopper for the chemical hydrogen route. Thus, the laboratory-scale demonstration of the entire regeneration process is crucial. Major emphasis should be placed on this.
- Activities are planned.
- This is an extensive and diverse effort, perhaps a little too ambitious. Increased focus may be desirable.
- Continued work on non-PM catalysts is of course encouraged, but the success of the recent work may be close enough to the targets for now.
- The flow reactor will help speed up catalyst screening.
- Proposed future work builds on progress achieved to date as well as continuing to search for new materials and catalysts.
- "Engineering-guided research" is an excellent approach at this stage of the project.

**Strengths and weaknesses****Strengths**

- Collaborative.
- Strong synthesis component and skills.
- Excellent mechanism/kinetic studies.
- Good understanding of chemistry and engineering issues.
- Work is well focused.
- Very solid theoretical and experimental work.
- Liquid ammonia borane fuels may be more practical for on-board storage systems.
- Downselect process is robust in concept and seems to be used effectively.
- Use of theory to accelerate progress is good.
- Excellent team and approach.
- Different versions of ammonia borane, very complementary to the PNNL materials.
- Practical engineering integration work.
- The prospect of direct onboard rehydrogenation ties very nicely into the Chemical Hydrogen Storage Center of Excellence.
- Good balance between materials research and engineering considerations.

**Weaknesses**

- PEM fuel cell studies are important, but the work to date does not address the issue of poisoning, and should not be presented as such. 100 ppm of CO, the prototypical PEM fuel cell poison, requires ~10 hours of exposure to kill the catalyst. Thus, the 2-3 hour data collected to date does not address catalyst poisoning from a real world point of view. Also, cell impact is better addressed using voltage/current ( $V \times i$ ) curves rather than current/time ( $i \times \text{time}$ ) curves.
- Work on a liquid system seems misplaced at this time. A workable solid-state system should be the focus and activities that detract from this goal should be deferred.
- Need to address methods to treat volatile by-products following hydrogen release.
- One of the barriers with liquid fuel is the formation of solid spent fuel that requires proper engineering treatment.
- Higher hydrogen release rate is desirable.
- Cost basis as noted above, max use of lower cost labor would be good.
- Might be trying to do too much at once.

**Specific recommendations and additions or deletions to the work scope**

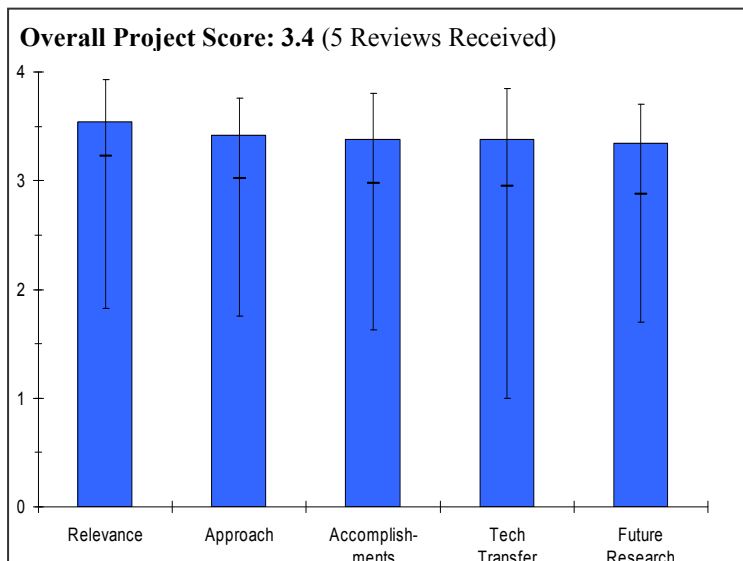
- Continue work with emphasis on mechanism, digestion, hydride reagents, PEM fuel cell poisoning. Defer other issues.
- A question: Could the hydrogenation be carried out electrochemically at a non-noble electrode (cobalt for example, which would produce a surface metal hydride)? This might provide a very clean system.
- Formulate methods to treat volatile by-products following hydrogen release.
- For the liquid fuel option, develop methods to address issues due to formation of solids in spent fuel.
- Effort on the on-board regeneration should be minimal in that, inherently that is going to be very hard in these sorts of systems due to the delta G being against you.
- Need to demonstrate some of these processes, in theory this looks good but need to demonstrate.
- Be careful of the amount of effort on fuel cell poisoning - this is valuable work but if it is to be done in depth, it needs a fuel cell expert's input. Also, I would suggest not.
- Heterogeneous catalyst work seems to be successful in nearly meeting targets. Maybe it is time to reduce that effort and focus more effort on the regeneration scheme - efficiency, cost and practicality.
- Given the clear impurity problem with ammonia borane, this reviewer suggests adding an engineering analysis of the in-line hydrogen purification process. What will an onboard purification process and associated apparatus look like on a vehicle? How often will it have to be regenerated? Initial cost?
- The fuel cell impact is better addressed using voltage/current ( $V \times i$ ) curves rather than current/time ( $i \times \text{time}$ ) curves.

**Project # ST-07: Amineborane-Based Chemical Hydrogen Storage***Larry Sneddon; University of Pennsylvania*

[Member of the Chemical Hydrogen Storage Center of Excellence]

**Brief Summary of Project**

The overall objectives for this project are to 1) develop methods for on-demand, low temperature hydrogen release from chemical hydrides that can achieve Department of Energy targets; and 2) develop high conversion off-board methods for chemical hydride regeneration. In collaboration with Center partners, the goal of this project is to develop new methods for hydrogen release and spent fuel regeneration that will enable the use of amineboranes for chemical hydrogen storage. Penn will use the activating effects of ionic liquids, chemical promoters and/or metal-catalysts to enhance the rate and extent of hydrogen release from amineboranes.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- Objectives in enhancing hydrogen release rate from  $\text{NH}_3\text{BH}_3$  and the mitigation of borazine formation is relevant to the DOE objectives due to the high weight percent of hydrogen in  $\text{NH}_3\text{BH}_3$ .
- This project is highly relevant to the Hydrogen Fuel Initiative because of its potential for high hydrogen capacities, high release rates at temperatures close to  $80^\circ\text{C}$ , and liquid forms of the storage medium.
- Project shows excellent orientation and relevance to DOE goals: weight, volume, rates, spent fuel regeneration efficiency, etc.
- The materials under investigation are important for reaching storage system targets and DOE program goals.

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- Approach correctly looks at both increasing the hydrogen release properties of ammonia borane, followed by a practical, efficient and economic spent fuel regeneration process, similar in objectives to the Pacific Northwest National Laboratory and Los Alamos National Laboratory projects.
- Utilization of the proton sponge to avoid  $\text{NH}_3\text{BH}_3$  foaming shows very good approach in indentifying and solving problems.
- The approach of using ammonia borane in ionic liquids, with chemical promoters and/or catalysts to enhance hydrogen release kinetics is a very good one.
- The approach in reducing the ionic liquid content is good as it enhances the weight percent of hydrogen.
- The regeneration approach of converting  $\text{BNH}_x$  dehydrogenation products to boron trihalides that are then converted to ammonia borane is a very good one because it avoids B-O or diborane intermediates.
- The release work is complimentary to Pacific Northwest National Laboratory and Los Alamos National Laboratory. It looks at accelerating release of hydrogen by ammonia borane through the use of ionic liquids, M-catalyzed ionic liquids and chemical promoters.
- The spent fuel regeneration process is also different and seems to be conceptually simpler than the Pacific Northwest National Laboratory and Los Alamos National Laboratory regeneration processes: acid-halide

digestion followed by 3-step, "one-pot" reduction and conversion. Importantly, the Penn process avoids the formation/use of troublesome  $B_2H_6$ .

- There is nice, innovative chemistry in this project.
- The PI is very qualified to conduct this project. However, the approach may be too reliant on homogeneous catalysts that have limited commercial prospects.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.4** based on accomplishments.

- Good progress has been made over the last year.
- A significant improvement in hydrogen release kinetics has been achieved in a 10.2 weight percent ammonia borane - ionic liquid material at 120°C. However, this material appears to be semi-solid in morphology.
- Foaming of the material during hydrogen release has been significantly reduced with a proton sponge addition.
- The use of proton sponges was important to show the increased decomposition kinetics, as well as eliminate the foaming problem.
- Reduction of the ionic liquid amount added to  $NH_3BH_3$  is good however potential formation of toxic gases such as  $NH_3$  and borazine needs to be checked.
- Solubility limitation of  $NH_3BH_3$  as the ionic liquid amount is reduced needs to be addressed.
- Presenting new regeneration processes of  $NH_3BH_3$  is good, however proof of concept needs to be illustrated, i.e., the reduction with silane step followed by reacting with  $NH_3$ .
- Progress has been made with the regeneration of dehydrogenation products via the boron trihalide approach.
- Decomposition kinetics of the enhanced ionic liquid ammonia boranes has been increased.
- The Penn regeneration approach has been largely demonstrated on a lab scale and seems to this Reviewer to be simpler and closer to practical than the Pacific Northwest National Laboratory and Los Alamos National Laboratory processes.
- The progress towards the objectives has been very good for addressing aminoborane dehydrogenation. The progress towards effective aminoborane regeneration has been limited.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.4** for technology transfer and collaboration.

- There is effective collaboration between the PI and other members of the Chemical Hydride CoE.
- Significant interactions occur with the other members of the Chemical Hydrogen Storage Center of Excellence.
- Good technology collaborations within the center, including important industry connections.
- Suggested to have more visible collaboration with other members.
- Unlike the National Lab projects, there seem to be no significant international collaborations.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.3** for proposed future work.

- Optimization of the ratio of ionic liquid:  $NH_3BH_3$  is a good step; however many other factors such as solubility limitation and formation of toxic gases need to be addressed more.
- It is suggested to measure the effects of using different ionic liquids to down select the better ones
- Focus of the superacid/halide reduction for the regeneration of  $MNH_2BH_3$  is good and needs to be illustrated
- Emphasis on improvements in the regeneration scheme, particularly the more effective conversion of dehydrogenation products to  $BX_3$  species, is crucial.
- Future work is a logical extension of the past.
- The project should focus on aminoborane dehydrogenation and the use of heterogeneous catalysts to effect the dehydrogenation.

### Strengths and weaknesses

#### Strengths

- Liquid form of the material is very strong when we design the reactor.
- Again, liquid phase has a potential of controlling speed of release.
- Synthetic approaches and considering reducing the penalties for solvating  $\text{NH}_3\text{BH}_3$  in ionic liquids
- Excellent PI.
- Very good technical approach.
- Excellent, practical chemistry.
- A promising, hopefully practical, efficient and cheap regeneration process.
- Low vapor pressure of ionic liquids has significant advantage for hydrogen separation from liquid.
- Optimization of ionic liquid/aminoborane ratio to increase overall material capacity.
- Non-precious metal catalysts are highly desirable.

#### Weaknesses

- The spent fuel regeneration approach must be proven to be viable on a laboratory scale.
- It is not clear how the release efforts compare in practicality to those in Pacific Northwest National Laboratory and Los Alamos National Laboratory.
- Catalysts can lower the temperature of hydrogen release but are homogeneous rhodium catalysts too expensive and fragile?

### Specific recommendations and additions or deletions to the work scope

- It is suggested to have more collaboration with other members working on catalyst design as the  $\text{NH}_3\text{BH}_3$ -ionic liquid systems are being optimized.
- The project showed good progress and enhancing the  $\text{NH}_3\text{BH}_3$ -solution weight percent should be pursued while improving the kinetics.
- Optionally consider reducing the decomposition efforts in favor of the regeneration efforts. Should there be some deference to the Pacific Northwest National Laboratory and Los Alamos National Laboratory approaches on release?
- Minor suggestion: Chemists may like equivalents and engineers may like weight percent. Suggest using dual scales to satisfy both.
- More emphasis on dehydrogenation work versus the aminoborane regeneration.

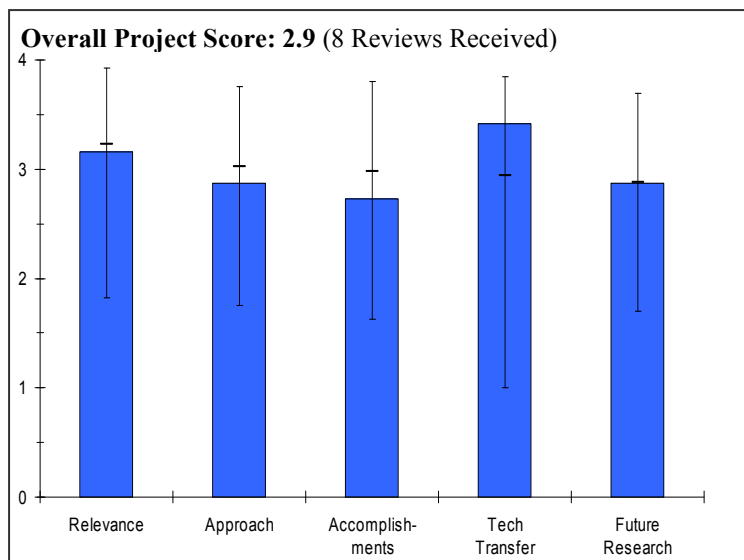
## Project # ST-08: Chemical Hydrogen CoE - Novel Approaches to Hydrogen Storage: Conversion of Borates to Boron Hydrides

Suzanne Linehan; Rohm and Haas

[Member of the Chemical Hydrogen Storage Center of Excellence]

### **Brief Summary of Project**

The overall objectives for this project are to 1) develop and advance novel hydrogen storage materials to meet the Department of Energy 2010 targets and with the potential to meet 2015 targets; 2) leverage expertise and experience across the Center; and 3) support the DOE Chemical H<sub>2</sub> Storage Systems Analysis Sub-Group. The Phase 1 goal is to define and evaluate novel chemistries and process for producing chemical hydrides. The emphasis will be on low-cost routes to regenerate sodium borohydride (SBH) from spent fuel leading to go/no-go review. The Phase 2 goal will be to identify cost and energy efficient pathways to “first fill” and regeneration for ammonia borane and other borane storage materials.



### **Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.

- The development of lower cost and scalable production methods for sodium borohydride (NaBH<sub>4</sub>) is key to the implementation of ammonia borane (ammonia borane) and other boranes as viable chemical storage media.
- This project plays a critical role, providing industrial expertise and perspective, to the Chemical Hydrogen Storage CoE.
- Low cost NaBH<sub>4</sub> synthesis from NaBO<sub>2</sub> is needed for first fill ammonia borane.
- Work is relevant to DOE objectives.
- Activity supports the initial processing of raw borate to storage precursor borohydrides.
- Focus on process and cost.
- Development of new chemistry leading to NaBH<sub>4</sub>.
- Work on NaBH<sub>4</sub> regeneration provided essential data for DOE Go/No GO decision in September 2007.
- After no-go decision for NaNH<sub>4</sub>, the project is aligned with hydrogen vision & DOE R&D objectives.
- Objective to select single pathway for low-cost NaBH<sub>4</sub> is important in the development of ammonia borane.
- The most relevant aspect of this project is the exploratory work towards low-cost sodium borohydride production.

### **Question 2: Approach to performing the research and development**

This project was rated **2.9** on its approach.

- Provided strong support for the sodium borohydride storage concept including potential regeneration pathways and played a key role in supplying important input to the sodium borohydride go/no-go decision process.
- Following the no-go decision this project has fully supported the redirection to study sodium borohydride preparation as a feedstock for other potential storage materials, e.g. amine borohydrides.



## HYDROGEN STORAGE

- Flow of approach looks good, identify possible processes, evaluate in the lab, and develop process models and costs.
- Process and cost models are being presented without key considerations or data (How do the three processes presented compare to each other, for example?)
- Open issues that may dramatically change the model includes: 1) What metal(s) and is metal recovery necessary (or could the metal oxide be left as a waste product); 2) What are product separation and work up costs; and 3) How large of a carbon footprint does carbo-reduction generate (syngas is a carbon burden as soon as it is burned).
- This project is focused on a single goal to identify more cost effective methods for large scale production of  $\text{NaBH}_4$  via analyses of alternative synthesis routes with limited laboratory scale testing to assess feasibility and limitation of the two approaches being considered.
- Emphasis has changed from regeneration of products from the hydrolysis of  $\text{NaBH}_4$  solutions to initial synthesis of lower cost feed stock material for making ammonia borane or other boranes.
- This project still emphasizes analytical evaluations of the general processes with relatively little assessments of more practical aspects such as efficient separation of reaction products to obtain pure  $\text{NaBH}_4$  and experimentally identify the by-products that could seriously impact either synthesis route.
- Very good experimental technique to demonstrate metal reduction pathway toward  $\text{NaBH}_4$  synthesis from  $\text{NaBO}_2$ .
- There are more uncertainties and practical barriers in the carbothermal reduction pathway than metal reduction pathway (proposed scheme is based on limited experimental data from Idaho National Labs).
- Comprehensive methodology established for costing.
- Rohm & Haas's contributions toward the development of low cost  $\text{NaBH}_4$  are important for first fill ammonia borane.
- Focus to look for best pathway for low cost  $\text{NaBH}_4$  is good.
- Focus on low-cost  $\text{NaBH}_4$  helps to meet DOE cost target.
- More technical results from the laboratory-scale production of sodium borohydride are necessary to meet the objectives of a scalable production process. There is too much emphasis on process modeling of production methods that may not be technically feasible.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- Has showed good progress in meeting roles and technical responsibilities as a fully participating member of the Chemical Hydrogen Storage CoE.
- Identification of potential process chemistries is an important accomplishment.
- Produced useful and helpful results in both energy and cost analysis for sodium borohydride go/no-go decision in September 2007.
- In the absence of specifics (metals under consideration or at least the parameters that would idealize a metal system) it is impossible to evaluate the proposed system(s).
- The investigators have demonstrated the feasibility of the metal-based reduction process to produce  $\text{NaBH}_4$  in good yields with at least one unidentified metal hydride. However, the cost of these hydrides does not seem to have been addressed nor has the methods necessary to separate  $\text{NaBH}_4$  from resulting oxides or other by-products.
- From the team presentation information, the carbothermal reduction reaction will require very high reaction temperatures with formation of copious quantities of carbon monoxide to be recovered as well as using the greenhouse gas methane as a feedstock. The team has given inadequate attention on impact of these issues to total system cost as well as the associated environmental and safety concerns.
- Important progress has been made on this project for the use of ammonia borane.
- Progress appears to be quite slow after September 2007.
- Cost analysis for two pathways show significant progress.
- There seems to be little progress towards finding scalable synthesis methods for sodium borohydride. The PI did not present much technical progress.

- Much of the process analysis work presented here was carried out previously in support of a Millennium Cell process.

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.4** for technology transfer and collaboration.

- Outstanding interactions and collaborations with members of the Chemical Hydrogen Storage CoE.
- The primary collaboration appears to be participation in the go/no-go decision on “hydrogen on demand” type systems. The input to the decision was highly collaborative.
- Most of the new work presented appears to be in-house work. However, that appears totally appropriate.
- The Rohm & Haas team has been interacting mostly with the two lead organizations of the Chemical Hydrogen Storage CoE but it has provided input regarding regeneration costs to the no-go decision for on-board hydrolysis of NaBH<sub>4</sub>.
- Has very close interactions with Chemical Hydrogen Storage CoE partners.
- Needed collaborations exist.
- There appears to be effective collaboration with other partners in the Chemical Hydrogen Storage CoE.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- Good plan for continued support of CoE activities including taking the lead in low-cost, scalable process for SBH (sodium borohydride) as precursor to ammonia borane.
- Key open questions have been noted above. It is unclear that key issues have been identified and approaches put into place to address these issues.
- To the point: a limited set of specific chemistries must be selected before a reliable process/cost analysis can be obtained. How high a priority is limiting the chemistries that will be considered?
- The team intends to assess both metal-based and carbothermal reduction routes for producing less expensive NaBH<sub>4</sub> for first fill ammonia borane usage.
- The emphasis still seems to be more on thermochemical trades and modeling assessments rather than laboratory testing of the reactions themselves and identification of practical and efficient methods for separating NaBH<sub>4</sub> from residual reactants and other by-products.
- Future work to support first fill ammonia borane and ammonia borane regeneration is relevant and crucial to ammonia borane hydrogen storage option.
- Plans are effectively built based on past progress.
- The plans for next year were not clearly presented. There appears to be more emphasis on experimental progress which is necessary to meet the project goals.

#### **Strengths and weaknesses**

##### Strengths

- The team provided systematic chemical production schemes for two reactions that may decrease cost for manufacturing industrial quantities of NaBH<sub>4</sub> as the intermediate material for ammonia borane and perhaps other boranes for chemical hydrogen storage options.
- An important issue if boron species are ever to become an accessible storage system.
- Approach considers both chemistry and cost in an interactive manner.
- Investigators are willing to move far away from the existing process to achieve breakout energy and cost efficiencies.
- They presented laboratory-scale test results that show significant yields of NaBH<sub>4</sub> can be achieved with at least one or two metal hydrides using the metal reduction approach.
- The analysis methodology tool developed for NaBH<sub>4</sub> production should be useful to assess ammonia borane and other storage materials.
- Step by step approach toward the cost estimation and regeneration of important material.

## HYDROGEN STORAGE

- Team of experts with broad range expertise.
- Strong experimental capability.
- Well established methodology for costing.
- The initiation has a good track record in this area.
- The project team has the capacity to perform very sophisticated process modeling and economic evaluation.
- Relatively modest budget for the work being performed.
- Strong internal team with extensive industrial experience and expertise in necessary chemical areas.

### Weaknesses

- Specific chemistries have not been elucidated.
- Much of the work presented appears not to involve new thinking, but is related to prior Millennium Cell related work.
- The cost analysis appears premature (and thus potentially not trustworthy), given the number of open questions related to chemistry and process.
- There was insufficient investigation into methods of separating NaBH<sub>4</sub> products for either reaction scheme.
- More laboratory testing and analyses of the reaction products should have been done to better establish practical yields and requirements for cost and energy effective synthesis.
- Inconsistent year over year progress.
- Impurity concern such as borazine has not been addressed.
- The stated experimental processes for sodium borohydride production (reactive milling and carbothermal) may not be suitable for large-scale production at levels that will enable the DOE program goals for hydrogen cost. From the equation for carbothermal production as shown in the presentation - delta G only goes negative at >1900 °C - can you really process large amounts of material at these temperatures?

### Specific recommendations and additions or deletions to the work scope

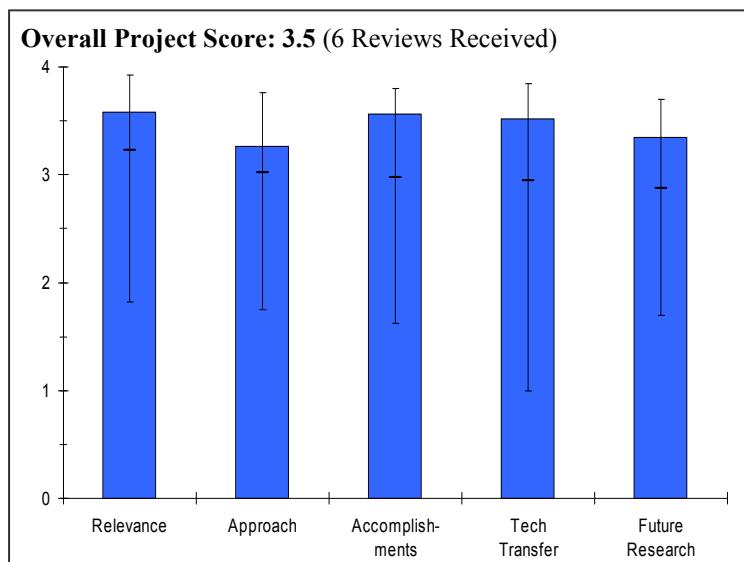
- Continue work by identifying specific chemical systems to evaluate.
- During the remainder of the project, the team should de-scope the system trade studies and cost estimating analyses until the actual chemical reactions and operating requirements are better established.
- The team should spend more time in the laboratory evaluating the reaction conditions and products generated by both synthesis schemes.
- If possible, consider lab-scale experiments to validate the carbothermal reduction pathway.
- The project should focus on validating the production processes before expending resources on process modeling.

**Project # ST-09: Main Group Element and Organic Chemistry for Hydrogen Storage and Activation***David Dixon; University of Alabama*

[Member of the Chemical Hydrogen Storage Center of Excellence]

**Brief Summary of Project**

The objectives of this project are to 1) develop promising approaches to chemical hydrogen storage for current and future Department of Energy (DOE) targets using computational chemistry and synthetic organic/inorganic chemistry; and 2) provide computational chemistry support (thermodynamics, kinetics, properties prediction) to the experiment efforts of the DOE Center of Excellence for Chemical hydrogen Storage to reduce the time to design and develop new materials that meet the DOE targets. Experimental focus is on organic and main group chemistries which may be able to perform better for release and regeneration by improving the energy balance. This will provide longer term alternatives.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.6** for its relevance to DOE objectives.

- This project couples strongly with many activities in the Chemical Hydrogen Storage CoE, and is helpful in understanding experimental results, guiding experiments towards new materials and catalysts, and plays a significant role in the success of the center.
- Addresses the DOE goals for hydrogen storage and regeneration of spent fuel.
- The theoretical work complements some aspects of the experimental activities in the center and is relevant to the DOE objectives.
- The project supports processes for regeneration of amino-borane which has a potential of high hydrogen release over 10 weight percent.
- The computational aspects of the project are highly relevant to a number of aspects of the Chemical Hydrogen Storage Center of Excellence activities.
- Highly relevant.
- How are system costs addressed by the project?

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- The University of Alabama team used a combination of molecular orbital theory and density functional theory implemented on advanced computer architectures to predict the electronic structure of molecules to obtain thermodynamic and kinetic information in support of the design of hydrogen storage materials and of regeneration systems – release and addition of hydrogen.
- Their technique for accurate and validated first principles computational chemistry is effectively incorporated in Chemical Hydrogen Storage CoE.
- The computational approach and the issues being addressed are excellent.

## HYDROGEN STORAGE

- The strength of this project include: 1) theory can certainly efficiently guide experimental work reducing R&D costs and efforts, and 2) efficiency issues are seriously considered. The weakness is that validation data has not been discussed in much detail.
- The experimental focus on carbene/TCNE and amino (imidazolo)-boranes is good, but must soon start to yield some significant improvements in hydrogen storage capacities.
- This project has the potential to link theoretical and experimental efforts at the same institution.
- Theory effort seems to be making bulk of contribution -- how does Arduengo tie in?
- The approach uses accurate quantum chemistry methods to explore a wide variety of materials' energetics. More accurate molecular orbital (MO) methods are used, as opposed to things like density functional theory (DFT). However, all calculations are for molecular systems, and some of the materials being simulated are condensed solid-state (or liquids). It would be useful to the other researchers in the computational hydrogen storage community (e.g., metal hydrides, or sorbent materials where DFT approaches are much more commonly used) to provide accurate comparisons between the errors associated with using DFT for the solid-state systems versus using MO theory for the molecular systems. And, it would be useful to characterize this "tradeoff" of errors for various types of systems (molecular solids, sorbent systems, as well as more typical ionic solids such as complex hydrides), to really try and understand where DFT approaches suffice, and where they do not.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.6** based on accomplishments.

- Examples of significant accomplishments and impressive body of knowledge generated so far include: (1) exploration of regeneration schemes and of new chemical storage systems, (2) improvement of efficiencies, (3) examining pathways to improved kinetics and (4) contribution to fundamental knowledge about mechanisms (etc.)
- The accomplishments include predicted reliable thermodynamics for more than 500 reactions for regeneration schemes. Impressive productivity!
- Many processes for amino-borane regeneration have been precisely evaluated. This information is considered to be effective to choose appropriate reactions and to analyze reaction mechanism in Chemical Hydrogen Storage CoE.
- Valuable theoretical results associated with ammonia borane regeneration.
- Produced a huge amount of data; large number of reactions, thermodynamics, kinetic mechanisms, catalysts, etc., surveyed.
- Alane shown to be an effective catalyst for hydrogen release from  $\text{NH}_3\text{BH}_3$ , but this work has also produced useful information for alane regeneration. A very significant synergy.
- Nice results for the Carbene/Cyanocarbon (particularly as it pertains to volumetric density).
- Interesting results on possible CBNH materials.
- While the accomplishments of the theoretical work are obvious, the experimental contributions are less well defined.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.5** for technology transfer and collaboration.

- Very large number of external collaborations. Seems to be the "central hub" for theory within the Chemical Hydrogen Storage CoE.
- Excellent theory calculation interactions with other members of the center.
- Theory work is clearly closely coupled with experimental work being done by center partners.
- Good interactions with partners within the center.
- Good collaborations with other team members.
- Collaboration with Los Alamos National Laboratory is effectively conducted in experimental confirmation of their prediction and process design at Los Alamos National Laboratory.
- However, a discussion on how theory and experiments interact precisely within this project should be provided.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.4** for proposed future work.

- Use computational chemistry to support overall center efforts in hydrogen release, spent fuel regeneration, new concepts including alternative inorganic and organic compounds, and mechanisms for hydrogen release and spent fuel regeneration. Improve hydrogen storage by mass stored and kinetics for hydrogen release for main group substituted organic compounds.
- Future work appears ambitious; however the team has generated an impressive amount of results so far and very likely will be able to do the job.
- Their prediction is still very important to the center.
- Future work includes studies of solids using density functional theory, and will systematically study 25 different exchange correlations to find which one works best for the solids.
- Would be nice to see the computations take on more of a "predictive" aspect by leading experiments in new directions. At the moment it appears as though the role of computation is strictly to \*follow\* experiments by "putting out fires." This is OK, as clearly computation is making a large contribution by operating in this fashion, but I think even larger impact would be possible by having computation take the lead in some areas.
- Seems to largely prioritize the huge amount of potential computations based on what is most urgently required by experimental colleagues.
- Computational future work looks well-focused.
- Experimental future work looks vague.

**Strengths and weaknesses**Strengths

- Appears to have a very strong and good connection with the experimental groups; maintains good contact, and gives very fast turnaround.
- Impressive body of knowledge obtained in direct support of DOE storage objectives.
- Efficiency and energetics are seriously considered by the team.
- Ability in highly accurate and validated first principles computational chemistry.
- Effective interaction with experimental groups.
- The theory and calculation portion of the project is very strong and useful to the center activities.
- Predicting spectroscopic properties for comparing with experiments.
- Good coupling with experiments.
- Strong communication with other center projects.

Weaknesses

- Validation of theory work has to be clearly established and discussed, interaction between theory team and experimental partners should be clarified.
- Although the accurate molecular properties are important, the overall accuracy of prediction will strongly depend on the model selected for simulation. The prediction from the model systems which better represent experimental systems may be more useful than the accurate molecular orbital calculations.
- The experimental portion of the project does not appear to be producing significant improvements in hydrogen storage capacity materials.
- Strength of contributions of Arduengo's project unclear.
- Very large budget for what appears to be largely a single PI project.

**Specific recommendations and additions or deletions to the work scope**

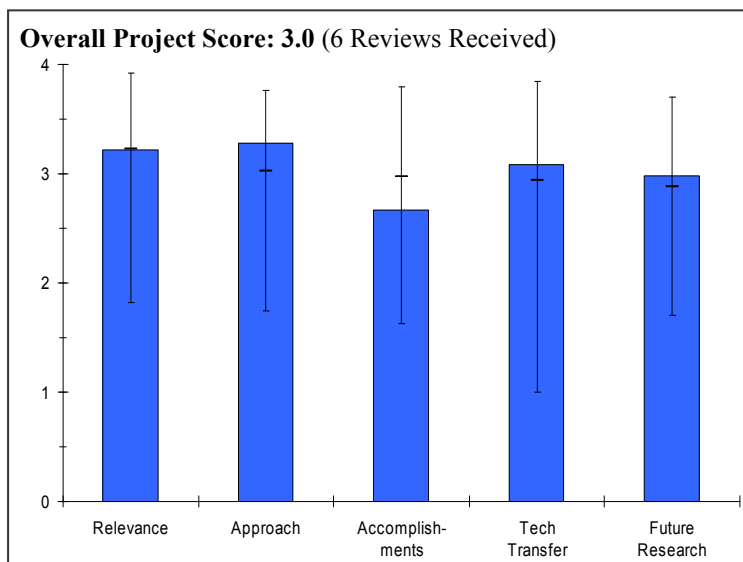
- Some validation of the simulations/calculations should be discussed in more details to show feedback between theory and experiments.
- Unless significant improvements are obtained soon, consideration should be given to a no-go decision on the continuation of the carbene/TCNE and amino (imidazolo)-borane work.
- Clarify role of Arduengo.

**Project # ST-10: Solutions for Chemical Hydrogen Storage: Hydrogenation/Dehydrogenation of B-N Bonds***Karen Goldberg; University of Washington*

[Member of the Chemical Hydrogen Storage Center of Excellence]

**Brief Summary of Project**

The Center-wide objective of this project is directed toward the use of amine borane (BN materials) as on-board vehicular hydrogen storage materials. The University of Washington objectives are to: 1) develop cost-effective metal catalysts for the dehydrogenation of BN hydrogen storage materials; 2) optimize catalysts to meet the Department of Energy target goals of hydrogen discharging rates from BN materials; and 3) identify and develop new BN materials to address challenges for automotive hydrogen storage materials.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.

- Designing catalysts for enhancing the performance of high capacity materials is related to the DOE objectives in increasing the dehydrogenation rates.
- Improved catalysts to increase the kinetics of ammonia borane-type hydrogen storage materials are important to meet storage targets.
- The exploration of combined exothermic and endothermic chemical approaches may lead to the possibility of on-board rehydrogenation.
- Amine-boranes are of no interest without good catalysts for both hydrogenation and dehydrogenation.
- The organometallic chemistry presented here is fundamental to generating a robust low cost catalyst for dehydrogenation.
- New CBN substrates may potentially dramatically improve the energy balance in the ammonia borane type of systems.
- Work is relevant to DOE objectives.
- Ammonia borane has high material capacity and the potential to meet DOE 2010 targets.
- New CBN materials have the potential for direct rehydrogenation on-board.
- Search for optimized catalysts is relevant.
- Finding solutions to ammonia borane regeneration, catalysis and liquefaction are key to the center objectives. These three subjects are the fundamental issues facing ammonia borane materials today. Perhaps the PI is stretched thin by working on three subjects at once.
- CBN materials work appears to be redundant with earlier work by Air Products.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- Original catalyst employed expensive iridium as the backbone - recent attempts have tried to replace iridium with cheaper metals such as cobalt with limited success.
- PI should incorporate some modeling guided theory to aid in catalyst design.
- The approach is focused on key issues.
- A good interplay of synthesis, calculation, and kinetic analysis is provided.

- Synthesizing low cost catalysts is important to the ammonia borane hydrogen storage option.
- What is the fall-back position of cobalt turns out not to work?
- What is the contingency plan if modifying ligand structure fails to yield a viable catalyst?
- Approach seems to have a significant trial-and-error component.
- The project indentified the barriers in the system studied and made decisions to downselect or modify approach.
- The idea to develop CBN materials that couple exothermic dehydrogenation BN bond to endothermic dehydrogenation CC bond is good. However, the benefit of such coupling may be reduced significantly if the dehydrogenation temperatures of these two bonds are too far apart. So, it is necessary to look at not only delta H but also reaction temperatures in the design of CBN materials.
- Is there a go-no/go decision point on the CBN materials?
- PI should reduce efforts on CBN regeneration and concentrate on catalysts.
- Liquid ammonia borane fuels have many advantages over solid fuels.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- PI made tremendous progress in synthesizing new catalysts and approaches - unfortunately they do not work as well as the original iridium systems.
- The previous and current catalysts still only work to remove the first equivalent of hydrogen- 2nd and 3rd equivalents are required if capacity targets are to be approached.
- Good progress on lowering the metals cost.
- Question: While the indicated tridentate ligands work, have you investigated the possibility that the first row systems may not require a tridentate system?
- It appears as though little progress has been made with catalyst development.
- Determined that cobalt catalyst is not stable at temperatures above 60°C.
- The technical approach in manipulating the ligands and moving from the iridium based catalyst is a good approach, however, as the catalysts are designed, the metals used need to be cheap and abundant.
- The attempts with development of the cobalt catalyst are very good, but the possibility exists that cobalt will not work, based on the present results.
- Determined that mixed ammonia borane/MeAB polymers are not suitable for direct rehydrogenation due to high exothermicity.
- Reasonable progress on synthesizing and investigating new BCN substrates.
- Developed concept and synthetic methods to obtain CBN materials.
- Considering the CBN compounds as new storage materials is good however, concerns on the potential formation of gases other than hydrogen, i.e. NH<sub>3</sub>, CH<sub>4</sub>, B<sub>2</sub>H<sub>6</sub> which could occur.
- How do the bond energies of B-H, N-H, and C-H compare? Is it possible to lower the C-H bond energy?

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- PI working well with the key strong players in aminoborane research (Los Alamos National Laboratory and Pacific Northwest National Laboratory).
- Strong collaborative interactions with theory group.
- Good interaction with Chemical Hydrogen Storage CoE partners and university.
- Suggested to have more visible collaboration with other members, i.e. for the CBN compounds, collaboration with the theory group and Air Products.
- Is there any benefit in strengthening interactions with Los Alamos National Laboratory for catalyst screening?
- For the CBN materials there is clear overlap (and possible duplication) with prior work by Air Products (Note: Air Products work was on CN materials.) However there appears to be no communication or collaboration with Air Products in acknowledgement of this.



### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- PI should defer CBN materials to Air Products or collaborate with them.
- PI should provide reviewers with some guidance as to the robustness of a ligand based material in such an ammonia borane environment.
- This is a strong program. It is pointed in the right direction with a promising trajectory.
- The researchers should include the determination of turnover numbers since the stability of the catalyst is an important unexplored parameter. It could turn out for example that the iridium catalyst is less expensive than the cobalt catalyst if they have widely different turnover numbers.
- Continue to develop and optimize inexpensive first-row transition metal catalysts.
- What is the plan to get more than one hydrogen equivalent from the cobalt-based catalysts?
- The development of CBN materials that meet the dehydrogenation and rehydrogenation criteria will be a significant breakthrough for the ammonia borane hydrogen storage option.
- PIs need to also consider cost of CBN materials in future work.
- The synthetic routes for the formation of CBN compounds need to be clarified. Also, the vapor pressures of the compounds prepared need to be tested.
- Given the pay-off if potentially on-board reversible CBN materials could be discovered, synthesized, and optimized, perhaps this should be a higher priority than the catalyst work.
- CBN work should be halted until a unique research plan (distinct from prior Air Products work) has been developed.

### **Strengths and weaknesses**

#### Strengths

- Good synthetic capability.
- Clever ideas related to reaction mechanism and substrate design.
- Key understanding of the underlying coordination chemistry.
- Good understanding of chemistry and ammonia borane dehydrogenation/rehydrogenation issues.
- Close collaboration with center partners.
- Research is very well focused.
- Synthetic approaches and catalyst designs.
- Attempts to develop non-precious metal catalysts.
- Exploration of novel CBN hydrogen storage materials.

#### Weaknesses

- Ligand approach and complex nature of catalyst might decrease the overall robustness. PI does not seem to have a plan or modeling guided approach to determine if cheaper metals can be substituted for iridium.
- A wider view of ligand systems should be considered.
- It is suggested to have more collaboration with other members as mentioned above.

### **Specific recommendations and additions or deletions to the work scope**

- Continue as is.
- The project showed good progress in designing catalysts and it's recommended to keep the project.
- Consider dehydrogenation/rehydrogenation temperatures of B-N and C-C bonds in search for the most favorable CBN materials.
- Provide some cost estimates of CBN materials.
- More emphasis on the CBN materials.
- CBN work should be halted until a unique research plan (distinct from prior Air Products work) has been developed. Note: Air Products work was on CN materials.
- Air Products is investigating similar CBN type materials. PI should coordinate activities with Air Products.

**Project # ST-11: Chemical Hydrogen Storage using Ultra-High Surface Area Main Group Materials & the Development of Efficient Amine-Borane Regeneration Cycles**

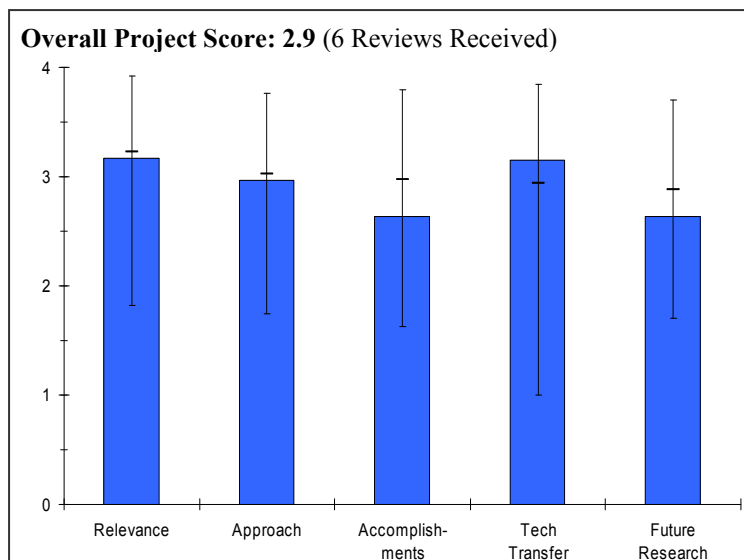
*Philip Powers; University of California - Davis*

[Member of the Chemical Hydrogen Storage Center of Excellence]

**Brief Summary of Project**

The objectives of this project are to: 1) provide new materials, compounds and support for chemical regeneration of amine-boranes or boran amides from B-X (X = halide or oxide) compounds; 2) develop a method of regenerating amine-boranes from spent fuel with use of a metal formate/hydride cyclable system; 3) develop light element hydride nanomaterials for spent chemical hydride regeneration such as ammonia-borane “AB” regeneration; and 4) enhance the hydrogen release for chemical hydrides such as ammonia-borane “AB” with light element hydride nanoparticles.

**Question 1: Relevance to overall DOE objectives**



This project earned a score of **3.2** for its relevance to DOE objectives.

- Strength: The project is relevant to regeneration cycles for chemical hydride materials and release mechanisms (and suppression of foaming) that could lead to a storage strategy that meets the DOE volume and weight targets.
- Strength issue: choice of cheap precursor materials.
- The work on light element nanoparticles for hydrogen evolution is strong science directly related to DOE objectives.
- The work of metal formates to hydrides is consistent with the original program goals, but has recently been jettisoned in revised goals based on thermochemical analysis of the proposed cycle.
- Though the metal formate work is not of current interest, the chemistry studied in these systems provides important basic science; so, there is a positive spin-off.
- The objectives of the project are to develop efficient methods to regenerate amine-boranes or boron amides, in support of the center’s selection.
- This project appears to have been successfully re-directed after the no-go decision on the silicon-based hydrides.
- The PI is pursuing innovative chemical cycles for ammonia borane off-board regeneration consistent with much needed efforts in establishing the practicality of chemical hydride approaches.
- A key factor in the inherently complex regeneration of ammonia borane is to incorporate low-cost chemical precursors in order to meet or exceed DOE cost targets. The PI has given a significant amount of thought to this challenge.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- The light nanoparticle approach for hydrogen evolution is excellent, but not well understood.
- An understanding of the chemical mechanisms associated with the hydrogen release process is needed.

## HYDROGEN STORAGE

- The work that addresses enhanced hydrogen release from ammonia borane by incorporating nanoparticles of boron nitride (BN) appears to immediately solve the foaming problem while reducing the temperature for desorption.
- What will be the basis for hydride formation?
- The team used main group formate small molecules or hydride nanomaterials as low cost reagents to convert B–O or B–X in one step to B–H.
- The regeneration aspects are closely interfaced with theoretical predictions.
- In the area of regeneration, the exploration of metal formates as ammonia borane regeneration precursors is intriguing and potentially viable for select metals. There are, however, unexpected thermodynamic consequences which the PI has encountered relative to the conversion of metal formate intermediates to the starting material via benzene dithiol (*vis-à-vis*, tin diformate). Further complications have been discovered with the choice of substituent for the metal formate which inhibits decomposition of the metal formate. Overall, the approach is clever as it permits exploration of a variety of substituents and establishes priorities for parallel modeling efforts prior to experimentation.
- No information was provided as to whether or not other hydride generation mechanisms would be explored now that the formate system has been abandoned.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.6** based on accomplishments.

- The hydrogen evolution side of the project appears on track with several "initial hits".
- More information on the effects of nanoparticles on ammonia borane hydrogen release kinetics would have been useful, since this appears to be a positive result.
- Consideration: project has been substantially modified recently so performance in relative terms is good if this is factored in.
- The technical accomplishments of this project are impressive. However, greater diligence is needed in screening the potential barriers associated with 1) tin monoformate substituent-interactions and 2) decomposition of the substituted tin monoformate. In this context, computational calculations need to progress more rapidly.
- Initial program goals were reasonably on track for being met, but has not actually been met.
- No information on reorientation of the program was provided.
- The research confirmed the Pacific Northwest National Laboratory prediction that boron formates eject carbon monoxide rather than carbon dioxide.
- Regeneration work, although useful, does not appear to have produced interesting results yet.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- Good inter-partner communication.
- Premature to evaluate technology transfer.
- The teams work closely with the other center members, including University of Alabama and Pacific Northwest National Laboratory groups.
- Close interaction with the theoretical portion of the Chemical Hydrogen Storage CoE.
- The choice and number of technical partners is consistent with the level of effort and expected outcome of the project.
- As mentioned above, greater interaction and collaboration with University of Alabama is needed to progress further in the modeling efforts.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.6** for proposed future work.

- Nanoparticle effects on hydrogen release of ammonia borane are the most interesting aspect of the future work.
- Future work in the area of hydrogen release from ammonia borane is appropriate based on the accomplishments up to this point.
- Further work on light nanoparticles on the release rate and foam reduction seems worthwhile.
- Reasonable program goals on hydrogen evolution catalysts.
- Plans build on the previous progresses.
- No information provided on the hydride synthesis project.

### **Strengths and weaknesses**

#### Strengths

- The project has adapted its task list to results and made go/no-go decisions when required and has proposed adequate modifications (to direct hydrogenation).
- Role of project partners is clear (e.g. nanoparticles input, energetics) and their input has been considered by the team.
- Preliminary results show positive effects of nanoparticles for release and foaming issues.
- Elimination of boron formates as hydride precursor (no carbon monoxide).
- Strategy for regeneration and release objectives seemed sound initially.
- Good science.
- Strong synthetic chemical component.
- Interesting initial observations with regard to light nanoparticle effects on hydrogen evolution.
- Nanoparticle effects on hydrogen storage.
- Innovative concepts for an ammonia borane regeneration cycle which take into consideration the cost targets (i.e., cheap starting materials), while simultaneously advancing new knowledge in an interesting field of chemistry.
- The project has demonstrated success in establishing low-cost routes to synthesis of target chemical precursors and in synthesizing a select number of such precursors.

#### Weaknesses

- In absolute terms, overall progress to meeting DOE objectives is modest considering the lifecycle of the project.
- Energetics of formate.
- Little understanding of nanoparticle effects.
- No revised goals given for hydride formation chemistry.
- The efficiency of the tin-formates route is questionable as the hydride formation requires hydrogen to migrate from carbon site to tin site via an O-bridge.
- Ammonia borane regeneration work may not lead to much that is useful for the regeneration process.
- The project plan does not take better advantage of computationally-based screening approaches for the selection of viable chemical precursors.

### **Specific recommendations and additions or deletions to the work scope**

- In the area of regeneration, the PI should consider adopting computations as a means of screening the choice of metal and substituent in the metal-formate-based regeneration cycle.
- More emphasis on nanoparticle effects on release.
- Recommend augmenting computational efforts for screening and predicting energetics associated with metal formate decomposition.
- Formate portion of project should be defunded unless a revised project is submitted for new hydride formation chemistry.

**Project # ST-12: Hydrogen Storage in Metal-Organic Frameworks**

*Omar Yaghi; University of California – Los Angeles*

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

The objectives of this project are to 1) research the relationship between MOF structure and binding energy (low pressure measurements at various temperatures); 2) conduct high pressure hydrogen adsorption measurement at room temperature (impregnation of polymer and metal complex); 3) move toward the practical use of MOFs (cycling and kinetics of hydrogen charge/discharge) and 4) coordinate with theory (prediction of hydrogen uptake capacity).

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.6** for its relevance to DOE objectives.

- Critical to develop an adsorbent designed from the ground up.
- The target of the project to explore the metal organic framework working at room temperature is adequate.
- This is very important work on a promising class of materials critical to the hydrogen initiative.
- While relevant and aligned with the Program, the presented work looks like attempts to repeat earlier success and does not seem to be poised to address the major barriers that were identified in the investigator's earlier successes.

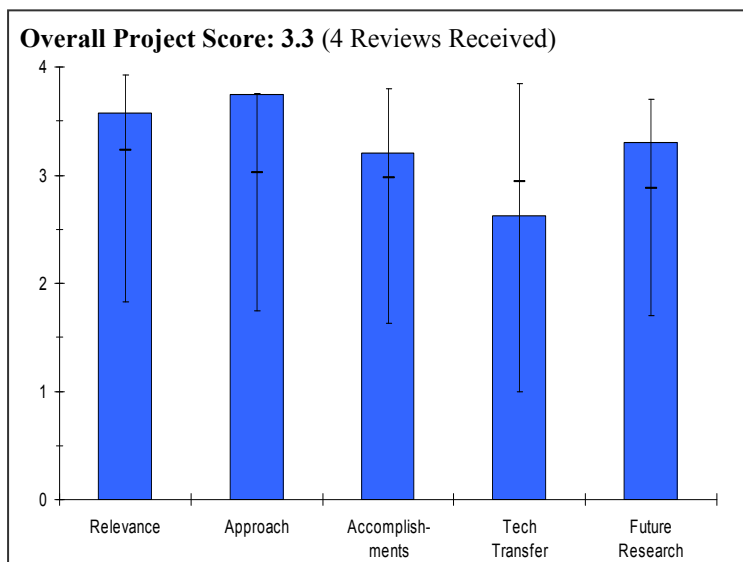
**Question 2: Approach to performing the research and development**

This project was rated **3.8** on its approach.

- Had a diverse comprehensive line of attack.
- The approach of “materials development” is proper.
- The approach is sound, and seeks to reach DOE system targets and is sharply focused on them (page 6-7 of the presentation).
- The group has tackled practical considerations concerning the actual use of sorbents (uptake, release, effects of impurities).
- It is clear that using metal organic frameworks for storage will require moving beyond incremental improvements, and pursuing substantially different/additional concepts. This project is working on such different/additional concepts.
- Intentionally developing interpenetrating networks that will increase the density of higher-energy unsaturated-metal binding sites could be one such different/additional concept, using polar atoms/bonds in the organic framework could be another, developing hydrogen-dissolving organics in polymer-filled metal organic frameworks and in carbon organic frameworks could be a third. Lithium incorporation could be a fourth.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.2** based on accomplishments.



- Marries theory with experiment.
- Good improvement in ambient temperature performance.
- Obtained hydrogen capacity at room temperature with room to improve.
- Substantial progress has been achieved over the last 5 years (volumetric density having risen from 14 to 58 gH<sub>2</sub>/L @50 bar and 77K).
- Preliminary work on potential chemisorbents initiated.
- Good cycling uptake/release, good reliability, fast charge rate.
- While providing materials of general interest, none of the different/additional concepts above has achieved, nor appears poised to achieve, the breakthrough needed to overcome the hydrogen binding energy / capacity barrier.
- The reported results for interpenetrating networks are both encouraging and discouraging. Encouraging in the sense that somewhat higher binding energies appear to result, discouraging in the sense that the improvement in binding energy and storage capacity appear to be incremental. Agreed, there is indeed an immense number of interpenetrating network systems that could be made and studied, but right now it appears that the concept is already close to "maxing out" its impact.
- Successful formation of materials that incorporate unencumbered lithium centers would be interesting, but so far the path is unclear.

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.6** for technology transfer and collaboration.

- Collaboration with four professors and BASF.
- In the presentation, collaboration with industry and academia was mentioned little.
- Input from the theory group of Goddard et al. guides R&D experimental efforts.
- Coordination with other program participants should be explained more clearly.
- Not clear that this project is closely collaborating or cooperating with any other. But neither is it clear that such would lead to more rapid advances.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.3** for proposed future work.

- Good plan.
- The future work is well organized. Especially, collaboration with computational scientists is effective to explore materials.
- Lithium-enhanced compounds show promise (theory; comment on slide 26: please indicate pressure and temperature info when mentioning uptake).
- Including lithium or other "lithium-like" open centers in the framework appears to be the most ambitious new/different concept in the future plans for this project, other parts of its future plans look incremental. Based on other presentations from the Program, such "open metal" centers appear to be the "final frontier" of sorption-based hydrogen storage, and this project appears better poised than some others to achieve materials that have such "open metal" centers.
- That said, a more systematic and determined approach to preparing "open metal" centers would be preferred. There is some old literature on preparing "coordinatively unsaturated" metal centers by first preparing ether-solvated compounds, using NEt<sub>3</sub> to displace ether (because the ether could not be removed by vacuum alone), then using vacuum and gentle heating to remove N.

#### **Strengths and weaknesses**

##### Strengths

- Good, dedicated researchers.
- Much work delivered.
- The research on metal organic frameworks has been initiated by this group and they have successfully prepared various metal organic frameworks.

## HYDROGEN STORAGE

- The team has performed an impressive amount of very relevant and interesting work which has had a considerable impact on the field.
- These investigators opened the field of metal organic frameworks and should have greater appreciation for the types of materials that are possible, and what modifications they can tolerate.

### Weaknesses

- Room temperature hydrogen capacity has not been improved.
- The field of sorptive hydrogen storage needs a fundamental breakthrough; the inclusion of additional open metal centers (whether by lithiation etc. or by interpenetration) seems the most likely way to achieve such a fundamental breakthrough; but do not see this receiving the emphasis it could warrant.

### Specific recommendations and additions or deletions to the work scope

- Should indicate the effect of different materials and processes on hydrogen uptake. Do these have a major effect on engineering properties?
- Combination of theory and experiments is strongly recommended.
- Per above, put additional emphasis on increasing density of open metal centers.

**Project # ST-13: Carbide-Derived Carbons with Tunable Porosity Optimized for Hydrogen Storage**

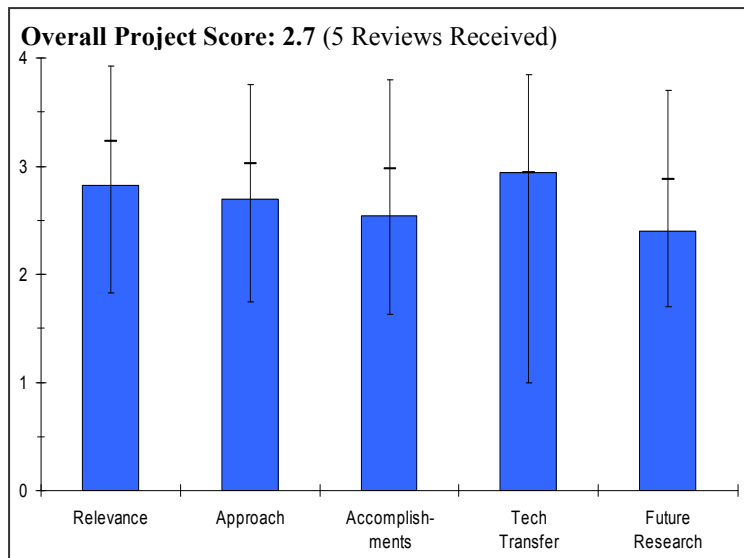
Jack Fischer, presenting, University of Pennsylvania; Yury Gogotsi, Co-PI, Drexel University; Taner Yildirim, Co-PI, NIST

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

The objectives of this project are to:

- Develop and demonstrate efficient, durable and reversible hydrogen storage in carbide-derived carbons (CDC) with tunable nanoporosity (2004-2005).
- Determine the optimum pore size for hydrogen storage using experiment and theory (2005-2006).
- Identify post-processing strategies and catalytic additives which maximize the performance of CDC-based hydrogen storage materials, using experiment and theory (2006-2007).
- Finalize the design of a CDC-based H<sub>2</sub> storage material that meets 2010 DOE performance targets and commercialize it (2007-2008).

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.8** for its relevance to DOE objectives.

- This project seeks to develop carbide-derived carbon (CDC) powders as hydrogen storage materials with higher levels of performance compared to other types of adsorption materials such as activated carbons or metal organic framework compounds.
- While this is an independent project outside of the Hydrogen Sorption Center of Excellence (HSCoE), it shares common objectives and approaches particularly with respect to increasing both hydrogen storage capacity for the mass and volume targets as well as increase operating temperatures towards ambient conditions.
- The objectives are well aligned with DOE R&D objectives.
- It is great to see the PI address scale-up issues in the project scope.
- Concern: Investigators have identified importance of small pores, but have not shown that even optimal materials would have a volumetric capacity sufficient to meet DOE objectives.
- To their credit, investigators have one of the best-understood "amorphous carbon" systems known to date, which should enable more sophisticated study and better understanding of such materials than will be provided by competing projects.
- CDCs might not exceed the gravimetric densities of activated carbons.
- CDCs need high temperatures and aggressive leaching chemicals [for synthesis].
- Research on new high surface area carbon materials is important for reaching the program goals for hydrogen storage.

**Question 2: Approach to performing the research and development**

This project was rated **2.7** on its approach.

- The prior empirical synthesis approach is now being supplemented by more theoretical modeling and neutron scattering studies via the National Institute of Standards and Technology [NIST] partner as well as exploring metal doping and alternative "activation" processing to improve capacity and hydrogen binding.



## HYDROGEN STORAGE

- The idea of tuning pore shape by choosing different precursors is really good.
- The "designer" pore structure approach is good in theory. It needs to be experimentally validated.
- Post treatment can create more pore volume. However it is important to know the size of the pores created in this step.
- It is not clear how to achieve the optimum pore size.
- The binding energy and volumetric uptake are not addressed.
- Although they have identified small pores as necessary, their route to developing materials with more such pores isn't clear.
- Sodium doping doesn't seem to have accomplished much, nor have preliminary experiments in titanium loading; what do they plan if further experiments do not pan out?
- The project has taken a comprehensible approach to design and create new CDCs.
- Usage of energy intensive temperatures and aggressive leaching chemicals is a critical path.
- The approach of activating carbide-derived-carbons (CDC) with CO<sub>2</sub> or KOH does not generate materials with any added benefits for hydrogen storage vs. conventional activated carbons. The significant added expense of CDC over activated carbons calls into question the logic of the PI's approach.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.5** based on accomplishments.

- The investigators have shown that KOH activation increases the excess hydrogen gravimetric capacity up by ~40 percent for adsorption at 77K primarily due to greater surface area and pore volume. However, binding energies of hydrogen have about the same values as the capacity was not improved at room temperature during limited assessments.
- Researchers looked into possible improvements via metal dopants where serious issues remain with efficient doping and blocking of the porous structure within the CDC powders that severely limited storage capacity.
- The PI does not have enough data to show the pore size distribution which is critical to correlate the data.
- It is not clear how doped titanium is distributed on the CDC.
- When comparing Ti-doped TiC-CDC with activated carbon, it is necessary to plot both of them on the same chart at same temperature (Slide #14).
- Within the scope of this project, there have been some interesting technical accomplishments, although, continued work within this scope appears to offer only diminishing returns. Were this project to be continued, this reviewer would recommend radical changes in scope.
- The presentation did not show comparisons between "old" and "new" results.
- It stayed unclear, whether chemical surface modifications could be successfully applied to CDCs.
- Usage of alkali metal doping showed "slight" or even "significant" reduction of gravimetric densities.
- The PI demonstrated progress in surface modification that increased the heat of adsorption. This is important for realizing practical hydrogen storage materials.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.9** for technology transfer and collaboration.

- The three partners within the team complement each other in conducting theoretical analyses and experimental assessments of the CDC materials as improved hydrogen storage materials.
- The involvement of the Spanish group with KOH activation led to significantly enhanced sorption capacity at 77K.
- Some collaboration exists but need more collaboration to achieve a fundamental understanding of the materials produced.
- It was not clear what parts of this project were done at which of the partner institutions. This could be because the partnership is working very well, or because the partnership is not working at all - difficult to judge.
- There could be significant advances were this team to collaborate with the Sorption COE on using their materials in "spillover hydrogenation" studies.
- The project has very good collaborations with a remarkable fraction of international and industry partners.

- Project has found an industry partner, who tries to scale-up the material manufacturing.
- There is little evidence of significant collaborations for this project.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.4** for proposed future work.

- Planned future work is consistent with past study with appropriate characterization and hydrogen adsorption measurements on titanium-doped CDC and investigation to alternative surface treatments to increase surface areas and porosities without compromising other properties.
- Lack of general understanding on how activation protocol can impact the pore size distribution which is critical for improved hydrogen uptake.
- 100 mg sample size is too small to obtain some meaningful results.
- Other metals than titanium should be explored.
- Continued work within the project scope as outlined in this presentation is likely to face diminishing returns. Optimization is very unlikely to greatly increase volumetric capacity.
- The project tries to fine-tune their materials with the already existing tools and measures.
- It stayed unclear, which extra measures would be applied to promote the project towards the envisioned objectives.
- It stayed unclear, how results of the theoretical modeling can be successfully applied to the production and generation of improved materials.
- It is doubtful, whether the project will reach its key milestone of "getting excess material capacities at the level of the best metal organic frameworks" within the short remaining project time and the remaining budget.
- The PI did not clearly present how the materials development will address overcoming the barriers of low adsorption enthalpy.

#### **Strengths and weaknesses**

##### Strengths

- The team has adapted its preparation and activation processes to enhance 77K sorption capacities.
- There is currently greater inclusion of theoretical efforts and structural characterization to assist in interpretation of adsorption of the CDC powders and to search for additives to increase hydrogen binding energies.
- CDC approach provides a valuable path of producing sorbent material with well controlled pore size distribution.
- The CDC materials and activation procedures offer some of the best understood of the "amorphous carbons" under study.
- Results of the project are showing an alternative way of possible hydrogen storage materials through hydrogen absorption.
- The PI has a very good understanding of microporous carbons and adsorption.

##### Weaknesses

- The best 77K sorption capacities are still equivalent to most activated carbons and metal organic framework compounds for hydrogen desorption that is leading to enhance performance wanted by DOE.
- Lack of fundamental understanding of how post-treatment can affect the material property design.
- Metal doping and further optimization of pore size distributions do not appear to offer a path to significantly improved hydrogen storage performance. More radical experimentation with the activated CDC materials could however provide new leads.
- For the preparation of CDCs, usage of chlorine at high temperatures up to 1200°C is needed. For the chemical activation, e.g. KOH at 1000°C is needed.
- The necessity of using leaching materials at high temperatures as a crucial process step is energy demanding.
- The necessity of using leaching materials at high temperatures as a crucial process step is raising safety issues.
- As mentioned by the project's presenter, CDCs might one day match the gravimetric densities of activated carbons, but will not beat them significantly.

## HYDROGEN STORAGE

- CDC are likely to be expensive and do not demonstrate any significant advantage over activated carbons for hydrogen storage.

### **Specific recommendations and additions or deletions to the work scope**

- Independent characterizations of pore size distribution and hydrogen occupancy is still needed.
- Additional external collaborations especially having in-situ nuclear magnetic resonance assessments of pore size with the University of North Carolina would benefit this effort.
- Team should measure adsorption isotherms at different temperatures to determine heat of reaction on the CDC materials especially to assess whether metal doping or surface processing can lead to stronger chemical bonding.
- Recommend that collaboration be started to characterize pore and slit dimensions via in-situ nuclear magnetic resonance.
- Try "spillover hydrogenation" with the activated CDC materials - what happens?
- Addition of an evaluation of needed process energies, ingredients and safety hazards during production of CDCs. Comparison of that evaluation with other sorption materials, especially metal organic frameworks and activated carbon.
- If CDCs might not exceed the gravimetric densities of activated carbons, the project should point out much clearer where the advantages of their CDCs are.
- The PI should focus on understanding the observed effects of surface activation on the heat of hydrogen adsorption. This may lead to materials with better adsorption properties.

**Project # ST-14: Effects and Mechanisms of Mechanical Activation on Hydrogen Sorption/Desorption of Nanoscale Lithium Nitrides**

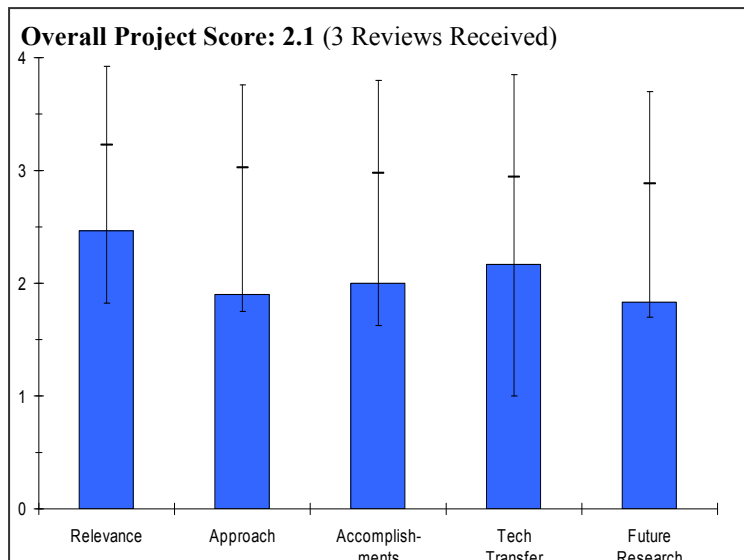
*Leon Shaw; University of Connecticut*

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

Project objectives in FY 07 were to: 1) identify hydriding/dehydriding reaction mechanisms and rate-limiting steps of (LiNH<sub>2</sub>+ LiH) systems; 2) enhance hydriding/dehydriding rates via nano-engineering and mechanical activation; and 3) improve hydriding/dehydriding properties via thermodynamic destabilization.

Objectives in FY 08 have been to: 1) further improve hydriding/dehydriding properties of (LiNH<sub>2</sub>+ LiH) systems via nano-engineering, mechanical activation, and thermodynamic destabilization; 2) establish the atomic level understanding of the reaction mechanism and kinetics of mechanically activated, nano-engineered (LiNH<sub>2</sub>+ LiH) systems; 3) perform nano-engineering and mechanical activation of LiBH<sub>4</sub>-based materials; and 4) demonstrate hydrogen uptake and release of (LiBH<sub>4</sub> + MgH<sub>2</sub>) systems with a storage capacity of ~ 10 wt% H<sub>2</sub> at 200°C.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.5** for its relevance to DOE objectives.

- The base material has a very high desorption temperature and a gravimetric capacity that will not achieve 2010/15 targets. Ball milling to decrease the thermodynamics has been thoroughly investigated with limited success and many drawbacks.
- LiNH<sub>2</sub>/LiH system: The MHCoe has discontinued consideration of this system due to low plateau pressure and slow kinetics, therefore the studies are relevant only to the extent that understanding this system will lead to improving other, systems under consideration. The particular phenomenological observations are intriguing but not well enough understood to offer great improvements to other systems.
- LiBH<sub>4</sub>/MgH<sub>2</sub> system: similar concern as with the LiNH<sub>2</sub>/LiH system, although as long as this system is still under consideration in the Program as a system with potential, performing the phenomenological studies has some value.
- The project supports the goal of developing high-density hydrogen storage with materials that have adequate kinetics to meet the program goals for refueling time.

**Question 2: Approach to performing the research and development**

This project was rated **1.9** on its approach.

- Ball milling may not be a viable process for large scale automotive manufacturing and their associated volumes. Creating nano size particles of most metal hydrides is only useful if they can be immobilized and prevented from agglomeration, sintering and etc. The PI does not address these requirements at all.
- Attempts to overcome diffusion barriers by mechanical treatment alone seem very unlikely to succeed. The empirical observation of improved reaction rates begs more questions than it answers, which the PI should be driven to address, for instance: How can the system possibly "remember" the temperature at which it was ball-

milled after several cycles at  $>200^{\circ}\text{C}$ ? What kind of "defects" could be durable through these cycles (ex.: maybe different amounts of iron or chromium slough off the ball mill onto the hydride material and serve as catalysts?).

- As long as the investigators are looking at thermodynamic phase destabilization by mixing metals, it seems surprising that they didn't also look at kinetic effects of mixing metal hydrides, e.g. combine  $\text{LiNH}_2/\text{LiH}$  (slow dehydriding) with  $\text{Mg}(\text{NH}_2)_2/\text{LiH}$  (rapid dehydriding) to see if the mixture exhibits intermediate dehydriding rates.
- The approach relies on simple modifications of known hydrogen storage materials. These hydrogen storage materials do not have a high probability of meeting the DOE program goals. The material capacity is very small unless the pressure is reduced to a vacuum which is not feasible for onboard hydrogen storage.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.0** based on accomplishments.

- Thermodynamics were predictably reduced by ball milling however the desorption temp of  $\sim 200^{\circ}\text{C}$  is still far too high for use in automotive systems. Little progress or direction has been demonstrated in improving the cycling performance of such materials.
- Progress appears to be limited to cataloging the effects of different milling conditions. The results do show that these are interesting to catalog, but the underlying understanding does not reach the level of sophistication to be broadly applicable.
- After some number of hydriding/dehydriding cycles, it would seem inevitable that the material will lose its "memory" of milling conditions. The investigators should establish how many cycles, and develop a more sophisticated understanding of the effects.
- The PI did not present any breakthrough results that indicate a high probability of reaching the project milestones. The project milestones are very aggressive.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.2** for technology transfer and collaboration.

- The PI appears to have strong collaborators however is perhaps not utilizing them to their full potential.
- Good use of nuclear magnetic resonance characterization in Pacific Northwest National Laboratory collaboration, but there is little evidence of other collaboration in this project. More detailed characterization of particle size and defect concentration would seem in order, are there collaborators who could provide this?
- The PI presented little evidence for collaboration or even understanding of the parallel efforts within the DOE hydrogen program.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **1.8** for proposed future work.

- The PI is not clear about what approach will be used to stabilize the nanostructure materials. It is clear that these materials are not stable with cycling and will need to be immobilized. It is not clear that the PI has a solid understanding of this and what tradeoffs will be incurred in capacity with various immobilization techniques such as scaffolds. The work proposal is proprietary at this point – he should at least provide a direction as to what routes will be pursued.
- It is not at all clear what "nano-engineering" means or what experimental path is intended. While it is true that understanding, and even more important, intentionally controlling, the interphasic reactions in these "thermodynamically destabilized" systems would be very useful, it is not clear the project has a clear path to the necessary level of understanding and control.
- The future research plan that was presented by the PI has little potential of meeting the system weight percent target with the existing hydrogen storage materials. New materials development will be needed to meet the project goals.

**Strengths and weaknesses**Strengths

- If the interphasic reactions can be fully controlled to give the necessary rates, these systems have some promise, although the heat of dehydrating needs to be lowered further.
- The PI showed characterization results that were of high quality.

Weaknesses

- Needs to move beyond observing and cataloging the effects of different milling conditions and particle sizes.
- The project approach of modification of metal amide systems is not likely to meet the project milestones.

**Specific recommendations and additions or deletions to the work scope**

- Proprietary nature of the scaffolding approach - this is clearly where all the focus and novel discovery of the project should be and should be elucidated / described up front.
- The PI should coordinate with other projects that attempt to destabilize metal hydrides and provide some kind of scaffold or support, such as aerogels, in order to fully understand the challenges and tradeoffs with such techniques.
- Either develop scope for a detailed understanding of the inter/intraphasic reactions within this project, or transfer scope to other projects.
- Novel materials development will be necessary to reach the project milestones. The capacity should be measured under realistic system operating conditions (e.g. desorption at 2 bar, not vacuum).

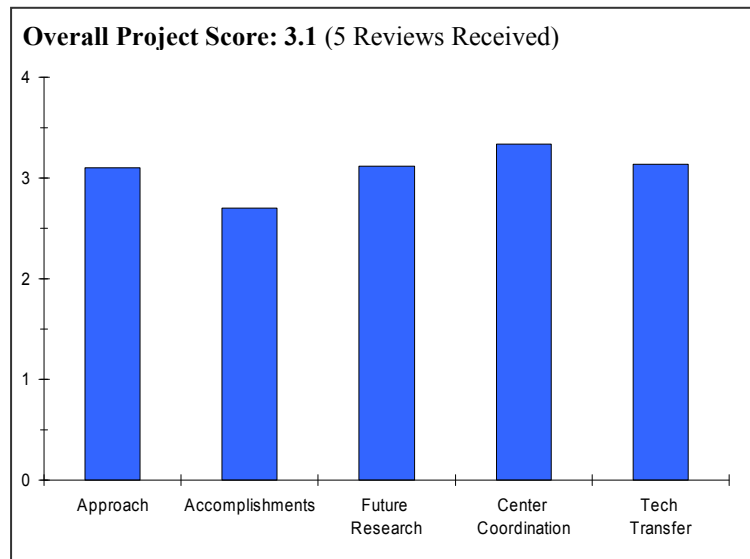
### **Project # ST-15: DOE Hydrogen Sorption Center of Excellence (HSCoE) Overview**

*Mike Heben; National Renewable Energy Laboratory*

[NOTE: This presentation was to evaluate the entire Hydrogen Sorption Center of Excellence as a whole. A separate review form was used and can be found in Appendix C. NREL's technical contribution to the center is evaluated in ST-19.]

#### **Brief Summary of Project**

The mission of the DOE Hydrogen Sorption Center of Excellence (HSCoE) is to develop materials that will enable close to room temperature storage of hydrogen on-board a vehicle at moderate pressure. The strategy used by the HSCoE is to design and synthesize materials which bind hydrogen as either (a) weakly and reversibly bound atoms or (b) as strongly bound molecules. Examples include nanoporous polymers, boron/carbon polymers, metal-organic frameworks (MOFs), carbon nanohorns, aerogels, carbon-metal hybrid nanomaterials, new materials “built from the ground up”, and new multi-component sorbents. Additional objectives are to understand mechanisms and the interplay between structure, binding, and material stability and storage densities (per volume and per weight) and develop the experimental and computational tools to speed discovery, development and testing of materials that meet DOE system goals. The final objective is to overcome barriers to 2010 Department of Energy system goals and identify pathways to meet 2015 goals.



#### **Question 1: Approach to performing the R&D including Center Management**

This project earned a score of **3.1**.

- The overall CoE effort is very well designed and technically feasible.
- CoE has a good balance between universities, DOE, national labs and industry.
- The separation of research work in research clusters shows a way how to reasonably divide the tasks into “digestible” parts.
- Some challenges in finding new materials are clearly addressed, like weight percent, binding for higher temperature storage, less so for volume which is the most significant challenge. The CoE seems to use partner skills well and is coordinated with only rare exceptions. Down selection has been done. Audits are unclear.
- Formation of the clusters is a good idea.
- Research cluster organization has gelled into an effective approach to enhance development in the different thrust areas of research.
- Good coupling between theory and experiment.
- Broad spectrum of research areas looking at different hydrogen surface interaction mechanisms.
- Center remains in discovery mode. Center doesn't use hard metrics for go/no-go decisions.
- The center consists of four research clusters that are led by senior National Renewable Energy Laboratory staff with a roadmap. This makes targets and research of each cluster and individual very clear.

#### **Question 2: Technical accomplishments and progress toward DOE goals**

This project was rated **2.7**.

- The significant amount of progress across the center is appreciated.
- Especially, the amount of publications, presentations and review work is outstanding.
- Yet, it was not clear enough, whether sorption materials will ever meet the DOE system targets, especially without using higher pressures and/or lower temperatures.
- Improvement in binding energy and volumetric densities is appreciated.
- Not clear about measurement to milestones but progress [observed] in several areas. Would prefer to see addressing the key remaining problems more quickly, for example kinetics in spillover.
- More emphasis on establishing the feasibility of materials synthesis estimated from theory by providing a plan and addressing key challenges at the beginning.
- Although spillover approach appears very promising, progress has been slow and many questions remain.
- Metal organic frameworks (MOF) – determined relation between binding energy and binding site on MOF-74.
- Have demonstrated a number of materials with binding energies higher than molecular physisorption.
- The major research topic of this CoE is “spillover” but the progress from last year [appears] little, especially in hydrogen capacity.

### **Question 3: Proposed future research approach and relevance**

This project was rated **3.1**.

- The future work plan is well planned and addresses the key technical barriers.
- Actual plan details are less clear but the areas are appropriate. Would like to see theory plans and theory interaction with experiment plans, but glad that something is intended.
- Proposed future work is finally beginning to focus on less exotic species (such as metal doped fullerenes) and towards cheaper, more readily available materials.
- Consideration of non-carbon based materials is a good expansion of current work.
- Lithium intercalated graphite may hold promise as a storage material.
- Future plan does not clearly show the direction of the material development. There is no “Kubas” compound any more. Scale-up in preparation and high-pressure measurements of spillover material, which is a major focus of the center, are only shown.

### **Question 4: Coordination, collaborations and effectiveness of communications within the CoE**

This project was rated **3.3**.

- There is no doubt that there is outstanding continuing cross-center communication and collaboration inside and also outside the CoE.
- The center coordinator seems to have the right means to leverage the right resources for the necessary research and has created a fruitful platform on which new ideas can be created.
- All partners seem to profit from the overall group effort.
- Generally good, mostly working together with maybe a single counter example, good structure to get communication between logical partners often and all partners on occasion.
- Collaboration with others is visible.
- Collaborations between center partners do exist, but there is some room for improvement.
- Individual PIs appear focused on their own research projects and there could be better interaction to facilitate developments in some areas.
- Practical and engineering inputs from the industrial partner, Air Products and Chemicals, Inc., are not apparent from the presentation.
- Coordination through research clusters works effectively. In addition, research of theory is coordinated across the clusters.

### **Question 5: Collaborations/Technology Transfer Outside the CoE**

This project was rated **3.1**.



## HYDROGEN STORAGE

- Like the previous work with the hydride center, there is a good degree of interaction with the world community.
- More collaboration is suggested to ensure testing reproducibility and the utilization of the Southwest Research Institute facility is recommended.
- International Energy Agency (IEA) [Hydrogen Implementing Agreement, HIA] and International Partnership for the Hydrogen Economy (IPHE) involvements are good.
- Collaborations outside of the center [are] on a personal PI basis, rather than being focused on a thrust area, material or process.
- Collaborations with other CoEs and institutes outside are few.

### **Strengths and weaknesses**

#### Strengths

- World-renowned researchers.
- Good mix of competencies and partners.
- Spillover methodology as one of the most promising storage material candidates.
- Powerful team.
- Visible collaboration between theory and experiments.
- Center leveraging others' work.
- The center explores novel materials in a large number including carbon nanotubes, "Kubas" compounds, spillover materials and so on for hydrogen storage.

#### Weaknesses

- It was not clear, whether sorption materials will ever meet the DOE system targets, especially without using higher pressures and/or lower temperatures.
- No significant effort in producing the desired material quantities for a 1 kg storage system. [NOTE From DOE: A 1-kg prototype is no longer part of the scope of work for this HSCoE effort.]
- Do not seem to be attacking the key problem in spillover – kinetics. However, it is not clear they have the power to tell partners to do certain things – they may not be able to push experimenters.
- Relying on modeling to down-select materials and not having a path forward and a plan towards materials synthesis while addressing key challenges.
- The materials predicted by theory are not synthesized in real experiments. "Kubas" compounds are one of the examples. One of the reasons is that the materials prepared have been too small in the amount for precise characterization.

### **Specific recommendations and additions or deletions to the work scope**

- While focusing resources on spillover, it is suggested to clarify/confirm this phenomenon and evaluate its potential for hydrogen storage experimentally with theory support.
- Center needs to ensure resolving testing discrepancies observed especially in the spillover topic.
- Attention should be paid to not confuse the difference between system and material densities especially at presentations.
- Presentations should contain an overview plot or list of the best achieved materials and measurements.
- Why is there "No significant effort in producing 1 kg system in agreement with new DOE goals"? [NOTE From DOE: A 1-kg prototype is no longer part of the scope of work for this HSCoE effort.]
- CoE Coordinator's answers in the "white paper" on low temperature focus at 77K should address the question, whether adsorption materials will ever be able to hit DOE targets at low pressures and room temperature.
- Is the storage density of the new materials independent of their surface areas?
- Somehow the raft of negative experimental results on the metal atoms needs desperately to be used to update the theory until the theory can predict reality and then turn the theorists loose again on predicting materials.
- Keep the center scope but suggest to devise plan towards targets while clearly addressing challenges.
- The materials that cannot be operated at ambient condition should be decided as "No-Go" like another CoE.

**Project # ST-16: A Biomimetic Approach to New Adsorptive Carbonaceous Hydrogen Storage Materials***Joe Zhou; Miami University of Ohio*

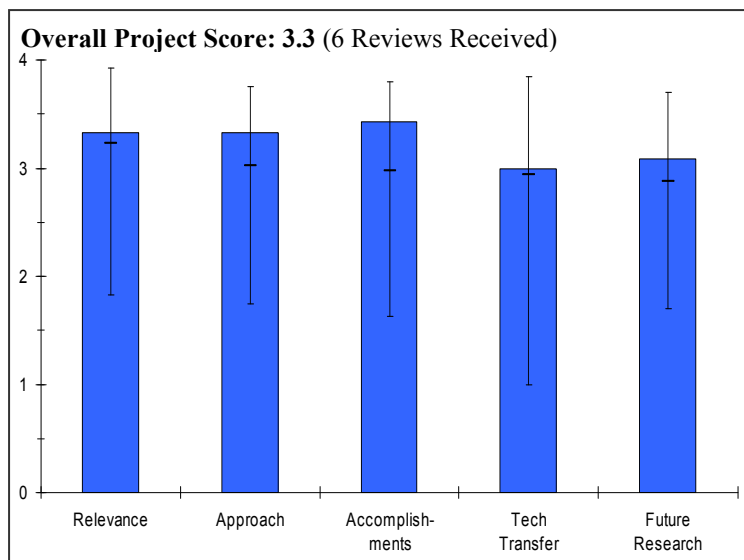
[NOTE: This project is part of the Hydrogen Sorption Center of Excellence; as of the Fall of 2008, Joe Zhou will be at Texas A&M University.]

**Brief Summary of Project**

The objective of this project is to design, synthesize and characterize MOFs with active (open site) metal centers aligned in porous channels and accessible by hydrogen molecules. Through optimized, cooperative binding, the MOFs are expected to have enhanced affinity or binding energy to hydrogen. These MOFs can help to reach the Department of Energy 2010 and ultimately the 2015 hydrogen storage goals.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.



- Project is aligned with DOE objectives and targets for hydrogen storage.
- The objectives are well aligned with DOE R&D objectives.
- Project is aligned with DOE objectives and targets for hydrogen storage.
- The work scope for this project aligns with the hydrogen vision and the DOE RD&D objectives in most respects.
- If relevance means that a project can either demonstrate achievement of the DOE targets for hydrogen storage or provide seminal new insights that assist in the identification of materials/concepts with the potential to meet one or more of the DOE targets for hydrogen storage, this project falls in the latter category.
- The project's objectives and strategy are sufficiently well aligned to the DOE program vision and aims. The idea of aligning coordinatively unsaturated metal centers (UMC) in order to obtain significantly stronger hydrogen-framework interaction is innovative and may provide fruitful insights and quite useful results.
- Though the work is nominally focused on the 2010 DOE storage targets, it's not completely clear how the PI hopes to achieve these targets. It does not seem as though increasing the binding energy alone will enable all the targets (e.g., they've already increased the binding energy to 12 kJ/mol, but only are able to get < 0.5 weight percent at room temperature). So, if the PI is able to achieve the targeted binding of 15 kJ/mol, will this really enable room-temperature storage?
- The volumetric densities of these materials are inherently low, and only some reference to future work on interpenetration seems to address this crucial issue.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- The approach to try to align metal bonding sites to increase interaction with hydrogen is sensible.
- The concept of aligning the metal center is good.
- It is not clear how theory can guide the experimental design.
- Is only aligning the metal center enough to achieve targets or do some other approaches need to be explored at the same time?

## HYDROGEN STORAGE

- This project applies biomimetic concepts and logics to extend the hydrogen storage capacity of metal-organic framework materials (MOFs), primarily by incorporating coordinatively unsaturated metal centers (UMCs) in the MOFs.
- The metal organic framework synthesis efforts are directed at compact, aligned, interpenetrating structures with hydrogen adsorption enthalpies in the desired range (ca. 15 kJ/mol) for DOE's hydrogen storage targets.
- The overall approach is indeed focused on the technical barriers addressed and leads already to tangible results. The project integrates well with other ongoing research on framework materials.
- Interesting, and unique approach to the design of novel MOFs for hydrogen storage. The connection between the approach of a close-packed array of metal sites, and the oxygen transport of hemoglobin (which seems to underlie the entire philosophy) is not completely clear.
- Would be valuable to see a more rational, directed approach to decide how the many variables in the synthesis will be optimized.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.4** based on accomplishments.

- Achieved relatively high storage density (5.5 weight percent, ~45g/L) at 77K and 50 bar pressure.
- Demonstrated increased heat of adsorption through alignment of open metal sites.
- The PI has shown some interesting results to prove the concept.
- The progress is reasonably good considering this is a new project.
- Metal organic framework structures with the desired aligned UMC deployments were successfully synthesized and hydrogen adsorption properties were measured.
- The hydrogen uptake properties of these new structures were marginally better than those of the best MOFs without UMCs; a heat of adsorption near 12 kJ/mol was obtained for one of the UMC-based MOFs.
- A limited amount of characterization (beyond hydrogen sorption measurements) was reported (i.e., inelastic neutron scattering (INS) results).
- Although the project is underway for a little under a year (started in July 2007), a number of promising results have been obtained. Several milestones have been reached in FY2007 and some significant technical accomplishments were presented (like the promising hydrogen uptake of PCN-12 following optimization attempts for the alignment of coordinatively UMCs). INS measurements have also shown strong hydrogen-metal organic framework interactions.
- Good progress in synthesis of proposed compounds and measurements of their storage capacities. Results are not entirely encouraging, but progress is strong.
- PI is to be commended for focusing on volumetric density, and reporting these numbers (even if they are somewhat "ideal" in the sense that they are based on the single crystal density). The volumetric density is at least as significant a challenge for sorbent materials as gravimetric density, though the latter gets much more attention.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.0** for technology transfer and collaboration.

- Some good collaborations exist.
- This project involves six partnering organizations.
- The nature of the collaboration with some (but not all) of these partners was spelled out in the presentation.
- The project seems to be well connected with the Hydrogen Sorption CoE.
- Collaborations through partnership with several research groups (including the industrial ones) are shown. They seem to complement nicely the work done by the PI's team. Of note are the collaborations with groups outside the United States (Korea Research Institute of Chemical Technology, Korea; University of Gottingen, Germany).

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Plans to increase metal center density and increasing metal organic framework stability are addressing proper barriers.
- Plans for interpenetrating metal organic framework networks have potential for significant increases in storage density.
- The general direction of the future plan is good.
- The absolute gravimetric and volumetric storage value should not be used as a single go or no-go decision point. The degree of improvement is more important to justify if the approach works.
- The proposed future research builds logically on the results of the past year's work.
- It must be said here that the hydrogen storage results presented at the review are not impressive in the context of DOE's storage targets for 2010 (and less so for 2015 targets) and it is hard to imagine what the research team could possibly accomplish in FY 2009 to change this.
- Future research plans for 2008 and 2009 build on the progress achieved so far. A milestone is rightly set for the 3rd quarter of 2009 (go/no-go decision) as to whether the project can substantially contribute towards the attainment of the DOE 2010 goals.
- For reasons stated above, it is not clear that the future research will result in materials that could enable the DOE 2010 goals (if 12 kJ/mol currently is only getting 0.5 weight percent at 300K, how will 15 kJ/mol really help?).

### **Strengths and weaknesses**

#### Strengths

- The PI appears to have a good handle on designing metal organic frameworks (MOF) of desired geometries, and how synthetic variations affect structures.
- All the appropriate characterization tools are in place for characterizing new MOFs.
- Novel concept.
- A very competent synthesis team has designed and then proceeded to produce some very interesting metal organic framework structures.
- The resources and facilities needed to perform the required synthesis and characterization work are available to the team.
- The overall level of the science produced by this project is very high; several high profile peer reviewed publications have appeared or are in press.
- Innovative idea, strong research team and partners.
- Promising initial results.
- Novel approach to design new metal organic framework materials for storage.
- More focus on volumetric density than other sorbent programs.

#### Weaknesses

- Lack of a general strategy on how to achieve the desired orientation in order to meet DOE targets.
- Lack of theory prediction and an overall experimental approach strategy.
- There is very little hope that any type of metal organic framework structure will be able to meet DOE's 2010 hydrogen storage "system" targets for ambient temperature operation; simple back-of-the-envelope calculations would prove this; there's just too many other atoms in the UMC/metal organic framework structure along with the stored hydrogen; if the project team disagrees with this statement, they should be prepared to demonstrate otherwise at the next Merit Review.
- A rational design strategy for improving capacity is lacking. It is not clear that increasing binding energy will really enable capacities that they are targeting.
- Budget seems excessive for what appears to be largely a single PI project.

#### **Specific recommendations and additions or deletions to the work scope**

- There exist a large number of available options regarding different parameters to be considered (e.g. metal nature, geometry, etc.). An effort should be made to narrow down these options based on a sound approach.
- Future work should have a stronger focus on improving volumetric densities.
- The PI needs to work more closely with the theory group to guide the experimental direction.

## HYDROGEN STORAGE

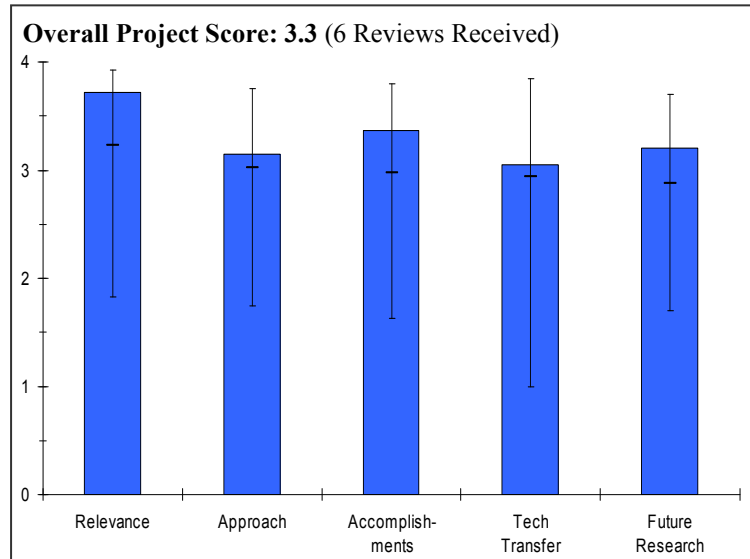
- At the next Merit Review, the PI should present an appropriately determined upper bound for the ambient temperature gravimetric and volumetric hydrogen storage capacities one could expect to achieve with the leading candidate unsaturated metal centers/metal organic framework structure for which the team has presentable test data.
- Alternatively, the presenter should make a compelling argument for why 77K results represent a useable condition for on-board hydrogen storage. It's time for the physisorption/chemisorption teams to show they are getting within range of the 2010 DOE system targets for gravimetric and volumetric hydrogen storage-December of 2010 is only 30 months away.
- The possible assessment of the porous coordination network (PCN) metal organic frameworks for spillover should be considered.
- The PI expressed concerns about the usable capacity (between e.g. 50 bar and 2 bar) of the materials. This may not be a real problem as temperature swing techniques may bypass the issue.

**Project # ST-17: Hydrogen Storage by Spillover***Ralph Yang; University of Michigan*

[NOTE: This project is part of the Hydrogen Sorption Center of Excellence.]

**Brief Summary of Project**

The objectives of this project are to 1) develop hydrogen storage materials with capacities in excess of 6 wt% (and 45 g/L) at ambient temperature by using the spillover mechanism; 2) develop and optimize the bridge-building techniques for spillover to enhance hydrogen storage in metal organic frameworks (MOFs); 3) develop direct doping techniques for spillover on carbons with ultra-high surface areas (higher than all MOFs); and 4) obtain a mechanistic understanding for hydrogen spillover in nanostructured materials for the purpose of hydrogen storage.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.7** for its relevance to DOE objectives.

- Addresses relevant DOE hydrogen storage targets and goals.
- This project is focusing on improving the room temperature adsorption hydrogen storage capacity towards the DOE mass and volumetric targets via a spillover process with metallic clusters/particles on the surfaces of adsorbent materials. The concept of building bridges between the metal species and carbon host materials was shown to significantly enhance these capacities although reaction rates are much too slow to meet DOE charging and discharging requirements. The observed 1-2 weight percent capacities are still too small but do point the direction for a viable adsorption storage system.
- This project is well aligned with the hydrogen vision and the DOE RD&D objectives; hydrogen spillover is one of, if not the key to meeting DOE hydrogen storage targets with sorption-type materials/processes.
- The insights that emanate from this work are having a profound impact on research directions within the Hydrogen Sorption CoE.
- If sorption-based processes were within range of meeting ambient temperature gravimetric and volumetric hydrogen storage targets, this project would get an even higher score for relevance.
- A sorbent with a high hydrogen capacity at room temperature would be a very significant breakthrough. Hydrogen spillover effects in carbon-based sorbents have real potential for the development of room temperature hydrogen sorbent materials with capacities suitable for vehicular applications.
- Project as presented and described is outstanding and attempts to understand kinetic issues limiting the use of carbon materials.

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- The approach has potential to meet DOE gravimetric storage targets for 2010.
- Use of platinum at anywhere near these levels will be too expensive – need nickel or a cheaper metal.
- Isotope studies can help define doping levels needed and effective distance of spillover effect.

## HYDROGEN STORAGE

- Need a mechanistic model and estimate of maximum - can you go beyond one hydrogen/carbon atom with spillover? Is the hydrogen atom occupying a carbon coordination site, or can more than one hydrogen atom occupy a coordination site?
- This project is empirically investigating the addition of platinum/carbon catalyst particles on several types of activated carbons in addition to metal organic framework (MOF) compounds to allow for hydrogen spillover onto the main carbon sorbent. They are also looking at the degradation effects of water and air on stabilities of the metal organic framework materials.
- They have also used deuterium isotope effects to investigate the mechanisms to the spillover effect into splitting hydrogen molecules into atoms for chemical adsorption on carbon materials and also facilitate reversible desorption. These analysis methods, as used by the investigators, are certainly informative but further in-situ spectroscopy would be useful.
- The methods of study applied in this research are very cleverly orchestrated; the demonstrated concept of bridge-building and the tracer experiments provide pathways for understanding and enhancing spillover.
- Spillover in the high surface area templated carbons and metal organic frameworks is an excellent approach.
- Efforts to develop non-noble metal catalysts for spillover are important.
- Understanding spillover is highly relevant and is the key to advancing the state-of-the-art in sorption materials. Why synthesize materials when so many others in the CoE are synthesizing novel carbons that could use used in your study?

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.4** based on accomplishments.

- Have achieved 1.5 weight percent at room temperature with platinum-doped metal organic frameworks.
- Have increased heat of adsorption in IRMOF-8 to 21 kJ/mol.
- Technical accomplishments to date are outstanding providing solid progress towards understanding storage systems costs.
- The PI showed several examples where the bridged 5%Pt/AC catalysts not only enhanced the room temperature storage capacity by factors of 2-3 but also leads to the desirable increase in the heat of reaction. The kinetics are still rather slow while the capacities are also beyond upper levels theoretically expected.
- Showed that spillover-storage is influenced by surface area and binding energy.
- Made the case that spillover-storage on nanostructured carbon is "far" from reaching theoretical limits.
- Presented data showing that ambient temperature discharge rates for selected sorption materials are now in the range of the DOE target.
- Performed some interesting deuterium tracer results that provide direct evidence of molecular hydrogen dissociation, and "last-in-first-out" behavior during spillover/reverse spillover procedures.
- Relatively little progress on room temperature hydrogen capacity since the excellent result of 4 weight percent hydrogen at room temperature in IRMOF-8.
- Current work with the templated carbon and new metal organic frameworks looks interesting for the possibility of increasing the hydrogen capacity at room temperature.
- Technical accomplishments to date are outstanding.
- Mechanistic understanding of spillover with deuterium isotopes will lead to a new understanding of how carbon sorbs hydrogen.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- Some collaboration with the National Renewable Energy Laboratory and National Institute of Standards and Technology, spillover seems to be spilling over to other projects in the sorption center.
- Collaborations extend across all CoEs and national laboratories.
- The University of Michigan investigators are interacting with several of members of the Hydrogen Sorption Center of Excellence for samples sources and characterizations.

- Numerous partners were listed on slide 2 of the presentation but it was not clear, as the PI went through the accomplishments/results, which ones were done at the University of Michigan and which ones were done by a partner.
- Other collaborations were mentioned by the PI during the presentation but are not well documented in the slide file.
- Clearly, many in the hydrogen storage community have picked up on the findings from this project.
- Relatively little interaction with other members of the Hydrogen Sorption Center of Excellence. This project would benefit greatly from increased center theoretical interactions, particularly as to the mechanisms of hydrogen spillover and how theory might guide experimental progress to increase hydrogen capacity at room temperature.
- Collaborations need to be elaborated upon, showing a list of collaborators is not enough.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- Future work should look at using nickel or cheaper metals; platinum use is price prohibitive.
- Proposed future work is very promising.
- The plans of this project to address mechanisms of the spillover kinetics with emphasis on understanding and improving the kinetics are just where they need to be as the details of the actual processes are still obscure and the models are not yet substantiated.
- Furthermore, development of improved metal dopants and dispersion methods on metal organic framework and other carbon compounds is also needed if hydrogen adsorption storage capacities above 6 weight percent are to be obtained.
- Spillover measurements with bridge-building for other promising metal organic frameworks and high surface area carbons.
- Synthesis of carbons with surface areas  $>3500 \text{ m}^2/\text{g}$ .
- Exploration of metal doping to facilitate spillover and enhance storage capacity.
- Emphasis on achieving 6 weight percent and 48 g/L hydrogen storage at ambient temperature.
- Will address fueling rate issues.
- The metal organic frameworks and templated carbons to be studied have significant potential.

#### **Strengths and weaknesses**

##### Strengths

- Broad-based collaborations with both private and public institutions.
- Observations of reversible hydrogen storage capacities greater than 1 weight percent at room temperature are promising for developing metal organic framework or activated carbon materials that might reach DOE storage targets.
- The demonstration of larger bonding energies with spillover suggests better sorbents may be possible.
- The PI is a world renowned expert in the field.
- All the essential expertise and facilities required to make significant progress on this project are available within the project team.
- Spillover optimization (perhaps maximization) is absolutely essential if sorption-based hydrogen storage "systems" are going to simultaneously meet DOE capacity and rate targets - so, this project has the right focus.
- Original discovery of the hydrogen spillover effects that may increase hydrogen capacities at room temperature in carbon-based sorbents.
- Isotopic studies to determine spillover charge and discharge mechanism and kinetics are beneficial to determining viability of carbon materials.

##### Weaknesses

- There is a great need for better understanding of the detailed spillover mechanisms that observations of just macroscopic adsorption capacities and general rates do not provide. While the isotope exchange experiments do indicate breaking of molecular hydrogen bonds, these do not give a complete picture.



## HYDROGEN STORAGE

- In general, it will be very difficult for any sorption-based material to meet the ambient temperature hydrogen storage targets set by DOE; to meet the 2010 "system" targets, a sorption material had better demonstrate at least 9 weight percent and 64 g/L at ambient temperature to give it a credible chance in a "system" context; December of 2010 is just 30 months away.
- Not enough theoretical guidance associated with this project.
- Kinetics of processes are currently too slow to be of use. Paths forward to solve this problem need to be explained.
- The real storage capacity of carbon is far from the theoretical limit. Need explanation on how to bridge today's results to tomorrow's achievement.

### **Specific recommendations and additions or deletions to the work scope**

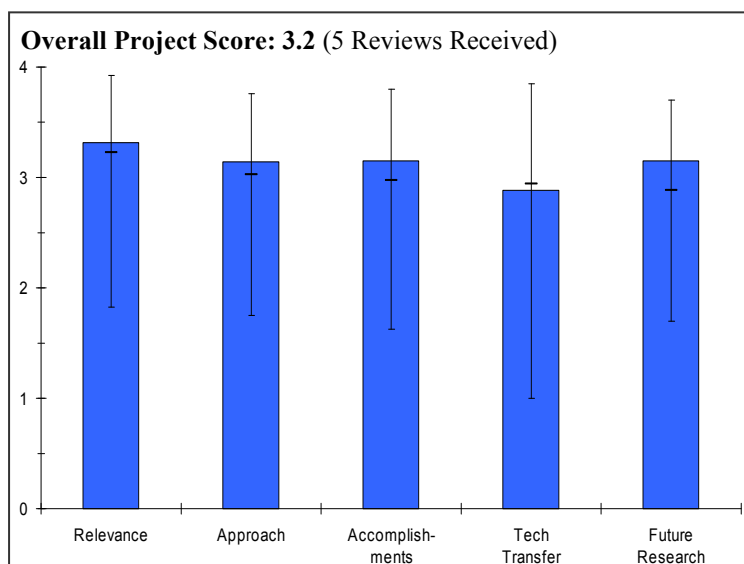
- Modeling of spillover on metal organic frameworks would be useful, because it not clear how "spillover" to an unsaturated metal center would improve adsorption; is it spilling over to the framework organic portion of the metal organic framework?
- Should look more closely at effects of metal catalyst particles (composition and morphology) on room temperature hydrogen storage via spillover.
- Strongly suggest this team work more closely with other HSCoE partners such as National Institute of Standards and Technology or University of North Carolina to include comprehensive spectroscopic characterization via neutron and nuclear magnetic resonance techniques.
- To what extent is it possible that the principles of spillover could be implemented in a meaningful way in chemical and/or metal hydride storage systems, e.g., to speed up the rehydriding rates?
- Could in situ small angle x-ray or neutron scattering provide any useful information on the spillover process, e.g., the effect on the morphology of the adsorbing surface? A real time, in situ measurement of the initiation and progression of spillover seems like something worth doing.
- Discontinue moisture effects on metal organic frameworks.

**Project # ST-18: Theoretical Models of H<sub>2</sub>-SWNT Systems for Hydrogen Storage and Optimization of SWNT**  
*Boris Yakobson, presenting; Robert Hauge (Co-PI) both of Rice University*

[NOTE: This project is part of the Hydrogen Sorption Center of Excellence.]

**Brief Summary of Project**

The overall objectives of this project are 1) to model materials structures' interaction with hydrogen, optimize their makeup for storage and assess the volumetric and gravimetric capacity; and 2) provide recommendation for the synthetic goals (e.g. pore/channel size, metal enhancement routes). The 2007-2008 objectives are to 1) identify the obstacles (thermodynamics and kinetics) for spillover and suggest material designs to overcome them; 2) enhance the binding of hydrogen by introducing charge into the carbon lattice by adding a highly stable superacid anion that also acts as a spacer; and 3) explore doping as an anchor to metal/metal cluster, role of bridges and dopants on the threshold of spillover.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- Relevant to DOE storage goals and targets.
- This project involves both first principles computations and simulations of hydrogen interactions with metal clusters and defects on carbon surfaces as well as production of various carbon nanostructures and foams to assess their hydrogen adsorption behavior via gas adsorption experiments. A major goal of the theory effort is to identify and define whether hydrogen spillover behavior can be enhanced to reach DOE storage targets as well as advance understanding of the mechanisms.
- The experimental work is exploring different options for producing carbon nanostructures and fluorination treatment to possibly enhance adsorption energies where hydrogen reaction would be assessed by their Sorption Center of Excellence partners.
- The project addresses the objectives of the storage program in general terms without reference to the specific goals set by DOE.
- Most of the theory work is relevant.
- Various tasks within this project have varying degrees of relevance; the work on spillover is quite important, and focused on materials that have the potential to have high capacities; the work on foams is not as clearly targeted towards materials which are likely to exhibit good storage properties (though the PIs have demonstrated a high gravimetric density at 77K).

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- Modeling approach using ab-initio and experimental potentials to bracket adsorption between maximum and minimum is OK, but feedback from adsorption experiments being done at the CoE should allow them to validate models and arrive at correct potential to use.
- The work on metal clustering effect is important.

## HYDROGEN STORAGE

- Modeling work suggests that vertically aligned nanotube arrays (VANTA) are not as productive an area to work on as carbon "sponges".
- Modeling of spillover starting with palladium clusters rather than platinum. I believe platinum is more active in hydrogen spillover in catalysis.
- While the theoretical and experimental tasks are not explicitly correlated, they do share common objectives and features to enhance effective reaction sites for the adsorbing hydrogen coupled to modifications of the host carbon matrix and metallic additives.
- Not much was presented on experimental approach, so this is hard to quantify.
- Good combination of theory/experiment; however, in many cases, the experiments and theory are working on different problems. It would be good to have a closer connection between the theory/experiment, e.g., particularly on the spillover work.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- Modeling is making good progress.
- Modeling results indicate carbon foams are a good area to pursue.
- Synthetic/experimental progress on vertically aligned nanotube arrays (VANTA) is slow (efforts focused on calculations?).
- The majority of information presented at this review concerned simulations of hydrogen adsorption where particular emphasis was on interactions with simple clusters of palladium metal. The trends are suggestive of possible spillover processes but future assessments are needed.
- Relatively limited experimental adsorption data was given for 77K tests. This data was mainly of zeolite-templated carbon foams, which yielded capacities similar to the better metal organic framework materials. The other suggested candidates remain to be prepared.
- Nice work on spillover modeling (score of 3.6).
- Little progress apparent on experimental work (score of 2.4).
- Theoretical/computational work has had a lot of excellent technical accomplishments this year; the experimental work has produced interesting new results on the foams, but in general, seems to be lagging behind the theoretical work.
- Work on spillover is highly imaginative, and is currently the only detailed proposed mechanism of this phenomenon in hydrogen storage. The implications of this nucleation-and-growth picture of spillover should be more fully explored.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.9** for technology transfer and collaboration.

- Collaborations evident.
- Collaborations/interactions with others modeling the effects of charged centers on hydrogen storage at other centers of excellence may be useful (for example, Hwang at Michigan Technological University).
- The presentation indicated fruitful collaborations and interactions not only with several partners within the Hydrogen Sorption Center of Excellence and other active carbon materials research groups being supported by DOE/EERE.
- The theory effort, while focused on an important topic (spillover) seems to be conducted largely in isolation.
- No experimental collaboration with center partners apparent.
- Theory work seems closely connected with external partners and the CoE. Not clear how the experimental work is connecting.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Modeling of spillover with less expensive metals like nickel is necessary.

- The theoretical efforts address a number of detailed mechanisms and possible diffusion processes involved with spillover behavior. These appear to be logical next steps.
- The proposed geometries and modified compositions for the carbon materials do not appear to be duplicated elsewhere where the rationale for improved hydrogen adsorption behavior is reasonable if not overwhelming.
- Computational study of impact of catalyst in spillover process is the next logical step.
- Experimental next steps are poorly defined.
- Good plans for the spillover work. This area should be the top focus for the theoretical work.

### **Strengths and weaknesses**

#### Strengths

- Extensive theoretical modeling effort of hydrogen interactions with palladium metal clusters and possible processes in the spillover mechanisms.
- Exploring methods to fabricate and alter bonding within carbon foams and nanophases are key features of the experimental growth of these materials as possible improved hydrogen adsorbents.
- Highly imaginative and differentiated from other efforts in the center (except for the metal-carbon work, which is somewhat redundant with other efforts).

#### Weaknesses

- Metal cluster sizes and geometries look to be chosen more for computational ease rather than reflecting actual configurations achieved during doping.
- Model calculation primarily involved palladium clusters rather than platinum clusters that are being used in most spillover studies and it is not evident that conclusions drawn in these calculations actually pertain.

### **Specific recommendations and additions or deletions to the work scope**

- It would be good to have a closer connection between the theory/experiment, e.g., particularly on the spillover work.
- Suggest that calculations of spillover mechanisms be extended to include platinum and nickel metal clusters to allow direct comparisons with current results obtained on palladium/carbon systems.
- Effort on "non-starter" approaches (e.g., storage within fullerene pores) to storage should be eliminated.
- Focus efforts on spillover.
- The spillover work should be the focus for theory; the metal-carbon work seems less important since (a) it is somewhat redundant with other efforts in the Center, and (b) it is proving extremely difficult to synthesize these theoretically-predicted structures anyway.

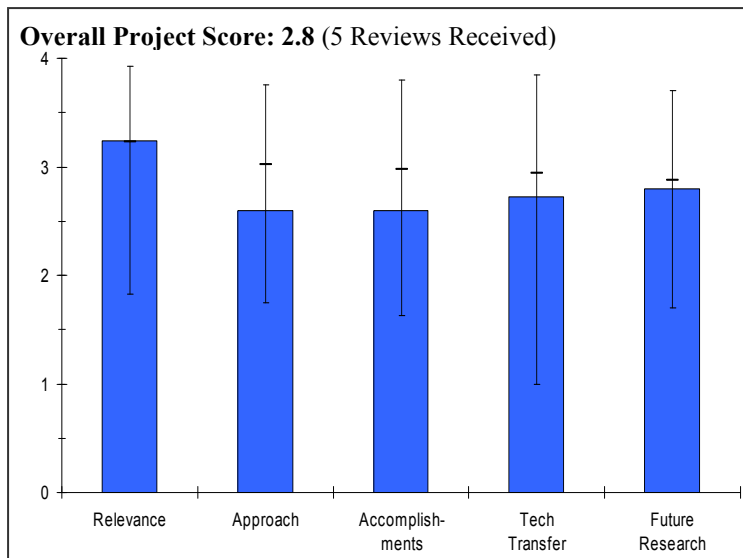
**Project # ST-19: National Renewable Energy Laboratory Research as Part of the Hydrogen Sorption Center of Excellence**

*Anne Dillon; National Renewable Energy Laboratory (NREL)*

[NOTE: This review is for NREL’s technical contribution to the HSCoE.]

**Brief Summary of Project**

The objectives of this project are 1) develop stable high surface area, minimally macroporous, light materials that can either stabilize large quantities of hydrogen directly (by physisorption), or provide frameworks for incorporating/stabilizing other species; 2) increase concentration of substitutional dopants (e.g. B and N) in lattices to adsorb dihydrogen directly (via donation), stabilize active species (e.g. transition metals) against agglomeration, or provide anchor points for building more complex sorbents; 3) synthesize sorbents which can bind multiple dihydrogen ligands through metals that are capable of “Kubas binding”; and 4) develop methods to prepare catalytic species, bridges, receptors and the activation processes to reproducibly prepare spillover materials with high capacities and good kinetics.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.

- Very relevant.
- The objectives are aligned with DOE R&D objectives.
- The project works toward enhancing the binding energy and the hydrogen weight percent to reach the DOE objectives.
- It is clear that the project is aimed at discovering new, high-density hydrogen storage materials.
- Emphasis of project is currently on binding energy, which is extremely important, but not the only consideration.

**Question 2: Approach to performing the research and development**

This project was rated **2.6** on its approach.

- Approach proved to be not particularly successful.
- General chemical behavior of fullerenes is not quite in line with calculations used to justify this research.
- The research cluster approach is OK in general and they are grouped together well.
- Some of the specific approaches in material design are not based on the fundamental understanding of material need.
- The PI seemed to still work on impractical material.
- The approach to support the four research clusters shows interaction and collaboration.
- The concept of using theory to guide experiments is a well-established and promising strategy. However, in practice, many (if not all) of the theoretical predictions produced by this project have focused on exotic materials which have not been amenable to experimental synthesis.
- It would be very helpful to have a set of criteria in place to guide whether a given theory prediction should be pursued experimentally.

- Theory seems to be operating only in a "forward prediction" mode. Theory could also be employed to help decipher why various experimental efforts have thus far not yielded synthetic or storage goals.
- NREL defines their own objective, "efficiency", which translates to binding energy of 15-20 kJ/mol.
- NREL contributes to all 4 research clusters in the center, so materials being studied cover a wide range of properties and characteristics.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.6** based on accomplishments.

- A lot of experimental work without sufficiently positive results.
- Model systems may need some additional adjustment.
- Only modest progress over last year, not proportional to the large funding.
- Lack of fundamental understanding and lack of the attempt for fundamental understanding of the material system.
- Difficulty in synthesizing materials per the theoretical estimation for enhancement the binding energy of hydrogen in  $C_{60}$  by adding dopants (organometallic fullerenes) was illustrated. It is suggested to have a clear path forward prior to materials selection based on solely theoretical estimation and to enlist challenges to achieving the targets as a first step.
- The concept of co-intercalation of Li/metal within graphite using THF/benzene has to be carefully considered to avoid hydrogen solubility situation or simply liquid evaporation!
- The discrepancy between the University of Michigan and NREL results is suggested to be resolved.
- Many systems have been explored, but there has been relatively little progress in identifying materials with promising properties.
- Wrapping up organometallic fullerenes and finally going to simpler structures. Theoretical structures found to be difficult to synthesize.
- Intercalated graphites have been synthesized. Li/THF shows some modest hydrogen uptake.
- Has expanded spillover approach using wet chemistry - NaSWNT shows ~4 weight percent.
- Provides measurements for center partners.
- Materials synthesis lab is operational.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.7** for technology transfer and collaboration.

- Very good collaboration.
- Some collaborations exist.
- The PIs should really extensively collaborate with some expert in catalysis field to get better understanding of the spillover effect.
- Collaboration with others within the center is visible.
- Good collaboration with center partners, but no external collaborations identified in the presentation.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- Reasonable plans; hope they will materialize.
- The material design should be based on the fundamental understanding of the system. There is little attempt in understanding the science behind the results.
- Path forward for the Li/solvent intercalated graphite is suggested to be more clarified to avoid the  $C_{60}$ /metal scenarios where calculations predictions do not match with synthesis/formation feasibility.

### Strengths and weaknesses

#### Strengths

- Strong expertise in chemical synthesis.
- Organized research cluster approach.
- Visible collaboration with others within the center.
- Trying to create truly new hydrogen storage materials.
- Collaboration between theory and experiment.

#### Weaknesses

- Model systems are not particularly efficient.
- Lack of fundamental understanding in material design.
- Relying on theoretical estimations.
- Lack of devising a strategy for material synthesis and identifying the challenges as the materials estimated by the theory are selected.
- The research direction is dictated too strongly by modeling predictions on "unrealistic" exotic compounds.

### Specific recommendations and additions or deletions to the work scope

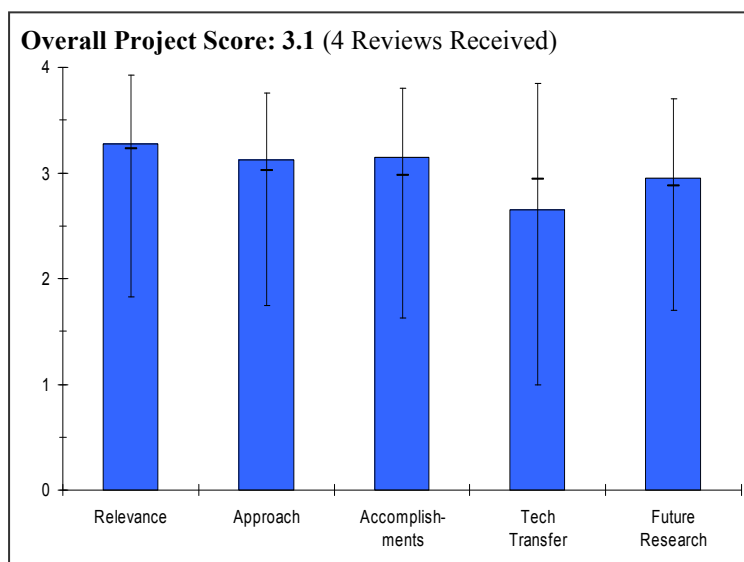
- Suggest keeping the project; however, a clear plan for materials selections and synthesis needs to be presented.
- Suggest increasing efforts on mechanistic studies of spillover.
- Suggest careful consideration of efforts exerted towards synthesizing exotic compounds.
- Overall, it is suggested to identify challenges as the materials are selected for synthesis based on theoretical estimations and create a plan towards achieving the targets.
- NREL could help the development of spillover for storage if they would include some studies related to understanding the phenomena, e.g., looking more at the temperature dependence of uptake and release, using analytical techniques to ascertain the hydrogen atom sites.

**Project # ST-20: Single-Walled Carbon Nanohorns for Hydrogen Storage and Catalyst Supports***David Geohegan; Oak Ridge National Laboratory (ORNL)*

NOTE: This project is part of the Hydrogen Sorption Center of Excellence.

**Brief Summary of Project**

The overall objective of this project is to exploit the tunable porosity and excellent metal supportability of single-walled carbon nanohorns to optimize hydrogen uptake and binding energy. The 2008 objectives are to 1) improve surface area to 2,200 m<sup>2</sup>/g for >3.0 wt% at 77K; 2) adjust pore size controllably to <1 nm; 3) quantify effects of pore size; 4) theoretically investigate origin of binding energy increase; 5) search for alternative metals to enhance binding energy; and 6) develop new synthesis/decoration approaches for these materials.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- Project addresses relevant hydrogen storage goals and targets.
- The objectives are aligned with DOE R&D objectives.
- The project addresses the objectives of the hydrogen storage program in general terms. Without specific reference to the DOE targets.
- Carbon nanohorn structures may provide an effective storage material, but there are many obstacles to overcome; specifically, volume and weight density, binding energy and other target-related metrics.
- The project involved both experimental and theoretical efforts in tailoring the pore size and morphology of carbon nanohorns and understanding the nature of bonding in metal coated fullerenes. High surface areas and small pore sizes were achieved, but the gravimetric density of hydrogen fell far short of the DOE target.

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- Addressing appropriate issues such as clustering and dispersion of metal dopants.
- Unclear how CaH<sub>2</sub> formation will be prevented at higher temperatures (room temperature and above - CaH<sub>2</sub> is thermodynamically favored) - CaH<sub>2</sub> is fairly stable and may trap hydrogen, not leading to spillover but leading to hydrogen that is not releasable until high temperature.
- The material synthesis approach is unique.
- The PI should work with theory group to predict the best pore size combination of this type of materials.
- Well orchestrated approach.
- The approach of using charge effects to enhance binding energy is a good, promising alternative to other techniques being examined in the center.
- The search for dispersed metal coatings is important for spillover development.
- Both experimental and theory have used state-of-the-art techniques, but there has been a disconnect between the two.



### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- Demonstrated spillover in single walled carbon nanohorns (SWNH). Demonstrated up to 3.5 weight percent hydrogen storage at 77K in short SWNH.
- Have prepared calcium decorated nanohorns but need to demonstrate enhanced adsorption with these materials
- Good progress toward objectives.
- Pathway to achieve higher capacity has been identified.
- Publications resulting from experimental work are not comparable with that of theory. The progress in overcoming barriers is modest although the progress in the synthesis of materials with small pore size and high surface area is good.
- Developed "short" nanohorns with high surface area; hydrogen capacity is consistent with C surface. Binding energy ~6 kJ/mol.
- Studied decorated long nanohorns.
- Charged nanohorns. Theory calculations indicate Ca, Sr can generate good binding energy and sites.
- Experimentally was able to decorate nanohorns with Ca that also may show some intercalation.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.7** for technology transfer and collaboration.

- Collaborations within the center are apparent.
- More collaboration with Ralph Yang's group [University of Michigan] could be beneficial.
- Some collaboration with group at Michigan Technological University looking at interactions with charged species (metal perhydrides) may be mutually beneficial.
- Some collaborations exist, but only in materials characterization part.
- The PI should expand the collaborate area to include some theory prediction.
- Tech transfer and collaborations not discussed in the presentation.
- Partnerships used for analytical work on materials.
- The team has worked well with other members in the center.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- People have looked at metal intercalated graphene previously – unless there is some new insight regarding optimum spacing, what will be new?
- The general research direction is good.
- The PI should include the theory prediction in defining what is the maximum pore volume can be created by this approach and which metal carbide can provide the best pore size desired.
- Focus on charged nanostructures and spillover is good, as is the objective for fundamental understanding of spillover.
- Consideration of kinetic properties of spillover good.
- Dispersion of metals on nanostructures an important aspect of using these materials for storage.
- Studies of graphene flakes and graphite nano-particles with metal doping will provide further insight into the effect of structure and composition on hydrogen binding but unlikely to lead to a material sought by DOE for hydrogen storage.

### **Strengths and weaknesses**

#### Strengths

- The research approach is novel.

- Addressing the efficiency and thermal management issue through design of materials with high thermal conductivity is important.
- Synergy between theory and experiment plus efforts to control pore size. Understanding of the spillover mechanism.

Weaknesses

- Lack of theory work in predicting what the technology limit is.
- Theory and experiment should be better coordinated. Experiment was carried on Ca coated nanohorns while theory was on Ca coated fullerenes. The stability of materials with Ca coated C<sub>60</sub> should be investigated.

Specific recommendations and additions or deletions to the work scope

None.

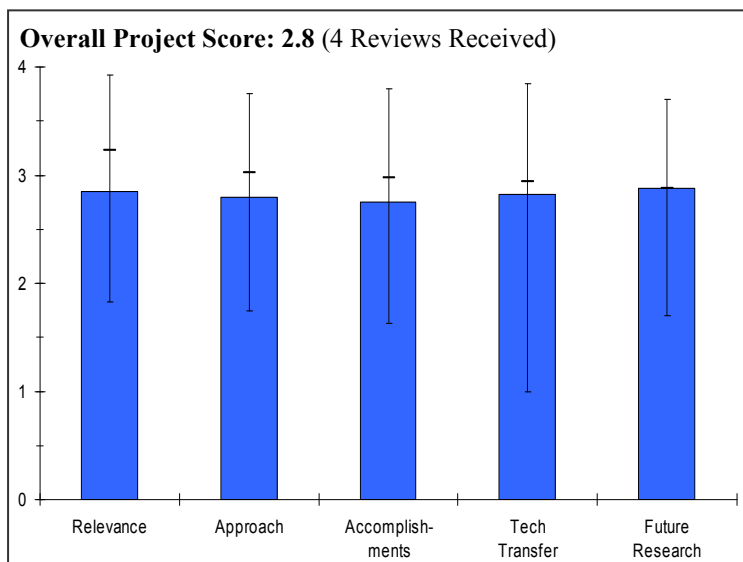
**Project # ST-21: Hydrogen Storage through Nanostructured Polymeric Materials**

*D.J. Liu, presenting; Argonne National Laboratory (ANL) and Luping Yu; University of Chicago, Co-PI*

NOTE: This project is part of the Hydrogen Sorption Center of Excellence.

**Brief Summary of Project**

The objectives of this project are to 1) design, synthesize and evaluate nanostructured polymeric materials (NPM) as new hydrogen storage adsorbents for transportation applications; and 2) support polymer materials development with modeling/simulation and advanced structural characterizations. Polymer surface properties such as specific surface area and porosity can be controlled at the molecular level. Polymer-hydrogen binding can be enhanced through incorporating different functional groups and atomically dispersed metals. Polymers are generally stable under the temperature and humidity required for hydrogen storage application.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.9** for its relevance to DOE objectives.

- This project has the objective of developing porous polymers from conductive and polyimide skeletons with various functional groups added to enhance hydrogen adsorption capacity. However, initial results indicate that rather low surface areas (i.e. < 1000 m<sup>2</sup>/g) are being formed and the hydrogen adsorption capacities measured at 77 K are not any larger than found for most other common carbon materials. While improvements are possible, the current materials will not meet the DOE mass or volumetric targets. There was no indication that any significant enhancement is available from these specific materials.
- Polymers are inexpensive materials with a number of tailoring options for improving hydrogen storage capacity.
- This project, based on designed nanostructured polymers, aims at the DOE targets and barriers, especially gravimetric capacity.
- The potential for meeting volumetric and other targets (e.g., kinetics) is not addressed in any quantitative sense.

**Question 2: Approach to performing the research and development**

This project was rated **2.8** on its approach.

- It does not appear that the program is absorbing the body of data on delta-H, spillover and other findings that have been established in the field.
- The Argonne National Laboratory and University of Chicago team is well balanced to address polymer design and synthesis and materials characterization and hydrogen storage measurements.
- The approach is a pretty conventional combination of selecting attractive functional molecular groups and components to produce a polymeric material that is then reacted with hydrogen gas at 77K. Based upon empirical observations and modeling analyses, iterations in components would be used to make further polymers for assessment of their hydrogen storage properties.
- At some point it might be interesting to look at hydrogen spillover effects in the polymers.
- What are the rationales being employed for enhanced hydrogen storage via the incorporation of "metallic" conductive features and selected functional groups?

- Are hydrogen permeability and polymer free volume being considered as possible guiding rationales for polymer hydrogen storage materials?
- The approach to explore new molecularly designed polymers, in particular controlled structures and porosity, is a convincing one.
- The ability to add metallic "backbones" will hopefully improve the storage capacities of the basic polymers via spillover-like phenomena.
- The direct collaboration between Argonne National Laboratory and University of Chicago is obviously synergistic.
- The project directions and chances for success will be helped by the modeling component.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- In comparison with the current state of storage the results appear well below the targets.
- Setting up and producing at least three series of polymers with moderate surface areas and narrow pore distributions were done within less than a year of this project.
- Initial storage capacities are OK but not suggestive of a high performance storage media even at 77 K.
- A good deal of progress has been made in a relatively short time, although initial hydrogen storage capacities are unremarkable.
- Although the project is new (< 1 yr), much preliminary work has been accomplished so far.
- Three multi-composition series of polymers have been synthesized and evaluated (along with a reference carbon material) in a relatively short time.
- The gravimetric storage results are not very good, so far, and may not bode well for the future. However good understanding has been made that should hopefully help to accelerate progress.
- Hydrogen testing well-established and is giving very credible results.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.8** for technology transfer and collaboration.

- Is it possible to interact with Southwest Research Institute for expedited and independent testing?
- Not clear how this project interacts with the Hydrogen Sorption Center of Excellence or perhaps there is no connection.
- The Argonne National Laboratory/University of Chicago team has been working with several members of the Hydrogen Sorption Center of Excellence on behavior during their first year and indicate plans for more detailed characterizations via neutrons, nuclear magnetic resonance, etc. in the future as they generate more favorable storage candidates.
- There appears to be little or no interactions with other hydrogen storage research organizations.
- Collaborations to identify hydrogen bonding sites in the polymers will be useful.
- The joint project combination of Argonne National Laboratory and University of Chicago seems excellent.
- There should be good collaborations within the Hydrogen Sorption Center of Excellence.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- There is divergence between the plans and the program goals.
- Will there be a critical analysis of the approach? A go/no-go decision at some point?
- In general, this team looks from their stated Fiscal Year 2008 and Fiscal Year 2009 plans to follow the course of analyzing and tweaking polymer designs to produce samples then test their hydrogen adsorption properties as they soldier on towards the goal of higher capacities.
- The plan seems good. Alternative directions are available.
- The milestones are good and have been met to date.

### Strengths and weaknesses

#### Strengths

- Complementary interaction between the University of Chicago polymer synthesis group and the Argonne National Laboratory characterization and modeling members to proceed toward possibly developing better hydrogen adsorption materials.
- Hydrogen storage in polymers is an area that has been little explored.
- Excellent knowledge of polymers and ability to design and synthesize old and new families.
- Project will be a thorough test of polymers and polymeric porosity.

#### Weaknesses

- The technical approach appears to be behind the current state of scientific discoveries in the field.
- At the moment, there does not seem to be any rationale for devising materials that could adsorb greater quantities of hydrogen gas at temperatures between 77K and room temperature (i.e., stronger H-C bonding with effective surface areas  $\gg 1000 \text{ m}^2/\text{gram}$ ).
- Predictive rationales for hydrogen bonding site construction in the polymers should be enhanced.
- Not enough focus on volumetric targets.

### Specific recommendations and additions or deletions to the work scope

- Do not spend too much time on polymers that do not show promise relatively quickly.
- The program needs to re-address the technical approach and streamline (eliminate) areas with limited strategic success.
- This team should more actively seek assistance of other sorption groups to explore feasibility of activation processing such as KOH processing and other methods to increase effective surface areas and internal porosity.
- Given the rather low H-capacities measured so far, it would be wise to start the metal-doping part of the effort sooner than originally planned (sometime in Fiscal Year 2009).
- There should be at least one quantitative go/no-go gate put in place for early Fiscal Year 2009.

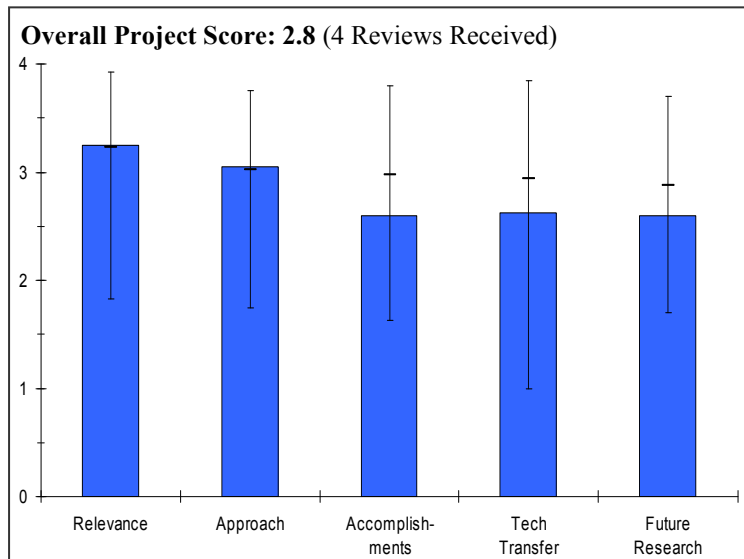
**Project # ST-22: Enabling Discovery of Materials with a Practical Heat of Hydrogen Adsorption**

Alan Cooper; Air Products and Chemicals, Inc. (APCI)

NOTE: This project is part of the Hydrogen Sorption Center of Excellence.

**Brief Summary of Project**

The objectives of this project are: 1) development and testing of new materials with high hydrogen storage density and appropriate enthalpy of hydrogen adsorption; and 2) development of enabling technologies for hydrogen storage materials development. Air Products' goal is the reversible adsorption of hydrogen at near-ambient temperatures at densities that will enable meeting the 2010 Department of Energy system-level targets for hydrogen storage. Air Products has leveraged existing materials science and chemistry capabilities in carbon materials and fluorine chemistry to generate new hydrogen storage materials for testing.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- Project as presented and described is good.
- The work is focusing on a key problem in the DOE hydrogen program - hydrogen storage. There is currently no effective means of storing hydrogen via chemical/physical storage techniques. Gas/liquid tank storage seems to be the best route which takes up valuable space. An effective alternative, such as what is proposed in this project, is necessary.
- Clearly trying to develop new hydrogen storage materials and improve understanding of existing materials (e.g., spillover).
- Much of the project supports the DOE objectives.

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- Approach is sound; project's results are poor.
- The project is attempting a relatively unique approach. The materials being examined are very novel, and this is probably necessary to achieve any success (F-based materials). Air Products and Chemicals, Inc. is proposing a number of unique concepts that are currently not be examined elsewhere - for example the effects of anion-hydrogen interactions in intercalated carbons. The approach is well thought out and appears to be scientifically acceptable. The approach is conceptually very solid.
- The project, as proposed, would use a balance of modeling and experimentation to achieve the project goals. This is a rational approach to develop new materials at a molecular level.
- The work is considering new materials that APCI has had success in synthesizing in the past.
- Unclear whether the  $C_{32}F_8$  compounds are thermodynamically stable or will be able to be synthesized in a morphology consistent with theory.
- Thermodynamic predictions (slide 10) suggest only weak bonding of hydrogen at high loading -- (~4kJ/mol at 8 weight percent hydrogen); this does not appear to be a viable material. Unclear why experiments conducted given expected poor performance.

## HYDROGEN STORAGE

- Modeling of mechanisms of spillover is valuable.
- Although the modeling of spillover phenomenon is important, its impact on the development of the approach for hydrogen storage is not clear.
- The emphasis on intercalated graphite materials may not lead to a viable storage material.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.6** based on accomplishments.

- Approach to add N to C is novel and should be explored as N tends to make C more basic in nature.
- The project has had some general success in developing computer based models for several different aspects (spillover mechanism, conceptual materials, etc.). The models appear to have a big value to the Hydrogen Sorption Center of Excellence.
- However, the work appears to lack any solid experimental results at this time. The only results appear to be some low level hydrogen results on the F-carbon materials. All are well below 1 weight percent - which is well below the DOE targets. It is unlikely that these materials will ever be developed up to a reasonable level. This is a major concern as this project has been ongoing for about 2 years and based on the opening slide - is 60% complete.
- It is not clear that APCI has yet been able to synthesize the necessary materials. Attempts have been made - but the analytical data tends to suggest that the attempts were unsuccessful.
- A balance of modeling and experimental work is a good approach - but this project needs to provide some experimental results.
- The surface area of the materials under consideration is too low (75 m<sup>2</sup>/g). Considering the poor hydrogen weight percent, it is unlikely that this material will have any use for hydrogen storage.
- Modeling work seems to be progressing at a reasonable pace.
- Several attempts at synthesizing materials have been performed, but no promising leads thus far.
- The intercalated materials may be promising candidates for storage, but they are a long way from the performance (e.g., capacity) achieved with other materials.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.6** for technology transfer and collaboration.

- Anticipated collaborations need to be explained or removed. When unexplained they appear as fluff.
- Tech transfer and collaboration are acceptable.
- The work appears to involve a number of outside participants with needed special skills.
- The work appears to be highly coordinated with the Hydrogen Sorption Center of Excellence. In particular, it appears that the modeling work is of considerable interest to the center.
- Seems to be significant overlap with Rice University's efforts on spillover on graphene. Redundant?
- Some interaction and collaboration with center partners, but external collaborations not apparent.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.6** for proposed future work.

- Consider adding more detail in work for next year and leaving out work for current fiscal year.
- The work is suggesting the investigation of some new materials - N based. However, it appears that the work is being conducted on few potential materials and others need to be considered.
- The work needs to concentrate on completing some experimental work.
- Unclear if using other graphitic carbons will increase accessibility of hydrogen
- Limited hydrogen accessibility could be endemic to these intercalated materials.
- Intercalation of N doped C may be promising.
- Not clear what the MD ab initio calculations on BC<sub>3</sub> intercalated compounds will yield in terms of developing these materials.

**Strengths and weaknesses****Strengths**

- The project is based on some unique scientific concepts that could have significant benefit if the work is successful.
- The modeling effort has been successful and is providing insight into potential mechanisms and conceptual materials.
- Good connection between theory and experiment.

**Weaknesses**

- There is a significant lack of any solid (or positive) experimental results.
- The results provided thus far tend to indicate that the current material has little chance of success.
- Theoretical predictions are for "exotic" compounds that may not be thermodynamically stable and/or realized experimentally.

**Specific recommendations and additions or deletions to the work scope**

- The project needs to identify (and test) other material compositions - including materials with high surface area.
- Consider balancing synthesis and characterization for hydrogen uptake. Project heavy on synthesis and light on results for uptake.
- Suggest clarifying role of Air Products and Rice University regarding spillover modeling to avoid redundancy.

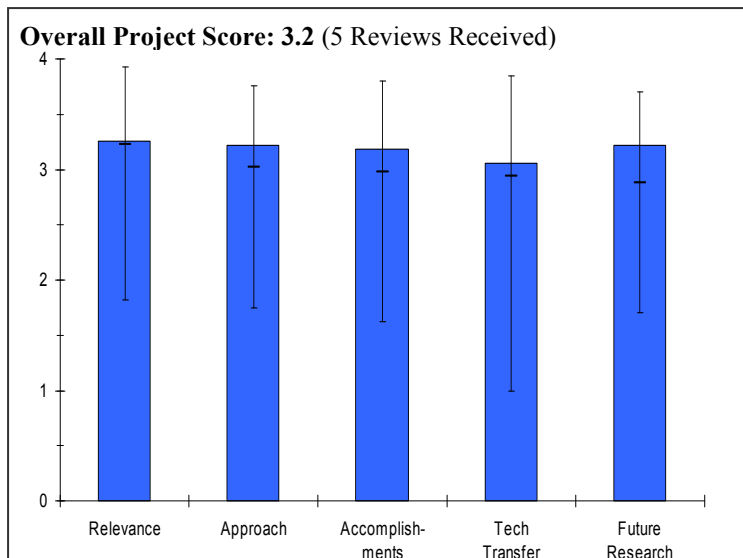


**Project # ST-23: Enhanced Hydrogen Dipole Physisorption: Henry's Law and Isothermic Heats in Microporous Sorbents***Channing Ahn, California Institute of Technology*

NOTE: This project is part of the Hydrogen Sorption Center of Excellence.

**Brief Summary of Project**

The objectives of this project are the 1) synthesis of framework structures via normal solvo-thermal routes; 2) evaluation of aerogel properties in collaboration with Lawrence Livermore National Laboratory; 3) evaluation of microporous activated carbon properties; 4) adsorption/desorption evaluation with volumetric Sieverts apparatus capable of measurements of samples at 77, 87, 195, and 298K temperatures; 5) thermodynamic evaluation of sorption enthalpies via Henry's Law region of isotherm and/or isosteric enthalpy of adsorption; and 6) neutron scattering (diffraction and inelastic) of promising systems in collaboration with the National Institute of Standards and Technology.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- The project is aligned with DOE R&D objectives.
- The objectives of this project need to be better defined.
- The project like so many others addresses the objectives of the hydrogen storage program in general terms without reference to the specific targets set by DOE.
- The emphasis of this project is on several key aspects of the hydrogen storage goals that align with the hydrogen vision and DOE RD&D objectives.
- More specifically, the project seeks to develop understanding of critical issues for hydrogen sorption processes.
- It appears that important new knowledge about hydrogen sorption is emerging from the work of this project.
- Synthesis of frameworks structures and measurement of the isothermic heats of adsorption and pore sizes is very relevant to DOE objectives in enhancing the room temperature weight percent hydrogen by increasing the binding energy.
- This program is highly relevant to the DOE Hydrogen Storage Program.
- It is concerned with improving the properties of high surface area materials with respect to hydrogen storage.
- Activated carbon, aerogels and metal organic frameworks (MOFs) are the materials of interest.
- This program has the capability to synthesize and characterize complicated MOF materials.
- This capability is highly relevant to the DOE objectives.
- Surface packing density of hydrogen was achieved in a newly synthesized MOF.

**Question 2: Approach to performing the research and development**

This project was rated **3.2** on its approach.

- The approaches are OK in general but nothing unique. The slit pores have been known for long time.
- Lack of systematic approach in selecting the materials for testing.
- Synthesis and characterization of framework structures, including electron microscopy where appropriate.

- Measurement and evaluation of the hydrogen sorption properties of framework structures, aerogels, and microporous activated carbons.
- Measurements include temperature dependencies and sorption thermodynamics.
- Neutron diffraction and scattering measurements to identify hydrogen positions.
- Good approach in identifying relevant materials properties.
- The approach is highly scientific and professional.
- While MOF-74 has a high surface packing density (SPD), the weight percent hydrogen is still well below that of competitive materials.
- Efforts to improve gravimetric density are planned and should be encouraged.
- A more negative adsorption enthalpy should be a goal.
- A less time consuming MOF synthesis should be devised.
- An important barrier is the low gravimetric density at room temperature.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.2** based on accomplishments.

- The PI made some progress toward objectives.
- Pathway to achieve higher capacity has been identified through the available data.
- Showed that sorption enthalpies approach a constant value as pore size distribution narrows.
- Elucidated several of the causes for sorption enthalpy heterogeneity.
- Found that when sorption enthalpy is high, a majority of the sorbed hydrogen is retained at pressures less than 2 bar and 77K; as temperature increases, a larger fraction of the sorbed hydrogen is available at pressures greater than 2 bar.
- Made projections about optimum pore size and size distribution.
- Identification of pore/slit geometry of 1 nm and careful examination of surface area effect is very good approach in the identification of key frameworks properties which would help in frameworks design.
- The successful synthesis of MOF-74 is an impressive feat. Its structural determination is also impressive.
- The determinations of the isosteric heats of adsorption for MOF-74 and activated carbon materials are of wide interest.
- Although still in the early research stage, the cost of the subject materials should be of concern.
- Similarly it appears that soon a choice must be made between MOFs, aerogels and activated carbon adsorbents.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- Some collaborations exist, but only in the materials synthesis and nuclear magnetic resonance measurement part.
- A substantial number of collaborations and interactions were mentioned during the course of this presentation.
- Some collaborators provide materials for study (e.g., Lawrence Livermore National Laboratory); others provide characterization capability (e.g., National Institute of Standards and Technology [NIST]).
- This research appears to be well recognized and respected within the Hydrogen Sorption Center of Excellence.
- Professor Ahn seems to have many collaborations within the Center of Excellence.
- Visible good collaboration with theory group at NIST.
- This program has extensive collaborations both within and outside the Metal Hydride Center of Excellence.
- A cited publication in "Langmuir" is a fine paper.
- Several presentations are also noted.
- Technology transfer with members of the Metal Hydride Center of Excellence as well as industry could be improved.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

## HYDROGEN STORAGE

- The general research direction is good.
- The PI should feed some of the experimental data into theory prediction.
- The PI needs to pay more effort in better understanding how to design a material with maximum usable hydrogen on board.
- Optimization of pore size and pore volume to maximize volume density. Otherwise, much of the future research will be a continuation of Fiscal Year 2008 activities involving framework structures, aerogels, and microporous carbons with emphasis on those materials displaying homogeneous sorption enthalpies.
- Continued evaluation of thermodynamic properties, including differential enthalpy of adsorption near zero coverage.
- Good plan to support several members in the center. However the approach towards enhancing the adsorption by tuning the pore sizes needs to be clarified and addressed more.
- Plans noted are logically based on past progress, but in view of the DOE time-line, it is time to choose the most advanced material and concentrate the effort on it.

### Strengths and weaknesses

#### Strengths

- Accurate experimental measurement techniques.
- The PI is very knowledgeable about the systematics of sorption processes and is keenly aware of the ongoing progress in the field regarding hydrogen sorption.
- The emphasis of this project is heavily weighted towards developing understanding of the influence of all relevant properties and parameters as opposed to just making lots of materials and doing lots of sorption measurements.
- Well established collaborations and well respected PI.
- Systematic approach.
- A very strong scientific effort.
- The resources appear adequate.
- The MOF effort is novel with implications beyond hydrogen storage.
- The expertise demonstrated in the thermodynamic studies is most impressive.
- The scientific credentials of the PI and his collaborators are excellent.

#### Weaknesses

- Lack of a general strategy in selecting the materials for measurement.
- No obvious weaknesses other than the daunting task of meeting DOE's ambient temperature hydrogen storage capacity targets using sorption-based materials and processes.
- Addressing materials design and synthesis by utilizing the results obtained.
- Practical problems involved in the use of microporous adsorbents as hydrogen fuel sources not addressed.
- Difficulty in synthesizing MOFs.
- Overall costs may be prohibitive.
- Cycling stability of MOFs not addressed.
- Low gravimetric capacity at room temperature.
- Safety issues have not been addressed.

### Specific recommendations and additions or deletions to the work scope

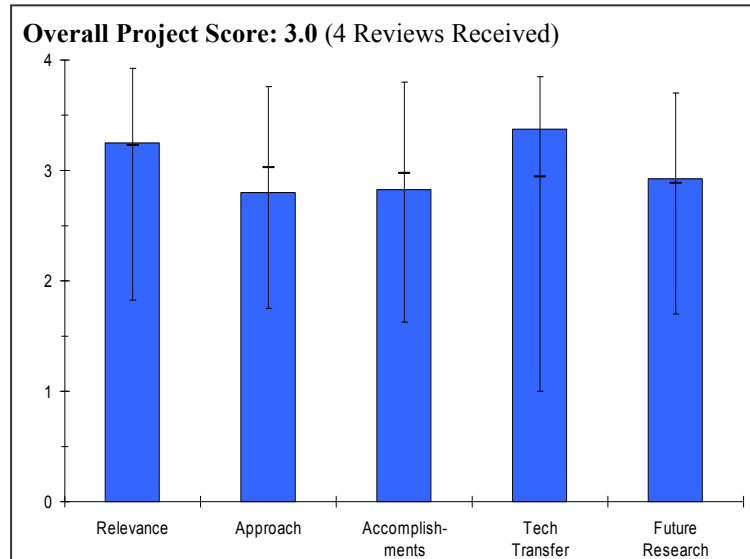
- The PI should expand the collaborations to include experts in other field, such as catalysis.
- Avoid expending too much effort on achieving high hydrogen uptake at ambient temperature; continue to focus on elucidating the interrelationships among the key parameters--pore size and pore distribution, enthalpies, temperature effects, and pressure effects--and how they collectively influence hydrogen uptake and release.
- The project showed good progress in designing catalysts and it is recommended to keep the project.
- The items discussed under "Project Weaknesses" should be addressed.
- While this effort is still in applied science stage the DOE time is short. Thus the following should be addressed; reversibility, cost, kinetics, storage capacity at 298K, and cycle stability.
- The above likely requires that a specific material be chosen.

**Project # ST-24: Carbon Aerogels for Hydrogen Storage***Ted Baumann; Lawrence Livermore National Laboratory (LLNL)*

NOTE: This project is part of the Hydrogen Sorption Center of Excellence.

**Brief Summary of Project**

The objective of this project is the design of novel carbon aerogel (CA) materials that meet the Department of Energy system targets (6 wt%, 45 g/L) for on-board vehicle hydrogen storage. The focus is in two areas: 1) engineering of CA-based spillover materials and 2) design of new CA materials as porous scaffolds for metal hydride materials. The specific objectives are 1) to optimize structure for enhanced hydrogen uptake and improved kinetics; 2) storage at reasonable operating temperatures; and 3) the potential to improve kinetic and thermodynamic performance of metal hydrides.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- Project relevant and addressing DOE goals and targets.
- Relevant in several ways, both as a storage media and a catalyst. Only lack is that the odds of meeting 2015 goals are low.
- The project is nicely focused toward the DOE goals and barriers, especially weight and volume.
- Future work will focus increasingly on kinetics.

**Question 2: Approach to performing the research and development**

This project was rated **2.8** on its approach.

- High surface area of carbon aerogels together with spillover effect has potential, overlap with use of carbon aerogels as scaffolds for metal hydrides.
- Use of platinum for spillover leads to cost issues, should focus on cheaper metals (nickel) for the spillover effect.
- Decision to discontinue work on undoped carbon aerogels (CA) is appropriate.
- The re-focus on spillover is indicative of good tactical change.
- Scaffolding appears to become less significant.
- ALD Vacuum Technologies approach does not appear of much value. It is not clear why the PIs decided to purchase their own system versus collaborating with other groups. This is not a good resource utilization and no justifications were made why this was done.
- Good that program has two routes to success.
- Methods used are suitable. Team is expert in doing this sort of material design.
- Project includes two worthwhile objectives: (1) M-doped carbon aerogels for maximum spillover performance; and (2) carbon scaffolds for containment and performance enhancement of metal hydrides.
- Aimed at optimization of pore structure for two applications.
- PI has long experience on the control of aerogel structures.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- With spillover, achieved only 1.2 weight percent at 100 bar at room temperature.
- Doubled thermal conductivity of carbon aerogels with carbon nanotubes composites.
- Increased kinetics for hydrogen uptake in platinum-doped carbon aerogels.
- Made spillover materials but not much success, but did show 1 nm diffusion distance likely a limit. Also apparently improved kinetics.
- Made highly regular pores in carbon for hydride scaffold.
- Starting to alter heat transfer character, though a long way from meaningful results in this area.
- Really great work on getting an incredibly tight distribution of pores in an aerogel.
- New M-doped aerogels have been developed and significant new data has been generated on their microstructure and hydrogen storage properties.
- Some structures show promise for spillover and some are disappointing. There has clearly been increased understanding during the last year.
- Understanding the needs for hydride-scaffold aerogels has developed considerably during this preliminary stage.
- Synthesis of nanoporous metal hydride-aerogel scaffolds has been improved by templating.
- The interesting possibility of including C-nanotubes for increased thermal conductivity has been explored.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.4** for technology transfer and collaboration.

- Collaborations within Metal Hydride Center of Excellence are good.
- Collaboration with Metal Hydride Center of Excellence for carbon aerogel scaffold work is present.
- Need more interactions with Southwest Research Institute (SWRI) for testing samples.
- Exemplary, working with 2 centers and outside people and making a difference to them all.
- Several useful collaborations have been established in the Hydrogen Sorption and Metal Hydride Centers of Excellence.
- Samples are being prepared for validation testing.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- Proposed spillover work with nickel is appropriate, platinum is too expensive.
- Plans to investigate stability/durability of carbon aerogels (either for scaffolds or with metal spillover) addresses a major barrier and need - with metal catalysts present, reaction with the carbon aerogel structure is a concern.
- Suitable.
- Given recent results, future work looks very reasonable and logical.
- Project will be completed during Fiscal Year 2009. At least one quantitative go/no-go gate (based on volume and weight) should be inserted for consideration of the concept beyond 2009.

### **Strengths and weaknesses**

#### Strengths

- High flexibility in approach.
- Several avenues to success.
- Good experience and skills in custom designing of aerogels.
- Project is concentrating on M-doping for spillover.
- Project provides good synergistic contributions to the CoEs. In particular, the HRL Laboratories hydride destabilization project should be greatly helped.

Weaknesses

- Really challenged on heat and cost.
- Volume efficiency in question, too.

**Specific recommendations and additions or deletions to the work scope**

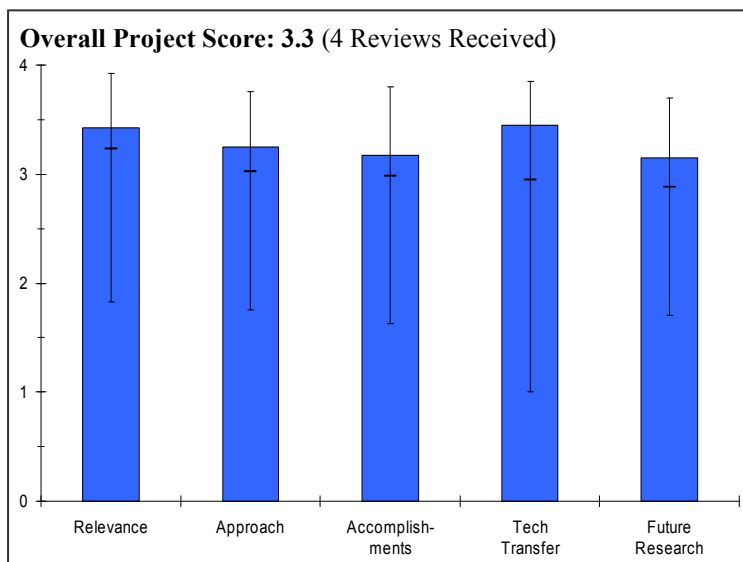
- If spillover is the pathway of future, need to establish more collaboration with University of Michigan and Rice University teams.
- Is there a synergistic effect between carbon aerogels and metal hydrides (LiBH<sub>2</sub> etc.)?
- ALD Vacuum Technologies may not be the right approach as the platinum/palladium clusters need to be loosely bonded with the substrate.
- The more pressing question would be is the carbon aerogel the right substrate with the spillover?
- Probably need to start looking for new catalysts. Need to start thinking about how to improve volumetric storage which may be inherently a problem.

**Project # ST-25: Characterization of Hydrogen Adsorption by Nuclear Magnetic Resonance***Yue Wu; University of North Carolina*

NOTE: This project is part of the Hydrogen Sorption Center of Excellence.

**Brief Summary of Project**

The overall objective of this project is to provide nuclear magnetic resonance (NMR) support to the Department of Energy Hydrogen Sorption Center of Excellence team members in developing reversible adsorbent materials with the potential to meet Department of Energy 2010 system-level targets. The 2008 objective is to use NMR porosymetry analysis to obtain detailed information on the micropore structures. This approach is based on the information of local magnetic field inside micro- and meso-pores probed directly by hydrogen.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.4** for its relevance to DOE objectives.

- Project as presented and described is good.
- Project is highly relevant and has a good potential for becoming critical.
- The approach developed should find applications in other energy related areas which employ porous material and hydrogen reactive gases including hydrocarbons.
- The microscopic characterization of pore sizes via nuclear magnetic resonance allows more detailed evaluations of the adsorption interactions of hydrogen with carbon surfaces as well as its binding energy and quantity of adsorbed hydrogen. While this information does not directly lead to higher performance levels for storage, it does let one compare local adsorption properties to predictions and modeling of structures. Hence, the more promising candidates can be emphasized in future development studies while less promising materials are down selected with greater confidence.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- Approach is sound.
- Not focused enough on promising systems or materials.
- Linkage to real need for this approach is missing.
- The project is well-designed, technically feasible, and integrated with other research.
- In-situ proton nuclear magnetic resonance provides unique information of hydrogen adsorption and porosity.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.2** based on accomplishments.

- Qualitatively, the results presented are quite convincing.
- Mass calibration requires further improvement, including calibration of a broader variety of systems and standards.

- A number of materials with different local structures have been evaluated using these proton nuclear magnetic resonance measurements and self consistent results were obtained.

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.5** for technology transfer and collaboration.

- Collaborations should be expanded to other CoE team members.
- Good coordination with other institutions; partners are participants.
- The nuclear magnetic resonance team has worked closely with several hydrogen sorption center groups to assess adsorption behavior and porosity.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Future research is not well defined.
- Is the group planning to wrap up the ongoing research only?
- The nuclear magnetic resonance group will look at a number of the more promising sorbent systems to assess their porosities and distribution between surface adsorbed and gas phase (bulk and confined) hydrogen species. These results will give useful insights into performance potential.

#### **Strengths and weaknesses**

##### Strengths

- Strong understanding of theoretical background and experimental techniques used.
- Good collaboration with other members of the CoE.
- A highly qualified nuclear magnetic resonance analysis team with dedicated spectrometer for evaluating hydrogen sorption behavior under in situ conditions over a range of temperatures.
- They have well established procedures and analysis methods to evaluate a variety of carbon-based adsorption samples.
- The use of nuclear magnetic resonance porosymmetry analysis is an innovative approach.

##### Weaknesses

- Project very limited in scope.
- Mass calibration requires further work.
- Future goals are not well defined.
- The current nuclear magnetic resonance porosymmetry analysis methodology lumps a complex distribution of interactions for the pore dimensions into a single parameter, which is OK for narrow size distributions but could be misleading for materials with complex wide or binominal distributions.
- The nuclear magnetic resonance shift depends strongly on the distance between hydrogen and the surface as pointed out by the presenter; L.E, the technique is sensitive only to surface layer. Is this a potential problem?

#### **Specific recommendations and additions or deletions to the work scope**

- Compare with nuclear magnetic resonance results with neutron scattering results where available (National Institute of Standards and Technology [NIST]).
- Consider isotopic studies to evaluate spillover and hydrogen or D in pores.
- The in-situ nuclear magnetic resonance facility should have its temperature range extended to lower temperatures (i.e., down to < 20K) to allow evaluations of more heterogeneous pore size distributions as well as more weakly bound hydrogen species.



**Project # ST-26: Hydrogen Storage Materials with Binding Intermediate between Physisorption and Chemisorption***Juergen Eckert; University of California - Santa Barbara*

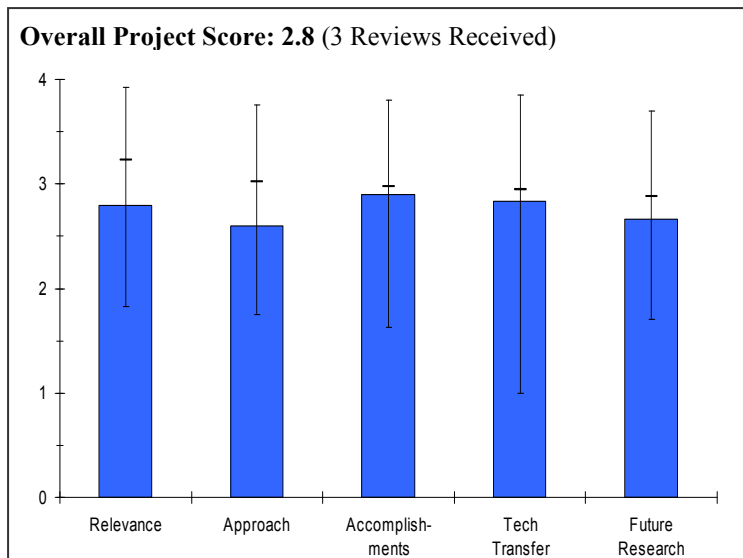
[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

The overall objective of this project is to develop hydrogen storage materials for reversible on-board application with hydrogen binding energies intermediate between physisorption and (dissociative) chemisorption. The University of California, Santa Barbara demonstrated the presence of molecular chemisorption of hydrogen in number of porous materials. Also, porous material with fluorinated organic and open metal sites was synthesized.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.8** for its relevance to DOE objectives.



- This project focuses on modifying the chemisorption properties of transition metals to either increase the number of bound hydrogen molecules or change their binding energies. Since stabilization of the active metals usually require large and massive organic support framework, these systems have very low storage capacity by either weight or volume. Unless, these metal complexes can either enhance hydrogen reactions with the framework group or serve as highly efficient catalyst to promote further adsorption, this approach has little potential to yield the needed improved hydrogen storage materials to meet DOE targets.
- The project addresses the objectives of the storage program in general terms without reference to the specific goals set by DOE.
- Relevant towards the discovery of a hydrogen reversible adsorbent with a " $\Delta H_2$ " of about 20-25 kJ/mole hydrogen.

**Question 2: Approach to performing the research and development**

This project was rated **2.6** on its approach.

- The approach to give enhanced chemisorption bonding on metal is primarily to alter the functional groups and framework geometry to alter electron density and accessibility for hydrogen molecules to bond.
- Structural characterization of these materials is by a combination of x-ray diffraction and neutron scattering with occasion hydrogen adsorption measurements.
- Good to excellent approach of focusing on the most critical property of hydrogen storage via adsorption - the heat that's associated with this reversible process, but capacity needs to be considered more.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.9** based on accomplishments.

- The PI indicated that changes in bonding energy at metal sites can be changed by ~50+ percent yet the total storage capacity for hydrogen storage is rather limited to surface areas of only a few hundred  $m^2$ /gram.

- While binding energies around 20 kJ/mol may be possible, the weight penalties seem to be substantial with little option for any real improvements.
- Excellent new science or materials which display a slight improvement in " $\Delta H$ " but unfortunately usually at a weight penalty. The mud touted effect of fluorinated linkages in metal organic frameworks is a case in point.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.8** for technology transfer and collaboration.

- The project has several international collaborators but relatively little interactions with the DOE hydrogen storage centers.
- The closure of the quasielastic QNES spectrometer at Intense Pulsed Neutron Source (IPNS)/Argonne National Laboratory has apparently restricted assessments of various samples by the PI and his collaborators.
- Good collaborative work.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.7** for proposed future work.

- The investigator has identified several candidate combinations of metals with organic linkers for evaluation of stronger bond formation that include chemical modification to increase surface areas as well as other properties.
- Needs more "new thinking" to focus on higher " $\Delta H$ " materials with a more favorable weight capacity.

**Strengths and weaknesses**

Strengths

- This project looks into details of single and multiple adsorption sites for molecular hydrogen as a possible method to produce bonding interactions that lie between conventional physisorption and chemisorption.
- The PI has long history in research and evaluation of the systems with insights into what modifications would alter adsorption behavior.
- The choice of Probins hydrogen interactions with host using inelastic neutron scattering is very sound.

Weaknesses

- There is little chance that practical high performance adsorption materials will be discovered from these combinations of transition metals and large framework of organic linkers.
- Project progress is highly depend upon accessibility to neutron scattering centers with limited capabilities or allocated testing times.
- The shut down of quasielastic neutron scattering capability at IPNS/Argonne National Laboratory will have a negative impact on the project.

**Specific recommendations and additions or deletions to the work scope**

- For near term neutron scattering studies, the PI should apply to the National Institute for Standards and Technology (NIST) neutron center for measurement time.

**Project # ST-27: A Synergistic Approach to the Development of New Hydrogen Storage Materials, Part I**

*Jeffrey Long, presenting; University of California-Berkeley. Jean M. J. Fréchet and Martin Head-Gordon, UC-Berkeley, and Sam Mao and Tom Richardson of Lawrence Berkeley National Laboratory (LBNL), Co-PIs*

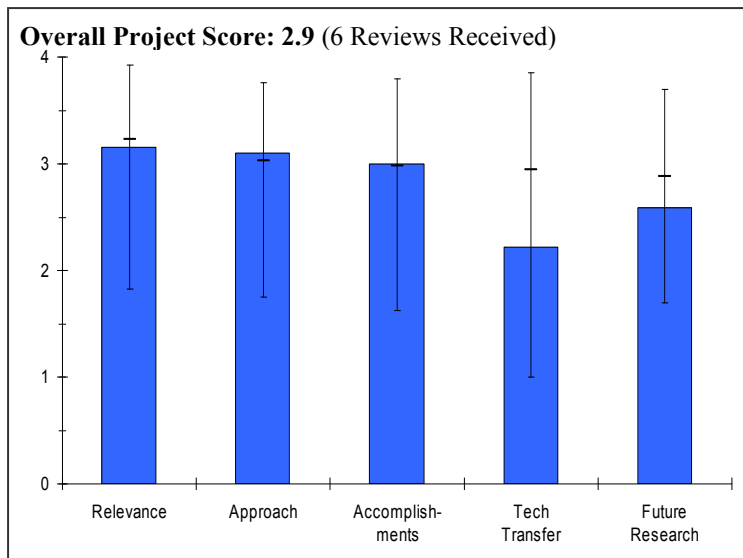
[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

The objectives of this project are the 1) synthesis of porous polymers; 2) synthesis of porous coordination solids; 3) calculations of hydrogen binding energies; 4) synthesis of destabilized hydrides; 5) hydrogen storage characterization instrumentation; 6) metal/metal hydride nanocrystals; 7) synthesis of nanostructured boron nitrides; and 8) theory for boron nitride materials.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.



- An apparent comprehensive effort out of Berkeley that addresses the programmatic efforts of the Office of Energy Efficiency and Renewable Energy.
- Long's group in particular synthesizes and analyzes a more interesting range of materials than other groups.
- Richardson and Head-Gordon appear to be contributing little relevance to this program and this is reflected in the publication record.
- No apparent contribution by Mao.
- Very innovative, cutting edge ideas about novel materials for hydrogen storage.
- Provides fundamental chemical insight into the molecular interactions that may optimize H<sup>+</sup> support interactions and thus H<sup>+</sup> storage density.
- Unclear whether or not improved hydrogen storage materials come out of this program since the concepts being explored are untested and in some cases unknown at this point.
- The goals of the research tasks that comprise this project are generally well aligned with the hydrogen vision and the DOE RD&D objectives.
- The nature of the work is mostly basic science aimed at identifying new types of materials with the potential to enable hydrogen storage systems that could conceivably meet the overall DOE hydrogen storage "system" capacity and performance targets.
- All the subtopics in this project do address and align with DOE objectives. Some aspects appear to be "hail Mary" efforts with little real hope of developing promising new leads (e.g., Cr doping), other aspects appear to be incremental efforts also with little real hope of promising new leads (e.g. differently-crosslinked polyaniline).
- Difficult to assess the "relevance" of this project, since it is composed of several distinct topic areas each of which have very different relevance to DOE objectives.
- Metal-organic framework materials (MOFs) are one of the most promising materials for hydrogen storage by physical adsorption and therefore are relevant to meeting the program goals.

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- Approach behind the work on porous materials is strong with interesting data. The volumetric densities that are calculated for the Zn benzene dicarboxylate are particularly interesting.
- Exploration of hypercrosslinked polymers looks like a good avenue to pursue.
- The work on destabilization should have a better grounding in thermodynamics/kinetics. It is not clear what the overarching theme is here. Many of the ideas at Mg destabilization are being addressed by other groups and in much more comprehensive ways.
- The computational effort also appears to be rather poorly focused. It appears to be directed at finding metals to put onto linkers but the rationale for this given the synthetic challenges and the gravimetric penalty associated with transition metal additions makes this pursuit of limited technological value and not very interesting from an intellectual standpoint. While the title of the presentation says synergistic, the integration with other parts of this program is weak.
- This is a basic science study grounded in the fundamentals of solid-state chemistry and coordination chemistry.
- The PI is a well-established young investigator in the area of coordination solid synthesis and is now demonstrating excellent skills in the area of organic polymer solid-state structures.
- The approach both for the metal-organic solids and the pure polymer systems are scientifically solid both from the synthesis and characterization points of view.
- Synthesis and characterization of porous polymers, porous coordination solids, and destabilized hydrides.
- Calculation of molecular hydrogen binding energies.
- Emphasis is placed on optimizing synthesis methods and on precise measurements of hydrogen uptake characteristics.
- Approaches to the R&D in the subtopics are generally sensible, but seem to be scattered and poorly integrated.
- It is difficult to review the "approach" for this project, because it almost seems like 3 completely disconnected projects (cross-linked polymers, MOFs, and destabilized hydrides).
- The destabilized metal hydride work does not seem to build on (but, rather seems to be redundant with) the considerable amount of work done on Mg-containing alloys and intermetallic systems in the metal hydride community.
- The cross-linked polymer and MOF work seems to be carefully thought out, and builds on (and surpasses) previous work in many respects.
- The efforts to increase the binding in MOF materials (e.g., via Cr incorporation) are likely to give a substantial penalty in gravimetric density.
- The PI has a well thought out approach to new materials development and has a good emphasis on new materials with high hydrogen binding enthalpy.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- The work on porous materials by Frechet and Long is interesting and very productive. Most of the presentation and the publications produced over the past year reflect this.
- The work of Head Gordon offers fewer physical insights and may be less relevant to the program.
- The work of Richardson does not cover any new intellectual ground from what has been articulated in this presentation.
- Program is meeting all scientific goals.
- New hydrogen absorption materials have been synthesized and characterized with respect to surface area and hydrogen uptake.
- Novel mechanisms of hydrogen support interaction have been explored.
- Understanding of the hydrogen uptake mechanism and improved solid-state synthesis of the conducting polymer systems.
- Presented results that showed the beneficial effect of polymer crosslinking on effective surface area, sorption capacity, and heat of adsorption.
- Clarified the required conditions for synthesis and stabilization of selected MOF materials; achieved record high effective surface areas with  $Zn_4O(BDC)_3$ .
- Attempted to incorporate metal carbonyls into MOFs with some preliminary evidence that hydrogen binding occurred.

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- Developed a new model for hydrogen binding that facilitates the study of how added metal centers influence binding of hydrogen in MOFs.
- Studied alloying of Mg to reduce the sorption enthalpy; preliminary results with fluoride addition look interesting.
- Seems to have "decent" progress in the subtopics.
- Porous polymers: the idea is intriguing, the reported results are sound but not yet exciting. Has there been any work on hydrogen uptake in crosslinked polyaniline as a function of extent of oxidation?
- MOF: Glad someone has paid attention to sample variability and stability. Ability to make Cr-hydrogen form is very interesting, its inability to release hydrogen is disappointing but not really surprising.
- Theory: Not clear that there is any new insight here.
- Hydride destabilization: Fluoride doping could be interesting but the reported results are not exciting.
- The work on cross-linked polymers seems promising, as this is a fairly unexplored area for hydrogen storage, and there is a huge "library" of possible polymers/crosslinkers.
- Very different surface areas found for MOF-5, depending on synthesis procedure, and found that exposure to air could be a controlling factor, and established a new synthesis and activation method, treating the samples as air sensitive (whereas others previously have not). This new synthesis procedure has led to substantially greater absorption than previous measurements on MOF-5.
- For MOF-5: Measured a volumetric density of 66 g/L at 77K and 100bar, approaching the density of LH<sub>2</sub>, though they are at 77K. Also found an excess absorption of ~7 weight percent, much larger than previously measured. However, the volumetric densities reported are a combination of the (measured) gravimetric density combined with the (ideal) single crystal density. So, actual volumetric densities will be reduced from this idea number by a factor of the packing density.
- Used quantum chemistry calculations to help identify more suitable binding metals. Similar to other predictions in other materials (e.g., at the National Renewable Energy Laboratory (NREL)), they are predicting things like transition metal (e.g., titanium). Synthesis is (like in the NREL predictions) a huge challenge.
- There has been good progress on making new MOF materials with higher hydrogen adsorption enthalpies. The conducting polymer materials do not show great promise for meeting the storage targets.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.2** for technology transfer and collaboration.

- Nature of collaborations has not been made very clear in any of this work.
- It appears that some collaboration takes place between the efforts of Long and Head-Gordon but they would benefit from better direction.
- Unclear that this requirement applies to the described study.
- Several partners are listed on slide 2 but it is not obvious how they interact with the project.
- Little was said about how this project connects to or communicates with the relevant CoEs.
- 5 investigators, 5 separate sub-projects. There is no evidence of any real attempt to integrate effort within this project itself, let alone with any other institution in the Hydrogen Program. This despite some potential opportunity.
- No collaboration/tech transfer identified. Also, the various portions of these projects (except the computational work) seems largely disconnected to the other parts of the project.
- Good collaboration with the National Institute of Standards and Technology (NIST) and other groups that perform characterization. Additional collaborations may be helpful for accelerating materials development.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.6** for proposed future work.

- Future work has not been addressed.
- The described studies are on track and will continue probing issues fundamental to synthesis and molecular interactions.
- The path is well defined and tracking well.

- The future plans are not well documented in the slide file.
- It was reasonably clear from statements made during the oral presentation that future work will proceed in directions that are sensible extensions of the work done in Fiscal Year 2008.
- Porous polymers: no communication of any future plans.
- MOFs: pi-complexation of different metals is further along in this project than in other projects of which this reviewer is aware, and some promising new directions are outlined. (If the dicarboxylate were anthracene-based instead of benzene-based, could Mg atoms be incorporated re Mg-anthracene? and what would happen then with hydrogen sorption?)
- Metal hydrides/fluorides: future plans seem rather pedestrian: more fluoride?
- No proposed future research was articulated.
- The PI's emphasis on new materials is very good and the attention to high adsorption enthalpy is consistent with the DOE program goals.

### **Strengths and weaknesses**

#### Strengths

- Work of Long and Frechet.
- Solid chemical foundations.
- Good molecular insight.
- Innovative materials and concepts for hydrogen-surface interactions.
- Successful identification of potential new hydrogen storage systems.
- Prof. Long and the other faculty working on this project are taking a scholarly approach to their research; the level of science is very high.
- The detailed study of what's important in the successful synthesis of MOF materials is much appreciated by the community.
- Well-known and respected investigators, excellent resources, further along in intentionally and advantageously functionalizing MOFs than other projects.
- The PI and his team have excellent capabilities in materials synthesis and characterization.
- The project is focused on new materials with high hydrogen binding enthalpies.

#### Weaknesses

- Work of Head Gordon and Richardson.
- Understanding of hydrogen-support interactions (proposed charge transfer mechanism appears unlikely) conducting polymer system.
- Synthesis of high surface area polyaniline systems.
- Misguided concept that a  $\text{Cr}(\text{CO})_2\text{H}_2$  system might be capable of releasing hydrogen under mild thermal conditions. (This idea violated known coordination chemistry). But, one can imagine other coordination systems where this might work.
- Needs better coordination with the CoEs; if substantive collaboration/communication does exist, it is not obvious from the presentation materials.
- Hydrogen storage based on sorption methods has no clear chance of meeting DOE's "system" storage targets at ambient temperature; the investigators working on this project are smart people who are capable of doing the type of back-of-the-envelope calculations that can readily show what it will take to store sufficient hydrogen by sorption methods at ambient temperature to meet DOE "system" targets for 2010 and more importantly beyond 2010.
- Sub-projects are too independent; insufficient effort to open new territory.
- Various portions of project are disjointed, and it's not completely clear (other than proximity) why they are together.
- The porous conducting polymer materials are unlikely to reach the necessary weight and volume targets for hydrogen storage materials.

### Specific recommendations and additions or deletions to the work scope

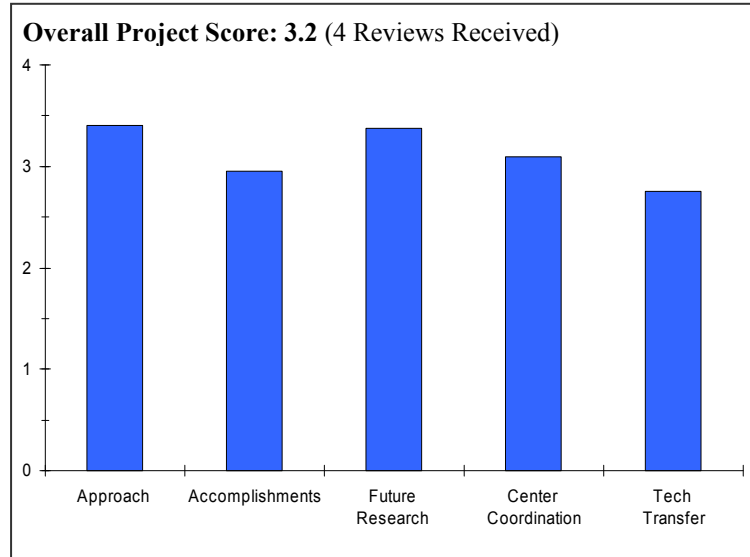
- Work of Richardson should not continue.
- Mao's contribution has not been presented and should not continue.
- Computational effort is poorly directed and doesn't appear to address program goals in any meaningful way.
- Continue program as is.
- Next year include summary slides for accomplishments and future plans.
- Elaborate on nature and effectiveness of collaborations with other related projects.
- Achieving Cr-doping by arene complexation in MOFs, begs the question of metal-arene complexation in the polymer systems. Could bis-arene-metal coordination be achieved as a "dehydrogenated" state, then the polymer subjected to strain while under hydrogen, resulting in metastable mono-arene-metal-(H<sub>2</sub>)<sub>x</sub> form? This is only one hypothetical example of how attempts to integrate the sub-projects might open new leads or concepts.
- Work on destabilized Mg alloys is not novel; this type of work has been extensively studied in the metal hydride community. No compelling justification was made to pursue this line, and it is not clear that the PI is aware of large amount of the previous work in this field.
- The PI should focus on new MOF materials and fundamental investigations on modifications to increase the hydrogen adsorption enthalpies.

**Project # ST-29: Metal Hydride Center of Excellence***Lennie Klebanoff; Sandia National Laboratory-Livermore*

[NOTE: This presentation was to evaluate the entire Metal Hydride Center of Excellence as a whole. A separate review form was used and can be found in Appendix C. Sandia's technical contribution to the center is evaluated in ST-36.]

**Brief Summary of Project**

The overall objective of the Metal Hydride Center of Excellence is to research, develop and validate reversible on-board metal hydride storage materials and systems that meet the 2010 DOE system targets for hydrogen storage, with a credible path forward for meeting the 2015 DOE storage targets. The approaches to meet the hydrogen capacity targets of 6 wt%, 45 g H<sub>2</sub>/L volume density are to 1) synthesize and characterize hydride materials with high hydrogen capacity and favorable thermodynamics; and 2) use state-of-the-art theory to guide the materials discovery effort. The approaches to meet the charge/discharge rate target of a 3 min system fill (5 kg) are to 1) develop materials that are fully reversible; 2) develop catalysts that aid reversibility; 3) assess nanoengineering promotion of kinetics; and 4) investigate the role of contamination on reaction rates. The approach to meet the hydrogen purity target of 99.99% is to assess release of NH<sub>3</sub>, B<sub>2</sub>H<sub>6</sub> and other volatile species from metal hydrides during desorption and cycling. The approach to meet the cycle life target of 1,000 desorption/adsorption cycles is to investigate durability of materials, cycling behavior, effects of contaminants, structural stability, and release of volatiles.

**Question 1: Approach to performing the R&D including Center Management**

This project earned a score of **3.4**.

- Materials go/no-go decisions that were done in September 2007 are extremely effective. The project is in a good shape.
- The center has demonstrated flexibility, for example dropping engineering focus based on new engineering center picking up the work but maintaining a liaison (exactly what was indicated); appropriate use of partners' skills and that partners have good skills in the area. The center has down-selected a large number of materials based on a combination of experiment and theory. They do review progress and ability to meet goals, and there are internal down-selects based there-on with clear criteria to get further support.
- Clearly focused on the key challenges and renewing that focus regularly.
- Work is being carried out by some partners on systems that initial favorable theoretical predictions have since been shown to have been in error.
- The theory team still needs to be pushed to include carbon compound outputs (methane).
- Based on the amount of work that has already been done on metal hydrides and the results achieved versus the challenging storage targets, including the results achieved in this center of excellence, it appears that metal hydrides have a significantly lower probability of meeting the on-board storage targets than other approaches. Although more is being learned about them, how to improve them, and to how find better metal hydride systems, they appear to have specific limitations that will be very difficult to overcome. Therefore funding this area of storage research to the extent it is funded may not be the best approach to meet the Department of Energy Hydrogen Program overall objectives.



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- This center of excellence is taking a broad, aggressive, and state of art approach to this research effort. The science being done is outstanding. They are including computational chemistry modeling to help screen and find new materials, nano-confinement, catalysis, as well as other important aspects to try to overcome the challenges for a metal hydride storage system. This is all very good work. This center of excellence is very well organized and following a good down-select process. There is an excellent process for gathering new ideas and materials, screening them against well defined criteria, and placing them in the appropriate part of the center of excellence if research on them is warranted.
- There is no mention of the storage cost target in the presentation. This also needs to be in the forefront of this effort.
- The center appears reasonably well managed. This reviewer's biggest concern is the amount of effort directed at a material system ( $\text{AlH}_3 = \text{Al} + \frac{3}{2} \text{H}_2$ ) that is already known to be irreversible; this effort is justified owing to this system being a potential learning tool. But this reviewer believes the effort would be better spent delving into the minute details of other systems that do have the thermodynamic possibility of being reversible: therein lies what really needs to be learned, what happens across solid-solid phase boundaries, how catalyst entities disperse and how they manage to function if non-dispersed, and etc.

### **Question 2: Technical accomplishments and progress toward DOE goals**

This project was rated **3.0**.

- The materials that meet the 2010 target and can be recharged on-board have not yet been proposed. However, the center of excellence has made go/no-go decisions and clearly selected potential materials to be studied.
- The confinement scheme is good progress. Determination of  $\text{B}_{12}\text{H}_{12}$  blocking intermediate is a key item that needs to be further understood. The alane ( $\text{AlH}_3$ ) work is important and looking at several ways to regenerate it. The theory group shows a good ability to learn and improve the quality of predictions based on experiment results and outside work. Calcium borohydride ( $\text{CaBH}_4$ ) work is important even if the material might not practical.
- The presentation could have done a better job of clearly stating in greater detail what the center of excellence has achieved over the past 12 months versus the Hydrogen Storage Subprogram's targets. Additionally it could have better described how and why the center of excellence believes it can fill the gap between current metal hydride systems' performance and the DOE targets.
- Based on the results that were presented, it is not clear that metal hydrides have a reasonable chance of achieving the DOE storage targets.
- There was no real detail in any area of the effort. The achievement statements were quite general and did not provide enough information as to the depth and level of the efforts. A few examples within the effort could have been very affective to clarify this.
- It is clear from the presentation that excellent science is being done in this project relative to computational chemistry modeling, nano-confinement, catalysis, and other areas. More detail on these would have been very welcome to get a better sense of these efforts.
- There is a decent record of publishable findings, however it has not been quite so good at focusing the "progress engine" toward making the vital findings in kinetics and thermodynamics of the hydrogen release/uptake cycle. One bright spot is Professor Robertson's demonstrated ability to focus on catalyst/material-phase interactions. Another is the apparently aggressive de-selection of some concepts that are not able to achieve DOE targets.

### **Question 3: Proposed future research approach and relevance**

This project was rated **3.4**.

- This year the center of excellence showed the go/no-go decision for the materials and distinguished individual scientists who lead each subject. It is a good direction that theoretical activities to explore novel materials will be coordinated by a talented scientist.
- Areas of future work are correct for their current position and the upcoming engineering center. In these areas the approach seems appropriate. I think it this is a good plan.
- The path forward and list of efforts for the future work fits well with what this center of excellence has accomplished and learned to date. The center of excellence efforts are well organized and utilize an excellent

process to gather new ideas and materials, screen them, and establish efforts on them in the appropriate parts of the center of excellence when warranted. The areas being pursued should yield continued advances in this area.

- There was nothing in the future work, nor details within the accomplishments to date, that suggests a strong likelihood that through these efforts, a metal hydride system could be developed that would meet the DOE on-board storage targets.
- Future plans appear reasonable. This reviewer accepts the premises of the Director, that only nanostructure and/or catalysis will improve the rates of hydrogen release/uptake for any material system, and that only composition (and perhaps nanostructure?) will improve the thermodynamic parameters for hydrogen release/uptake. Given the capacity requirements, a focus on boron materials appears sensible. Nitrides do not look as promising owing to the need for additional complexity (in material & chemistry, possibly also in system engineering) to mitigate ammonia (NH<sub>3</sub>) loss.

#### **Question 4: Coordination, collaborations and effectiveness of communications within the CoE**

This project was rated **3.1**.

- There are a large number of collaborations among projects under the Metal Hydride Center of Excellence.
- The partners are communicating regularly. This is good. The intellectual property (IP) agreement does seem to lead to less than full disclosure and thus inhibits cross fertilization. Structure is good. Interaction outside is quite good. There is a history of experiment guided by theory. Now that the communication going both ways between the experimentalist and theoreticians, it is clearly paying off in better theory.
- There appears to be good interaction, coordination, and communication within the members of the center of excellence based on the presentation, the project organization, and the results to date.
- Coordination and cooperation among partners appears to be good. Other center partner talks (e.g., Robertson, Johnson) offer more insight into the communication/coordination than the center talk itself.

#### **Question 5: Collaborations/Technology Transfer Outside the CoE**

This project was rated **2.8**.

- International collaboration has not been included in the presentation.
- Very good outside collaboration. Collaboration is on several fronts and not isolated to one area. Work with other centers (e.g., Vajo-Baumann) is great. They are also publishing with outside groups.
- The project has resulted in an impressive number of publications and talks at important conferences.
- It is not clear if there is any collaboration outside of the center of excellence. The center of excellence is quite large by itself but some collaboration with the private sector, especially perhaps with the OEM stakeholders could be very valuable.
- There is little evidence that the center is coordinating outside of itself.

#### **Strengths and weaknesses**

##### Strengths

- The go/no-go decision is a very strong point of the Metal Hydride Center of Excellence. This is a good example that the management of the center of excellence works effectively. There are a large number of world-class scientists in the center of excellence and they carry out their research intensively.
- The center has strong players.
- They are willing to learn from errors.
- Theory, experiment, and to some extent engineering all interact.
- A large collaborative group of excellent scientists are applying state of the art techniques and chemistry to try to find a metal hydride system that can meet the very challenging targets of the DOE on-board Storage Program.
- This center appears to be the best one poised to orchestrate the discovery and development of a lightweight, high capacity, truly rapidly reversible, metal hydride storage system.

### Weaknesses

- The engineering part will be dissolved and the activities will be moved to the new Engineering Center of Excellence. Therefore engineering applications, such as large scale preparation, may be lost. Collaboration with the new Engineering Center of Excellence will be indispensable.
- There is more secrecy internally than is good with some partners not appearing to fully collaborate.
- There is still a need to upgrade theory to be fully helpful.
- Metal hydrides have been studied for some time. There may be fundamental characteristics of this approach to hydrogen storage that make it unlikely that it can ever meet the DOE on-board Storage Program targets.
- It is not at all clear that Nature will cooperate in allowing the existence of a metal-hydride storage system that meets all DOE expectations.

### Specific recommendations and additions or deletions to the work scope

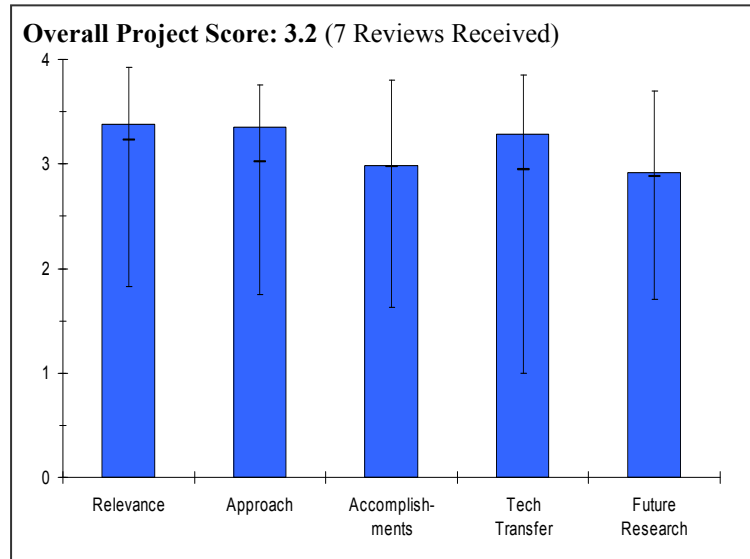
- Strong collaboration with the new Engineering Center of Excellence is highly recommended.
- Include carbon products in the theory package.
- Discontinue work on materials that will never be reversible.
- De-emphasize this storage center of excellence relative to other storage research and development by reducing its funding level.
- Recommend the Center give very careful consideration to whether Al/alane really makes sense, and to whether the work on it will give truly useful knowledge. Put more emphasis on atomic-scale understanding of interphase and intra-phase atom mobilities and catalytic effects.

**Project # ST-30: Thermodynamically Tuned Nanophase Materials for Reversible Hydrogen Storage***Ping Liu; HRL Laboratories*

NOTE: This project is part of the Metal Hydride Center of Excellence.

**Brief Summary of Project**

The overall objective of this project is to develop and demonstrate a safe and cost-effective light-metal hydride material system that meets or exceeds the DOE goals for reversible on-board hydrogen storage. The 2007-2008 objectives are to 1) identify and test new high capacity Li- and Mg-based destabilized hydrides; 2) screen candidate  $\text{LiBH}_4 + \text{MgX}$  destabilized systems and evaluate energetics and kinetics; 3) down-select systems for additional work; 4) evaluate sorption kinetics and thermodynamics of  $\text{LiBH}_4$  and Mg in carbon aerogel scaffolds; 5) investigate effects of pore size and pore size distribution on reaction rates of  $\text{LiBH}_4$ ; and 6) incorporate Mg into the aerogel and measure its kinetics.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.4** for its relevance to DOE objectives.

- This program is highly relevant to the Department of Energy Storage Subprogram.
- It is concerned with novel, thermodynamically destabilized, nanophase materials for hydrogen storage.
- The introduction of carbon aerogels as scaffolds to preserve the nano-scale properties of the active materials is innovative.
- Systems of interest are  $\text{Li}(\text{BH}_4)$ ,  $\text{MgH}_2$ ,  $\text{Li}(\text{BH}_4)/\text{Mg}_2\text{NiH}_4$ ,  $\text{MgX}$  ( $\text{X}=\text{Ni}$  or  $\text{Si}$ ) as well as aerogel properties.
- This program has the capability to synthesize and characterize these materials. This capability is highly relevant to DOE objectives.
- The project is very relevant.
- The project objectives and respective work plan are very well aligned to the hydrogen vision and they are of high relevance to the DOE research and development strategy.
- This project to develop and test new high capacity lithium- and magnesium-based destabilized hydrides is clearly contributing to DOE's objectives.
- The project is aligned with the hydrogen vision and DOE research and development objectives.
- The objective to screen lithium- and magnesium-based hydrides is good.
- Incorporating magnesium into the carbon aerogel is a unique objective.
- The project is focused on  $\text{LiBH}_4$  system, which has a potential for high hydrogen capacity.

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- The approach is highly scientific and professional.
- A compilation of attractive destabilized systems was carried out.
- The pertinent properties of selected systems were characterized.
- Aerogels of various pores sizes were synthesized.

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- The selected systems were or will be incorporated into aerogels.
- This is an interesting experimental approach that focuses on existing barriers.
- The project is well-designed.
- This is a solid, well thought-out approach. The project is moving with clear steps to address the key issues and closely following up progress against set milestones and implementing go/no-go decisions.
- They are fully exploring possibilities offered by advances in hydride destabilization methods and nanoengineering.
- The approach for MH destabilizing and nanoengineering seems to be well thought-out and feasible.
- The principal investigator presents adequate experience to perform the proposed research.
- The focus to enhance reaction rate by nano-engineering is good.
- The focus on destabilized system will help in lowering enthalpy ( $\Delta H$ ).
- This project is focused on kinetic enhancements that are critical to practical use as well as thermodynamic destabilization and hydrogen content.
- A much stronger integration with other efforts within the center is needed, specifically with respect to advanced characterization.
- There is little to no focus on efficiency.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- The system  $\text{Li}(\text{BH}_4)/\text{Mg}_2\text{NiH}_4$  was found to be reversible at  $350^\circ\text{C}$  with a hydrogen storage capacity up to 8 weight percent.
- The reactions and product phases were determined.
- A  $\text{Li}(\text{BH}_4)$  - aerogel system was characterized.
- High loadings of magnesium in an aerogel were achieved with no change in thermodynamics with an associated improvement of reaction kinetics.
- Aerogel temperature and pore size effects were determined.
- Good progress.
- The approach may require a significant adjustment if degradation of the hydrogen storage component is due to the formation of  $\text{B}_2\text{H}_6$ .
- Satisfactory accomplishments and sound progress, particularly taking into account the degree of complexity and level of challenge of this research.
- Encouraging data from the use of aerogel scaffolds with destabilized hydrides for lowering desorption temperatures and improving kinetics.
- Screened a new class of destabilized material systems; progressed in nanoporous scaffolds and starting to understand the effect of pore size and distribution.
- The principal investigator has made significant progress towards developing a new  $\text{LiBH}_4/\text{Mg}_2\text{Ni}$  system for hydrogen storage.
- The success of the destabilizing and nanoengineering techniques in lowering reaction temperatures and improving kinetics contributes towards improving the performance of these materials.
- Significant progress has been made as evidenced by publications and presentations.
- Improvement in kinetics by use of nanopore materials is demonstrated in this project. This result is very instructive to research and development activities of metal hydrides with practically high desorption temperature.
- Finding of ternary borides shows possibility of other metal hydrides with high capacity and low desorption temperature.
- Successful impregnation of aerogels with magnesium.
- No improvements in dehydrogenation temperature of magnesium hydride.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- This program has extensive collaborations both within and outside the Metal Hydride Center of Excellence.
- A total of two refereed publications over the period of 2007 to 2008 have been produced.
- Similarly a total of three presentations have been given.
- A provisional Patent application "Metal Filled Porous Carbon" has been filed.
- Good collaboration.
- Limited industrial collaboration.
- Strong collaborations within the Metal Hydride Center of Excellence, but also with other DOE-funded projects (carbon scaffolds work) and international collaborations (access to unique testing facilities and expertise).
- The cross-center collaboration is particularly important when expertise developed in one center can benefit the others.
- There is a large degree of interaction between the principal investigator and partner institutions in this project.
- Impressive collaboration with center of excellence and other intuition.
- This project has contact with research groups of nanomaterials in other centers of excellence as well as the theoretical research group in the Metal Hydride Center of Excellence.
- Even though multiple partners are listed, actual partnering is obscure, if at all existent.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- The incorporation of  $\text{Li}(\text{BH}_4)\text{-MgH}_2$  in an optimized aerogel scaffold.
- The following systems will be candidates for scaffolding:  $\text{Li}(\text{BH}_4)\text{-Mg}_2\text{NiH}_4$ ,  $\text{Li}(\text{BH}_4)\text{-MgF}$ ,  $\text{Li}(\text{BH}_4)\text{-MgS}$ ,  $\text{Li}(\text{BH}_4)\text{-MgX}$  where  $\text{X} = \text{O}, \text{OH}, \text{Ni}$ .
- Adopt nano-engineering to improve kinetics.
- Research plans are well defined and realistic.
- The approach presents a clear idea of current material system limitations and is well structured, with carefully drawn future plans. Very useful project progress and future direction matrix.
- Opening a new research avenue with the exploration of oxide-based destabilization reactions supported by the theory group.
- The principal investigator seems to have a good plan for building on the work already accomplished.
- The research should continue as planned.
- Plans built on past progress.
- Nano-engineering to reduce diffusion distance should help reaction rates.
- Theory to address oxide-based destabilization is essential.
- Future research into new destabilization agents is lacking reason. Why  $\text{MgX}$  with  $\text{X} = \text{O}, \text{OH},$  and  $\text{Ni}$ ? Especially  $\text{Ni}$  since the  $\text{LiBH}_4/\text{Mg}_2\text{NiH}_4$  system has been already investigated. Is there a reason to expect that  $\text{MgO}$  will be so much different from  $\text{MgS}$ ?
- How will the fully destabilized  $\text{LiBH}_4/\text{Mg}_2\text{NiH}_4$  system be incorporated into scaffolds? How will the stoichiometry be controlled/varied from one pore to another? With an expected broad distribution of stoichiometries, what will be the utility of future work?

#### **Strengths and weaknesses**

##### Strengths

- A very strong scientific effort.
- The resources appear adequate.
- The technology transfer is good.
- The use of a scaffold to preserve physical integrity and prevent dissemination nano particles.
- The realistic appraisal of critical problems and issues.
- The demonstrated reversibility of the  $\text{LiBH}_4/\text{Mg}_2\text{NiH}_4$  system.
- Solid experimental work.
- Good collaboration.
- Strong team, highly skilled, with an open mind and a clear vision.
- The principal investigator presents adequate experience to make the project successful.

## HYDROGEN STORAGE

- Nano-engineering.
- The results in this project are totally analyzed according to appropriate structural and thermal analytical data.
- This project considers kinetics, thermodynamics, and hydrogen capacity.
- Using scaffolds to control diffusion distances.

### Weaknesses

- The prospect that any of the scaffold systems will meet the 2010 DOE targets is unlikely.
- The possible evolution of borane has not been addressed.
- The question arises, what are the safety issues involve with aerogels and their incorporated materials?
- Due to high processing temperature, carbon aerogel offers limited opportunities for functionalization/doping.
- Practical considerations with respect to aerogels, capacity limitations and, cycling performance, have not yet been addressed. Is it possible to have scaffolds of high enough specific porosity volume to “balance”/mitigate the capacity penalty for instance?
- Feasibility of developing a destabilized material system able to meet all thermodynamic targets for application; theoretically calculated values have not been experimentally confirmed.
- Even if the project succeeds, the materials barely have enough hydrogen holding capacity to meet DOE's 2010 goals.
- Lack of theory group.
- Conclusion that lowered kinetics in 4nm pores is due to limited access of hydrogen is unsupported by the data. 40 angstrom holes are still much larger than hydrogen molecule.
- A claim about "beginning to understand pore size/distribution effects" is unsupported by the data. No actual understanding provided.
- Dissemination of results (publications/presentations) is low.
- NMR, FTIR characterizations have been planned but have not been done.
- Work on scaffolds appears to be separated from work on destabilized systems.

### Specific recommendations and additions or deletions to the work scope

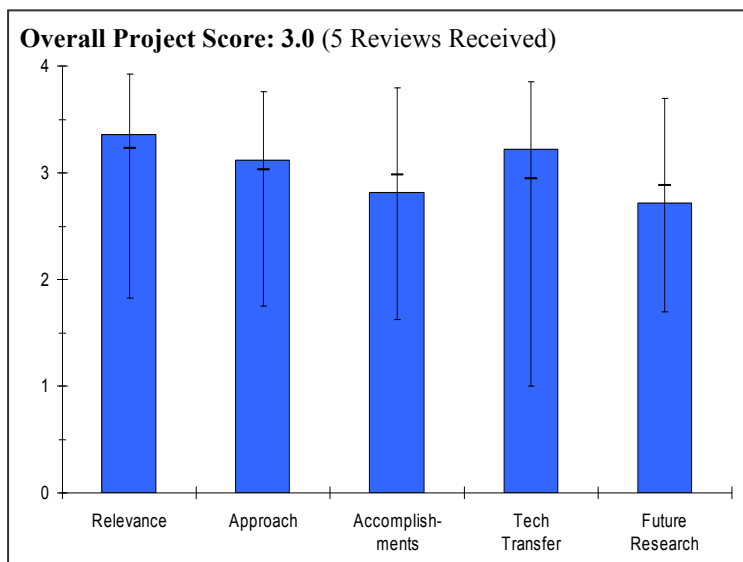
- It is likely that high melting point alloys will have very poor phase separation kinetics when the product phases require long range metal atom rearrangement. Thus some effort should be diverted to low melting point systems that do not require large metal atom diffusion distances. In the latter case very small nano particles ameliorate such problems as shown in this project but they also introduce other difficulties.
- Further emphasis on borohydrides should include the determination of whether evolution of borane is a problem.
- At this point the type of safety issues which may arise should be addressed.
- Increase emphasis on the  $\text{LiBH}_4/\text{Mg}_2\text{NiH}_4$  system.
- Closely collaborate with theoreticians and modelers to refine the destabilization predictions so as to better guide further investigations.
- Explore the effects of incorporated catalysts on the sorption kinetics.
- Much better integration with theory.
- Focus on scaffolds and nanostructuring.

**Project # ST-31: Chemical Vapor Synthesis and Discovery of H<sub>2</sub> Storage Materials: Li-Al-Mg-N-H System**  
 Zak Fang; University of Utah

NOTE: This project is part of the Metal Hydride Center of Excellence.

**Brief Summary of Project**

The overall objectives of this project are to 1) discover new solid hydrides that meet reversibility and kinetics requirements; 2) develop the chemical vapor synthesis process (CVS) for production of nanosized solid metal hydrides; and 3) demonstrate the effectiveness and unique properties of nanosized solid hydride materials. Objectives for fiscal year 2007-2008 are to 1) understand reaction mechanisms of materials based on lithium alanates destabilized by light metal amides, and LiMgN; 2) establish capability and quantify NH<sub>3</sub> co-production during dehydrogenation; 3) synthesize new materials using high-energy, high-pressure reactive milling process; and 4) synthesize nano precursor and hydride powders using the CVS process.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.4** for its relevance to DOE objectives.

- The project is partially aligned with Department of Energy research and development objectives.
- Based on the stated objectives, this project seems to be highly relevant to DOE's goal of discovering new high capacity materials for hydrogen storage.
- Enhancement of compound reversibility is relevant to the DOE objectives.
- Project is quite relevant to DOE program objectives, especially in relation to the Metal Hydride Center of Excellence work program and aims. Important results are expected with respect to the applicability of certain material types (especially Li-Al-Mg-N-H systems).
- Materials based on the Li<sub>3</sub>AlH<sub>6</sub> + <sub>3</sub>LiNH<sub>2</sub> system should be abandoned from further consideration since the temperatures required to achieve reversibility are much too impractical.
- The principal investigator has made a good effort to realign the program objectives by focusing on the LiMgN system, which has proven to be reversible with a theoretical capacity of 8.2 weight percent. However, the dehydrating temperature for this system also appears to be impractically high (~200°C) and, hence, may warrant focusing efforts on a different, more promising system.

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- The approaches are good in general if these reactions can ever work for on-board usage.
- The chemical vapor synthesis and high-pressure high-energy synthesis route are effective.
- There is a lack of overall structure in approach.
- There is a lack of creativity.
- The project is well designed and incorporates rapid screening tools such as TGA, XRD and FTIR as well as PCI and NMR for in depth characterizations.



## HYDROGEN STORAGE

- The principal investigator plans to demonstrate feasibility based on characterizations of the thermodynamics and kinetics. This is important.
- Good usage of the theoretical estimation results with regards to the LiMgN compound.
- Mechanistic understanding and visible collaboration with other center members (i.e. NMR, effects of O<sub>2</sub>) is good.
- Overall approach is sound and focused on the project aims. Important milestones lie ahead (September 2008) and quite rightly a go/no-go decision on LiMgN and (Li<sub>3</sub>AlH<sub>6</sub> + <sub>3</sub>LiNH<sub>2</sub>) suitability is to be taken in September 2009.
- While chemical vapor synthesis of hydride materials is a potentially useful approach, it is not evident from the presentation what scale of throughput may be achieved by the system. If found to be important in synthesizing nano-sized powders of a highly-active metal hydride, what is the practical scalability of the process?

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- The principal investigator made some good progress toward objectives.
- Some new synthesis routes have been validated.
- It was confirmed that LiMgN is reversible with 6.6 weight percent capacity. This is good but the ammonia production poses a significant problem that must be solved.
- MgLiN could not be reversed such that the total 8 weight percent was obtained. This could imply a multi-step decomposition with observed ammonia formation. For future work, it is not clear how this could be improved.
- Promising results have been obtained on two fronts (Li<sub>3</sub>AlH<sub>6</sub> + <sub>3</sub>LiNH<sub>2</sub>) and LiMgN (although the latter is relaxed to the (MgH<sub>2</sub>+LiNH<sub>2</sub>) system that is no longer pursued at the Metal Hydride Center of Excellence level). Rehydrogenation of the former system is found to depend on heating rate and this should be further explored. LiMgN is shown to be a 6.6 weight percent reversible material and this justifies further work on it.
- Now that the principal investigator appears to have both analytical and synthetic capabilities well in hand, progress toward discovering and screening new hydride materials with acceptable sorption temperatures should proceed at an accelerated pace. More frequent collaboration with the theory group of the Metal Hydride Center of Excellence is strongly encouraged to aid in the selection of potentially promising systems for experimental studies.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.2** for technology transfer and collaboration.

- Some collaborations exist.
- The PI works closely with the theory group.
- Collaboration with the Metal Hydride Center of Excellence Theory Group to identify promising candidates has been an asset to this project.
- Collaboration with the other center members researching amide-hydride mixtures is suggested to avoid duplication.
- Good interaction for mechanistic understanding, such as NMR.
- Several collaborations exist and complement nicely the work done at the University of Utah. Close interaction and good coordination is shown.
- As mentioned above, more frequent collaboration with the theory group is encouraged in order to help select additional hydride chemistries of potential interest.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.7** for proposed future work.

- The general research direction should be aligned with potential on-board usage.
- Chemical vapor synthesis is a proven approach for synthesizing nano-sized. However, the principal investigator needs to expend more effort in determining what is the phase and chemical composition of the end product.

- The plan to focus on LiMgN and  $\text{Li}_3\text{AlH}_6 + 3\text{LiNH}_2$  and to develop techniques to minimize the release of  $\text{NH}_3$  are reasonable and this will address a key barrier to using these materials for hydrogen storage.
- Nano particles of LiMgN: Using methods such as CVS could help solve the kinetics problem initially but sintering as the material is cycled could occur. Careful tracking of particle size is highly recommended. It is also not clear how the particle size relates to the potential multi-step decomposition path.
- Overall path forward for  $\text{NH}_3$  mitigation needs to be more clarified (i.e., to avoid scenarios similar to  $\text{LiNH}_2:\text{LiH}$ ).
- Future research plan makes sense and builds properly on progress achieved so far.  $\text{NH}_3$  emission is an issue but the finding that it depends on heating rate provides interesting hints on how to fight it. The high pressure, high energy ball milling process can be further explored. The Mg-Ti system on which it is applied is an interesting one, especially with regard to the differences observed between film and bulk material.

### **Strengths and weaknesses**

#### Strengths

- Experimentally validated the predictions from the theory group.
- The applicant has the resources needed to complete the proposed work.
- Utilization of theory to guide materials selection and following systematic approach.
- Promising results on the two systems investigated. Findings about heating rate dependence of rehydration process and ammonia release may have important implications.
- The principal investigator has strived to obtain detailed, mechanistic characterization of candidate metal hydride systems, leading to a better understanding of the attributes and pitfalls of such systems.
- Establishment of an apparatus for chemical vapor synthesis of nano-size hydride precursors provides a potentially useful venue for rapidly synthesizing new materials and screening their viability.

#### Weaknesses

- There is a lack of a systematic approach in selecting the materials to be studied.
- The use of a pH meter to detect  $\text{NH}_3$  formation is not the best way to do this. An RGA has more sensitivity and it can detect a variety of other gases that may be produced. The principal investigator could send samples to a partnering institution for RGA analysis if one is not available on site.
- Further clarification of path forward and how current problems will be tackled is needed.
- Further collaboration with other members working on amides and alane is needed.
- Issues related to  $\text{NH}_3$  emission need to be dealt with. Maximum capacities expected range between 6.6 to 8.0 weight percent and are therefore low.
- Materials that are found to be thermodynamically non-viable are not being abandoned early enough in the program to allow a more aggressive pace in the investigation of other candidate materials/chemistries.

### **Specific recommendations and additions or deletions to the work scope**

- A go/no-go decision should be made within the current fiscal year on whether or not  $\text{NH}_3$  evolution from the LiMgN system exceeds acceptable limits. If the results show that  $\text{NH}_3$  exceeds acceptable limits, further study of this system should also be abandoned in favor of new chemistries as predicted by theory (e.g.,  $\text{Li}_2\text{CN}_2$ ).
- Further characterization studies on the  $\text{Li}_3\text{AlH}_6 + 3\text{LiNH}_2$  system should be abandoned.
- Potential formation of  $\text{CH}_4$  from the amide-carbon mixture should be carefully addressed.
- Clarification on how the nano structures, for both Al and LiMgN, could enhance the decomposition temperature and decomposition route is suggested.
- The Mg-Ti system presents interest. It would be nice to explore further the HPHE milling facility to try to understand the observed differences between films and bulk material in this case.
- Abandon the  $\text{Li}_3\text{AlH}_6 + 3\text{LiNH}_2$  from further study.
- Abandon the LiMgN system if  $\text{NH}_3$  evolution is confirmed to exceed the acceptable limits.

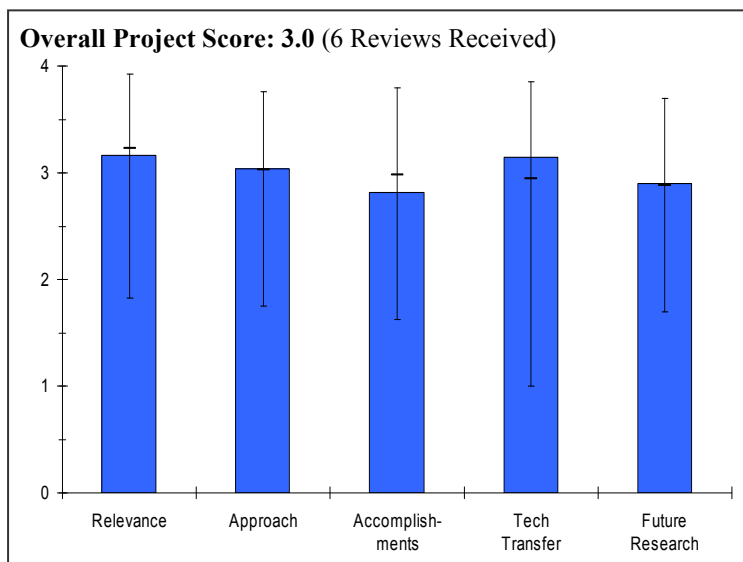
**Project # ST-32: Reversible Hydrogen Storage Materials – Structure, Chemistry and Electronic Structure**

*Ian Robertson, presenting; Duane Johnson, Co-PI, University of Illinois-Urbana-Champaign*

NOTE: This project is part of the Metal Hydride Center of Excellence.

**Brief Summary of Project**

The main objectives of the University of Illinois, Urbana-Champaign within the Metal Hydride Center of Excellence (MHCoe) are to 1) advance the understanding of the microstructural and modeling characteristics of complex hydrides; 2) provide feedback and knowledge to partners within MHCoe framework; 3) provide more reliable theoretical methods to assess hydrogen-storage materials, including key issues affecting materials under study; and 4) help achievement of specific targets and milestones.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.

- The project supports the DOE objectives.
- Catalyst study (distribution) in response to barrier A; theory work in response to barrier C; not clear how barrier B has been addressed directly by the project.
- This project to develop new theoretical models for studying hydrogen storage systems aids partnering institutions in their efforts to understand these materials and therefore supports DOE's goals.
- Experiments on catalyst dispersion are relevant (score 3.0).
- Theoretical calculations are mostly irrelevant since it is not clear they add anything beyond what Georgia Tech/Pitt project is already providing (score 1.0).
- Claims that they have developed a "new theoretical method" are unfounded.
- Quite good. Comes closer than other projects to developing a nano-, almost atom-, scale understanding of how the material constituents and their catalysts function in a metal-hydride storage system.
- Experimental work on micro structural analysis and location of catalyst particles is critical towards improving these materials, and making current high-capacity (but irreversible) materials more practical. Theoretical work does not have as clear a relevance to the Hydrogen Fuel Initiative.
- Project is essential to supporting materials discovery efforts within the Metal Hydride Center of Excellence by providing advanced characterization and theoretical modeling capabilities.
- The project provides scientific support for characterization and microstructural analysis of complex hydrides and theoretical work aimed at prediction of new crystal structures.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- The project is technically feasible and is well integrated with other research in the Metal Hydride Center of Excellence. It contributes to overcoming some barriers.
- Experimental approach score 3.0.
- Theory score 1.5.

- Also quite good. Very impressed by the emphasis on detailed understanding at the scale of smallest-detectable phases, and below.
- Experimental work combining a variety of techniques to locate catalyst particles in various hydride materials is really unique and important work. However, it would be helpful to see more of a connection as to how this information is being used to guide experimentalists towards new catalysts, processing, materials, etc. At the moment, this connection is not clear.
- Not clear how the theory work here is differentiated from other work in the center of excellence, and what true value it is providing.
- Imaging techniques developed to characterize catalyst-particle dispersal will provide much needed information about the effectiveness of processing steps, such as ball milling.
- The development of DFT-based methods to predict reaction enthalpies and, ultimately, the Van't Hoff plots are a significant accomplishment that should find broad use for predicting such properties in novel materials prior to experimental measurements.
- It is not clear what specific new methods were developed in connection with this project.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- The development of a theoretical model suggesting that reversibility is affected by intermediates is valuable information to researchers who seek to understand the mechanism.
- Since last year there seems to be only minimal experimental progress, and essentially zero theoretical progress.
- Good techniques developed in electron-microscope imaging, but could use more progress toward exploiting the understanding of catalyst and phase effects in improving kinetics.
- Measurement of catalyst dispersal in a variety of materials is an excellent accomplishment.
- Theoretical work on  $\text{LiBH}_4$  seems very similar to what was presented last year (the figure is the same), and even to what was presented in 2006.
- Significant technical accomplishments have been made thus far in the program.
- Understanding of intermediate phases and prediction of reaction enthalpies.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- The principal investigator has worked closely with partners within the Metal Hydride Center of Excellence to provide a theoretical framework for their investigations.
- There are some minor collaborations with Dr. Ronnebro and Sandia National Laboratories on materials. Wider collaboration with other center partners should be encouraged.
- Appears to coordinate and communicate well with other center partners.
- Experimental work is closely connected with other portions of the center of excellence. Theoretical work seems largely unconnected.
- Imaging methods developed to characterize catalyst dispersion are relevant to physisorption materials, and collaboration should be extended to the respective center.
- Collaboration between theory and experiment, particularly leading to joint publications, should be improved.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- The principal investigator plans to continue the modeling work that is underway and to build on past progress.
- The proposed future work is okay but seems on the "passive" side.
- The aim is to continue work as before. While the previous published work is of good quality, I would have liked to see some novel approach towards discovering new materials/catalysts.

### Strengths and weaknesses

#### Strengths

- The team operates in support of the center and in close coordination with other center partners.
- Determination of catalyst distribution (and Alane precursor).
- Characterization methodology is versatile and has qualified and quantified the efficiency of the dispersion of the catalysts.
- Reaction enthalpy calculations have been validated.
- Accurate and better prediction of reaction enthalpies in molecular solids by adding corrections.
- Demonstrated ability to quantify efficacy of ball-milling and mixing for dispersion of catalyst reversibility and starting phases.
- Integration with center activities.
- Accurate predictions of reaction enthalpies of destabilized reactions.
- None noted.
- Good experimental techniques. Good at asking important questions about the materials and driving toward some answers.
- The methods being developed under this project are capable of providing important insights into the structural and thermodynamic properties of candidate storage materials, and would serve as important screening tools for many investigators.
- The project benefits from theoretical input and seems to be driven by theory. The prediction of alloy phase diagrams is an asset to the program.

#### Weaknesses

- There are some limitations due to beam damage in “low-dose” STEM mode.
- The project is currently understaffed.
- None noted.
- Theory project seems to be irrelevant.
- Theory component does not seem as well advanced nor integrated nor as adept at asking the critical questions.
- The project's ability to ask critical questions has led to some improved understanding, but the next steps (from understanding to improvement to breakthrough) does not seem to have happened - yet.
- No significant weaknesses on which to comment.
- The record of publications is disappointing, particularly from the experimentalists.

### Specific recommendations and additions or deletions to the work scope

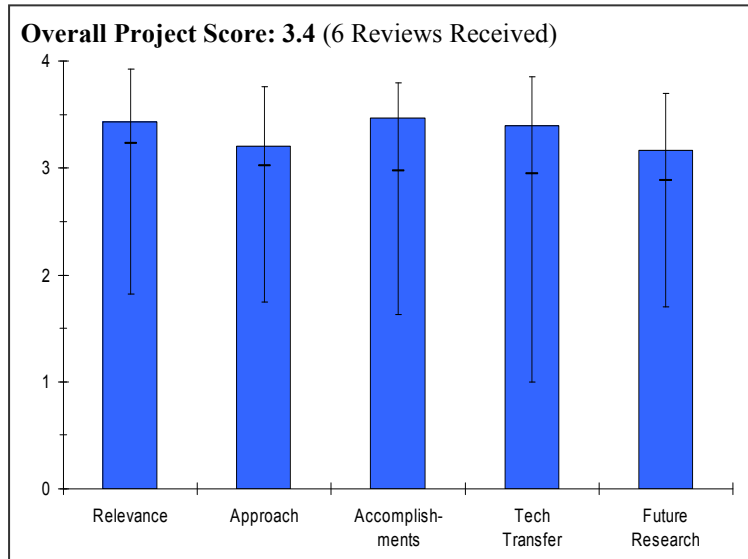
- Expand interaction with the Metal Hydride Center of Excellence efforts to help individual investigators screen the predicted properties of new materials under consideration.
- Given the strong contributions of the Georgia Tech/Pitt and Majzoub (U. Missouri) theory projects, it is recommended to eliminate this theory project and redirect efforts towards experiments.
- The dehydrogenated form of boron-based materials is usually a boride, and most borides have extended boron-boron networks that are absent in the hydrogenated form. The need to disrupt and re-form such boron-boron networks has to be a contributor to poor kinetics. Find a new way to mobilize boron atoms and facilitate the formation/disruption of boron-boron networks. Or find a boron-based material that doesn't need to have them.
- The PI's should broaden the scope of their research. I do not see how more funding can enable the PI's to be more innovative.
- Coordinate with the physisorption center. Plan for future work should be expanded to include characterization studies on promising physisorption materials; namely, such materials that take-up hydrogen via a spillover mechanism. Structural characterization relative to catalyst dispersion and interfacial region between catalyst and substrate in these materials is needed.

**Project # ST-33: First-Principles Modeling of Hydrogen Storage in Metal Hydride Systems***Karl Johnson, presenting; University of Pittsburgh, David Sholl, Georgia Tech*

NOTE: This project is part of the Metal Hydride Center of Excellence.

**Brief Summary of Project**

The overall objectives of this project are to 1) compute the thermodynamics of metal hydride systems; 2) compute interfacial properties of hydrides; and 3) address fundamental processes in hydrogenation. Specific objectives for fiscal year 2007-2008 were to 1) develop an automated approach for screening complex hydrides by gravimetric densities and heats of reaction,  $\Delta H$ ; 2) explore nanoparticle thermodynamics through calculation of surface energies and Wulf construction calculations; 3) screen doped hydrides for phase stability; 4) compute surface reactions as relating to poisoning and initial kinetics of hydrogenation/dehydrogenation; and 5) investigate the structure and thermodynamics of  $\text{Mg}(\text{BH}_4)_2$ .

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.4** for its relevance to DOE objectives.

- Highly relevant in that it can greatly reduce the experimental load in identifying new tests to do with higher chance of getting good thermodynamics and hydrogen capacity.
- This project addresses aspects of hydrogen storage that are crucially important to meeting the hydrogen vision and Department of Energy research and development objectives.
- Specifically, these computational studies greatly facilitate the screening of candidate hydrogen storage materials, thus simplifying and accelerating the process of selecting materials for development and testing.
- Computational prediction of effectiveness of solid state hydrogen storage materials.
- Clearly relevant.
- Theoretical work is focused on predicting high capacity reactions with suitable thermodynamics; this is exactly what theory is most useful for at this "materials discovery stage."
- The work is relevant to DOE objectives as it deals with predictive theory and directs experimentalist toward discovery of new materials.

**Question 2: Approach to performing the research and development**

This project was rated **3.2** on its approach.

- The team has a good approach and is doing all the right things. Could use more validation of modeling approach.
- DFT and temperature scan is a good a method as is known. Using libraries of functions calculated to make things more efficient is wise.
- Limiting to single step reactions is not appropriate and the movement to multi-step reactions is an improvement.
- Theoretical studies are based mainly on density functional theory methods; thermodynamic and interfacial properties are calculated.
- Reaction screening is a major focus of this work.
- Investigating nanoscale effects on the reaction thermodynamics of metal hydride particles.

## HYDROGEN STORAGE

- A creative application of computational methods for screening hydrogen storage materials limited to solids of known structure.
- Many of the predicted reactions, in particular those involving elemental carbon as a reactant, are clearly incorrect. Because of the large exothermic formation enthalpy of methane, all carbon will be converted to CH<sub>4</sub> as a first thermodynamic step in these reactions. Hence the proposed reactant combination is unstable, and for all practical purposes the hydrogen bound in CH<sub>4</sub> will be inaccessible at temperatures of realistic interest.
- Use of DFT to screen through many reactions is a good idea.
- The approach is focused on overcoming the barriers of high storage capacity at reasonable (de)hydrating conditions. The computational approach is built on the work of others (which the principal investigators credit adequately), and is an excellent use of theory to screen through a large number of candidate reactions.
- The PI is using standard codes and DFT-formalisms for the calculations. No new methodology is being developed.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.5** based on accomplishments.

- Addition of considering multi-step reactions correctly is a big improvement.
- The project scanned a huge number (millions) of discreet compositions and narrowed those of interest to dozens grouped by major chemical classes.
- Evaluated nanometer-sized particles for improved thermodynamics and only magnesium and sodium are better and then only at 3 nm or less.
- Millions of dehydrating reactions have been screened since inception of this project.
- The project has identified 43 single step reactions with greater than 6 weight percent H and dehydrating enthalpies in the 15 to 75 kJ/mol range.
- Several interesting multi-step reactions have been identified.
- The effect of particle size on dehydrating temperature and thus dehydrating thermodynamics has been elucidated.
- Excellent progress on a large-scale computational search for hydrogen storage materials - not previously published. Would like to see a more explicit indication of correspondence with experimental data.
- Good progress.
- Good use of the linear programming approach to predict new reactions; excellent discussion of the "caveats" associated with these predictions, and where they might go wrong. This is a very important, candid, discussion to have for the experimentalists.
- Screened millions of possible reactions along with studying nano-size effects through surface.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.4** for technology transfer and collaboration.

- Good tie-in with universities, national labs, and companies. There is no apparent corporate tie-in now that General Electric is no longer a center partner.
- Very good both within the center and outside the center, and more to the point is that there is two-way exchange of information.
- Many institutions within and outside the Metal Hydride Center of Excellence have taken direction from this project in formulating their work plans.
- This work has had major impacts on the choice of materials for study and on developing understanding of the dehydration of metals.
- The principal investigator and his team seem to be readily willing to make computations for systems proposed to them by other organizations where ongoing work can benefit from computational studies, e.g., planned computations on Mg(B<sub>12</sub>H<sub>12</sub>).
- Good collaborative work - particularly as stimulating experimental studies on the computationally predicted systems.
- Project seems to be well-connected to experimental efforts within the Metal Hydride Center of Excellence.

- Work seems to be well-connected within the center of excellence and obviously excites many of the experimental groups to test the predictions.
- The PI has worked very well with others in the center and the synergy between theory and experiment has been very good.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- Continuing predictions for multi-step reactions is appropriate.
- The proposed contaminant work is also good.
- Plans to search for metastable/multi-step dehydriding reactions.
- Plans to continue work on dehydriding thermodynamics at the nanoscale.
- Plans to investigate the energetics and kinetics of surface reaction pathways involving poisoning agents, like H<sub>2</sub>O and O<sub>2</sub>.
- Hopefully, they will continue to be responsive to the community at large as interesting issues arise that theory may be able to address in a substantive way.
- Good future work plan shown. Suggest relating more to experimental data, even if it involves applying persuasive effort to experimentalists for acquiring it!
- The future plans are somewhat vague.
- The proposed future work is a bit weak. The discussion of the caveats associated with these predictions was really excellent, but the future work does not really provide a clear pathway to address these caveats. The future plans really look like largely a continuation of the activities, with no clear plans for where the future critical needs will come.
- The PI plans to continue work as before. The publications have been modest and no publications exist jointly with experiment.

#### **Strengths and weaknesses**

##### Strengths

- This is important work that should be funded.
- This is a strong team with good “bang-for-the-buck”.
- Continuing upgrade of the theory and the mechanism of implementation is a major strength.
- The efficiency of the library method.
- Recognition of limits of technique.
- Scholarly, enthusiastic, collegial principal investigator.
- Very effective and extensive collaborations.
- This project is saving the metal hydride program lots of time and effort.
- Automated approach for screening complex metal hydrides and understanding their phase-stability.

##### Weaknesses

- There are no obvious weaknesses.
- Calculations of properties of nano-particles through consideration of surface energies and Wulf construction may not be valid for small nano-particles. Effect of detailed surface structure is important.
- Lack of inclusion of hydrogen carbon products in the thermodynamic database may lead to incorrect conclusions.

#### **Specific recommendations and additions or deletions to the work scope**

- More tie-in to experimental work.
- Keep up the good work.
- The first priority for future work should be inclusion of CH<sub>4</sub> into the thermodynamics database.
- The database of phases should be periodically updated so that the proposed reactions can be re-assessed. This will aid in the accuracy of the predictions.
- The PI should be critical of using standard techniques for nano-particles.



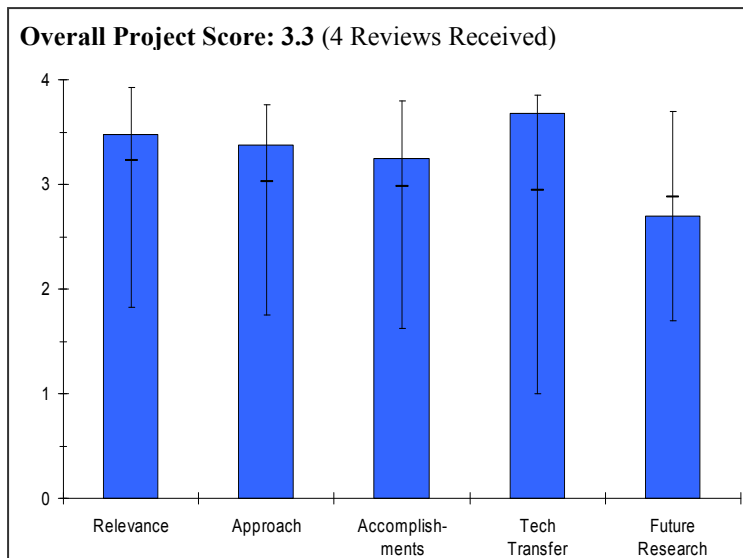
**Project # ST-34: Development and Evaluation of Advanced Hydride Systems for Reversible Hydrogen Storage***Bob Bowman; NASA Jet Propulsion Laboratory*

NOTE: This project is part of the Metal Hydride Center of Excellence.

**Brief Summary of Project**

The overall objective of this project is to develop and demonstrate light-metal hydride systems that meet or exceed the 2010/2015 DOE goals for on-board hydrogen storage.

The Jet Propulsion Laboratory objectives are to 1) validate storage properties and reversibility in light element hydrides including: a) nanophase, destabilized hydrides based upon LiH, MgH<sub>2</sub>, and LiBH<sub>4</sub>; b) complex hydrides (e.g., amides/imides, borohydrides, and AlH<sub>3</sub>-based hydrides); and c) samples provided by numerous Metal Hydride Center of Excellence partners; and 2) support developing lighter weight and thermally efficient hydride storage vessels.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- The principal investigator employs a valuable analytical technique [nuclear magnetic resonance (NMR)] to assist metal hydride center partners in characterizing new materials. The principal investigator's experience, knowledge and lab skills are clearly a benefit to the whole center.
- The project addresses fundamental aspects of hydrogen storage.
- As a general service to the Metal Hydride Center of Excellence members and their project groups, this particular project indirectly supports the Department of Energy objectives to the high extent the center of excellence itself does.
- Very relevant to DOE objectives. Finally someone is sorting out the chemical species that participate in, and perhaps disrupt the desired pathways of, hydrogenation/dehydrogenation.

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- NMR is a valuable technique to characterize amorphous type materials (many of the materials studied in the metal hydride center are amorphous rather than crystalline in structure). Even crystalline materials may begin to exhibit amorphous characteristics after cycling or other undergoing other stresses. The NMR technique should better help researchers to understand these mechanisms and design more robust materials with improved capacity.
- Systematic approach is effective.
- This project provides much needed services to all five project groups of the Metal Hydride Center of Excellence: (A) Destabilized Hydrides, (B) Complex Ionic Materials, (C) Amides-Imides, (D) Alane, (E) Engineering Analyses and Design.

- The main support effort is in the specialty field of NMR, valuable for understanding hydrogen-bonding, phase content, and reaction pathways. The principal investigator is a high-level expert in this field and has access to valuable NMR equipment and services.
- The other principal area of center of excellence contribution is hydride container design, evaluation and modeling, very useful to Project Group E.
- Done right, NMR is a magnificent method for identifying chemical constituents that elude diffraction and other means.
- Identification is only a part of the battle, who is going to use effectively this identification?

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- The principal investigator's work has been crucial to the identification and understanding of  $B_{12}H_{12}$  intermediate kinetically inhibited compounds in the cycling of borohydride based materials. The mechanism of this intermediate step must be understood in order to overcome many of the cycling issues currently associated with boron-based materials.
- An overview of state-of-the-art of storage systems is important.
- The identification of  $B_{12}H_{12}$  as a key intermediate is significant.
- During the relatively short time this project has existed, a large quantity of new data has been generated on a variety of storage media.
- The extensive NMR data obtained has added to the fundamental understanding of most of the materials being developed within the center of excellence. For one example, it has been useful in phase identification of amorphous species (not amenable to XRD or Neutron Diffraction study) and reaction pathways.
- The confirmation that  $B_{12}H_{12}$  is an intermediate in the decomposition of borohydrides may help to set the directions for the development of practical reversibility of same.
- The Metal Hydride Storage Survey Report will be useful when it is completed.
- The container modeling effort is new, but it is not yet clear what it will add to other DOE-supported efforts or other similar worldwide efforts.
- Identifying  $[B_{12}H_{12}]^{-2}$  as a borohydride dehydrogenation product is an important accomplishment and identifying different M-BH<sub>4</sub> entities will prove to be useful in understanding dehydrogenation of mixed-metal borohydrides.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.7** for technology transfer and collaboration.

- The principal investigator clearly communicates with nearly every other principal investigator in the Metal Hydride Center of Excellence.
- The project has collaborations across the Metal Hydride Center of Excellence.
- The project provides important characterization to significant number of center of excellence members, as well as to other researchers.
- The collaborations within the center of excellence and outside are outstanding. Information is getting transferred.
- Publications are quickly getting out to the public.
- Project appears to be collaborating and cooperating well with a number of the Metal Hydride Center of Excellence partner institutions.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.7** for proposed future work.

- Continue work and continue to offer characterization techniques to the center as a whole.
- Both the relevance and approach are good.

## HYDROGEN STORAGE

- Given that the principal investigator is leaving, the future work is in doubt.
- Future work follows along the same directions as the recent past.
- Many things are being worked on at once. Some down-selection may be necessary as other center of excellence projects may falter.
- The principal investigator is soon to "retire."
- Hydride-bed design: This work appears to be useful, but not as essential as understanding how the hydriding/dehydriding material chemistry is happening, and how to improve it.

### **Strengths and weaknesses**

#### Strengths

- Excellent technique for characterizing amorphous type materials.
- Project offers a means of characterization which is independent on material morphology.
- Project offers support to all center of excellence researchers.
- Provides a much-needed and powerful NMR service.
- Works well as a service within the Metal Hydride Center of Excellence.
- The NMR studies, and the discoveries thereby enabled, are extremely important. Keep this capability!

#### Weaknesses

- The project is not incorporated in upfront strategy of the center.
- Technique is limited to NMR active nuclei.
- It is difficult to do in situ characterization.
- The project does not seem to be fully integrated with other projects aimed at exploiting the chemical reaction discoveries.

### **Specific recommendations and additions or deletions to the work scope**

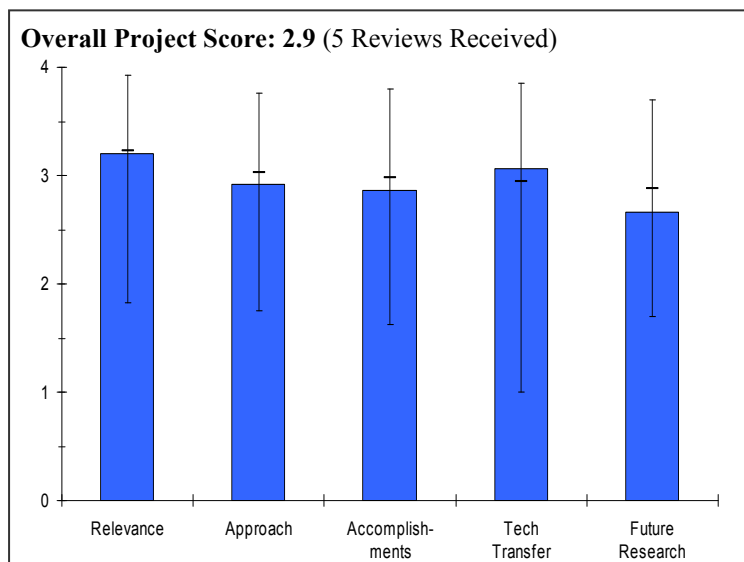
- Perhaps the center could incorporate the principal investigator in upfront discussions about material strategies, etc.
- The project should be prepared to abandon any materials that do not show promise.
- Leave a time slot for possible new materials that are suddenly discovered.
- Consider offering NMR services to the other centers of excellence.
- Be prepared to transfer the engineering services to the Engineering Center of Excellence, if and when it is established.
- Send the bed-design scope to another project. Add more solid-state boron chemistry to the scope of this project.

**Project # ST-35: Complex Hydrides for Hydrogen Storage Studies of the  $\text{Al}(\text{BH}_4)_3$  System***Gilbert Brown; Oak Ridge National Laboratory (ORNL)*

NOTE: This project is part of the Metal Hydride Center of Excellence.

**Brief Summary of Project**

The overall objective for this project is to develop the chemistry for a reversible hydrogen storage system based on borohydrides, amides/imides, alane, and the light alanates. Target materials and processes are 1) complex anionic materials (Metal Hydride Center of Excellence [MHCoE] Project B); 2) amide/imide (M-N-H) systems (MHCoE Project C); and 3) regeneration of alane (MHCoE Project D). The Oak Ridge National Laboratory goal is to employ solvent-based procedures appropriate for scale-up to production and practical application with a focus on high hydrogen content materials (>10 wt% hydrogen).

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.

- The materials studied are those given a "go" by the go/no-go decision.
- The project is very relevant.
- The project covers the correct area of materials but unclear what they really intend to do.
- The project is relevant in that it is investigating fundamentals of hydrogen storage materials. However, there seems to be a lack of focus or urgency.
- Discovery of new ways to utilize aluminum-borohydride and aluminum-hydrides is relevant to the Department of Energy objectives as these materials are hydrogen-rich compounds.

**Question 2: Approach to performing the research and development**

This project was rated **2.9** on its approach.

- To understand the reaction mechanism is critical to explore novel materials and to improve performance of existing materials.
- The project focuses on technical barriers.
- The strong chemical component is a plus.
- The approach or plan is fairly obscure, they will use schlenk lines to make materials and test it, but the actual chemical approach or guiding principles were not at all clear.
- The project seems very curiosity driven. No energy analyses were performed to see if they are technically feasible.
- The presenter demonstrated a very good approach and new ways towards overcoming diborane gas formation from aluminum-borane.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.9** based on accomplishments.

## HYDROGEN STORAGE

- The reaction mechanism of  $\text{Al}(\text{BH}_4)_3$  and  $\text{Mg}(\text{BH}_4)_2$  has been clarified.
- Good progress.
- Interesting experimental results.
- I am not sure that  $\text{Al}_3\text{Ti}$  is the true catalyst; what happens to Ti-H compounds, which may form as intermediates?
- $\text{B}_2\text{H}_6$  often forms during thermal decomposition of metal borohydrides (shown by VV. Volkov et al.).
- Looked at  $\text{Al}(\text{BH}_4)_3$  and confirmed previous results of large  $\text{B}_2\text{H}_6$  formation and extended to various temperatures.
- Initial work on ammonia adduct of the aluminum borohydride seems to have less diborane.
- Claim that  $\text{B}_2\text{H}_6$  is inherent but the method and evidence was very sketchy at best. They may well be right but they have assuredly not proven it!
- Suggestion that hydrogen pressure suppresses diborane has been known for some 4 years.
- Progress is slow and all over the map. They need to focus and use energy analysis to guide activities. The work seems very preliminary and more suited for Basic Energy Sciences.
- Remarkable progress in understanding mechanisms and materials performance needs.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- This work is carried out in the network of the Metal Hydride Center of Excellence.
- Good collaboration with DOE partners.
- Collaborating well and in fact much of the value in what was presented was from partners however it is not clear that partners are benefiting though!
- The collaborative aspects are not apparent in the presentation.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.7** for proposed future work.

- The future plan presented is not clear about the research targets.
- Future work is well defined.
- Probably suitable but the plan again is not clear.
- Future work plans were not very clear.
- Understanding intermediate steps towards decomposition is a very good proposal.

### **Strengths and weaknesses**

#### Strengths

- The reaction mechanism of borides has been analyzed experimentally.
- The advantage of expertise in handling air/moisture sensitive materials is well utilized for the activities of the Metal Hydride Center of Excellence.
- Very solid experimental work.
- Good understanding of chemistry involved.
- Good lab technique.
- Very good synthetic approach.
- Devising methodologies to allow for  $\text{Al}(\text{BH}_4)_3$  utilization by mitigating  $\text{B}_2\text{H}_6$  formation.

#### Weaknesses

- The mechanism analysis did not show the research direction for material development. Suggestions and proposals for other material scientists are highly recommended.
- An additional theoretical component may be a plus.
- The project seems to be just wandering around looking for something to do, there seems no underlying plan or understanding.

- Presentation probably obscured what progress and understanding they have.
- It was not clear they are up to date on the literature.
- By this time the project should have settled on something to go with. It is still at very preliminary stages.
- Insufficient interactions with theory group.

**Specific recommendations and additions or deletions to the work scope**

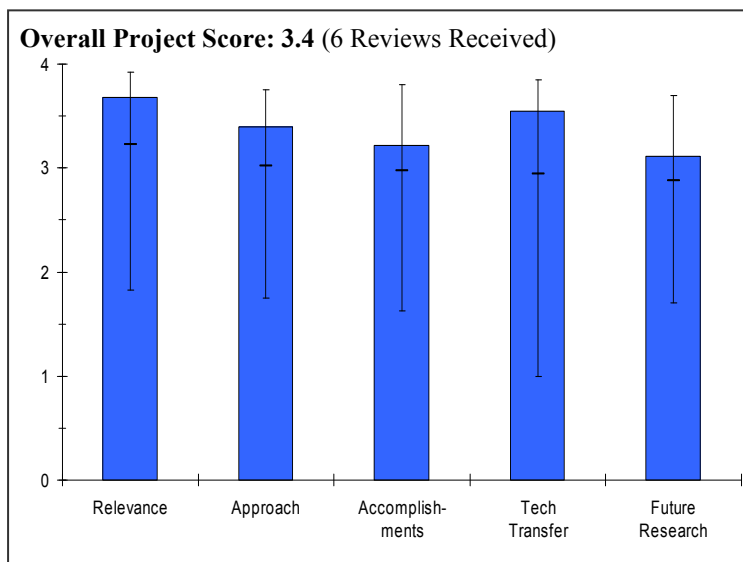
- The results of the mechanism should be transferred to the scientists who explore novel hydrogen storage materials.
- The PI needs to develop a clear plan and direction.
- The project should choose a system and go with it.
- Definitely keep the project.
- For the  $\text{AlB}_4\text{H}_{11}$  compound decomposition, diborane formation needs to be tracked and checked.
- Collaboration with the theory group within the Metal Hydride Center of Excellence is recommended.
- Close collaboration with the alane reversibility groups is also recommended.

**Project # ST-36: Discovery and Development of Metal Hydrides for Reversible On-Board Storage***Ewa Ronnebro; Sandia National Laboratory-Livermore*

[NOTE: This review is for Sandia's technical contribution to the MHCoe.]

**Brief Summary of Project**

The primary objective of this project is to discover new complex hydride materials. The experimental objective is to establish a synthesis route that combines high-energy milling followed by hot-sintering under high H<sub>2</sub>-pressures. A new start as of July 1, 2007 was work on improving kinetics, cycling life and desorption properties by incorporation of hydride materials in nanoframeworks. The theory objectives are to 1) employ the Prototype Electrostatic Ground State technique for structure determination and  $\Delta H$  estimates to provide Metal Hydride Center of Excellence partners with theoretical support regarding Al-N bond energies for AlH<sub>3</sub>.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.7** for its relevance to DOE objectives.

- This project is very important for the Hydrogen Fuel Initiative and fully supports Department of Energy objectives.
- Efforts to synthesize new borohydride related materials for hydrogen storage supports the DOE's objectives.
- Discovery of metal hydrides which are reversible (moderate  $\Delta H$ ) is an important activity and relevant to the DOE targets.
- This project is clearly relevant.
- There is a correct focus on high capacity materials.

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- The project focuses on new materials and barriers.
- There is a good combination of theory and experiment.
- The principal investigator has several well designed projects that are integrated with other research going on with partnering institutions in the Metal Hydride Center of Excellence. These efforts utilize the strengths of each institution.
- The principal investigator presents more than adequate experience to perform the proposed research.
- It is likely that the characterizations of Ca(BH<sub>4</sub>)<sub>2</sub> will be completed and that nanoengineering will improve the hydrogen storage properties of these new materials.
- Some activities have been terminated. To try new material based on new ideas is quite important for finding better hydrogen storage materials. No-go decisions do not indicate a poor job.
- The presenter demonstrated good integration between theory and experiment which is well guiding their discovery work.
- The PEGS approach is promising.
- There is a nice connection between theory and experiment.
- The project address kinetics and reversibility.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.2** based on accomplishments.

- Significant progress in 2007 and 2008.
- The regeneration mechanism for  $\text{Ca}(\text{BH}_4)_2$  still requires explanation.
- Group reports interesting research on multi-metal systems, which have limited applications potential.
- The principal investigator has made significant progress towards the objectives of synthesizing new hydrogen storage materials.
- Reversible re-hydriding for  $\text{Ca}(\text{BH}_4)_2$  system with an additive is an outstanding result in this field which may solve the reversibility problem in complex metal hydrides, although the present results do not achieve the DOE 2010 target.
- Enhancements of the kinetic performance of  $\text{Ca}(\text{BH}_4)_2$  with additives is interesting.
- Utilizing the PEGS modeling to discover a potential alane adduct is a good effort.
- There have been no breakthroughs experimentally. It appears that only modest progress has been made on  $\text{Ca}(\text{BH}_4)_2$  after more than a year's worth of effort. Disappointing that the enthalpy for  $\text{Ca}(\text{BH}_4)_2$  has yet to be measured by experiment.
- Theory work seems to be the headliner.
- Experiment:  $\text{Ca}(\text{BH}_4)_2$  has been shown to be reversible. Reversibility optimized with several additives.
- Theory: Numerous useful predictions that are being verified by experimentalists.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.6** for technology transfer and collaboration.

- Good collaboration that includes international collaboration.
- The collaborations and interactions with other the Metal Hydride Center of Excellence partners are excellent and ongoing.
- The presenter showed very good collaboration with others for  $\text{Ca}(\text{BH}_4)_2$  (i.e. discovery of the polymorphs).
- Its advisable for the modeling to have a closer collaboration with the experimental Brookhaven National Laboratory group working on alane adducts.
- Good job with collaboration.
- This is a well coordinated effort. Numerous useful collaborations.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Insufficient details about future work were presented.
- It is not clear how the nanoframeworks will be created.
- What are alternative "nanostructured metal hydrides"?
- The principal investigator has several projects planned for the future that involve additional studies on borohydrides, nanoengineering and continued collaboration with the theory group.
- The research should continue as planned.
- Fundamental studies for kinetics and reaction mechanism (rate determining step) of  $\text{Ca}(\text{BH}_4)_2$  system is required to judge its practicality for a hydrogen storage tank. Its cycle life is also important to know its practicality, but it is the second priority.
- Emphasis on the kinetic enhancement for  $\text{Ca}(\text{BH}_4)_2$  is very important.
- Will  $\text{Mg}(\text{BH}_4)_2$  be explored experimentally?
- Future work is based on prior results.



### Strengths and weaknesses

#### Strengths

- Good experimental work.
- Good combination of theory and experiments.
- Good collaboration.
- The principal investigator has access to all the equipment and financial resources needed to complete the proposed work.
- Intimate collaboration between the experimental group and the computational group.
- Experience in synthesis of complex hydrides and their analysis.
- $\text{Ca}(\text{BH}_4)_2$  is an illustration of excellent interaction between theory and experiments.
- Enhancement of kinetics with different additives for  $\text{Ca}(\text{BH}_4)_2$  is a very good progress.
- Good connection between theory and experiment.
- Thorough analysis of results obtained to date.
- Right decision-making about what to pursue and what not to pursue.
- Excellent coupling with theory.
- Strong publication record.

#### Weaknesses

- The project has somewhat slowed down compared to the previous year.
- New materials ideas are needed.
- Collaboration with industry is still insufficient.
- None noted.
- Interactions with the group working on alane synthesis and reversibility.
- The high throughput screening facility is not functional and therefore could not be used for combinatorial work.
- Vaguely stated "alternative nanostructuring." What would be the alternative(s)?

### Specific recommendations and additions or deletions to the work scope

- Definitely keep the project.
- Incorporate experimental comparison of thermodynamic stability of  $\text{Ca}(\text{BH}_4)_2$  polymorphs to validate theoretical predictions.
- Incorporation of materials inside nanostructures could lower the gravimetric and the volumetric capacities and therefore it is suggested to have this addressed as the frameworks are researched.
- None.

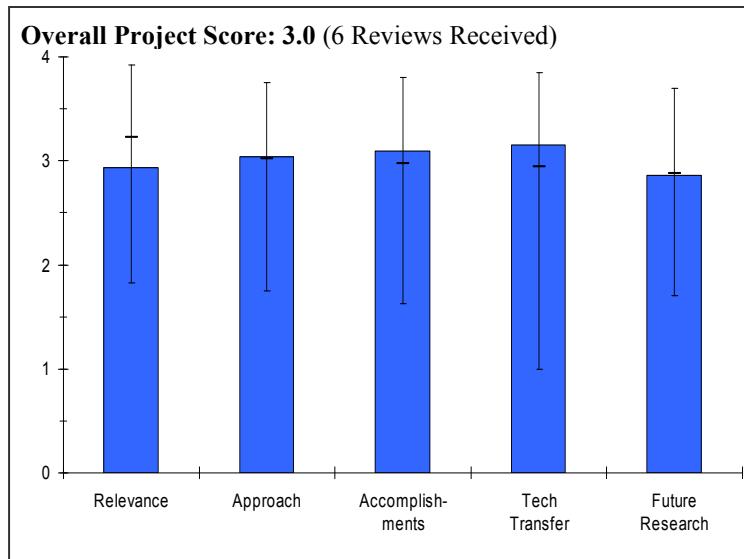
### Project # ST-37: Effect of Trace Elements on Long-Term Cycling and Aging Properties of Complex Hydrides for Hydrogen Storage

Dhanesh Chandra; University of Nevada-Reno

NOTE: This project is part of the Metal Hydride Center of Excellence.

#### Brief Summary of Project

The primary objective of the project is to determine the effects of gaseous trace impurities such as O<sub>2</sub>, CO, H<sub>2</sub>O, CH<sub>4</sub>, etc. in H<sub>2</sub> on long-term behavior of the complex hydrides/precursors by pressure cycling and/or thermal aging with impure H<sub>2</sub>. Secondary related objectives are 1) vaporization behavior of hydrides; and 2) crystal structure studies. Earlier objectives have included 1) construct high pressure (up to 100 bar) cycling equipment; 2) perform hydrogen cycling studies on amide-imide and mixed alanates; 3) initiate vapor pressure behavior of Li<sub>3</sub>N and Mg(BH<sub>4</sub>)<sub>2</sub>; and 4) perform HP DSC experiments, in situ neutron, and X-ray diffraction studies. Objectives for 2007 and 2008 (May 15, 2007 – April 1, 2008) have been to perform thermodynamic and crystal structure studies.



#### Question 1: Relevance to overall DOE objectives

This project earned a score of **2.9** for its relevance to DOE objectives.

- The project addresses issues of storage material degradation.
- The material studied is problematic when it is unclear which material will find future applicability.
- The project is aligned with hydrogen vision Department of Energy research and development objectives.
- The objective to determine the effects of gaseous impurities in hydrogen is essential on long-term behavior of hydrides/precursors.
- The project is relevant to DOE goals.
- It is not clear whether this should be done when there is still a need for better and new materials that may be susceptible to other impurities.
- Although this project itself contributes little to the improvement of hydrogen capacity of materials, durability against impurities and loss of materials by vaporization are important to estimate "practical" capacity over the life time of the tank using the materials.
- The scope of work for this project addresses several important aspects of hydrogen storage material behavior that are well aligned with the hydrogen vision and DOE research, development and deployment objectives.
- This project specifically addresses impurity effects on storage material performance and cycle life issues.
- The effects of trace impurities on the long-term performance of candidate storage materials is an important aspect of the program that should be investigated judiciously using standard practices.
- The choice of complex hydrides for study should be selected among materials that have a reasonable chance of meeting the thermodynamic targets.

#### Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The approach is reasonable.
- A larger number of different materials should be studied.

## HYDROGEN STORAGE

- The approach of the project is focused.
- The approach is uniquely addressed using Knudsen Torsion Effusion Method.
- The project adequately addresses targeted technical barriers and demonstrates technical feasibility.
- The effects of trace impurities on the stability and cyclability of metal hydride storage materials are being investigated.
- Vaporization thermodynamics are studied at moderate temperatures.
- The long-term behavior of metal hydrides and their precursors during pressure cycling and thermal aging are tested.
- In situ phase transformations are studied by high-resolution x-ray diffraction.
- Analytical approaches are excellent, but choice of candidate materials is not compatible with thermodynamic targets. For example, while the theoretical capacities of amide-imide and amide-alanates are high, the desorption temperatures are unrealistic relative to the targets. Hence, detailed impurity studies for these systems seem moot.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- Identification of O<sub>2</sub> as a major impurity is important.
- More materials need to be addressed.
- Significant progress was made in addressing the effect of impurities in hydrogen.
- Progress is good. The project demonstrated effect of common contaminants on hydrogen sorption and desorption properties.
- The durability against impurities obtained in this project is instructive to the research and development of similar hydrogen storage material, although the materials tested do not meet the DOE target.
- Lots of testing and measurements were performed in the past year.
- The effect of gaseous impurities on Li<sub>2</sub>NH-LiNH<sub>2</sub> cycling properties was determined.
- The vaporization behavior of Mg(BH<sub>4</sub>)<sub>2</sub> was studied.
- Phase transformations in Ca(BH<sub>4</sub>)<sub>2</sub> were investigated by synchrotron x-ray diffraction.
- Technical accomplishments for the materials selected for study is excellent.
- Further progress could be made on materials exhibiting more promising thermodynamic properties than those selected up to this point in the project.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- There is collaboration with some center of excellence researchers.
- Collaboration with more researchers would provide access to more/different materials.
- Some coordination with partners exists.
- Good collaboration with ESRF, Grenoble, and Sandia National Laboratories.
- Technology transfer appears weak. Are the results being applied?
- The information coming from this work answers many of the kinds of questions that have been raised in prior merit reviews.
- The breadth and the nature of collaborations are obvious and impressive.
- This research impacts many of the other research projects conducted under the umbrella of the Metal Hydride Center of Excellence.
- The principal investigator has established and planned broad collaborations with other investigators, particularly in the area of theory.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- The scope of future work is good.
- The next stage of where to go with this work is not clear.
- The project is lacking in optional paths.

- The plans are built on past progress.
- Addressing phase diagram determination of mixed complex hydride will be useful but may take away from the main program.
- This project is still very academic. Where is the technology transfer?
- Influence of impurities to the materials studied in the Metal Hydride Center of Excellence is predicted.
- The proposed future work (Slide 17) is very ambitious; it extends in a logical way and expands upon the fiscal year 2008 accomplishments.
- Several new types of measurements (neutron diffraction, differential scanning calorimetry, phase diagram determinations) are in the future plans.
- Broadening of the collaboration profile to include International Energy Administration [Hydrogen Implementing Agreement] and the International Partnership for the Hydrogen Economy inspired interactions is also planned.
- The principal investigator has made reference to "other" borohydrides for future studies. These undefined systems should be selected judiciously relative to thermodynamic targets.

### **Strengths and weaknesses**

#### Strengths

- Addressing the effects of impurities on materials will be important in the future.
- The principal investigator is well suited to address the problems stated in the project.
- The project contains good science and well designed experiments.
- Cycle durability of reversible hydrogen storage material can be tested with impurity under practical conditions.
- The principal investigator seems very knowledgeable and most aggressive in tackling the impurity, cycling, and aging issues.
- The cadre of tools being employed in this work provides the flexibility to study a broad range of issues; some of the research involves state-of-the-art measurements at neutron and synchrotron x-ray sources.
- The project team has access to excellent sources of well characterized materials to examine through its participation in the Metal Hydride Center of Excellence.
- Project has the potential to provide much-needed data on the stability of candidate storage materials when exposed to real-world levels of common gas impurities.

#### Weaknesses

- The type and number of materials studied for impurities effects should be broadened to better cover future possibilities.
- It is difficult to study the effects of impurities on storage materials, when the type of storage material which will ultimately find merit is as yet unknown.
- Future plans are too ambitious.
- The project is academic in that it is not connected to the end user.
- There are no obvious weaknesses.
- Evaluation of the effects of gas impurities on storage materials with sorption-temperatures within practical ranges has not been achieved.

### **Specific recommendations and additions or deletions to the work scope**

- Further studies (e.g., cycling, impurities, and thermodynamics of vaporization) on  $\text{LiBH}_4$  should be abandoned since the sorption temperature for this system is much too remote from the targets.
- Impurity studies in the future should focus on materials exhibiting sorption temperatures at or near practical targets.
- Add some customer input.
- Keep up the good work but don't out stretch your resources.
- Try to resolve lingering uncertainties in some of the results (like in the  $\text{H}_2 + \text{O}_2$  versus  $\text{H}_2 + \text{H}_2\text{O}$  results) as discussed during the question period.
- Abandon further work on pure  $\text{LiBH}_4$  and  $\text{Mg}(\text{BH}_4)_2$ .
- Conduct impurity studies on the  $\text{LiMgN}$  system, which has been shown to be reversible at temperatures slightly below  $200^\circ\text{C}$ .

**Project # ST-38: Fundamental Studies of Advanced High-Capacity Reversible Metal Hydrides/ Recharging of Light Metal Hydrides Through Supercritical Fluid Hydrogenation**

*Craig Jensen, presenting: University of Hawaii, Sean McGrady, University of New Brunswick, Canada, Co-PI*

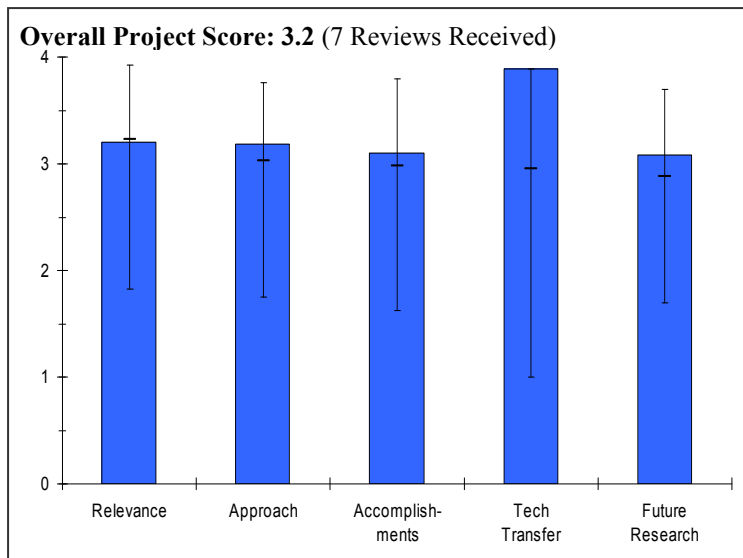
NOTE: This project is part of the Metal Hydride Center of Excellence.

**Brief Summary of Project**

The objectives of this project are to 1) develop new materials with potential to meet the DOE 2010 kinetic and system gravimetric storage capacity targets such as novel borohydrides that can be reversibly dehydrogenated at low temperatures and Al and Mg nano-confined in carbon aerogels; and 2) develop a method for the hydrogenation of Al to alane,  $AlH_3$  at moderate pressures in hydrogen containing supercritical fluids.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.



- This program is highly relevant to the Department of Energy Hydrogen Storage Program.
- This project is concerned with novel, reversible metal hydrides with the potential to meet 2010 DOE targets with respect to hydrogen storage.
- Aluminum and magnesium nano particles in aerogels, transition metal borohydride complex, hydrogenation and reaction catalysts, and alanes are the materials of interest.
- This program has the wide capability to synthesize and characterize these materials.
- This capability is highly relevant to the DOE objectives.
- A novel effort concerns the synthesis of alane ( $AlH_3$ ) and Mg alanate in supercritical fluids.
- The project is well aligned with the hydrogen vision addressing key issues for overcoming some of the main barriers.
- The project objectives are dynamic and flexible enough to continuously remain of high relevance to DOE research and development strategy, as demonstrated by the down-selection performed and the inclusion of a new promising research area in this project on alane regeneration with supercritical fluids.
- This project is clearly contributing to, and is in good agreement with, DOE's goals.
- The project is aligned with the hydrogen vision and research and development.
- The objective to develop new material to meet DOE 2010 system gravimetric capacity and kinetic targets is essential.
- Both objectives address key problems in promising routes to storage.
- Work is scattered among many subjects, some of which are not really relevant to the Hydrogen Fuel Initiative (e.g., LiSc-borohydride which may be a good ion conductor, but is irrelevant to the Hydrogen Fuel Initiative simply because of the cost of scandium).

**Question 2: Approach to performing the research and development**

This project was rated **3.2** on its approach.

- The approach is highly scientific and professional.
- The reduction of borane contamination in the decomposition of anionic borohydride is an objective of the program.

- Efforts to improve reversibility of borohydrides are also addressed.
- Borohydride reaction products are characterized by panoply of techniques.
- Various supercritical fluids are of interest for synthesis reactions under relatively mild conditions.
- A rather well-focused approach, with set milestones and decision points, is employed. This is valid for both the novel borohydrides discovery subproject and for the development of a hydrogenation method of aluminum to alane, at moderate pressures in hydrogen containing supercritical fluids.
- There are at least three distinct projects underway, each of which is well-designed and integrated with research going on at partner institutions within the Metal Hydride Center of Excellence.
- The approach to develop new materials is sharply focused.
- The program's neat organometallic approach to achieve high loadings of carbon aerogels is unique.
- Another unique approach employed is hydrogenation of aluminum in supercritical media.
- Supercritical method is unique and worth trying.
- Confinement is known but a good approach.
- The use of ions to change stability makes sense.
- Synthesis of  $\text{AlH}_3$  under mild condition is strongly expected to improve energy efficiency of its off-board rehydrogenation path.
- A whole slew of borohydrides is being synthesized but sometimes without enough rationale. For example, it is not clear why these syntheses are relevant and which barriers they are addressing.
- Actual syntheses have not been described in enough detail to determine whether or not they are geared towards addressing any of the technical barriers.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- $\text{Na}_2\text{Zr}(\text{BH}_4)_6$  has undergone decomposition up to  $110^\circ\text{C}$  with no detectable  $\text{B}_2\text{H}_6$  contamination.
- The structure of  $\text{LiSc}(\text{BH}_4)_4$  was determined.
- The reaction  $\text{MB}_x - \text{M}(\text{BH}_4)_x$  was found to be reversible at 1000 atm and  $230^\circ\text{C}$ .
- High loadings of magnesium in carbon aerogel were achieved.
- Initial supercritical syntheses indicated the presence of small amounts of alane produce from aluminum.
- The project is making excellent use of powerful experimental techniques and of its collaborations with expert groups in the field. As a result, sound progress is being made toward objectives.
- A particularly interesting result is the confirmation that there are low levels of diborane contamination as hydrogen evolves from anionic borohydride complexes, at relevant temperatures for operation.
- The work with supercritical fluids is innovative and very interesting and could offer new ways for improving the thermodynamics of the system.
- It is noteworthy that some new reversible borohydride materials have been identified and that a new method for rehydrogenating [spent] alane has been identified.
- Excellent progress has been made as evidenced by publications and invited presentations.
- Mixed transition metal  $\text{BH}_4$  complexes have been shown to desorb hydrogen with no  $\text{B}_2\text{H}_6$  loss and at low desorption temperatures.
- A good lithium ion conductor was found in the bargain.
- The program was able to get magnesium into carbon aerogel.
- The project was able to make surface hydrogenated aluminum using supercritical fluids.
- Synthesis in supercritical fluids has been demonstrated as a promising technique for  $\text{AlH}_3$  production.
- Work on alane in supercritical  $\text{CO}_2$  is positive. If alane may be synthesized this way in high yields this would present a much needed breakthrough.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.9** for technology transfer and collaboration.

- This program has extensive collaborations both within and outside the Metal Hydride Center of Excellence.
- A total of 10 refereed publications over the period 2007 to 2008 have been produced.

## HYDROGEN STORAGE

- Similarly a total of 14 invited presentations were given.
- Technology transfer with members of the Metal Hydride Center of Excellence as well as industry should be improved.
- Impressive lengthy list of strong collaborators including international experts in the field. Such interactions really reinforce the project and return high value for money.
- The degree of interaction and collaboration with other institutions is outstanding.
- Impressive collaborations with the center of excellence and other institutions.
- Good connections to many groups with mutual benefits.
- The project is conducted with interaction of the International Partnership for the Hydrogen Economy countries as well as the laboratories of the Metal Hydride Center of Excellence.
- A highly collaborative work.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Borohydride calorimetric studies are planned.
- Collaboration with Sandia National Laboratory (Ronnebro) in the dehydrogenation of borohydrides is planned.
- The effects of catalyst compositions upon borohydride reactions will also receive attention.
- The effect of aerogels upon the enthalpy and reaction kinetics will be addressed.
- The exploitation of the properties supercritical fluids for synthesis of alane and magnesium alanate will continue.
- Solid future plans, building on past experience and taking the research steps forward. There may be too many areas to cover now given the resources available and the time left.
- Looking forward to hearing more next year about the collaborative discovery with Sandia National Laboratories on the reversibility achieved for one compound through high pressure experiments (patent pending).
- The work planned for the future with partner institutions is well thought out and feasible.
- Continue the work as planned.
- Plans are clearly built on past progress.
- The project focus seems diversified.
- Future plans seem suitable. Preference would be for more clarity of plan rather than general area of work.
- Strategy for improvement of  $\text{AlH}_3$  yield is not clear. Fundamental study of the behavior of  $\text{AlH}_3$  and etc. in supercritical fluids is required.
- There is no contingency planning.
- No go/no-go decision points are foreseen.

### **Strengths and weaknesses**

#### Strengths

- A very strong scientific effort.
- The resources appear adequate.
- The technology transfer is outstanding.
- The use of supercritical fluids for synthesis of metal hydrides is very innovative and should be vigorously pursued.
- The principal investigator's expertise in the field is a strength. He has a strong team and a well-organized, consolidated network of collaborators.
- The large number of partnering institutions adds strength to the project.
- The principal investigator is well suited to address the problems stated in the project.
- This is the best presentation of their work that this reviewer has seen.
- An interesting, new approach that there is reason from industrial practice to think that it could work.
- Strong team.
- International cooperation is actively conducted.
- The project leader has much experience in organometallic, organic, and inorganic chemistry.
- The project is broad in scope.
- Innovative approaches, especially for the synthesis of alane.

Weaknesses

- The prospects of borohydrides meeting the 2010 targets are dim.
- Similarly dim are magnesium intercalated carbon aerogels.
- Rather ambitious future plans - probably too many areas to cover given the available resources.
- None noted.
- Focus is too diversified.
- The project falls out of focus with so many subjects and research avenues.
- There is not enough concentration on the promising candidate materials, except for work on alane.

Specific recommendations and additions or deletions to the work scope

- The items discussed under "Project Weaknesses" should be addressed.
- The DOE time is short, thus, the following should be addressed: reversibility, cost, kinetics, storage capacity at 298K, and cycle stability.
- The above likely requires that a specific material be chosen.
- The program should increase the effort on super critical fluids even if it decreases the effort in other areas.
- It is recommended that it would really be good to do some sort of thermodynamics to show there is sufficient energy in the process to actually accomplish the regeneration of aluminum to alane.
- Identify the most promising research avenues and concentrate the efforts there.
- This program would benefit from an analysis of the energetics. What sort of energy must the supercritical process provide into the aluminum to make alane and compare that to what can be provided (at reasonable energy input required to generate the supercritical fluid).
- Likewise it would be good to see some more quantified analysis of the use of ionicity to alter the stability, and perhaps a ranking of logical ions to try based on that theory.
- There is no need to continue work on pure magnesium in aerogels. This may be relevant for basic science but has little relevance to the Office of Energy Efficiency and Renewable Energy mission.
- Focus and expand the effort on improving yields of alane.
- Establish quantitative go/no-go targets, especially with regard to improved yields of alane. If 10 percent or more conversion can be shown, then pursue further improvements with vigor.



**Project # ST-39: Aluminum Hydride Regeneration**

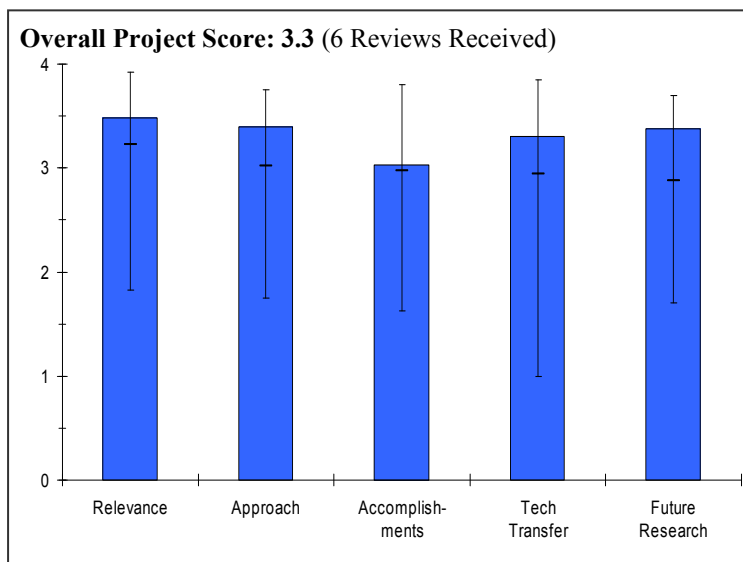
*Jason Graetz, PI, presenting, Jim Wegrzyn, co-PI; Brookhaven National Laboratory*

NOTE: This project is part of the Metal Hydride Center of Excellence.

**Brief Summary of Project**

The overall objective of the project is to develop a material that supports the 2010 DOE technical performance targets using aluminum hydride (AlH<sub>3</sub>), by fully elucidating the nature of hydrogen desorption from AlH<sub>3</sub> and developing an efficient regeneration method. Objectives are to 1) develop new routes to prepare pure crystalline α-AlH<sub>3</sub> from Al (spent fuel) with minimal energy cost; and 2) assist the engineering design for an off-board system based on AlH<sub>3</sub>. The challenge is that AlH<sub>3</sub> is thermodynamically unstable below 7 kbar (at 300K). In an AlH<sub>3</sub> system H<sub>2</sub> evolution is controlled by temperature (rather than pressure) so the ability to tune decomposition kinetics will be critical.

Various routes exist to adjust kinetics (e.g. size, coatings and catalysts). The key issue is regeneration (hydrogenation of Al metal), and multiple regeneration pathways are being investigated.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- Very relevant and timely project, clearly addressing the goals of the Hydrogen Program.
- The project is exploring possibilities for new cost-effective and energetically efficient methods to regenerate or recycle the hydride from the spent fuel and reaction products.
- This project is responsive to the Department of Energy's objectives in so far as the principal investigator plans to develop ways to regenerate alane, a very promising hydrogen storage material.
- The project addresses a fundamental step in the adoption of hydrogen technologies, according to the Hydrogen Fuel Initiative.
- AlH<sub>3</sub> is one of the few materials with a realistic chance at achieving storage gravimetric, volumetric, and kinetic targets. Regeneration is one of the key obstacles and deserves substantial focus.

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- The results with LiAlH<sub>4</sub> are encouraging.
- The success metrics are not clear.
- The project uses a systematic approach appropriately using the expertise from the Metal Hydride Center of Excellence.
- The link to and integration with the Metal Hydride Center of Excellence is instrumental for overcoming the scientific and technical barriers in aluminum hydride regeneration.
- The titanium was shown to be well dispersed, but does the form matter? The form of titanium might be titanium particles, TiAl<sub>3</sub>, solid solution or even change during use. Does it matter? At some point this should be looked at.
- There needs to be costs estimates done, such as for adduct formation.

- Very good overall.
- The technique of alane harvesting is a novel technique for overcoming the technical barriers that may prevent it from being a reversible storage material.
- The approach is clear and concise.
- The project integrates with other research.
- Highly imaginative schemes (both at the Brookhaven National Laboratory and elsewhere within the center) towards the regeneration of  $\text{AlH}_3$ . One question I have about the Brookhaven National Laboratory approach of regeneration of solvated  $\text{AlH}_3$  that I would have liked to hear discussed is: The temperatures for separation of the solvent and dissociation of hydrogen will need to be clearly separated in any future process (i.e., one cannot have the  $\text{AlH}_3$  dissociating during the process of removing the solvent) and, the dissociation temperature for hydrogen cannot be brought down too low, since the equilibrium pressure above it is so high. What is the plan to deal with these thermodynamic/kinetic issues?

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Clearly much technical work is done and much has been accomplished but it is difficult to gauge how much closer the project is to its internal milestones.
- Satisfactory progress has been made with respect to objectives.
- Theory guided choices of adduct were made, and overall energy cost considerations were attempted, following up on last year's recommendations.
- Further progress was made with the hydrogenation occurring at lower pressure of less than 13 bar and at room temperature. Separating the alane from the organometallic without decomposition is still challenging.
- The program managed to reverse the reaction of lithium alanate at moderate pressure and temperature. It will be interesting to see how this develops.
- The principal investigator has worked with others to identify and test organic stabilizers that may be suitable for alane harvesting. Results from gas phase calculations can be used to predict the most likely prospects for this.
- There are a number of significant technical accomplishments.
- The work has been done effectively and efficiently.
- Good progress with the TEDA, showing a complete reversible cycle, and also in the analogous work regenerating  $\text{LiAlH}_4$ . It would be nice to more clearly compare this latter work to the analogous work from Ritter's group at the University of South Carolina.
- The use of theory to predict new ligands is quite useful; it will be interesting to see whether these predictions are verified.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- This research work is strengthened by the collaborations established within the Metal Hydride Center of Excellence, the Chemical Hydride Center and by the interaction with international partners, through the International Energy Administration.
- Close collaborations with partnering institutions is adding overall strength to the project.
- The number of collaborations, both within the Metal Hydride Center of Excellence and externally is good.
- Good connections with other partners within the center. As this regeneration scheme is "off-board", it might be useful to have a closer connection with some of the regeneration efforts in the Chemical Hydrogen Center of Excellence.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.4** for proposed future work.

## HYDROGEN STORAGE

- Clear work program was presented with set down-selection pathways and go/no-go decision points for the regeneration via organometallics and for recovering of the hydride from alane-adducts. Identifying the energy penalties also planned.
- Milestones planned for 2008 and 2009.
- The principal investigator has a well thought out plan for continuing the alane harvesting, building on past progress.
- The proposed future work is well thought out.
- It is nice to see some self imposed go/no-go targets.
- The inclusion of a process energy efficiency goal is nice.
- Proposed future research seems like a reasonable path forward.

### **Strengths and weaknesses**

#### Strengths

- Networking and inter-collaborations within the center of excellence.
- Good team, good approach.
- The key personnel in this project have the experience working with alane that is necessary to make this project successful.
- The concise methodology used is impressive.

#### Weaknesses

- The alane on-board/off-board storage concept requires a radically different infrastructure system. While regeneration is correctly identified as one of the barriers, there are many other significant barriers which could diminish the probability of the success of this concept (under Grand Challenge program). So this begs the question that at what point and under what conditions a go/no-go decision should be made. This comment reflects on all alane regeneration projects and not just this work. What are the success metrics?
- Engineering aspects and associated regeneration costs, respective energy penalties, remain an issue.
- The applicant does not appear to have much experience or expertise in working with organic stabilizers, which are essential materials for this project.

### **Specific recommendations and additions or deletions to the work scope**

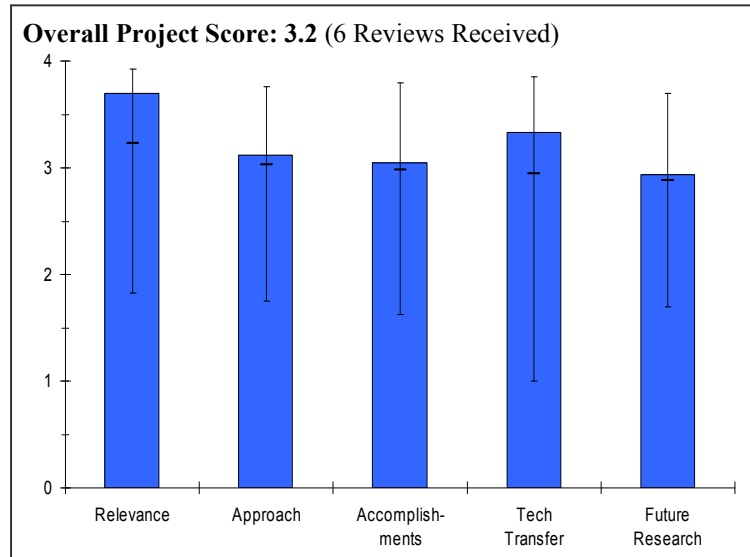
- This comment is for the entire effort on alane (not just this project). Would it be more appropriate to fund these projects under the Office of Basic Energy Sciences?
- While the alane concept is far from storage device development, can the system analysis project review the feasibility of the concept (under optimistic assumptions) and obtain the well to tank (WTT) efficiency and on-board storage metrics?
- Need to conduct even at this stage a preliminary energy analysis, over the life cycle, to get a feeling where the project stands and how it progresses with respect to regeneration costs and energy penalties.
- This project needs to be connected to the soon to be established Engineering Center of Excellence to investigate the alane system engineering aspects and practical application issues.
- There needs to be costs estimates done, such as for adduct formation.

**Project # ST-40: Fundamental Reactivity Testing and Analysis of Hydrogen Storage Materials and Systems**  
*Don Anton; Savannah River National Laboratory*

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

The objectives of task 1 – risk assessment are to 1) assess the potential risks of using solid-state hydrides; 2) develop test protocols and experimental designs to aid in characterization of hypothetical accident scenarios; and 3) test six compounds in three discharge states using standardized semi-quantitative test methods. The objective of task 2 - thermodynamics and chemical kinetics is to quantitatively assess chemical reactions of compounds with air, water and other engineering materials. The objectives of task 3 - risk mitigation are to 1) quantitatively assess chemical reactions of compounds with potential inhibitors; and 2) evaluate efficacy of inhibitors in laboratory scale tests. The objective of task 4 – prototype system testing is to design assemble and test prototype storage systems to evaluate effectiveness of inhibitor systems.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.7** for its relevance to DOE objectives.

- The project is critical to Department of Energy’s hydrogen initiatives.
- The overall objectives of this project are well defined although most of them are premature.
- It is very important to determine the chemical and environmental reactivity characteristics of the materials and systems to be used for on-board storage which is the overall objective of this project.
- It may be too soon to initiate significant effort on the chemical and environmental reactivity characteristics of the materials and systems to be used for on-board storage. Most of the effort should be after materials have been identified that have a high probability of meeting the storage requirements.
- Critical to the Hydrogen Program both for risk mitigation and an effective down-selection process.
- A highly relevant project, addressing the development of solid low-pressure hydrogen storage via metal hydrides, chemical hydrides and sorption hydrides.
- As a materials characterization center, this project helps to put the various DOE storage projects on an even plane.
- This project is critical to ensuring that systems can be developed for safely utilizing hydrogen storage materials and fully supports the relevant multi-year program plan.
- Tasks 3 and 4 are imperatives for assessing the potential risks of solid-state hydrides and other materials as well as the mitigative technologies/techniques.
- Important work to (as UTRC pointed out) put more meaning in the DOE safety target of “Meets or exceeds applicable standards.”

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- The approaches are good and effective in general.

## HYDROGEN STORAGE

- The principal investigator should also consider the difference between pelletized material and powdered material at early stage of the project.
- United Nations methods and procedures are being used to measure pyrophoricity, self heating, burn rates, and impact of water contact. These methods do not appear to be state of the art approaches. Savannah River National Laboratory is developing additional more scientific methods as well. It seems that there should be more scientifically based tests that have been previously developed and standardized to characterize the chemical and environmental reactivity of solid materials that could be used.
- Many of the methods being used do not include capturing the products of the reactions and determining their composition. It would seem this would be possible and important to do. Separate calorimetry experiments are being developed that include identification of the reaction products but these do not seem to be state-of-the-art either. For example there are differential scanning calorimetry (DSC) instruments connected to gas chromatography-mass spectrometry (GC/MS) that could be used.
- Future work includes developing some predictive models relative to material chemical and environmental reactivity in on-board vehicle applications. These will be empirically based. This may prove to be very challenging at best.
- Mitigation strategies are discussed in the future work but no examples are provided. The speaker mentioned pelletizing and the use of inhibitors or retarders but admitted there had been little thought about this aspect of the project.
- The approach is very safety-centered – a major positive.
- Very thorough approach in determining thermodynamic and kinetic properties of materials.
- Involving the centers of excellences is a plus.
- Good combination of standard tests and innovative self-developed tests.
- If they are going to look at sorption materials, they may need a different set of tests.
- The technical approach is good and will systematically address key properties of the materials being studied.
- The "connections" and interactions with the storage centers of excellence are functioning well, but it is less clear how the material down-selects from the centers of excellence are taken into consideration. The approach of looking at classes of materials seems very reasonable at this point in time.
- Testing of a few specific metal hydrides following standard United Nations protocols for the transport of dangerous goods. Augmented by developing a scientific basis for the often arbitrary criteria for these United Nations tests.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- The principal investigator made some good progress toward objectives.
- The established thermodynamic and kinetic database will provide valuable insight for material development work.
- The experimental data really helped the theory group to build an effective model.
- Given the approach taken, significant effort has been made and considerable results on one metal hydride system has been obtained, all of which is in keeping with the funding available to date.
- The value and extent of the results could be much greater if better approaches were taken (see comments under the approach section).
- Small comment: Reviewer is not convinced that the reaction of the storage solid after hydrogen evolution is pyrolysis only. It can also be diffusion limited oxidation, where the reaction and heat release rate is limited by the rate of oxygen diffusion into the powder. This is the same as ash combustion.
- A very thorough assessment of thermo-sensitivity of  $\text{LiBH}_4/\text{MgH}_2$ .
- Work with this material sets out a good protocol for future testing.
- Predictive modeling should help to determine a pathway to mitigation.
- It may have been valuable to have seen some comparative results with other materials.
- Progress on tasks to date is good.
- Good, careful studies of a few metal hydrides. Instructive results for the thermal and other behavior of the particularly examined compositions, information which is not confidently transformable to other than the most closely related systems. Nevertheless, at least the demonstration and use of the standardized U.N. tests for metal hydride materials is of broader value.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- Some collaborations exist.
- The collaborations should be expanded to include some combustion experts outside the center.
- There is some good collaboration with other members of this International Partnership for the Hydrogen Economy project and with the DOE Storage Subprogram centers of excellence.
- Working with United Technologies Research Center and Sandia National Laboratories provides a thorough characterization of materials.
- There appears to be good coordination with the centers of excellences.
- Very good international component.
- This project has a very strong team of partners that includes international participation through the International Partnership for the Hydrogen Economy.
- Good collaboration with partners.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- The general research direction is good.
- Small scale system-level testing should be considered at current stage of the project.
- The mitigation strategies should be considered at an early stage of the project.
- There is a well-defined plan for additional work that will continue to characterize on-board storage materials for their chemical and environmental reactivity, utilizing the approaches that have been taken for metal hydrides that have been evaluated.
- The project plan includes work on mitigation strategies but very little thought has gone into this part of the project.
- Since the principal investigator is doing the primary effort in understanding risks and mechanisms for reactivity, it is important for the principal investigator to suggest mitigation strategies.
- Task 2 seems somewhat limited. It would be good to do more testing of various storage materials from all the centers.
- Risk mitigation task is next logical step, and this group is well qualified to perform it.
- Priority attention should be given to Tasks 3 (Risk Mitigation) and Task 4 (Prototype Systems Development).
- Since we are far from practical hydrogen storage materials, investigators should try to make the results of this work as broadly applicable as possible. Focus more on the development and "illustration" of techniques than in-depth analysis of a few specific hydrogen storage materials.

**Strengths and weaknesses**Strengths

- The overall approach of accessing potential risks of solid state hydrogen storage materials is effective.
- Good set of experiments done well to identify chemical and environmental reactivity issues with metal hydrides using UN test procedures.
- Generally good approach to understanding the reaction risk factors for hydrogen storage materials.
- Very strong project leader.
- High safety consciousness.
- Thorough set of tests.
- The principal investigator and partners have the requisite expertise to achieve the project goals.
- The principal investigator fully recognizes the importance and need to develop sound and even novel technologies and techniques for risk mitigation associated with the use of these materials.

Weaknesses

- The scope of this project should not only be limited in material level testing. Small scale system-level testing should be considered at early stage.

## HYDROGEN STORAGE

- It does not appear that this project is utilizing state-of-the-art test methods and analytical techniques that are likely already well established for testing the chemical and environmental reactivity aspects of solid materials.
- It may be too soon to initiate a significant effort on the chemical and environmental reactivity characteristics of the materials and systems to be used for on-board storage. Most of the effort should be after materials have been identified that have a high probability of meeting the storage requirements.
- There needs to be some comparative tests with other materials to at least better understand the qualitative tests (e.g., water drop, surface contact).
- Less specific attention has been given to-date to the specific risk mitigation technologies/techniques than I think is desirable.
- The principal investigator did not include feedback comments on 2007 Annual Merit Review recommendations in the back-up slide section of the presentation material.

### Specific recommendations and additions or deletions to the work scope

- Find and utilize the best state-of-the-art test methods and analytical approaches available for this effort.
- To the three water tests: Immersion, Surface Contact, and Water Drop, the project should add a credible 4<sup>th</sup> test. A Dense Slurry test, which is an extension of the Immersion test, where the possible heat release in immersion is not quenched by the water heat capacity, and there is a potential for ignition, with larger heat release per unit volume should be added. It is suggested to drop 1-10 ml solid powder into 1-10 ml of water. The results of "contact" and "drop" tests imply this immersion could ignite, possibly with "interesting" results. The mechanics expected may be where ignition occurs at the interface, where some of the powder has yet to sink and propagates into dry powder. The released heat diffused downward may evolve hydrogen and/or evaporate water, allowing combustion propagation downward into slurry as well.
- In the "Predictive Models" slide (slide 27): add tasks of "Predict combustion rate during hydrogen evolution" and "Predict reaction rate during pyrolysis or diffusion-limited combustion of material."
- Use these tests as screening tests for more materials.
- Work on identifying and testing appropriate fire suppression agents for these classes of materials should be considered in cooperation with the other companion projects being funded by the Storage Subprogram.

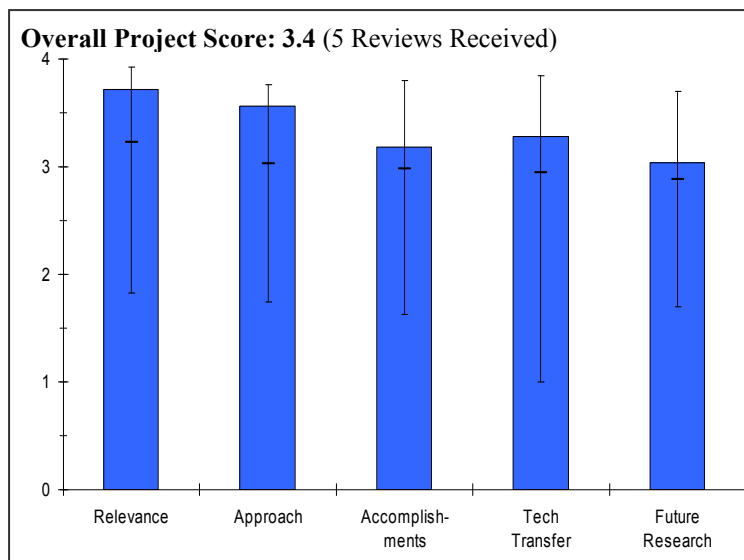
## Project # ST-41: Quantifying and Addressing the DOE Material Reactivity Requirements with Analysis and Testing of Hydrogen Storage Materials and Systems

Dan Mosher; United Technologies Research Center

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

### Brief Summary of Project

The objectives of this project are to 1) quantify the DOE On-Board Storage Safety Target: “meets or exceeds applicable standards”; 2) evaluate reactivity of key materials under development in the Materials Centers of Excellence; 3) establish generalized and specific risk analyses between reaction characteristics and satisfaction of acceptance criteria; 4) reduce reactivity consequences of candidate materials and systems through development of mitigation methods; 5) determine the trade-offs between performance and residual risk; and 6) support risk informed choices for codes and standards activities.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- This program is highly relevant to the Department of Energy’s Hydrogen Program.
- It is concerned with the chemical and environmental reactivity analysis and testing of hydrogen storage systems.
- Candidate systems are based on  $2\text{LiBH}_4/\text{MgH}_2$ ,  $\text{AlH}_3$ ,  $\text{NH}_3\text{BH}_3$  and activated carbon materials.
- This program has a wide capability to test and characterize these materials.
- This capability is a valuable asset to the Metal Hydride Center of Excellence effort.
- The project is critical to DOE hydrogen initiatives.
- The overall objectives of this project are well defined although most of them are premature.
- The project attempts to quantify and address the DOE Material Reactivity Requirements with Analysis and Testing of Hydrogen Storage Materials and Systems.
- The presentation stated that the project addressed code and standards as well as system weight and volume but it is not clear from the materials presented how the system weight & volume were addressed.
- Setting "meet/exceed standard," mitigation strategies, trade-off process, and codes and standards efforts in this project are critical to meeting overall program objectives.
- This project is also critical to ensuring that systems can be developed for safely utilizing hydrogen storage materials and fully supports the relevant multi-year program plan.

### Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- The approach is highly professional.
- It is concerned with risk analysis, material testing, reaction kinetics, risk mitigation and prototype implementation.
- There are four material candidates;  $2\text{LiBH}_4/\text{MgH}_2$ ,  $\text{AlH}_3$ ,  $\text{NH}_3\text{BH}_3$ , activated carbon which will be tested as charged/uncharged, as synthesized, both with and without contamination, before and after risk mitigation.
- A task structure has been set up the program partners and collaborators.



## HYDROGEN STORAGE

- Risk analysis will be carried out on a quantitative basis.
- The approaches are good and effective in general.
- The mitigation strategy and results need feedback to modeling work.
- Ball milling agglomerated materials is counter to automotive experience.
- The approaches used appear to be adequate.
- Risk analysis framework effort is well done and valuable to program success.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.2** based on accomplishments.

- Finely divided  $2\text{LiBH}_4/\text{MgH}_2$  hydrided was tested with respect to various criteria.
- This material was found to be highly reactive and comparable to  $\text{NaAlH}_4$ .
- In the partially discharged state, coarser powder (100-200 mesh) was less reactive.
- Air exposure tests in the hydrided and partially dehydrided state of  $2\text{LiBH}_4/\text{MgH}_2$  were carried out. A complex reaction sequence involving  $\text{H}_2\text{O}$  was defined.
- The principal investigator made some good progress toward objectives.
- The experimental data helped theory group to build an effective model.
- The risks need to be distributed and prioritized over different factors, especially at system level.
- The project is making adequate progress.
- The dust explosion work was well done, and integrating the testing with Sandia National Laboratories modeling and Savannah River National Laboratories TR-XRD is very well done.
- The project has made reasonable progress.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- This program has many collaborators both within and outside the Metal Hydride Center of Excellence. These include Savannah River National Laboratories, Sandia National Laboratories, Forschungszentrum Karlsruhe (FZK, Germany), the National Institute of Advanced Industrial Science and Technology (AIST, Japan), and the University of Quebec at Trois Rivières (UQTR, Canada) each of which are responsible for several tasks.
- An expert panel will advise on the organization of the Risk Analysis Framework.
- No reports or papers were listed in the presentation, but the program began June 2007 and as of March 2008, is only 10 months old.
- Some collaborations exist.
- The collaborations can be expanded to include some combustion experts outside the center.
- Well integrated into DOE the centers of excellences and International Energy Administration and International Partnership for the Hydrogen Economy programs.
- This project has an extensive and strong set of collaborators.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- For fiscal year 2008, plans include: Compile input from the expert panel on risk assessment for on-board storage; Initiate quantitative ETA/FTA risk assessment; Define  $\text{AlH}_3$  and  $\text{NH}_3\text{BH}_3$  system configurations and perform risk analysis; Material testing and modeling for the  $2\text{LiBH}_4/\text{MgH}_2$  will be completed. Modeling will involve collaboration with Sandia National Laboratories and Savannah River National Laboratory; and Initiate testing of  $\text{AlH}_3$ .
- For fiscal year 2009 plans include: Involve risk studies of activated carbon for on board and off-board regeneration; Conduct dust explosion and air reactivity tests for activated carbon,  $\text{AlH}_3$  and  $\text{NH}_3\text{BH}_3$  and Develop risk mitigation methods.
- The general research direction is good.

- Small scale system-level testing should be considered at current stage of the project.
- The cycled materials might have different behavior compared to fresh materials. Therefore the proposed test should include accessing the cycled material behavior.
- The proposed future research builds on the past progress.
- Increased emphasis should be placed on ensuring that the system configuration which drives the failure mode and effects analysis (FMEA) for components and sub-systems is truly representative of what is likely to be designed/built as a first generation.

### **Strengths and weaknesses**

#### Strengths

- A very strong engineering effort.
- The resources are adequate.
- The collaboration arrangement is exceptional.
- The principal investigator is highly respected and has prior experience in conducting similar studies with  $\text{NaAlH}_4$ .
- This program is very relevant to the storage program's Centers of Excellence effort and should be vigorously supported.
- The overall approach of accessing potential risks of solid state hydrogen storage materials is effective.
- The project involves a wide range of new materials that were not routinely dealt with. Developing codes and standards to handle the materials in research and development and in future wide-spread application is critically important.
- The principal investigator and collaborators have established a methodology and assembled a team capable of meeting the objectives of quantifying and addressing the material reactivity requirements.
- The principal investigator clearly explained and illustrated the task breakdown for various collaborators. (Note: It would be more effective if this overview were given before the first talk or as part of the first talk, rather than in the second talk.)

#### Weaknesses

- Other than the lack publications or written reports, there are no weaknesses.
- The scope of this project should not only be limited in material level tests. Small scale system level testing should be considered at early stage.
- Although the work of all partners is relevant and well-illustrated in the task matrix, it is less clear how this interaction is managed, how technical progress is integrated and how priorities are set in a coordinated fashion.

### **Specific recommendations and additions or deletions to the work scope**

- I have no recommendations for either additions or deletions to the program scope at this time.
- The team should focus on one type of material and develop a complete set of codes and standards.
- The activated carbon effort may have moving targets regarding the pressure, presence of metals and lower temperatures that should be included in analysis and testing.

**Project # ST-42: Chemical and Environmental Reactivity Properties of Metal Hydrides within the Context of Systems**

*Dan Dedrick; Sandia National Laboratory-Livermore*

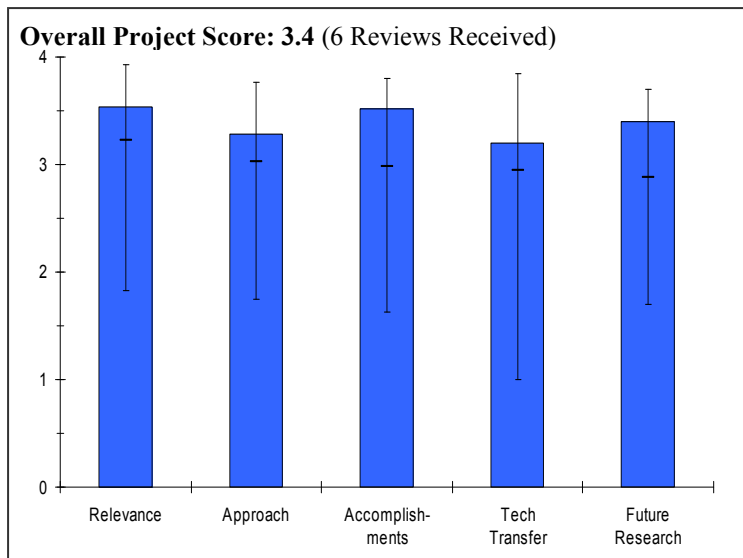
[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

The objective of this project is to develop generalized methods and procedures required to quantify the effects of hydrogen storage material contamination in an automotive environment. The eventual impact of the project will 1) provide technical basis for C&S efforts when appropriate technology maturity has been attained; and 2) enable the design, handling and operation of effective hydrogen storage systems for automotive applications.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.



- The project is critical to the Department of Energy’s hydrogen initiatives.
- The overall objectives of this project are well defined although most of them are premature.
- This project seeks to develop fundamental tools for quantifying the chemical reactivity related hazards of hydrogen storage materials is critical for committing their ultimate safe implementation. However, their work does not relate to health and environmental concerns of hydrogen storage materials.
- The project is addressing important basic material behavior characteristics from a chemical and environmental reactivity standpoint that should enhance the development of appropriate hydrogen storage safety requirements.
- The project addresses hydrogen storage in low pressure systems - a high Hydrogen Program need.
- Trying to look at real world contamination scenarios - this is also appropriate.
- This project is critical to ensuring that systems can be developed for safely utilizing hydrogen storage materials and fully supports the relevant multi-year program plan.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- The approaches are good and effective in general.
- The off-road of developing generally applicable tools, providing a scientific basis for standard United Nations tests (rather than testing individual hydrogen carriers) is appropriate at the present state of the development of the field of hydrogen storage.
- The four tasks in project, experimental methods and analysis will be effective in understanding the contamination effects for hydrogen storage materials.
- Task 4, mitigation strategies appropriate for a broad spectrum of storage materials may not provide the best mitigation strategy for a particular storage material finalist. Some attention to material specific mitigation strategies should be considered.
- The project plan is well-structured but could better address how to migrate results to standard or code requirements.
- The project focuses on contamination scenarios and has developed their own group of scenarios essentially covering tank breach and contamination. Breach and then air or moisture entry is a good scenario pathway.

- Contaminated refueling is a separate scenario that is not necessarily connected to others; it is fine to look at this, but it should not be made to look like part of same scenario path. (It's just a problem with the way the approach is presented rather than a real approach fault.)
- In the project plan, it is not entirely clear from the presentation that Sandia National Laboratories is addressing all four tasks.
- This project specifically adds contamination aspects to work of the associated partners in the areas of mechanism studies, life-cycle implications, etc.
- Task 4 (assessing the fundamental usefulness of fire suppression chemicals) acknowledges the importance of this topic as referenced in the white paper recommendation of the Hydrogen Safety Panel ("Potential Fire Suppression Agents for Metal Hydride Fires") and in the April 2008 report of the NFPA Hydrogen Research Advisory Council, "Research Needs in Support of Hydrogen Safety Standards."

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.5** based on accomplishments.

- The principal investigator made good progress toward objectives in a relatively short time frame.
- The generalized methods and procedures developed in this project to quantify the effects of hydrogen storage material contamination are very useful.
- Impressive development of techniques, in particular the STMBMS apparatus which may be regarded as the scientific data providing equivalent of the U.S. Kaemen Test for the effect of heating in a confined environment.
- Generally good results. Results for reaction products from alane heating in air exposure are well done.
- The project, in its early stages, is making good progress against the project plan.
- New flow cell seems to be a powerful tool to measure effects of contamination.
- Very interesting result on differences between alanes. (With many labs investigating alanes, this system could be very useful.
- Scale-up bulk reactor is also very appropriate.
- It is unclear how the dust cloud combustion effort fits with the rest of the work. It is not addressed sufficiently in the presentation.
- Project team's progress is milestone-based and appears to be appropriate for the one-year point.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.2** for technology transfer and collaboration.

- Some collaborations exist.
- The collaborations can be expanded to include some combustion experts outside the center.
- Good coordination.
- The project team is well-designed to address the project plan.
- Later in the project, representatives from Code Development Organizations (CDOs) and Standards Development Organizations (SDOs) should be engaged to help address issues related to migration of results to codes and standards.
- Collaboration with the United Technologies Research Center (UTRC) and the Savannah River National Laboratory is very good.
- Good international component with the International Partnership for the Hydrogen Economy.
- The principal investigator fully recognizes the importance of sourcing materials from collaborators to ensure relevance and continuity.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.4** for proposed future work.

- The general research direction is good.
- System level testing is not addressed at current stage of the project.

## HYDROGEN STORAGE

- The predicted accident scenarios need to be validated by OEMs.
- Continuing the development of tools. It is suggested to provide where possible some "linkages" to standardized United Nations tests.
- The future work plan is appropriate but later stages need to engage codes and standards experts.
- Risk mitigation work is a logical next step.
- It was not adequately explained as to whether existing systems will be used, new ones built, or etc.
- Task plan fully embraces milestones and go/no-go decision points.

### **Strengths and weaknesses**

#### Strengths

- The overall approach of accessing potential risks of solid state hydrogen storage materials is effective.
- The project represents an opportunity to build an appropriate technical structure from which future safety requirements can be developed.
- Seems like very good development and use of powerful diagnostic tools.
- Strong collaboration.
- The project is addressing an important area.
- The principal investigator has considered credible contamination scenarios based upon NFPA, ISO and SAE draft language.

#### Weaknesses

- The scope of this project should not only be limited in material level tests. Small scale system level testing should be considered at early stage.
- Once sufficient progress has been made, experienced codes and standards representatives should be engaged.
- The presentation needed to be a little clearer on what diagnostics were being applied to what tasks.

### **Specific recommendations and additions or deletions to the work scope**

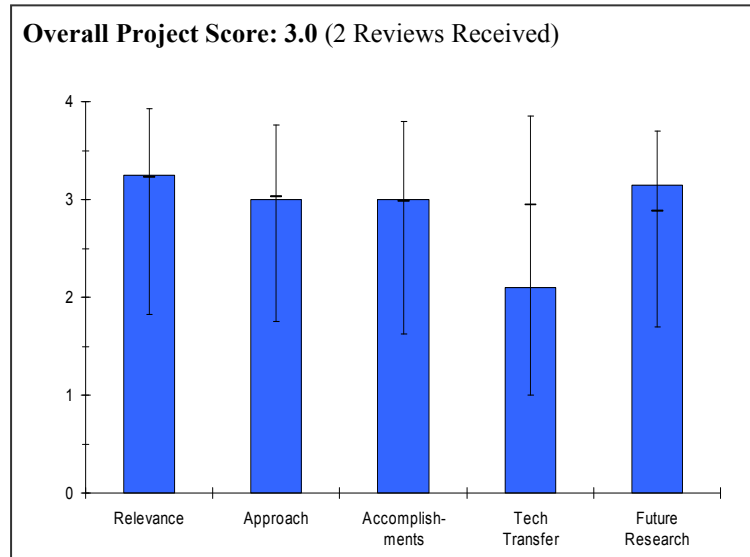
- For dust cloud combustion, the approach for step one of predicting gas/particle flow field needs to be done for several failure scenarios. Resulting burn velocity data for step two will likely depend somewhat on failure mode.
- Addition of a consultation link to CDOs and SDOs is recommended.
- The principal investigator/project team should consider outlining (perhaps in a short white paper) how they would approach the study of fire suppression agents. Such a document, which could incorporate other collaborators, could be provided for external review and feedback in advance of specifically planning Task 4.

**Project # STP-04: Purdue Hydrogen Systems Laboratory***Jay Gore; Purdue University*

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

The objectives of the project are to 1) improve the extent, rate and control of hydrogen release from ammonia borane (AB) by hydrolysis reactions; 2) discover practical uppermost hydrogen storage density of the AB hydrolysis approach; 3) understand engineering properties of the AB hydrolysis approach; 4) characterize the dehydrogenation products and develop new methods for AB regeneration; 5) investigate reaction mechanism and effect of process parameters on yield of hydrogen generation by novel noncatalytic AB hydrothermolysis; 6) determine parameters that maximize anaerobic biological hydrogen production; and 7) understand energy balance for a local modular energy system using biological/solar technology.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- Only the storage portion of this project is evaluated - not the hydrogen production portion.
- Addresses the Department of Energy hydrogen storage targets.
- Apparently no consideration of cost of this storage approach.
- Ammonia borane slurry storage research shows promise as a high hydrogen capacity storage method, which is clearly relevant to overall DOE objectives.
- The relevance of the "local modular energy system" using anaerobic biological hydrogen production was not made clear.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- Clearly aware of the DOE storage performance targets.
- Appears to be focused except for the work on hydrogen production which deflects attention and effort from the hydrogen storage effort.
- Has looked at two approaches for hydrogen release of hydrogen from ammonia borane and also regeneration of ammonia borane from spent fuel.
- Engineering analysis of ammonia borane storage shows focus on meeting DOE system weight goals.
- Experimental results appear to be conducted using good practices.
- Ambient temperature ammonia borane hydrolysis and noncatalytic ammonia borane hydrothermolysis (at ~117-170°C) being researched in parallel.
- The anaerobic biological hydrogen production part of this project lists feedstock cost and hydrogen yield as technical barriers and neither seemed to be addressed in the report.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Progress seems to be slow. Results to date indicate hydrogen material storage capacity that is marginal to meet system capacity targets and needs to be improved.
- Thermal release under increased pressure appears to be interesting.
- Experimental data indicates high storage density of ammonia borane hydrolysis approach at ambient temperature.
- Promising preliminary results for noncatalytic ammonia borane hydrothermolysis approach, provisional patent application filed.
- Demonstrated hydrogen production from waste using fermentation, and developed initial "modular local energy system."

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.1** for technology transfer and collaboration.

- General Motors and General Atomics are claimed to be partners in this project but no detail is given and it is not clear what contributions, if any, these partners have made.
- This work needs to be coordinated with the Chemical Hydrogen Center of Excellence.
- The ammonia borane storage research team is aware of the Pacific Northwest National Laboratory ionic liquid approach as a lower energy regeneration approach.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Future plans appear to be reasonable but are stated only in general terms - need to be more specific. From a hydrogen storage perspective, there is nothing to be gained from the plans to develop a storage system that is integrated with a fuel cell stack. This seems to be a diversion. The emphasis should remain on improving hydrogen storage capacity and regeneration.
- Team recognizes the need to improve regeneration yield, and thus reduce energy. Currently at 64 percent yield, goal of 80 percent by January 2009.
- They have a plan to reduce the water/ammonia borane mixture ratio.
- Optimize parameters for noncatalytic ammonia borane hydrothermolysis for maximum hydrogen yield.
- Maximize anaerobic biological hydrogen production.

### **Strengths and weaknesses**

#### Strengths

- Identification of system level targets, and understanding that the material capacity needs to be well above system targets.
- Parallel approaches to ammonia borane hydrogen storage (hydrolysis and hydrothermolysis).

#### Weaknesses

- Lack of coordination with other DOE efforts in hydrogen storage - coordination with the Chemical Hydrogen Center of Excellence.
- Energy requirements for regeneration not clearly stated.
- Anaerobic biological hydrogen production yield status/baseline/benchmark not reported; feedstock cost not addressed at all.

**Specific recommendations and additions or deletions to the work scope**

- Develop a relationship with the DOE Chemical Hydrogen Center of Excellence.
- Make regeneration energy requirements (and carbon emissions) more transparent.
- Show similar systems analysis for volume target, as you have done for weight.
- As hydrothermolysis research progresses, keep track of the amount of energy needed to sustain temperature and pressure requirements. Identify if this energy can be provided by fuel cell waste heat.
- Clearly address anaerobic biological hydrogen barriers of hydrogen yield and feedstock cost.

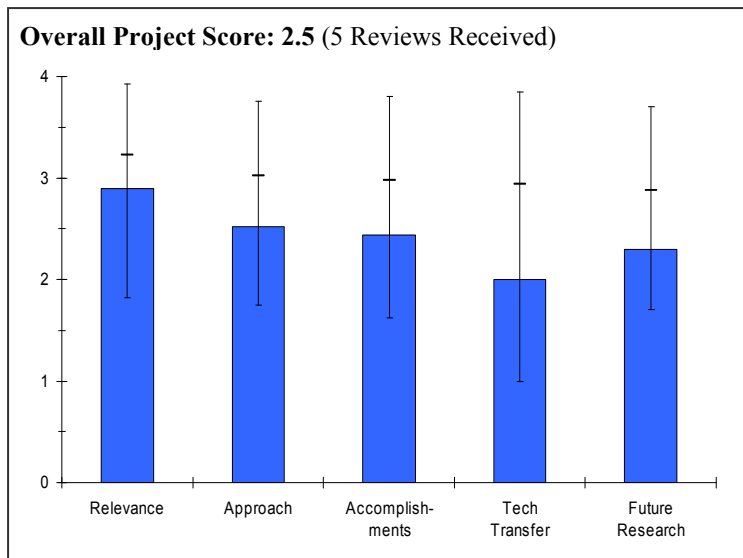


**Project # STP-05: Development of Regenerable, High-Capacity Boron Nitrogen Hydrides For Hydrogen Storage***Ashok Damle; Research Triangle Institute*

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

The overall objective of this project is to develop a boron-nitrogen hydride-based hydrogen storage system to meet U.S. DOE's 2010 technical (6 wt%) and cost targets (\$4/kWh). The hydrogen release objectives are to: 1) develop an energy efficient process of on-board thermal decomposition of ammonia-borane (AB) ( $\text{NH}_3\text{BH}_3$ ) to release pure hydrogen suitable for proton exchange membrane fuel cells; and 2) discover catalysts to improve efficiency of hydrogen release and to produce decomposition products that are amenable to regeneration of AB. The AB regeneration objectives are to 1) develop an energy efficient process for catalytic regeneration of AB decomposition products; and 2) discover catalysts to promote regeneration of partially dehydrogenated products, preferably using only  $\text{H}_2$  pressure and temperature.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.9** for its relevance to DOE objectives.

- Project is relevant to the main objectives of ammonia borane hydrogen storage option.
- Ammonia borane has high hydrogen material capacity and the potential to meet DOE 2010 targets.
- OEMs have stated their strong dislike for cartridge based storage systems- principal investigators should concentrate on liquefying storage materials if they cannot be charged on-board the vehicle.
- Regeneration of ammonia borane systems is key to the use of these materials as hydrogen storage media. Today, the lack of a good catalyst for this process is a major weak link to any practical implementation scheme. This work offers one approach to solving this critical issue. While the approach being explored in this grant is of interest, the current work has not identified any potential catalyst systems at this point.
- This project was redirected into catalyst development for ammonia borane hydrogen release and regeneration.
- Hydrogen storage using ammonia borane.

**Question 2: Approach to performing the research and development**

This project was rated **2.5** on its approach.

- Characterize non-catalytic thermal decomposition of ammonia borane.
- This process has long been a well understood phenomenon.
- This process clearly does not operate within the envelope of automotive operating conditions.
- Conduct combinatorial high-throughput screening of the catalyst libraries to identify catalysts. This is an important task however there are many more qualified principal investigators conducting this work in the Chemical Hydrogen Storage Center of Excellence.
- Evaluate promising catalysts and process conditions for regeneration of decomposition products to AB (with up to two moles of hydrogen released). This process will likely require more than just catalyst work to achieve reversibility.

- The cartridge approach should be abandoned completely. OEMs strongly prefer to avoid such systems to system complexity – (seals connections, logistics at the forecourt, etc.).
- The thermochemical analysis employed is good.
- The high throughput screen that has been developed is very clever.
- The concept of an internal multifunctional catalyst in continuous intimate contact with reactants and products is a well developed idea.
- Combinatorial high throughput screening is a sound approach to address hydrogen release and Spent fuel regeneration.
- Good integration of theory and experiment.
- Intematix screens catalysts and RTI determines their effects on release and spent fuel regeneration.
- There appears to be no clear rationale for catalyst selection for release and spent fuel regeneration.
- Reasonable approach to the catalytic and non catalytic dehydrogenation ammonia borane. Futile attempts to directly re-hydrogenate "spent" ammonia borane-due to the unfavorable thermodynamics.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.4** based on accomplishments.

- The principal investigator is utilizing a high throughput screening of ammonia borane using a 16 cell library method sputtering different catalysts. Using an RGB signal to implicitly determine if hydrogenation/dehydrogenations are occurring although they can't elucidate on exactly what reactions are truly occurring (potential undesirable side reactions). The technique is limited to hydrogen inert materials which is desirable however they will not be able to determine how the catalyst is behaving on hydrogen.
- Library screening techniques have been implemented (but not totally perfected).
- One potential catalyst has been identified and carried through a bulk analysis that indicated it was not a successful candidate.
- The accomplishments indicated above appear less than expected for a project that is time marked to be 70% complete.
- Good accomplishments in hydrogen release tests up to 500°C.
- Only one set of catalysts screened for dehydrogenation and one set for rehydrogenation, would have liked to see more.
- Spent fuel regeneration is a major hurdle for ammonia borane as a hydrogen storage material, while disappointing yet not too surprisingly, the first attempt at catalytic rehydrogenation of decomposition residue failed.
- Much of the work on the ammonia borane release looks like a duplication of effort with the Pacific Northwest National Laboratory work.
- Has done a good job at finding ways to release hydrogen from ammonia borane and demonstrating the considerable exo-thermicity of this process. But it should have been evident from their thermodynamics that the spent fuel regeneration process, a direct re-hydrogenation with hydrogen, would be futile.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.0** for technology transfer and collaboration.

- Neither the principal investigator nor the partner Intematix is significantly connected to the Chemical Hydrogen Storage Center of excellence.
- This project has not proceeded to a point where technology transfer can be considered.
- The limited work completed to date is collaborative in nature.
- Intematix is the only external collaboration partner (for catalyst screening).
- There appears to be no interactions with the solid ammonia borane work at the Pacific Northwest National Laboratory.
- RTI and Intematix.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.3** for proposed future work.

- With screening techniques in hand, work will now focus on the search for a catalyst. However, with the very limited data that has been produced to date, it is unclear if the selected search parameters have merit.
- Future plan is appropriate.
- Need to focus on rehydrogenation and demonstrate some success, absence of which renders the project less relevant to DOE objectives.
- This project ends in November 2008. It is unlikely that significant catalyst development will take place between now and then.
- As said there is no point in searching for catalyst to effect the highly thermodynamically unfavorable one step rehydrogenation of "neat" ammonia borane.

### **Strengths and weaknesses**

#### Strengths

- High throughput library technique should allow the principal investigator to evaluate many catalyst combinations quickly.
- A good high throughput screening for hydrogen evolution and catalyst oxidation state have been developed.
- Good experimental methods.
- Ability to generate large number of metal catalyst compositions.
- None.

#### Weaknesses

- Lack of collaboration with leaders of ammonia borane catalysis and regeneration.
- No catalyst or potential catalysts have been identified, and an updated strategy has not been presented that might improve the productivity of the project.
- Limited interactions with the Metal Hydride Center of Excellence partners.
- RTI does not have a rationale for catalyst development.

### **Specific recommendations and additions or deletions to the work scope**

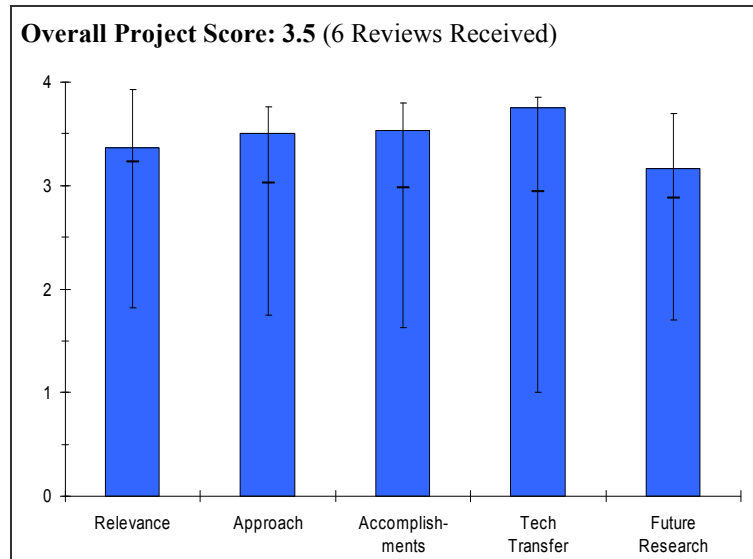
- Continue high throughput screening. Either the rate of screening must be upgraded or a more clever parameter space needs to be identified (or both).
- None.

**Project # STP-06: Neutron Characterization in Support of the Hydrogen Sorption Center of Excellence**  
*Dan Neumann, presenting Terry Udovic and Craig Brown, Co-PIs, NIST*

[NOTE: NIST is a member of the Hydrogen Sorption and Metal Hydride Centers of Excellence.]

**Brief Summary of Project**

The overall objectives of this project are to 1) support the development of hydrogen storage materials by providing timely, comprehensive characterization of center-developed materials using neutron methods; and 2) use this information to speed the rational development and optimization of hydrogen storage materials that can be used to meet the 2010 DOE system goal of 6 wt% and 45 g/L capacities. Objectives are to 1) provide Calphad calculations of phase relationships of potentially promising hydrides (Metal Hydride Center of Excellence only); and 2) contribute within the Center and with independent projects if it furthers the Center goals.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.4** for its relevance to DOE objectives.

- Strength: NMR is a wonderful tool, critical to understanding the mechanisms of adsorption in physisorbents by providing detailed structural information, binding locations, binding energies and even transport (diffusion) information. [DOE NOTE: NMR work is done at UNC, a partner of the Hydrogen Sorption Center of Excellence.]
- This project is providing a fundamental understanding of the structures of some hydrogen storage materials. To the extent that this understanding leads to developing new materials, it supports the Department of Energy's objectives.
- This project is providing outstanding structural and other analysis to the Storage Hydrogen Sorption Center of Excellence, is a key enabler to understanding these sorption materials and designing improved materials. Sorption-based materials offer perhaps the greatest chance of meeting the very challenging on-board storage targets for hydrogen fuel cell vehicles.
- Neutron scattering is critical to understanding the behavior of hydrogen in materials.
- The project scope is to provide a set of uniform characterization techniques applicable across multiple material samples. Within this scope, the project is quite relevant as the techniques definitely provide useful information on how and where hydrogen is sorbed. Whether this information leads to breakthroughs in achieving hydrogen storage goals rests in the hands of collaborators; it seems unlikely that this project itself will lead directly to such breakthroughs.

**Question 2: Approach to performing the research and development**

This project was rated **3.5** on its approach.

- This project is a critical tool in support of Hydrogen Program sorption-based storage projects. It provides deep insight into the sorption phenomena and can contribute significantly to determining go/no-go decisions.
- The neutron facilities for determining the elemental composition of materials and for determining the locations and bonding of adsorbed hydrogen are state-of-the-art. The principal investigator presents adequate experience to do the work.

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- The project's neutron scattering and other techniques are elucidating the exact structure and hydrogen placement of the sorption materials being researched. This is elucidating the reasons for the thermodynamics and performance being achieved; greatly advancing the science in sorption based materials for hydrogen storage and should enable the development of improved materials.
- The project provides much needed basic understanding of which centers are critical for improved hydrogen absorption.
- Again, within the project scope, the characterization techniques are well-focused on providing the expected information, and the project is reasonably well integrated with other activities.
- Greatest concern: This project's capabilities appear to have been applied most heavily to systems that are already reasonably well understood, and that are unlikely to be improved despite the additional understanding these capabilities provide. Can these capabilities be applied to more controversial materials where higher-than-typical capacities are claimed? That way, erroneous claims might be corrected sooner, and genuine new leads might be recognized and advanced more rapidly than has been the tendency.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.5** based on accomplishments.

- Strength: Technical achievements such as the experimental identification of adsorption sites in MOF-74, the effect of binding on the length of the H-H bond, the observation of a "denser than solid hydrogen" monolayer for MOF-74, and the confirmation of the breathing effect in materials such as the MIL-53 are very impressive.
- Strength: The results are outstanding and show pathways to achieving higher storage densities using physisorbents.
- Strength: The use of NMR as a non-destructive element analytical method to determine the degree of incorporation of various elements in nanoporous carbons before and after activation is interesting. (To what degree is this technique unique in that respect?)
- The work done to determine the structures of MOFs, including a "breathing" MOF, is excellent.
- The neutron methods have provided a valuable service to partnering institutions in the center.
- Has shown packing densities of hydrogen greater than in solid hydrogen in MOF-74 and has helped elucidate how and why this occurs through neutron scattering as well as BET surface area measurements along with sorption measurements.
- Discovered "breathing" in MOF MIL-53. This is a newly identified phenomenon that may enable further improvement in sorption material for hydrogen storage.
- Elucidated how boron and platinum affect nanoporous carbon hydrogen sorption through neutron scattering experiments.
- The project provides highly reliable structural data that can be and are used by partners in their materials design work.
- The project provides rapid access to neutron scattering facilities as requested by partners.
- The principal investigators are highly qualified experts in neutron scattering.
- There has been good progress using the techniques and capabilities, within project scope. Perhaps the most promising progress has been in contributing to understanding "phase breathing" material modes; a complete understanding of these modes may lead to new temperature/pressure cycles that can be exploited for storage. Also intriguing is the hint from inelastic scattering (slide 13) that "free" 1-d motion of hydrogen might occur in longer channels, although how this will contribute to meeting DOE capacity goals is unclear.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.8** for technology transfer and collaboration.

- The project is by its nature collaborative and fulfills its mandate with the Sorption Center of Excellence and other partners.
- The National Institute of Standards and Technology (NIST) has fulfilled one of its major objectives by providing characterization of materials, using neutron methods, to several institutions in the center.
- This project is collaborating with and aiding many parts of the Sorption Center of Excellence.

- The project is publishing many papers and presenting at conferences so that the knowledge being gained is getting transferred to a broad scientific community.
- The nature of work is highly collaborative.
- Excellent relationships with the Hydrogen Sorption Center of Excellence.
- Collaboration is inherent in this project's scope, and appears to be happening as intended. As mentioned in other comments, applying these capabilities to more controversial samples could be valuable.
- Some coordination exists.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- Strength: The project has a clear plan for future research that is consistent with past research and partner and program requirements.
- Strength: Infirmiting/confirming the role of "Kubas" interactions in doped physisorbents would be an important contribution.
- The principal investigator presents adequate experience and capability to continue neutron scattering studies on various adsorbents.
- Some contingencies to the future work could have been mentioned.
- A well defined plan for future work is in place for fiscal years 2008 and 2009.
- It is suggested that this project might try to define a clearer strategy with the Sorption Center of Excellence as to the areas, types of samples, etc. it should focus on to most efficiently aid in the development of sorption based hydrogen storage materials.
- The project clearly builds on prior accomplishments.
- Within the present scope, this project may not have much room to overcome barriers. The project appears to be constrained to provide more "service" than "guidance."

#### **Strengths and weaknesses**

##### Strengths

- This project has managed to achieve important technical achievements.
- This project is an essential characterization method in support of understanding sorption properties and mechanisms, performing non-destructive element analysis of modified materials, and guiding the development of materials that could attain DOE storage goals.
- NIST is providing access to neutron facilities to a large number of partners in the centers, as well as to several external partners.
- This project is providing outstanding structural and other analyses to the Sorption Center of Excellence that is a key enabler to understanding these sorption materials and designing improved materials. Sorption-based materials offer perhaps the greatest chance of meeting the very challenging on-board storage targets for hydrogen fuel cell vehicles.
- A whole suite of neutron scattering capabilities is utilized.
- Excellent publication record.
- High visibility of research.
- Solid and reliable data are disseminated quickly.
- Very good characterization within defined scope. Provides interesting insights into phenomenology of hydrogen sorption; insights that appear to be uniform and readily compared across different samples and sample types.
- Theoretical calculations look interesting.
- Some experimental results may be of certain practical value.

##### Weaknesses

- Weaknesses (refer mostly to the presentation provided for the review): Are the storage densities referred to net or excess densities? How are they obtained?
- Pressure and temperature information should be stated everywhere a storage density is mentioned.

## HYDROGEN STORAGE

- NIST should make more of an effort to extend its collaborations and partnerships to include some small independent DOE-funded institutions that are not part of the Hydrogen Sorption Center of Excellence or the Metal Hydride Center of Excellence.
- I noted that collaborations with the Metal Hydride Center of Excellence have not been presented. If these were simply not reviewed, this is fine. If these have been discontinued, then I think they should be restored.
- Insights into phenomenology, especially phenomenology of materials already empirically optimized, are unlikely to teach how to proactively design new, breakthrough, materials.
- The poster focuses on a limited set of materials provided by a few collaborating institutions. If possible, studies of a more diverse set of materials could lead to a greater likelihood of advancing progress toward DOE goals.
- I am not sure that this project is presented in the best possible way.

### **Specific recommendations and additions or deletions to the work scope**

- The SPD analysis provided in the slides is very interesting; it would be nice to compare with pure carbon nanostructures as a baseline reference (activated carbon for example).
- This method could likely make an important contribution in understanding and characterizing the spillover effect.
- It is suggested that this project might try to define a clearer strategy with the Sorption Center of Excellence as to the areas, types of samples, etc. It should focus on how to most efficiently aid in the development of sorption based hydrogen storage materials.
- Given the excellent results, I recommend expanded collaborations with the Metal Hydride Center of Excellence, and if possible, with added funding.
- If possible, put these capabilities to work on controversial samples or materials. That way, erroneous claims of unusually high capacity can be disproved sooner, and accurate claims can sooner be recognized and advanced.

**Project # STP-08: Optimizing the Binding Energy of Hydrogen on Nanostructured Carbon Materials through Structure Control and Chemical Doping**

*Jie Liu; Duke University*

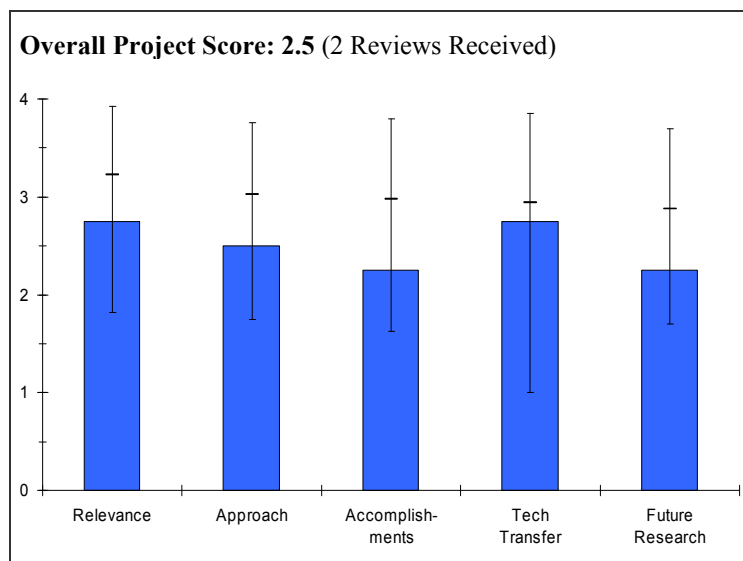
[NOTE: This project is part of the Hydrogen Sorption Center of Excellence.]

**Brief Summary of Project**

The objectives of this project are to 1) design and synthesize carbon-based materials with optimized binding energy to hydrogen molecules that will show storage capacity meeting the Department of Energy 2010 goal in hydrogen storage; and 2) design and synthesize microporous carbon-based materials with enhanced binding energy to hydrogen including: pore size control; surface area increase; metal doping of microporous carbon materials; and B-doping of microporous carbon materials.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.8** for its relevance to DOE objectives.



- This project as presented and described does not appear unique. Needs direction by center of excellence leadership to improve relevance.
- The project objectives are aligned with Department of Energy research and development objectives.
- Improving the binding energy of hydrogen and carbon is one of the critical factors to improve the hydrogen uptake for carbon-based materials.
- One aim is to increase surface area: but generally this will decrease volumetric density (which is already low for these materials); is there any way to achieve the 2010 volumetric densities with these materials? The PIs do not report any measurements of volumetric density, and do not comment on this issue. Thus, it seems as though they are unaware of this important drawback of their materials?

**Question 2: Approach to performing the research and development**

This project was rated **2.5** on its approach.

- Objective does not set this project apart from others in the Sorption Center of Excellence - what new research and development is this project doing?
- Micropore activation can be accomplished by steam, CO<sub>2</sub> or chemical means. Steam leaves OH<sup>-</sup> on surface, KOH tends to leave both K<sup>+</sup> and OH<sup>-</sup> and CO<sub>2</sub> leaves dangling oxygen bonds. The principal investigator needs to characterize surface to determine if there is an impact of microchemistry on outcomes. There are numerous tests to characterize the carbon surface within the center of excellence and correlation of the surface chemistry would strengthen this project and shed light on hydrogen sorption.
- The approach does not demonstrate how this project will add to the state-of-the-art.
- The principal investigator did not show how theory group can help them in the design of nanostructured carbon.
- The experimental approach is more like a trial and error approach rather than an engineered bottom-up approach.
- Very interesting surfactant approach to control pore size; it appears that the researchers have achieved sub-nanometer pore sizes using this approach!



## HYDROGEN STORAGE

- The PIs assert that continuous control of the binding energy should be possible by controlling pore size. However, they have not demonstrated that the binding energy is actually a function of the pore size (and since they have different pore sizes in their samples, it seems that this demonstration should be possible).
- The PIs say that there are problems associated with too weak or too strong a binding energy, and that they are trying to tailor their materials towards the optimum binding energy. However, they don't give any indication of what this optimum binding energy is? Could the PIs comment on this?

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.3** based on accomplishments.

- Technical progress is minimal for a project in its second year.
- Data presented does not look like new additions to art or literature. Most of data presented can be found in existing literature.
- The principal investigator has demonstrated modest progress on overcoming the barriers.
- There is not enough data to demonstrate the relationship between surface area, pore size, and binding energy.
- Though PIs show hydrogen weight percent adsorbed higher than the "Chahine rule," they still do not have any results above 2.5% at 77K, which is not anywhere near even state-of-the-art for activated carbons.
- Why are all the "super high surface area" samples tested at a different facility than the National Renewable Energy Laboratory? This raises some suspicions about the consistency of the various surface area measurements.
- The 8kJ binding energy is substantially higher than is typical for sorption materials; so this result is significant. However, the process used to obtain this binding energy [NMR measurements by HSCoE partner UNC] seems to have the strong possibility of experimental error (i.e., peaks from voids/pores first have to be separated, then integrated, and the resulting intensity from the pores is then fit to a Langmuir isotherm). It seems as though the experimental error bars on this binding energy are likely to be quite large, but the PIs do not report this error.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.8** for technology transfer and collaboration.

- Need to establish stronger collaborations within the Sorption Center of Excellence. Some collaborations are listed but could not be fully explained.
- The principal investigator did not demonstrate a close coordination with a theory group in defining the design parameters of a nanostructured sorbent material.
- The experimental results need to be independently verified, especially when a sample showed higher hydrogen uptake than expected.
- Good to see they are sending samples to the National Renewable Energy Laboratory for testing. Why are all of the samples not sent there?

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.3** for proposed future work.

- Proposed future work (boron doping) duplicates on-going work at Penn State carried out by T. C. Chung and needs to be re-evaluated and relevant.
- The current experimental method is based on lab scale 1" diameter tube furnace. The potential scale-up issue of optimized experimental parameters needs to be addressed at this stage.
- The sample lost about 80 percent weight during activation process alone. The low yield will in turn increase the product cost and the issue should be addressed in future research plan.
- The proposed future work is not sharply focused on overcoming the barriers associated with these materials. The PIs are focused on achieving 6 weight percent (presumably at 77K) in their materials, but this is not the DOE 2010 target (which is a system target for \*useful energy\*, not a material target at 77K). Also, the proposed future research does not mention any attempts to increase volumetric density, which is just as important a DOE goal as the gravimetric target.

- Theoretical modeling work is proposed to study the effect of doping on binding energy. However, this modeling work is already ongoing in other parts of the CoE. (And, the PIs say they will collaborate with Rice and Air Products on this.) So, it is not completely clear whether or not this modeling is proposed to be part of the Duke project, and if so, what is the rationale for duplication of this effort?
- The work on doping of these carbons (e.g., with boron) seems to be somewhat redundant with other efforts in the CoE.

### **Strengths and weaknesses**

#### Strengths

- The concept is aligned with DOE Hydrogen Program objectives and some of the results will help in understanding the relationship between binding energy and surface morphology.
- The main strength of this project is the successful synthesis of microporous carbons with variable pore sizes. This is an interesting accomplishment, and its implications towards hydrogen storage in these materials are not fully explored.
- Relatively modest budget for the work being performed.

#### Weaknesses

- The project has shown minimal progress and characterization of the carbons synthesized is lacking. The project could be strengthened by carbon microchemistry, surface activity/basicity, and other relevant characterization.
- Future work needs to be completely rethought and realigned to avoid duplication and to improve relevance.
- Lack of theory guided experimental design.
- The main weakness is the complete focus on gravimetric density (with a lack of attention on the volumetric density). The PI's approach for increasing gravimetric density is highly likely to actually reduce the volumetric density, which is arguably a larger obstacle for these materials.

### **Specific recommendations and additions or deletions to the work scope**

- The principal investigator can also try to activate the carbon with  $\text{NH}_3$  other than  $\text{CO}_2$ .
- It is not clear whether the PIs are proposing to do theoretical modeling work in the future, but if so, I would recommend deleting this from the project scope. The PIs do not have expertise in this area, and it appears to be redundant with other activities within the CoE.

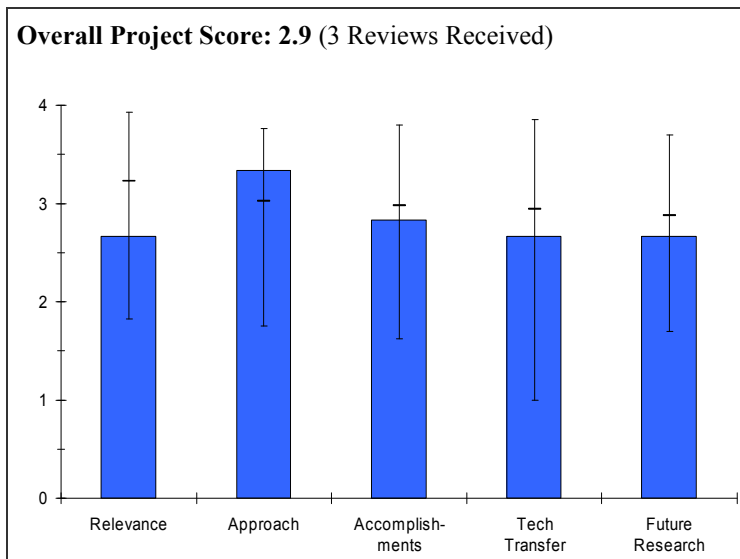
**Project # STP-11: Advanced Boron and Metal Loaded High Porosity Carbons**

*Mike Chung, Presenting; Peter Eklund, Hank Foley, Vincent Crespi, Co-PIs, Pennsylvania State University*

[NOTE: This project is part of the Hydrogen Sorption Center of Excellence.]

**Brief Summary of Project**

The primary objective of this project is to achieve the 6 wt% H<sub>2</sub> storage goal by increasing binding energy (10-30 kJ/mol) and specific surface area (SSA) (>2,000 m<sup>2</sup>/g). Boron substitution in carbon structures has the advantages of: lightness of boron, enhancing H<sub>2</sub> interaction, no serious structural distortions, catalyzing carbonization, and stabilizing atomic metal. Activities for FY 2008 include 1) synthesizing the desirable B/C and M/B/C materials with B content (>10 mol%), M content (>3 mol%), and SSA (>2,000 m<sup>2</sup>/g), and 2) studying structure-property relationships.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.7** for its relevance to DOE objectives.

- This project offers a unique approach to modifying the carbon structure with boron that could be an important breakthrough in understanding structure changes on hydrogen binding.
- The project claims to be ultimately aimed at a variety of DOE barriers, but only gravimetric capacity and adsorption enthalpy are covered in the presentation. Information on volume and kinetics would have been helpful to hear, even in a preliminary sense.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- Very good approach demonstrating strong modeling coupled with novel synthesis.
- Could/should be strengthened by broadening approach to consider other dopants to graphite structure and their impact on hydrogen binding energy.
- The overall approach, to increase the enthalpy of hydrogen adsorption on carbon, is good.
- Substitution of boron into the carbon structures has a good theoretical basis.
- The subsequent substitution of metal atoms provides a catalytic (spillover) component.
- Interesting approach to boron incorporation, and demonstrated significant levels of incorporation, coupled with a better than "Chahine-like" adsorption behavior.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- Good accomplishments.
- When is the go/no-go to determine when boron does not improve hydrogen storage and whether project should move on?

- The project has been successful in developing techniques to partially substitute boron for carbon in the structures.
- The addition of fine metal particles (~2 nm) has also been successful.
- The project has been successful in increasing the hydrogen adsorption enthalpy by 100 percent, a significant achievement and the confirmation of theoretical predictions.
- In spite of this, the 77K hydrogen-capacities seem on the low side relative to DOE targets, at least at 1 bar pressure. It would be interesting to see some higher pressure data.
- Have produced boron-doped materials with approximately 10 percent boron.
- The boron/carbon structure obtained as a function of pyrolysis temperature seems quite unusual. Do the principal investigators have some hypothesis to explain the proposed model? Is this model based solely on the XRD data of the d-spacings? If so, are there alternate explanations?
- The principal investigators have achieved a significantly increased binding energy of 11-12 kJ/mol. However, they should report error bars associated with the process of extracting these numbers.

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.7** for technology transfer and collaboration.

- Collaborations are not clear. Need to elucidate collaborations, not just list or explain.
- There are some collaborations within the Hydrogen Sorption Center of Excellence, but they seem somewhat limited.
- There are no apparent collaborations outside the center of excellence, or internationally.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.7** for proposed future work.

- Proposed future work needs to be clearly delineated and expanded upon. Much of future work looks similar to work already ongoing in the center of excellence. Show uniqueness.
- Future work is a logical extension of the past results.
- The description of the actual work planned is not very detailed.
- There should be a go/no-go target.
- The proposed future work is not sharply focused on overcoming the barriers associated with these materials. The principal investigators are focused on achieving 6 weight percent (presumably at 77K) in their materials, but this is not the DOE 2010 target (which is a system target for \*useful energy\*, not a material target at 77K). Also, the proposed future research does not mention any attempts to increase volumetric density, which is just as important a DOE goal as the gravimetric target.
- The future work relies on "finding the right metal M". How do the principal investigators propose to find this metal?

#### **Strengths and weaknesses**

##### Strengths

- This project offers a unique approach to modifying the carbon structure with boron that could be an important breakthrough in understanding structure changes on hydrogen binding.
- The project is looking in detail at the boron approach for increasing hydrogen adsorption enthalpy.
- The project combines synthesis advances with property evaluations.
- The group has excellent synthesis capability and understanding.
- Interesting approach to boron and metal incorporation; good synthetic approach.

##### Weaknesses

- Catalyst decoration needs to be expanded past current materials (i.e., Ti and Zr). Look at more relevant catalysts.

## HYDROGEN STORAGE

- Carbon structure can be modified with more than boron. Other cations have been shown to change surface catalytic properties and should be evaluated in this project.
- Apparently not working on specific properties other than weight.
- It seems this approach will have difficulty reaching any system target. Carbon may have insurmountable limits.
- Progress seems somewhat slow, given the amount of time spent, and the budget involved.
- The project should have an equal focus on volumetric and gravimetric densities (right now, volumetric densities are not mentioned).
- No rational course is proposed for deciding which metal is the best to incorporate in these materials.

### **Specific recommendations and additions or deletions to the work scope**

- Look past boron to other additives to carbon.
- More consideration to cost, volumetric capacity, and kinetics.
- Add some higher pressure measurements, if necessary through Hydrogen Sorption Center of Excellence partners.
- Add one or two measurements at room temperature. Would boron show some advantage there?

**Project # STP-12: Nanoengineering the Forces of Attraction in a Metal-Carbon Array for H<sub>2</sub> Uptake at Ambient Temperatures**

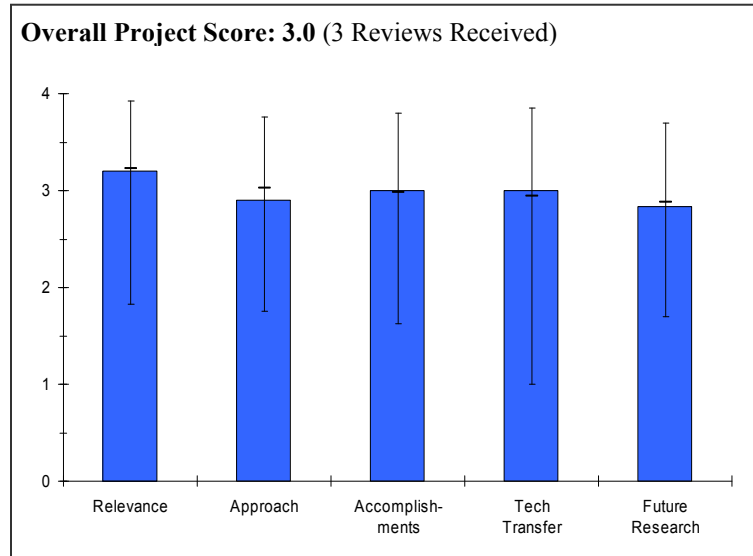
*James Tour, PI; Carter Kittrell, co-PI; Rice University*

[NOTE: This project is part of the Hydrogen Sorption Center of Excellence.]

**Brief Summary of Project**

The primary objective is to design and produce layered carbon-metal media with nanoengineered attractive forces capable of exceeding 80 g/L volumetric uptake of dihydrogen at -20°C. Nanoengineering the structure is conducted to effect the forces of attraction for dihydrogen. Four attractive forces are designed to act cooperatively to “pull dihydrogen” into the pore; these include: 1) Van der Waals attraction to a pi cloud of sp<sup>2</sup> (graphene or CNT) carbon surface; 2) dipole induced-dipole attraction between a charge separated (+) metal atom layer and a (-) graphene layer; 3) charge induced-dipole attraction near charged metal atoms; and 4) “Kubas-type” interactions for transition metal atoms.

Regarding force design parameters, each of the binding energies are intentionally chosen to be inadequate to bind H<sub>2</sub> at room temperature, but collectively will “pull H<sub>2</sub>” into the pore.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.

- A large number of promising and unique nanoengineered materials have been designed and synthesized. However, as observed last year, virtually no hydrogen storage measurements were presented. While the materials synthesis and characterization efforts are understandably time-consuming, some preliminary hydrogen storage data is highly desired. If it is a matter of coordinating with the sorption CoE to facilitate these measurements, then these interactions should be better developed.
- The project has a sharp focus on the need to develop hydrogen storage materials with volumetric hydrogen densities and enthalpies of dehydrogenation that are adequate to meet US DOE targets. However, this project suffers from a lack of careful consideration of the gravimetric hydrogen densities and the cost of the envisioned materials. The cost issue has not been addressed including presenting an estimate of the cost of the final, functionalized, metal-loaded material.
- Layered nanostructures assembled from well-studied graphene and further modified to elicit higher binding affinities for dihydrogen in the pore structure is precisely the theme of research on which the Sorption CoE should focus its efforts.
- Effort is consistent with other researcher's renewed interest in the manipulation of graphene or graphitic carbons to prepare oxide functional groups.
- Proposed concepts for modifying internal pore structure merge well with other, highly ordered nanostructures such as metal organic frameworks, thus establishing a common tactic for future research efforts.

**Question 2: Approach to performing the research and development**

This project was rated **2.9** on its approach.

## HYDROGEN STORAGE

- It was not clear in the presentation how meaningful and to what extent Rice is interacting with other collaborators in the sorption CoE.
- It is anticipated that additional collaboration with center partners would be particularly valuable in the area of hydrogen storage measurements. Could/should be strengthened by broadening approach to consider other dopants to graphite structure and their impact on hydrogen binding energy.
- The project is directed towards establishing a synergism between hydrogen-graphene Van der Waals interactions and the coordinative interaction in dihydrogen metal complexes. This is an interesting premise. The investigators seem to be very knowledgeable in the art of functionalization of CNTs and graphene. However, the project suffers from the lack of any real understanding of dihydrogen ("Kubas") complexes. As Kubas himself has repeatedly pointed out, a very special electronic environment must be established at the metal center in order for dihydrogen to bind to a metal center without rupture of the H-H bonding. There seems to be no appreciation of this in the planning of this project as it is proposed to introduce Pd(0) (which very unlikely supports dihydrogen ligands) into a ligand environment that is not conducive to stabilization of dihydrogen ligands.
- The approach, though ambitious, should establish a benchmark for comparing surface- and pore excess effects in "doped" physisorption materials as it is aimed at employing all non-bonded (classically) forces of attraction which, heretofore, have been studied only individually.
- One potential pitfall of the approach is that the end product becomes over-engineered to the extent that the cost of synthesis is prohibitive even though the starting materials and proposed dopants may be of low cost.
- Need to accelerate synthetic and bulk analytical efforts in order to validate at least one or two aspects of the energy "tunability" of the layered pore structures.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- In general, future plans are a logical extension of current work. This reviewer would advise placing much more emphasis on testing storage properties (e.g. uptake, binding energy calculations, cycling, etc). Additionally it is recommended that collaborations with center partners be clarified.
- Excellent progress has been made in single sheet graphene functionalization chemistry and the introduction of lithium into the modified materials. It remains to be seen if this progress is an important step towards overcoming technical barriers in the hydrogen storage problem.
- Very significant and impressive progress relative to the development of the nanoengineered slit pore concept, but more rapid transition of chemistries from nanotubes to graphene is needed to validate conceptual approach
- Overall program is 60% complete of budget or milestones (not indicated). If 60% complete of budget, the remaining 40% must be expended on probably the most labor and time consuming aspects of the technical approach. Should this be of any concern?

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.0** for technology transfer and collaboration.

- It was not clear in the presentation how meaningful and to what extent Rice is interacting with other collaborators in the sorption CoE.
- It is anticipated that additional collaboration with center partners would be particularly valuable in the area of hydrogen storage measurements.
- Limited collaborations within the CoE.
- Collaboration with other important theory- and experiment-based teams (e.g. NREL, ORNL, Air Products, etc) is evident.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- In general, future plans are a logical extension of current work. This reviewer would advise placing much more emphasis on testing storage properties (e.g. uptake, binding energy calculations, cycling, etc). Additionally it is recommended that collaborations with center partners be clarified.
- Future plans address several fundamental issues that will contribute to a finer fundamental understanding of the nature of the interaction of hydrogen in functionalized graphene. However, a sharper focus to bring these materials towards a go/no-go decision is necessary.
- Proposed future research adequately addresses concerns about the need to obtain experimental validation of proposed "nanopump" concepts.
- It will become particularly important to assess, theoretically and experimentally, the relative contributions of attractive forces engineered into the pore of the layered structure. For example, dipole-induced-dipole interactions may prove to be sufficient for dihydrogen pumping without charge or "Kubas-type" functionalities. This delineation should be included in the plan.

### **Strengths and weaknesses**

#### Strengths

- Diverse approach and strong materials synthesis capabilities/expertise.
- Recognized leader in nanoengineered carbon-based materials.
- The PI is clearly working toward room temperature storage and high volumetric capacity, two of the major challenges with this class of materials.
- Expertise in graphene functionalization chemistry.
- Concepts are well thought out and supported, in part, by theoretical predictions.
- Engineered layered structures of the kind proposed enables one to explore many different options to enhancing room temperature uptake of dihydrogen in nanoporous materials. The best options which emerge are likely to be relevant to engineering storage materials based on other highly ordered nanostructures.

#### Weaknesses

- Hydrogen storage property evaluations need to be performed routinely for all promising materials.
- The whole project rests on the to be assessed premise that the dihydrogen metal complexes will be formed within these materials and if they do, that the materials will have adequate gravimetric hydrogen storage densities at room temperature.
- The weakness in the approach is one of potential over-complexity if all modes of binding are eventually implemented. This may lead to a costly material to synthesize even if it meets or exceeds the storage goals.

### **Specific recommendations and additions or deletions to the work scope**

- In the next year it should be established if these materials actually storage hydrogen at room temperature and if so, what gravimetric and volumetric capacities have been achieved.
- While the goal of nanoengineering the forces of attraction in pores of metal-carbon layered structures is to attract dihydrogen without dissociation, the realization that dissociative uptake of atomic hydrogen is possible should be explored further as an alternative mechanism. In particular, one should ask whether or not a dissociative mechanism would be more favorable, thermodynamically, than non-dissociative binding within layered pores, and should structures be engineered to purposely affect this mechanism?



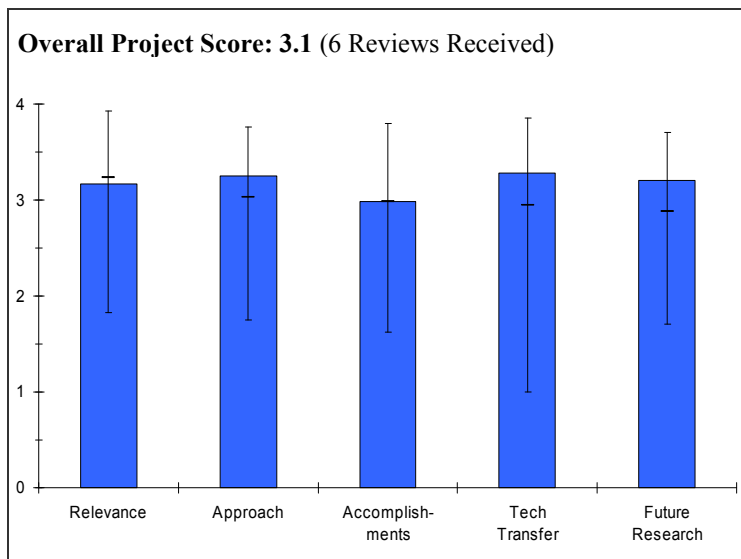
**Project # STP-16: Catalyzed Nano-Framework Stabilized High Density Reversible Hydrogen Storage Systems**

*Dan Mosher; United Technologies Research Center*

[NOTE: This project is part of the Metal Hydride Center of Excellence.]

**Brief Summary of Project**

The objectives of this project are to: 1) design and synthesize hydride/nano-framework combinations to improve a) reversible capacity, b) desorption temperature, and c) cyclic life; and 2) build upon successes previously demonstrated in the community and extend to a wider range of doped, functionalized and catalyzed framework chemistries to a) advance the understanding of behavior modification by nano-frameworks, b) obtain/maintain nano-scale phase domain, c) tune hydride/framework interactions to decrease desorption temperature for highly stable compounds, stabilize high capacity compounds – ligand elimination, and influence desorption product formation, and d) activate H<sub>2</sub> dissociation on highly dispersed catalytic sites.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.

- The project is well aligned to the program objectives and relevant to the President's Hydrogen Fuel Initiative. It is well committed to reach the Department of Energy objectives and focused on addressing the big challenge of improving reversibility of high capacity hydride candidates.
- Work is relevant to DOE objectives.
- Development of nanoframework is one of the ways to increase kinetics in metal hydrides.
- Partially supports the hydrogen vision and DOE research, development and deployment objectives in the areas of charging/discharging kinetics, reversible capacity, and cycle life.
- Seeks to lower desorption temperature, stabilize desired phases, and increase rehydrating rates.
- Is focused on exploring metal hydrides that have relatively high hydrogen weight percentages (e.g., LiBH<sub>4</sub>).
- The project is well-directed toward solving the weight, volume and thermodynamics targets and needs defined by the Program.
- Reversibility is a troublesome, yet very important property to achieve for on-board vehicular storage applications. Project correctly aims at this property.
- Mostly relevant.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- Well thought out, reasonable approach, with a clear direction and focus on technical barriers, using atomistic, thermodynamic modeling to identify promising as well as unfavorable system characteristics to guide the work.
- Getting the most out of previous experience and expertise and fully engaging modeling and experiment.
- Theory and experiment are well integrated. Atomistic and thermodynamic modeling to screen framework design and interaction with metal hydrides is very helpful before synthesizing materials.

- Experiments are well designed and conducted.
- Ability to tune nanoframeworks with dopants to enhance stability and interaction with metal hydrides is important to research.
- Conceptually interesting approach that involves dispersing metal borohydrides in nanoframework structures (NFSs) formed by aerogel techniques; this methodology provides an enhanced surface-area-to-volume for the borohydride that facilitates dehydrating and rehydriding.
- Theory (simulation) and experiment are combined to identify compatible NFSs.
- The NFS approach also offers the possibility to incorporate catalysts and to take advantage of beneficial interactions between the borohydride and the NFS.
- Eventually they hope to identify NFS/borohydride systems that exhibit target level cycle life and kinetics.
- Carbon NFSs have shown promise for some storage media. This project should help in testing the generality of the concept, such as extending it to oxide NFSs.
- There is a good coupling between theoretical prediction effort, synthesis and experimental verification.
- A nice spectrum of experimental techniques is in use.
- The inclusion of catalysts into the NFS will be an important component of the project.
- Unclear if theory is really "guiding" the experiment considering the complexity of the sorbent/scaffold interface structure. Have all reasonable interfaces been examined?
- Are the theoretical predictions on slide 13 for the lowest energy pathway? For example, the second reaction has bare Li and H bonded to  $\text{Al}_2\text{O}_3$  -- is this more favorable than having all Li and H in  $\text{LiH}$ ?
- There seems to be a trial-and-error aspect to the experimental approach of choosing what sorbents to use for scaffolding.
- The approach is based on the hope is that the scaffold will stabilize weakly-stable sorbents, and destabilize strongly-bound sorbents, but there does not appear to be a clear pathway for achieving the desired effect for a given sorbent.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Some progress already achieved despite that this is a rather new project. NFS material systems have already been developed, and down-selection of the hydrides to be incorporated has been made.
- This is a new project (starting July 2007), yet impressive accomplishments have been achieved in both modeling and experiments.
- Initial data on hydrogen release is very slow. Need to demonstrate faster kinetics as a primary focus.
- Used simulation methods to down-select NFS candidates.
- Identified and investigated a stable combination of  $\text{LiBH}_4$  in  $\text{ZrO}_2$  aerogel;
- $\text{LiBH}_4$  compatibility with a series of NFSs was tested.
- This project comes across as a work in progress. (They are one year into the current scope of work.)
- Although the project just started at the beginning of fiscal year 2008, good progress has already been made (e.g., defining the suitability of  $\text{ZrO}_2$  and non-suitability of  $\text{SiO}_2$  as NFS for Li- and Ca-borohydride).
- Relative values of various screening techniques are being defined.
- No apparent work yet on catalyst inclusion into the NFS.
- I expected to see some preliminary calculations or suggestions as to how much loss in volumetric and gravimetric capacities might be expected from NFS.
- New project - not ranked.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- Good cooperation with the partners from the Metal Hydride Center of Excellence; a coordinated effort, engaging theory, material synthesis methods and characterization tools for tackling the challenge of improving reversibility of high capacity promising hydrides via advanced NFS chemistries.
- Extensive collaborations with the Metal Hydride Center of Excellence, partners, and industry.

## HYDROGEN STORAGE

- Principal investigators may want to consider some interactions with Lawrence Livermore National Laboratory on carbon aerogels.
- There are three partners and each has a clearly defined role to play in the project.
- The project is integrated into the Metal Hydride Center of Excellence, so presumably it is coordinated with other related activities in the center.
- This is a good fit for the Metal Hydride Center of Excellence.
- Good collaborations among United Technologies Corporation, Sandia National Laboratories, Albemarle Corporation, and Aspen Aerogels. Duties of each are well defined.
- Collaborations allow access to a very nice array of screening and test equipment.
- Collaboration with Aspen Aerogels will help to quantify ultimate costs of the composites.
- New project - not ranked.
- Since there are now several projects pursuing scaffolding, need to be careful about duplication of effort.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- Future work planning builds on past results and includes critical go/no-go decision points.
- The plan for future research is very solid.
- Modeling studies will focus on  $\text{Ca}(\text{BH}_4)_2$  and  $\text{NaTi}(\text{BH}_4)_4$  with emphasis on interactions with the  $\text{ZrO}_2$  NFS and catalyzed versions of the  $\text{ZrO}_2$  NFS.
- Experiments/testing will focus on  $\text{ZrO}_2$  NFS, on identifying other stable NFSs, and on interactions of  $\text{Ca}(\text{BH}_4)_2$  and  $\text{NaTi}(\text{BH}_4)_4$  with NFSs and catalytically augmented versions of selected NFSs.
- Future plans follow the original contract aims.
- Plans are rather vague.
- Milestones are good.
- Go/no-go criteria are not quantitative enough.
- New project - not ranked.

### **Strengths and weaknesses**

#### Strengths

- Strong team with demonstrated expertise in their respective areas of responsibility - very good, complementary.
- Combining theory and experiment for fine tuning the work program.
- Unique approach with the combination of metal hydride and framework.
- Potential production of cheap, easy mass productions.
- Very solid and promising work.
- Extensive collaboration.
- Good understanding of important issues.
- The lead organization and partners have the facilities and capabilities needed to succeed in this project
- The project is emphasizing metal hydrides that have relatively high hydrogen weight fractions.
- It is a good combination of theoretical modeling, synthesis and screening.
- Collaborative interactions are excellent and provide equipment and expertise.
- The people involved are very well experienced in the field.

#### Weaknesses

- Need to clarify the path to use for controlling the hydride incorporation into the nanoframework and the associated mass transfer issues
- Approach to reach the target is not clear.
- None identified.
- Very little is apparent in the experimental work done to date that the NFS-based concept will actually work as expected.

- Because of the diluting effect of the NFS, the NFS-based concept is not likely to lead to a material embodiment that will meet DOE's system weight percent and volume percent targets; but it might meet some of the rate and cycle life targets.
- I estimate that roughly \$500K was expended on this project over the past year; if that is indeed the case, I would have expected more testing results to have been completed; the score in box 3 above would be higher if more results were obtained in the past year.
- The project is focused entirely on borohydrides, a tough challenge from the perspectives of thermodynamics, reversibility and potential boranes in the exit hydrogen.
- Go/no-go criteria are rather vague.

**Specific recommendations and additions or deletions to the work scope**

- Consider establishing a cross-center collaboration and interaction to benefit from the expertise developed in the Hydrogen Sorption Center of Excellence on aerogels
- Interact with Lawrence Livermore National Laboratory on carbon aerogels.
- Increase productivity.
- Stick with metal hydrides that have weight fractions on the high end of the possible range (nominally greater than 10 weight percent) because the nanoframework structure will diminish the overall weight and volume percentages of contained hydrogen.

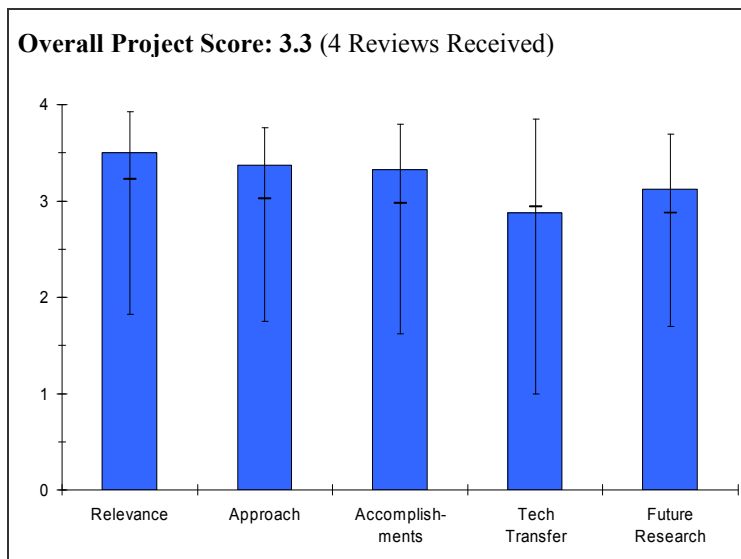
**Project # STP-18: Thermodynamically Tuned Nanophase Materials for Reversible Hydrogen Storage: Structure and Kinetics of Nanoparticle and Model System Materials**

*Bruce Clemens; Stanford University*

[NOTE: This project is part of the Metal Hydride Center of Excellence.]

**Brief Summary of Project**

The objectives of this project are to 1) develop fundamental understanding of metal hydride reaction kinetics; 2) develop understanding of metal hydride nanostructure thermodynamics; and 3) develop understanding of metal hydride structures during phase change. Little is known about the kinetic mechanism present in many promising metal hydride material systems including Mg, Mg<sub>2</sub>Si, Li<sub>4</sub>Si, NaAlH<sub>4</sub>, LiBH<sub>4</sub>+MgH<sub>2</sub>, etc. In order to improve the kinetics for any of these metal hydride systems, a sound understanding must be developed. Many systems suffer from inappropriate thermodynamics (equilibrium pressure), including Mg and Al, and continuum modeling suggests that reaction thermodynamics should be modified by reducing particle size to the nanometer regime. Material structure can play important role in reaction kinetics, especially during solid-state phase transformations such as those in metal hydride reactions, and understanding the interplay between material structure and reaction kinetics may provide insight on how to successfully engineer new materials with improved kinetics and storage properties.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- Understanding effects of crystal structure on thermodynamics and kinetics of materials is necessary for the design of improved materials for the Hydrogen Program.
- Project as presented and described is outstanding and attempts to understand kinetic issues limiting the use of carbon materials.
- This is a science-based project that seeks to develop insights concerning reversibility, capacity enhancement, physisorption, and chemisorption in hydrogen storage systems.
- The project's principal relevance lies in the opportunity to educate the next generation of scientists needed to advance fuel cell development through at least the first half of the 21<sup>st</sup> century.
- The results should contribute new knowledge concerning hydrogen reaction kinetics and the thermodynamics of hydrogen uptake and release at the nanoscale.
- This project is developing novel and potentially excellent experimental tools to better understand metal hydride reaction kinetics, thermodynamics, and structural phase changes that should enable the development of improved metal hydride systems for on-board hydrogen storage.
- The techniques being developed in this project are directed only at metal hydride research. Metal hydrides have been researched for a relatively long time. The considerable amount of data already available suggests that metal hydrides have a low probability of meeting the challenging DOE on-board storage targets.

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- Elegant approach (bottoms up) to understand how crystal structure affects kinetic, etc. Other approaches have used a more brute force of grinding materials to nanoscale and then immobilizing them without truly understanding the morphology of those particles. This technique should help the producers of scaffolds, etc. design more intelligent materials that could perhaps take advantage of effective structures discovered by this work.
- Very good approach demonstrating strong theoretical understanding coupled with strong experimentation and verification.
- While the approach is good, this project is still evaluating pristine surfaces with idealized metal clusters. What is the role of the size and morphology of the metal cluster on spillover? How do intentional changes in the carbon structure through doping with boron or nitrogen or defects affect metal.
- Surface science in a very low oxygen impurity environment.
- The principle research tools are comprehensive x-ray diffraction, quartz crystal microbalance, and neutron scattering with emphasis on oriented and/or epitaxial films, with most work to date done on Mg and Mg containing films.
- The insights from this research could be beneficial to interpreting hydrogen kinetics in ordered structures and nanoscale phases.
- The approaches taken in this research are not likely to identify new types of hydrogen storage materials, but could shed light on novel concepts for kinetics enhancement.
- This project is developing thin film growth techniques, an in-situ hydrogen pressure chamber for use with x-ray studies for real time structural change observations during hydrogen charging and discharging, and quartz crystal microbalance techniques to measure hydrogen uptake on thin films and nanoparticles. These novel techniques should in theory elucidate structural changes and thermodynamic properties of metal hydrides during hydrogen charging and discharging that should enable the development of improved metal hydride hydrogen storage materials.
- The techniques being developed are challenging to develop and it is challenging to prove the results and data interpretation are valid. Results to date on model systems are intriguing but some do not agree with other available data.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- A few thin films have been prepared with sputtering of Mg particles on a sapphire substrate. Proof-of-concept has been demonstrated. The principal investigator must demonstrate the technique on a wider range of substrates and complex hydrides for the technique to be useful to a wide range of material researchers.
- Technical accomplishments to date are outstanding.
- Mechanistic understanding of spillover being developed will lead to a new understanding of how carbon sorbs hydrogen. Identification of spillover as a phase nucleation process allows the temperature and pressure barriers to be modeled. Further allows predictive path forward to overcome barrier to be developed.
- Showed how hydriding/dehydriding of Mg films with preferred orientation causes loss of the preferred orientation, the extent of this loss depending on the degree of hydriding; the interpretation of this result as being related to the retention of some underlying (presumably unhydrided) template layer is an interesting and understandable finding.
- Presented data that indicated hydrogen uptake by nanoscale particles "might" deviate from predictions based on bulk phase thermodynamics.
- Also presented some preliminary neutron scattering data that look very interesting but have not been fully analyzed to derive the attendant surface morphological information.
- Completion/confirmation of measurements done to date will earn a higher score here in the future.
- The development of the novel and potentially excellent experimental tools within the project is progressing well.
- It has taken 3 years to reach the point of beginning to get potentially meaningful data from the techniques being developed.
- The information obtained from the in-situ hydrogen pressure chamber with real time x-ray studies shows evidence of mixed crystal re-growth for the Mg/MH<sub>2</sub> system which may explain its poor performance.

- The quartz crystal microbalance combined with the thin film and nanoparticle techniques is being used to begin to developing information supporting the theory that the smaller the material particle size the better the performance will be, but some of the data being generated is not in line with other available data.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.9** for technology transfer and collaboration.

- Great interaction with Dr. Ralph Yang at Michigan.
- Technology transfer for this project is basically collaborations that provide materials, facilities, or supporting calculations.
- This project is already within the preview of the Metal Hydride Center of Excellence, so insights gained from the Stanford University research should flow smoothly into the center of excellence as a whole.
- Papers are being published and presented relevant conferences.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Continue to expand material and substrate library. The principal investigator should begin to seek partners that can design scaffolds, etc. to stabilize these structures since the materials are not stable under cyclic conditions.
- The future plans build appropriately on where the project stands at this time; several of the experiments presented at the review need to be repeated and there are data analyses that need to be completed.
- Future work will emphasize materials at the nanoscale which is recommended.
- Moving on to new materials compositions will take place, presumably after all the observations presented at the review have been confirmed, formally reported to the center of excellence, and published.
- The future work plan is to complete the development of the techniques and to start to examine metal hydride materials that are more promising relevant rather than the model systems used to date. This is good.

### **Strengths and weaknesses**

#### Strengths

- Elegant approach (bottoms up) to understand how crystal structure affects kinetic, etc. Other approaches have used a more brute force of grinding materials to nanoscale and then immobilizing them without truly understanding the morphology of those particles. This technique should help the producers of scaffolds, etc. design more intelligent materials that could perhaps take advantage of effective structures discovered by this work.
- The graduate student who presented the poster did so in a scholarly and enthusiastic manner; clearly, he is well directed and is fully engaged in the project - that's a very good sign this project is being conducted the way a university program should be and bodes well for the availability of the cadre of bright young scientists and engineers needed to take fuel cell development through the coming decades.
- The facilities, experimental/computational skills, and understanding needed to study hydrogen interactions at the nanoscale are in place at Stanford and/or through their collaborations.
- Once it is reconfigured and its functional features are fully understood, the QCM should become a very useful tool for exploring hydrogen uptake and release at the nanoscale in well controlled environments.
- This project is developing novel and potentially excellent experimental tools to better understand metal hydride reaction kinetics, thermodynamics and structural phase changes that should enable the development of improved metal hydride systems for on-board hydrogen storage.

#### Weaknesses

- The principal investigator has not investigated templates that can be overlaid over these new structural configurations in order to maintain performance with cycling. This should be the future focus or at least transfer the knowledge to someone who can perform such work.
- This project is on the verge of producing some nice science, but the confirmatory experiments and the unfinished data analyses need to be completed.

- Reducing the oxygen impurities in experimental systems to levels low enough to allow pristine study of hydrogen in easily oxidized metals is not a trivial problem; clever ways to exclusively getter oxygen in the presence of hydrogen may be needed to effectively measure hydrogen metal interactions.
- Apparently, no peer reviewed publications have been submitted for this work.
- It is not clear exactly how the particular techniques being developed can be best applied to the most promising metal hydride systems.

**Specific recommendations and additions or deletions to the work scope**

- While very interesting and valuable work, perhaps this should be moved into the Basic Energy Sciences scope.
- The neutron scattering measurements being done with NIST look like they could produce many seminal insights about the impact of hydriding on surface structure - this aspect of the project deserves emphasis.
- Bring reported results to the point where publication is in order.
- The plan to integrate the QCM with the deposition system, characterization of the functional features of that integrated system, and subsequent utilization on nanoscale particles and films is encouraged.
- It might be worthwhile to base the selection of new materials on choices that have already survived down-selection at the centers of excellence.



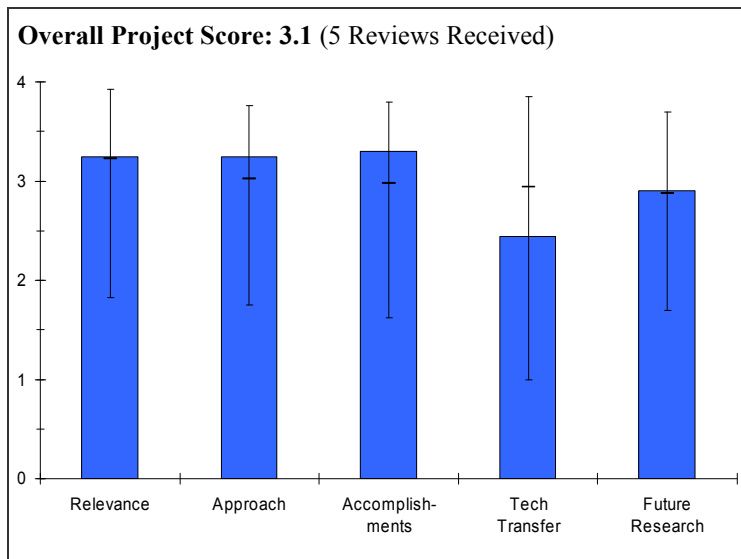
**Project # STP-19: Alane Electrochemical Recharging**

*Ragay Zidan; Savannah River National Laboratory*

[NOTE: This project is part of the Metal Hydride Center of Excellence.]

**Brief Summary of Project**

The objectives of this project are to 1) develop a low-cost rechargeable hydrogen storage material with cyclic stability and favorable thermodynamics and kinetics fulfilling the DOE onboard hydrogen transportation goals; and 2) determine that aluminum hydride (Alane- $\text{AlH}_3$ ), having a gravimetric capacity of 10 wt% and volumetric capacity of 149 g/L  $\text{H}_2$  and desorption temperature:  $\sim 60^\circ\text{C}$  to  $175^\circ\text{C}$  (depending on particle size) meets the 2010 DOE targets for desorption. The specific objective of this project is to avoid the impractical high pressure needed to form  $\text{AlH}_3$  by utilizing electrochemical potential to increase hydrogen activity and/ or drive chemical reactions to recharge  $\text{AlH}_3$ .



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.

- To synthesize  $\text{AlH}_3$  with around 10 percent capacity is one of the major focuses of the Metal Hydride Center of Excellence.
- This project addresses programmatic goal of hydrogen storage systems to meet 6 weight percent storage with the storage system cost less than 30 percent of the hydrogen cost.
- Alane has high material capacity (10 weight percent) and has the potential to meet Department of Energy 2010 targets.
- Alane regeneration is crucial to its viability as a hydrogen storage material.
- This project is narrowly focused on low temperature/low pressure regeneration of  $\text{AlH}_3$ , a 10 weight percent hydrogen material that has the potential to meet 2010 hydrogen vision and DOE research, development and deployment targets for gravimetric hydrogen storage.
- Meeting regeneration efficiency and cost targets is also an objective.
- The project is highly focused on one particular topic, that of using electrochemical potential to drive hydrogenation of Al to form alane. Built into this scope is the fact that the project cannot be any more relevant to the Hydrogen Program than alane itself may prove to be. If other difficulties with alane, such as safety considerations or air/moisture sensitivity, force a no-go decision, the project will have little impact on the Program.

**Question 2: Approach to performing the research and development**

This project was rated **3.2** on its approach.

- Instead of high pressure direct reaction and complicated chemical reactions, simple electrochemical reaction is one of the ideal methods to synthesize  $\text{AlH}_3$ .
- The project is an electrochemical approach to developing a rechargeable storage media (aluminum hydride) that has the potential for storing greater than 10 weight percent hydrogen.
- The system will be implemented off-board.

- Very clever approach to avoiding oxide formation by forming chloride protective layer
- Electrochemical recharging of Al offers an alternative method to regenerate  $\text{AlH}_3$  spent fuel
- Use of ionic solution electrolysis to form  $\text{AlH}_3$  is a significant improvement from past years efforts
- Experimental work is consistent with electrolysis technique.
- The calculation of energy consumption need to include energy required to recover  $\text{AlH}_3$  that dissolves in ether/THF.
- Electricity requirement to form  $\text{AlH}_3$  by electrolysis of  $\text{NaAlH}_4$  (8.44 kWh/kg  $\text{H}_2$  experiment, 5.66 kWh/kg  $\text{H}_2$  theoretical minimum) is significant. Regeneration by electrochemical means will not meet the DOE well to tank (WTT) efficiency target of 60 percent.
- Devising methods to electrochemically regenerate  $\text{AlH}_3$  and alkali metal alanates using nonaqueous electrolytes.
- Attempting to elucidate reaction mechanisms, and to calculate overall process yields, efficiencies, and alane/alanate production costs.
- Characterizing products of electrolysis tests.
- Technical work has been well focused on identifying and overcoming the initial barriers to electrochemical formation of alane. This reviewer is favorably impressed by the researchers' demonstrated ability to make advances in this complex and difficult system.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- $\text{AlH}_3$  was synthesized but it was mixed with raw material  $\text{NaAlH}_4$ . The hydrogen capacity of the product is about 9 percent. However, there is no direct evidence that  $\text{AlH}_3$  is clearly formed.
- Good progress demonstrating potential for over 8 weight percent system storage.
- Developed an understanding of optimal phase for alane.
- Focused in on appropriate solvent system and electrochemical parameters.
- Developed an understanding of the electrochemical cycle and identified reaction products.
- Developed an understanding of dendrite formation and how to avoid (using hydrogen overpressure).
- Demonstrated electrolytic alane formation in small quantities.
- New work using  $\text{NaAlH}_4$  solution electrolyte is a significant improvement over past years efforts.
- Have successfully demonstrated formation of  $\text{AlH}_3$  in  $\text{NaAlH}_4$  electrolyte, even though the rate and yield are still very modest.
- Despite the success with  $\text{NaAlH}_4$  electrolysis, unfortunately the WTT regeneration efficiency, even in the best case, has little chance of meeting the 60 percent target (electricity supply based on U.S. grid 2015).
- Demonstrated reversible alane formation and electrodeposition of  $\text{NaAlH}_4$ .
- Provided data that show the hydride production costs are in the range of DOE targets.
- Determined electrolyzer characteristics (e.g., electrode area) required to produce alane at meaningful rates.
- Good progress, within the tightly-defined scope. Investigators have identified "rate" as one critical barrier; using ether to dissolve and remove  $\text{AlH}_3$  is one improvement (although it makes removing the ether a necessary subsequent step). Formation of  $\text{Na}_3\text{AlH}_6$  may be another critical barrier; if so, the path to overcoming it is not presently clear. (Perhaps increasing amount of hydrogen available at cathode, to increase rate of capturing "Na" as  $\text{NaH}$ ?)
- Minimizing electrochemical overpotential will be important for energy efficiency, but this reviewer didn't see this topic mentioned.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.4** for technology transfer and collaboration.

- This is almost an independent project. There are other approaches to synthesize  $\text{AlH}_3$  which are being conducted by other members of Metal Hydride Center of Excellence.
- There is one university collaborator and no industry involvement.
- At this stage there seems to be little direct collaboration with industry, universities, or laboratories.

## HYDROGEN STORAGE

- This project is part of the Metal Hydride Center of Excellence but it is not clear how well integrated into the center of excellence it is at this time.
- Two partners are listed but it is not clear how these partners contributed to the work at Savannah River National Laboratory in fiscal year 2008.
- Collaboration does not appear to be a major component of project scope. If there were similar "electrochemical hydrogenation" needs elsewhere in the Hydrogen Program, collaboration with this team could be useful. The poster mentions partnerships with Brookhaven National Laboratory and Hawaii but not much about what these partnerships entail.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- The target reaction is not direct regeneration of  $\text{AlH}_3$  from spent Al but synthesis of  $\text{AlH}_3$  from alanate.
- Proposed future work focused on developing larger surface area electrode and use of catalysts to improve efficiency.
- Demonstration that larger surface area electrodes and catalysts can generate larger quantities of alane in larger electrochemical system.
- Will develop more efficient methods of extracting alane.
- The proposed future work to upgrade the electrochemical cell will accelerate the rate and increase yield.
- Working with other partners will be beneficial to the project.
- The proposed future plans build logically on what was done and what was learned in fiscal year 2008.
- Building and testing a larger electrolyzer is in the plan.
- Process optimization will be a major area of emphasis.
- So far, has been focused on "succeed or fail" with the  $\text{NaAlH}_4 + \text{Al} + \text{H}_2$  process. While the "scale-up" barrier to operating this process is likely to be overcome, the ultimate workability of alane is hard to predict.

### **Strengths and weaknesses**

#### Strengths

- To use electrochemical reaction to regenerate  $\text{AlH}_3$  is a good idea.
- Sound electrochemical principles. Electrochemistry allows excellent process control capability through the applied voltage.
- Low desorption temperature (60 to 175°C) partially within range of fuel cell waste heat.
- Good understanding of electrochemistry.
- Good experimental techniques.
- The results so far are encouraging.
- The hydrogen storage materials under study are among the more promising ones for meeting DOE hydrogen storage capacity targets.
- The system appears to have formidable experimental challenges. Progress to date appears good.

#### Weaknesses

- The reaction studied is not  $\text{AlH}_3$  regeneration from spent Al.
- Aqueous solution is electrolyzed if the voltage exceeds around 1.4 V considering the over potential.
- At present, hydrogen gas generated by electrolysis is the hydrogen source to regenerate  $\text{AlH}_3$  from alanate.
- Off-board regeneration creates potential infrastructure issues.
- Attention must be paid to organic solvent clean-up to avoid unwanted electrochemical reactions/system inefficiencies.
- Overpotential greatly decreases efficiency of process. Need to concentrate on ways to overcome through catalysts. With overpotential, the storage cost for hydrogen approaches that for liquefaction, which is a potential significant drawback
- Electricity cost used for the process (\$0.05/kWh) is not realistic in many parts of the country but could be achieved with nuclear.

- Regeneration of  $\text{AlH}_3$  using electrochemical recharging will have difficulty meeting the DOE target for WTT efficiency of 60 percent.
- There is little external collaboration.
- A state-of-the-art approach to electrochemical cell design and electrochemical measurement might produce results and understanding beyond what has been established in this project to date and should contribute to making the proposed "optimization" effort in the coming year more successful - systematic electrochemical engineering is required.
- It is questionable whether a process that requires both hydrogen and nontrivial electrical power can be practical on a large scale. If it could be operated so as to need only electrical power it might be more attractive. It would also help if there were more momentum in favor of widespread use of  $\text{AlH}_3$ .

#### **Specific recommendations and additions or deletions to the work scope**

- Proper non-aqueous and stable electrolyte should be selected for further work.
- Close contacts with other  $\text{AlH}_3$  regeneration people are strongly recommended.
- Get an industrial collaborator on board to evaluate potential for practical commercialization and costs.
- Accelerate understanding a choice of catalysts.
- Lifecycle systems costs should be examined, including cost of electricity to operate, solvent clean up, etc.
- Need to demonstrate more rapid alane formation rate using higher surface area materials. This should be a go/no-go in next year.
- Demonstrate electrolysis with  $\text{AlCl}_3$  solutions, the other ionic solution system proposed by the principal investigators.
- Calculate energy requirement to recover  $\text{AlH}_3$  from THF/ether.
- It would be good to show more comprehensive characterization results for the electrolysis products.
- Eventually, more detailed electrochemical measurements will be needed to elucidate electrode kinetics in a manner that defines the rate limiting electrode reaction (e.g., transient electrochemical measurements); such measurements can provide insights that aid the design and configuring of practical electrode arrays.
- There is considerable expertise and experience in the design of electrodes for continuous production of a solid deposit. Much has been published on this type of technology.

**Project # STP-20: LiMgN Sorption Kinetics and Solid State Hydride System Engineering for the MHCoe**  
*Don Anton; Savannah River National Laboratory*

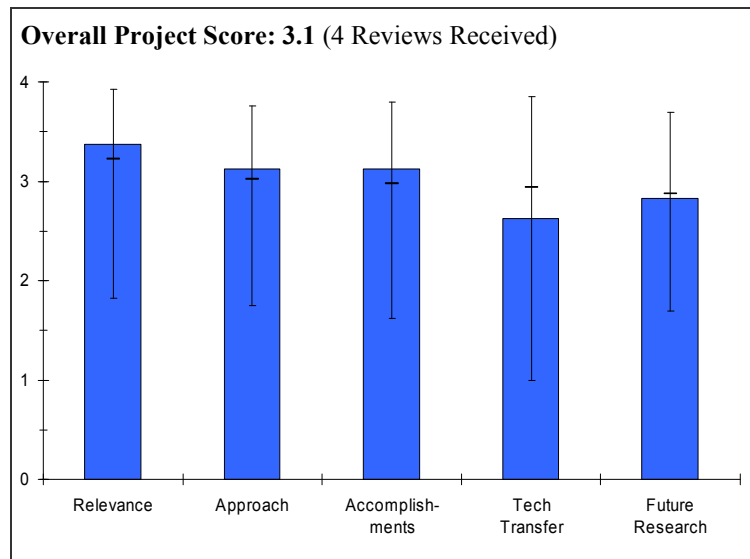
[NOTE: This project is part of the Metal Hydride Center of Excellence.]

**Brief Summary of Project**

The objectives of this project are to 1) determine heat management requirements for a refueling station based on metal hydrides; and 2) determine sorption kinetics for LiMgN. In 2008, the project will determine the hydrogen sorption kinetics and mechanisms of LiMgN over the temperature and pressure range of interest to DOE for automotive hydrogen storage applications.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.4** for its relevance to DOE objectives.



- Both efforts fit to the Department of Energy’s research and development objectives.
- The heating engineering aspects of the project seem more relevant to gas station aspects rather than vehicle aspects.
- The heat engineering work appears more relevant to the new Engineering Center of Excellence and one wonders why it is being pursued at this point in time.
- This project includes two distinctly different efforts of specific value to the Metal Hydride Center of Excellence. Both are aimed at DOE’s needs for the Hydrogen Fuel Initiative and DOE’s research and development objectives.
- The refueling station heat and mass analysis is critical to answer the question if three minute refueling can be accomplished and how much it will cost in terms of heat removal requirements and cooling costs.
- LiMgN is a new center of excellence material with potential to meet DOE weight and volume storage targets.
- The project will provide confirmation of center of excellence preliminary results by others and obtain required charging and discharging kinetics for future heat load studies needed to achieve the three-minute refueling target.
- Understanding cooling requirements of a fast fill with exothermic materials is important towards developing a material based storage technology for an automotive infrastructure. However the PI proposes nothing new that wasn't understood 5 yrs ago.

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- The approach of heat management is very reasonable even though heat management of refueling is only considered.
- The LiMgN study that just started is well organized.
- System analysis, especially from the view point of heat management, is very important to judge practicality and reality of hydrogen storage systems and infrastructure for them.
- This project appears to involve two disparate objectives, which have little interaction. The only thing that they have in common is that they are both engineering-related. That being said, the approach for each of the disparate activities is good.

- The refueling station was modeled in a relatively conventional way to provide useful insight into the massive reaction heat removal needed.
- The synthesis and kinetic work on LiMgN is routine and straightforward.
- Experimental details and planned kinetic parametric analysis are not clearly stated.
- It should be made clear that the kinetic studies on LiMgN will ultimately be used to address the three-minute on-board refueling target.
- PI used typical fueling station to provide model inputs. However, the PI only investigated using an evaporative cooler. Such systems were understood to be impractical due to size and water consumption many years ago- no new information was provided. A more interesting approach would have been investigating other heat sync such as metal hydride beds (as in metal hydride air conditioning systems) etc. An elegant solution to transferring such large amounts of heat must be realized for such systems. Evaporative cooling is not an elegant technique.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- Heat management has been well done.
- The results for LiMgN are preliminary.
- Real system image of infrastructure for hydrogen storage material tanks is very instructive for considering requirements for materials and tank designs.
- Why was LiMgN selected for investigation? Initial results show that its reversible capacity does not seem to be that high, the take-up/release temperatures are on the high side, and it appears to have cyclability problems.
- The heat engineering study has provided useful results for the cooling tower requirements that might be necessary at a hydrogen fueling station.
- The heat/mass transfer modeling work for the refueling has been completed, at least in a first cut. The results are useful in confirming the massive cooling water requirements and associated cooling system investments.
- The basic refueling plant requirements are defined. The bottom line is clear: the plant will work, but will be much larger than a gasoline plant.
- Preliminary LiMgN synthesis work has been reasonably successful.
- The cyclic work has not defined the pressure-temperature-time conditions for complete recharge yet.
- This calculation could be completed in one day by a talented heat exchange designer. Furthermore, a rough estimate could be completed in 15 minutes by almost any engineer sufficient to realize that such a technique for cooling is not feasible. This project should have investigated alternative approaches from the beginning.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.6** for technology transfer and collaboration.

- Input for heat management work has been done but the collaboration and technology transfer is not significant.
- Most of the collaborations are associated with the LiMgN work. No collaborations indicated for the service station work.
- Technology transfer and collaborations are limited to a few partners within the Metal Hydride Center of Excellence.
- Giving the “industrial” nature of the refilling station, an industrially experienced partner should have been included.
- Minimal interaction was required for this analysis. Results won't benefit forecourt designers since the results are self evident and don't provide novel insight to solving this heat rejection problem.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- The heat management work has been finished.

## HYDROGEN STORAGE

- The future plan of LiMgN is reasonable.
- The diameter of pipe to feed coolant to a hydrogen storage material tank should be also estimated.
- Identifying uses for the waste heat seems like the most important aspect for the heat engineering work.
- For the LiMgN, what is the plan for increasing the reversible hydrogen storage capacity?
- The refueling station work is to be continued, but the plan is vaguely focused.
- It is not clear why any further work is needed on the refueling at this time. The basics plant questions have been answered for now and it is probably more important to move toward heat/mass transfer studies of the on-board hydride tank itself.
- The future work on LiMgN seems logical, per se, but not detailed very well.
- Validation of data is always important. The question not clearly answered is to what extent the future work is confirmative in nature. Is similar work being done by others within the center of excellence?

### **Strengths and weaknesses**

#### Strengths

- In fact, engineering work has only been done in this project.
- None.
- The project has provided much needed information on the refueling plant design and heat requirements.
- Ad hoc work of engineering, validation and fine tuning should be useful to the center of excellence.
- A project which has the ability to respond to center of excellence needs not otherwise available has good value.

#### Weaknesses

- Only analysis for the heat management has been presented this year. Experimental work to develop total system and/or components of the systems is indispensable.
- Two disparate, non-interacting project activities are being pursued.
- It would seem that the real objective of this project is to enhance competitive posture for the new Engineering Center of Excellence.
- Proposed continuation of work on the refueling plant is doubtful and probably better placed into one of the analysis groups: TIAX or Argonne National Laboratory.
- The present and future LiMgN work is not clearly described: What exactly will be done and how will that generate the data that fits into the upcoming tank study?

### **Specific recommendations and additions or deletions to the work scope**

- The activities will be continued at the new Engineering Center of Excellence.
- Pick only one of these activities and concentrate on it.
- Delete any planned work on refueling plant modeling; transfer that to the established analysis groups.
- Set a quantitative go/no-go limit on the NH<sub>3</sub> level reductions of the exit hydrogen gas.

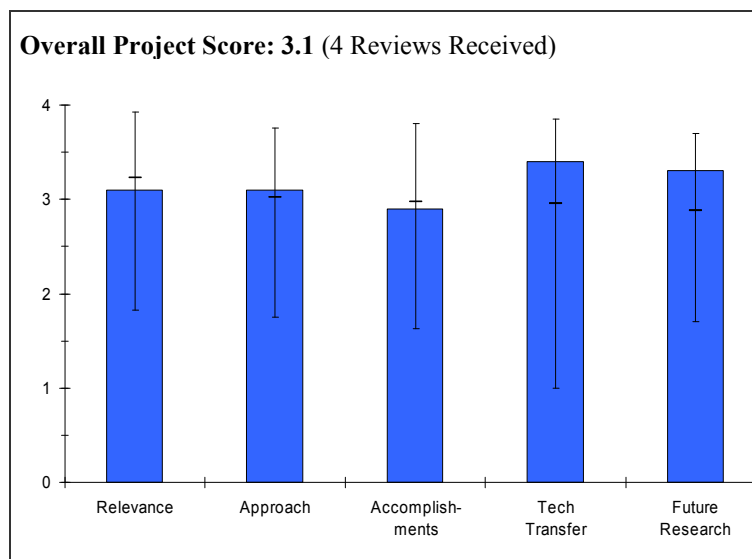
## Project # STP-21: Synthesis of Nanophase Materials for Thermodynamically Tuned Reversible Hydrogen Storage

Channing Ahn; California Institute of Technology

[NOTE: This project is part of the Metal Hydride Center of Excellence.]

### Brief Summary of Project

The objectives of this project are to 1) understand if thermodynamically tractable reactions based on hydride destabilization, that should be reversible but appear not to be, are kinetically limited; 2) enable short hydrogenation times associated with refueling, that will require short solid-state and gas-solid diffusion path lengths; 3) address the problems associated with large, light-metal-hydride enthalpies (hydrogen fueling/refueling temperatures) and develop strategies to address thermodynamic issues surrounding the use of these materials through hydride destabilization.; 4) understand issues related to grain growth and surface/interface energies, which are vital in order to understand the kinetics of hydrogenation/dehydrogenation reactions; and 5) follow up on previously studied reactions with phase identification via X-ray diffraction, nuclear magnetic resonance and transmission electron microscopy.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- The work is in line with the overall Department of Energy program objectives and of relevance for the attainment of research and development goals.
- Addresses some of the most challenging hydrogen storage targets for overcoming the barriers (B), (M), (N).
- There is a potential for high hydrogen storage capacity in mixed  $\text{LiBH}_4$  - other hydride systems.
- The project provides technical information on key aspects of some of the potential routes to high capacity hydrogen storage materials.
- Materials studied, in all cases, have the potential to reach DOE weight and volume objectives.
- The project focuses on fundamental mechanisms in relation to reversibility and kinetics.
- The project is relevant to DOE objectives, but not very quantitatively so.

### Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- This is a well-planned approach where material systems are chosen through theoretical screening by Metal Hydrides Center of Excellence partners and then predictions are checked in the laboratory.
- It explores the possibilities offered by the coupling of powerful experimental techniques.
- The project may be more sharply focused: either destabilized hydrides or Mg in aerogels.
- Concentrating on potentially reversible systems would improve the project quality.
- A sound approach of applying appropriate experimental studies to the key materials issues.
- There are two distinct experimental efforts to understand reaction mechanisms for materials generally derived from a priori predictive calculations. Both efforts involve nano-sized materials and both are valuable.
- One effort focuses nicely on the reaction pathways and reversibilities of destabilized mixtures.



## HYDROGEN STORAGE

- The second effort focuses nicely on infusing Mg into nanoporous carbon for potential thermodynamic improvements.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.9** based on accomplishments.

- Good screening of systems and progress towards objectives despite the not so encouraging results.
- In contrast to the calculated reaction enthalpies the large heats of formation of the reactant phases in the systems studied, are, as shown experimentally, still determining the overall kinetics. Additionally the formation of undesirable, stable intermediate phases are jeopardizing the reversibility of the system.
- The direct thermal decomposition reaction pathways are not easy to predict and overall there is still a strong need for understanding the reversibility mechanism.
- Interesting first results on the wettability of Mg in carbon aerogels and the effect of pore size on the reaction enthalpies. New avenues of investigation are now opening.
- Progress on  $\text{LiBH}_4$ -other hydride systems is good.
- Only overall reactions are shown. How about intermediaries? These may be extremely important in identifying rehydrogenation pathways.
- Confusing statements about  $\text{AlB}_2$ : it is shown as a final product, but x-ray powder diffraction data are inconclusive.
- The destabilizing effects of aluminum-containing species on  $\text{LiBH}_4$  are interesting.
- Perhaps understanding why liquid  $\text{LiBH}_4$  wets and infiltrates carbon aerogels so well might be useful in getting other species into the aerogel. What about Mg compounds or alloys with low sessile drop contact angles on graphite or graphene?
- Studies of the  $\text{ScH}_2$ - $\text{LiBH}_4$  destabilized mixture have shown it does not work nearly as well as predicted and why.
- The reversibility of  $\text{LiBH}_4$  was improved by mixture with  $\text{AlH}_3$  or  $\text{Ca}(\text{AlH}_4)_2$ . A potentially useful new Al "catalyst" effect was discovered.
- Progress was made on techniques to infuse Mg into carbon aerogels.
- Unfortunately, the principal investigator has not projected his new and interesting fundamental understandings of the materials studied toward the best paths forward to achieving the weight, volume and rate improvements needed for reaching DOE needs.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.4** for technology transfer and collaboration.

- Good collaboration record involving a number of laboratories and partners with diverse expertise.
- Not entirely clear if the experimental findings are effectively incorporated by the theorists for fine-tuning their models.
- Collaborations with others appear to be excellent.
- Systems being studied are identified by the Metal Hydride Center of Excellence theorists.
- Good collaboration with aerogel synthesizers.
- There are several good collaborations within the Metal Hydride Center of Excellence.
- With more transfer of information back to the partners, this can develop into a good example of the value of the center of excellence concept.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.3** for proposed future work.

- The project's future plans are logical, reasonable, building up on past experience and moving the research forward. Probably a bit ambitious given the resources available.
- There is some lack of focus. I believe that future work is too vaguely defined.

- Most of the future work appears to concentrate on carbon aerogels, rather than on systems that could destabilize  $\text{LiBH}_4$ .
- Future work should include further studies of the effects of aluminum on the stability of  $\text{LiBH}_4$ , particularly as to mechanisms of beneficial results.
- The proposed future work is reasonable.

### **Strengths and weaknesses**

#### Strengths

- An enthusiastic team with access to powerful characterization tools.
- Exploring collaboration possibilities with the other Metal Hydride Center of Excellence partners and particularly with the theory group.
- Using a variety of characterization techniques.
- Potentially very high hydrogen capacity materials are under study.
- Excellent knowledge of and experience with carbon materials.
- The principal investigator and his personnel have excellent abilities to do nice, potentially very useful, fundamental work.

#### Weaknesses

- Investigating systems which may not meet the targets - reversibility, kinetics are limited.
- It is not clear whether the experimental findings are fed back to the theorists for fine tuning their prediction models.
- Relevance of work with Mg in aerogels to future work with "hydrides" is unclear.
- Hydrides may be difficult to impregnate into aerogels using thermal methods/
- None.
- It does not seem to be converting mechanistic results into suggested directions to the rest of the center of excellence for moving these materials toward the meeting of DOE goals and targets.

### **Specific recommendations and additions or deletions to the work scope**

- Future plans may be ambitious given the resources available. Could consider to reprioritizing future activities and focus on the few tasks of utmost importance, based on the findings of the rest of the Metal Hydride Center of Excellence groups.
- Keep the communication channels with the theorists open and encourage the feedback of the experimental findings to the models.
- Could benefit from a closer cross-center of excellence interaction with the Sorbents on the aerogels work.
- Concentrate on the reversibility of  $\text{AlH}_3$  -  $\text{LiBH}_4$  system.
- Look into other sources of Al (beyond  $\text{AlH}_3$ ) leading to effective destabilization of  $\text{LiBH}_4$  and potential reversibility.
- Work with aerogels adds little to none, so it may be discontinued to better use available resources.
- Keep the focus on just a few key aspects identified by other members of the Metal Hydride Center of Excellence. Don't get too overextended.

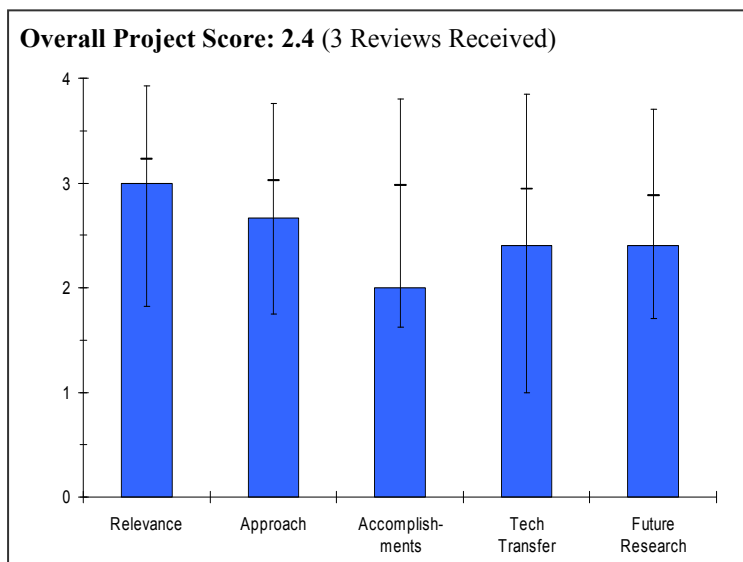
**Project # STP-24: Center for Hydrogen Storage Research at Delaware State University**

*Andrew Goudy; Delaware State University*

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

The overall objective for this project is to establish a Center for Hydrogen Storage Research at Delaware State University for the preparation and characterization of selected complex metal hydrides and the determination their suitability for hydrogen storage. The 2007 objectives are to 1) identify the most promising types of destabilized hydrides and demonstrate the optimum temperature/pressure range and sorption kinetics of the hydrides under a variety of conditions; and 2) determine their cyclic stability and develop improved sorption catalysts. The 2008 objectives are to 1) extend the studies to include other complex hydrides that have greater hydrogen storage potential than the destabilized hydrides, such as ternary borohydride systems; and 2) perform kinetic modeling studies and develop methods for improving kinetics and lowering reaction temperatures.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.0** for its relevance to DOE objectives.

- The project supports the President's Hydrogen Fuel Initiative.
- One of the objectives of the project, to establish a center for hydrogen storage research at Delaware State University for preparation/characterization of hydrides, was met.
- The identification of potential complex hydrides with improved kinetics and a lower reaction temperature are not satisfactory.
- The project is focused on high capacity LiBH<sub>4</sub>/CaH<sub>2</sub> systems.

**Question 2: Approach to performing the research and development**

This project was rated **2.7** on its approach.

- The technical approach is well designed.
- Technical barriers are not addressed to overcome.
- The research and development efforts are not well integrated.
- Weaknesses are described below.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.0** based on accomplishments.

- Results are presented without much insight.
- Publications and presentations are very poor. There was only one presentation at the Materials Research Society meeting in November 2007.

- Technical accomplishments are quite modest. A few "additives" have been examined by using thermogravimetric analysis, but none show improved reversibility or improved capacity.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.4** for technology transfer and collaboration.

- Collaborations are limited in scale.
- Collaborative relationships with other teams/investigators are non obvious.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.4** for proposed future work.

- The proposed future research approach is not addressed adequately based on the results of other Department of Energy projects.
- The approach to future research needs to consider contingencies.
- Future work is vaguely defined. It is unclear how and why future research will lead to meeting DOE objectives.

**Strengths and weaknesses**

Strengths

- The principal investigator has been involved in hydrogen storage activities for a long time.
- Kinetic modeling is a plus.

Weaknesses

- There is a lack of alignment between the project approach and the DOE goals.
- The project is trailing.
- The provided thermogravimetric analysis data appear to be unreliable.
- The future work is poorly defined. (It is extremely vague and unclear whether it can be accomplished, especially the first two listed goals).
- Due to loss of some B<sub>2</sub>H<sub>6</sub>, cyclic stability should be continuously deteriorating and low.
- No attempt to understand why the addition of LiNH<sub>2</sub> to an apparently reversible CaH<sub>2</sub>/LiBH<sub>4</sub> system suppresses reversibility. Is it due to a formation of a stable nitride? Are there other reasons?
- It appears that there is no systematic approach.

**Specific recommendations and additions or deletions to the work scope**

- The approach needs to be realigned with DOE program goals. For example, a storage system that requires 300-500°C for hydrogen release with say approximately 5 to 9 weight percent should be quickly reviewed and dismissed as it will not meet the 2010 overall system goals.
- In deciding on an alternate storage material, one has to consider the end-use system design and functionality. This needs to be shown in the approach.
- Based on the project management plan, the principal investigator is capable but needs to put more effort into the project.
- Given the current status of the project, it is difficult to suggest any meaningful additions/deletions.

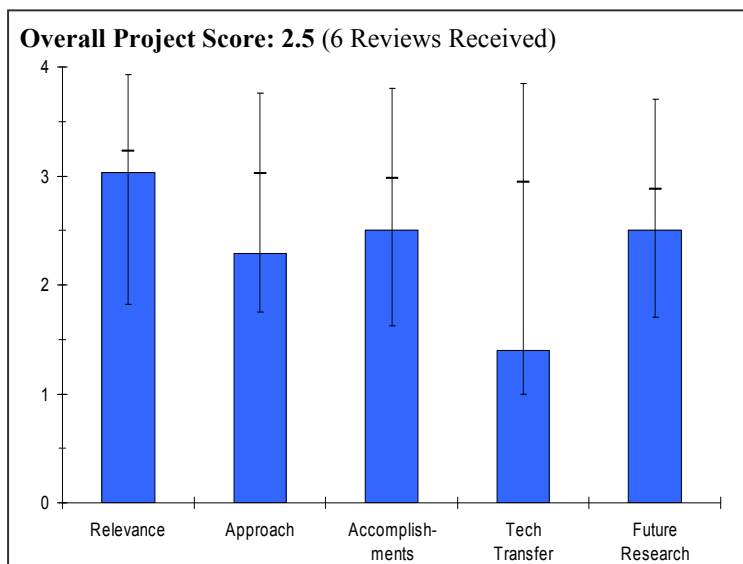
**Project # STP-26: Novel Metal Perhydrides**

*Jim Hwang; Michigan Tech University*

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

The overall focus of this project is to: 1) develop new kinds of materials that are able to bind hydrogen molecules into clusters; and 2) enhance hydrogen adsorption/desorption by means of hydrogen cluster formation/decomposition so that the capacity of materials for hydrogen storage and the kinetics for hydrogen release have the potential to meet the DOE 2010 and 2015 targets. The objective over the past year was to 1) study the potentials and roles of charged/polarized species on hydrogen cluster formation; and 2) examine the interaction behavior of charged species with hydrogen.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.0** for its relevance to DOE objectives.

- This project addresses hydrogen storage capacity and adsorption and desorption using a unique approach.
- The project addresses relevant goals.
- This is an exceptionally creative idea that is worth evaluating.
- If successful, a totally new mechanism for controlled hydrogen uptake and release will be available.
- High relevance to programmatic goals.
- The concept of charge-induced hydrogen cluster formation has a lot of question based on scientific fundamentals.
- Achieving the President's Hydrogen Fuel Initiative goals seem remote.
- While apparently aligned, it seems exceedingly unlikely that this method can actually work. Therefore it is not really aligned because the money spent here could better be spent on other aligned work.
- The project addresses relevant goals.
- The project supports a major research need for the Hydrogen Fuel Initiative – on-board storage with sufficient volumetric capacity.
- This is an interesting novel concept at the university exploratory research scale.
- Meeting the 2010 target by 2010 will be a challenge based on the technical status. (The principal investigator is optimistic.)
- The 2015 goal should probably be addressed.

**Question 2: Approach to performing the research and development**

This project was rated **2.3** on its approach.

- Novel approach to hydrogen storage looking at hydrogen adsorption by charged species.
- Calculations of cation perhydrides show promise for this type of material, but not sure how the systems looked at can be approached experimentally without forming some stable metal hydrides. The alkaline earths all form fairly stable hydrides.

- It is not clear from calculations and discussions whether the calculations are performed on isolated cations and anions, or if the conditions simulate cations and anions in a crystal structure, with limited space and geometry for hydrogen molecules in the crystal and additional interactions from neighboring ions.
- There is not much in the way of precedent to support (or not support) the concept.
- There is a potentially supportive mix of density functional theory calculations on molecular metal hydrides and experimental "electrochemical" data.
- It is unclear if the molecular model systems that have been calculated are a reasonable model of the hydrided surfaces that are sought. Given that the rationale for the project is based on the calculations, it is critical to know if the models employed are valid.
- Dissociative adsorption of hydrogen on metal surfaces is well documented, but not considered in this study.
- Presently the electrochemical studies (which are only recently initiated) only monitor electrode potential. Current is not monitored and no surface sensitive techniques are employed to establish the molecular nature of the process(es) being observed. This represents a major weakness of the study.
- The approach to investigate change-induced hydrogen cluster formation is not based on good fundamentals.
- This is unlikely to contribute to overcoming the barriers.
- The approach puts off testing the least probable portions to the end when the money is all spent.
- The use of theory and experiment together is good, but here the theory is not getting any feedback and so it is entirely unchecked for accuracy.
- It is not at all clear that the team has any real idea of the possible storage of the system. They could not clearly tell what the surface to mass ratio was nor the amount of hydrogen on the surface. Nor did they seem able to say if or how much hydrogen would go into the bulk.
- Novel approach to hydrogen storage looking at hydrogen adsorption by charged species.
- The principal investigator is cognizant of the technical barriers that need to be met. The project is focused on addressing feasibility of the concept followed by addressing the technical barriers.
- This is in the exploratory phase of research. The approach is to explore and validate the adsorption and desorption of clusters of hydrogen on anode and cathode materials using an external voltage source, and to evaluate performance of materials screened by computational chemistry. Solid materials will also be included in the hydrogen space between the electrodes.
- External voltage source would be supplied by battery.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.5** based on accomplishments.

- The project looked at the effects of hydrogen pressure on potential but did not measure any hydrogen adsorption in electrodes as a function of applied voltage. Hydrogen uptake needs to be measured directly to determine if there is any, not changes in potential versus a vacuum which could be affected by very small surface adsorption.
- Hydrogen bonding capacities in the cluster calculations appear to be for isolated charged species. Future calculations should look at larger clusters and include interactions with surrounding cations, anions and neutral metal atoms.
- The project has only had serious funding for about one year according to the presenter. Thus, accomplishments must be evaluated in light of the financial limits that have been placed on the project. (But, this comment appears inconsistent with the funding data provided.)
- Laboratory results are very preliminary.
- Two accomplishments exist: 1) density functional theory calculations on molecular hydride models (of questionable value since it is unclear if the systems selected represents what realistically might occur on a metal surface); and 2) Construction and preliminary testing of a capacitive charge/discharge cell to test the hydrogen uptake concept.
- The two noted tasks do not prove (or disprove) the concept at this point.
- Based on computational screening, a number of promising candidates were selected.
- The results are confusing.
- Publications are limited to the proposed work.
- Theory states these materials can be made and will store hydrogen, but at present there is no reason to trust or distrust this theory as there is no confirmation.

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- Did not have a very clear explanation of data, nor had they tested for other explanations of the voltage drops.
- Looked at effects of hydrogen pressure on potential but did not measure any hydrogen adsorption in electrodes as a function of applied voltage. Need to measure hydrogen uptake directly to determine if there is any, not changes in potential versus a vacuum which could be affected by very small surface adsorption.
- Hydrogen bonding capacities in the cluster calculations are for charged species which cannot exist in isolation apart from an anionic species.
- Phase 1 is scheduled for five years - with completion stated at 50 percent. (No performance schedule is shown with subtasks.)
- Computational analysis was accomplished for screening materials for anodes and cathods. Conducted initial tests for adsorption and desorption.
- Now planning concurrent electric polarization and hydrogen sorption reactor and new electrode structures to increase hydrogen storage.
- Progress appears to be moderate and meant to be addressing barriers.
- It is too early in research to really address the possibility of meeting the key challenges as identified by the performer (cost, weight and volume, and efficiency).

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **1.4** for technology transfer and collaboration.

- Collaborations are not apparent.
- Nature of the collaboration is unclear.
- Given the state of the project, a consideration of technology transfer is premature.
- Collaborations are mentioned but seem limited.
- There are no clear beneficial interactions.
- Collaborations are not apparent.
- The role of collaborators is to provide materials for testing and evaluation.
- There is no technology transfer collaboration as of this time.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.5** for proposed future work.

- Proposed future work involves experiments to perform needed adsorption measurements.
- Proposal to add pressure change detection to the capacitive cell is important.
- Proposal to add surface analysis is important. (But what analytical techniques will be used?)
- Ideas about adding a "contaminating" gas phase species does not seem to be sound.
- Independent of the calculation results, the reaction of hydrogen with a metal oxide species will likely lead to the formation of metal + water (smelting) not hydrogen storage. This is a not a high probability research track.
- The approach is fundamentally not good.
- Appropriate if and only if they show that the current results mean what they think they do.
- Proposed future work involves experiments to perform needed adsorption measurements.
- The future experimentation will continue to conduct work to achieve an exploratory basis for this novel idea.
- Investigate the effects of applied electric potential on hydrogen adsorption and verify the charge induced hydrogen adsorption/desorption process using a dedicated instrument that is able to measure hydrogen sorption in the hydrogen filled electrode reactor.
- Develop electrodes with large surface area and study the adsorption/desorption enhancement effect.
- Further study the adsorption/desorption enhancement effects of applied voltage and hydrogen pressure, and explore the optimization approaches.
- Examine the adsorption/desorption enhancement effects of different electrode materials (starting from the metals explored by computer calculation), and screen the best candidates.
- Investigate the hydrogen adsorption capability of materials with naturally polar bonds directed by computer simulation, including the exploring of the following material compounds: BeO, Cr<sub>2</sub>O<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub>, NiO, and CoO.

- Investigate the hydrogen adsorption capability of materials being electrically polarized, materials being explored will include: a) Inorganic ferromaterials, b) Organic ferromaterials, and c) Other materials having charge carriers that can be electrically separated. Materials will be placed in the hydrogen space between the electrodes.

### **Strengths and weaknesses**

#### Strengths

- This is a novel idea
- Some calculation support is provided.
- Reasonable progress over the past year.
- This is a good group of people to address the problem.
- Unique, certainly not just what everyone is doing.
- Unique, exploratory research to investigate the potential and roles of charged/polarized species to form hydrogen clusters - to thereby store significant quantities of hydrogen. The hydrogen would be adsorbed by electric charge and desorbed with the removal of the charge.
- The project has utilized computational chemistry to screen potential material for forming hydrogen clusters.
- Early experimental data shows that the concept may be feasible.
- The goal is to achieve storage capacity of greater than 0.06 Kg H<sub>2</sub>/Kg storage system - the Department of Energy 2010 target.
- The principal investigator is competent and knowledgeable, confident of making progress.

#### Weaknesses

- Lacking measurements showing proof-of-principal.
- No evidence has been obtained that hydrogen uptake or discharge is occurring in the target systems.
- No surface characterization studies are presently in place to demonstrate whether or not hydrogen is interacting with the electrode surfaces and whether or not an observed interaction is consistent with the model systems selected.
- The proposed chemistry is not well-supported by known coordination chemistry.
- The observation of a voltage variation is not proof that hydrogen is being absorbed or desorbed by the system.
- Scientifically weak approach.
- The key problems regarding whether this material be made are not being addressed
- Other interpretations of the data are not being looked at, which is indirect evidence, not direct evidence. This is a major concern.
- Lacking measurements showing proof-of-principal.
- This project needs significant additional information to show the feasibility and to provide a workable concept for use.
- Defining costs for this storage approach will need the additional information.
- Meeting the 2010 Department of Energy target by 2010 seems aggressive overall.

### **Specific recommendations and additions or deletions to the work scope**

- Continue the work, but focus strongly on determining if hydrogen uptake/release is occurring via a direct measurement (such as pressure swing or IR spectroscopy).
- If hydrogen uptake can be demonstrated (hopefully quickly) then the amount of uptake must be determined.
- Given the accomplishments of points one and two, analytical studies of the surface hydride structure will be important. This will then validate the density functional theory model(s) employed or suggest new models.
- The program needs to prove its assertion and calculate the storage that might be truly possible, not just a proposed stoichiometry.
- No recommendations are made.



**Project # STP-27: Glass Microspheres for Hydrogen Storage**

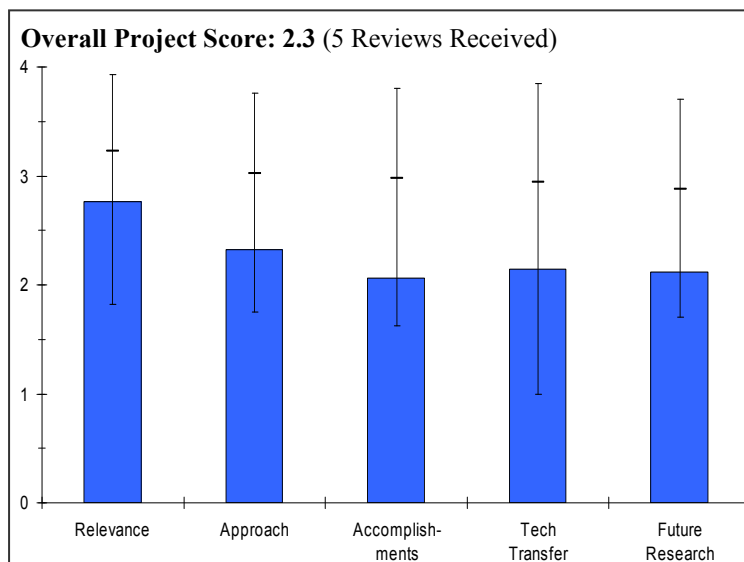
*Jim Shelby; Alfred University*

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

The objectives for this program are to: 1) demonstrate that hydrogen storage in hollow glass microspheres is a viable, safe method to meet DOE’s hydrogen storage targets; 2) prove that photo-induced hydrogen diffusion results in rapid release of hydrogen on command; and 3) optimize the composition of the glass used to produce hollow glass microspheres for hydrogen storage for maximum crush strength (maximize fill pressure) and minimum reaction time for response to changes in light intensity.

**Question 1: Relevance to overall DOE objectives**



This project earned a score of **2.8** for its relevance to DOE objectives.

- Project partially supports Hydrogen storage goals and vision, unlikely to meet the Department of Energy’s research and development objectives.
- Hydrogen capacity must be shown as favorable to meeting DOE targets.
- This project addresses the DOE programmatic goal of developing a solid state hydrogen storage system to meet 2010 target of 6 weight percent on-board storage.
- This project partially supports the hydrogen storage goals and vision, but it is unlikely to meet DOE research and development objectives.
- This project addresses a key barrier - weight percent of hydrogen storage.
- This project does not adequately address hydrogen storage volumetric density.
- The project has the capability to address cost, but has not yet addressed it.
- The project is addressing durability and operability.

**Question 2: Approach to performing the research and development**

This project was rated **2.3** on its approach.

- This is a well studied approach for storing hydrogen that is unlikely to meet the technical targets for volumetric storage density.
- The approach appears to be unable to meet 2015 gravimetric storage goals at reasonable pressures.
- The study does not appear to be focusing on the relevant issues such as maximum fill pressure of microspheres, optimal sphere diameters and thicknesses, maximizing packing densities, etc. that would maximize storage densities.
- Studies of photo-release of hydrogen do not appear to be addressing mechanism of release, and it is likely release is due to heating of the microspheres. Mechanism of release and things like the extinction coefficients, will determine what size container this type of activation would be effective in. If the distance it is effective over is too short (due to all the light being absorbed or scattered) it will not be useful.
- Other organizations have looked at hydrogen storage via microspheres.
- The project is focused on developing hydrogen storage system using hollow glass microspheres. Several previous investigations have focused on similar systems (without much success).

- The approach is to develop a more rapid method for hydrogen release (photo-induced) and optimize dopants.
- Hollow glass microspheres (HGMS) materials are commercially available, which is an advantage.
- With only 2.2 weight percent (materials only) demonstrated, it is quite a stretch to see how this approach can reach the desired goal of greater than 10 weight percent materials only (necessary to meet 6 weight percent system goal).
- Their approach is based on material weight percent rather than system weight percent. Why?
- The low pressure work is a good screening tool.
- They recognize the importance of size distribution of microspheres.
- Their Phase I/Phase II approach is logical in leading to pressure limits/scale up.
- The length of the project seems rather long, with Phase II lasting an additional four years to get to a working demonstration.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.1** based on accomplishments.

- Made some progress in increasing kinetics of release over thermally activated glass microspheres.
- Progress in demonstrating gravimetric storage density improvements are slow – only 2 weight percent has been achieved. The plan to use 10,000 psi should only lead to a gain of a factor of two; other plans to reach the target were not apparent.
- Progress appears to be very slow. Very low hydrogen capacity has been demonstrated.
- After over three years, only ~ 2 weight percent hydrogen capacities has been demonstrated, indicating it is probably impossible to reach DOE system capacity requirements.
- No spheres have been filled, to date, to 10,000 psi as proposed in project objectives.
- The author presents interesting results for a 5 weight percent CoO doped system with finely divided particles that has rapid hydrogen release rates.
- The mechanisms for photo-induced hydrogen release are not known; no appreciable heating of system was measured.
- Demonstrated fill of microsphere at 5000 psi; 10,000 fill is in progress.
- Demonstrated the ability to obtain 2.2 weight percent hydrogen in HGMS system.
- Narrowed the wavelength region of interest for the photo-induced effect to 1500-2300 nm to see an effect.
- Made some progress in increasing kinetics of release over that of thermally activated glass microspheres.
- They have shown no data that indicate they are reaching the weight targets - especially system weight percent.
- They need to show/produce more data on the effect of type of glass.
- They need to show the effect of hydrogen cycling on capacity.
- Good comparison of dopants.
- They are seriously compromised by the high pressure filling process. They need to better coordinate with Savannah River National Laboratory (SRNL) for the high pressure fill HGMS work.
- They make a statement about the wavelength of light to be used to facilitate the hydrogen diffusion process, but show no data. I would think that the wavelengths used would be more dependent on the type of glass.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.1** for technology transfer and collaboration.

- Collaborations to get microspheres filled to higher pressures are not smooth- delays in getting work done
- Other collaborations are not outlined.
- SRNL has been a partner in this project - but it is not clear what contributions SRNL has made to the accomplishment achieved thus far.
- Commercialization pathway is not clear.
- Collaborations to get microspheres filled to higher pressures are not smooth – there are delays in getting work done.
- Other collaborations are not outlined.

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- The coordination with SRNL seems to be a major stumbling block in getting high-pressure fills accomplished and staying on some kind of schedule.
- Appears to be good coordination with Mo-Sci for development of glass microspheres.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.1** for proposed future work.

- Plans do not address a path to meet or address volumetric storage targets.
- Develop an understanding of photo-induced effect is a logical goal.
- Develop a working prototype is a desired goal.
- There is no clear off-ramp decision point in case storage weight percent cannot be increased to more applicable levels.
- Plans do not address a path to meet or address volumetric storage targets.
- They will be addressing some key needs: glass optimization, other dopants, and fill pressure vs. microsphere survival.
- Fill temperature study must include a reality check. That is, refueling at non-ambient conditions may not be practical, and data gathered at these temperatures may not be relevant.
- Doubling the storage capacity will still leave the system short of targets.
- This project is facing a near-term go/no-go decision to proceed to Phase II. Phase II plans seem to address project objectives that should have been demonstrated in Phase I.

### **Strengths and weaknesses**

#### Strengths

- Demonstrated much more rapid photo-induced hydrogen release rates than from purely thermal.
- Discovery of optimal dopants is quite useful.
- Can use as a base for conventional materials that are sold commercially. The materials are durable and inexpensive.
- The method allows very good control over hydrogen release rates.
- This is a new twist (photo-induced hydrogen diffusion) on an old concept (glass microspheres) that had more or less been discarded years ago.

#### Weaknesses

- The system will not meet volumetric storage targets.
- The approach does not seem viable to achieve DOE performance targets.
- It is very difficult to determine the hydrogen storage capacity of materials as the researcher is supplied the materials pre-charged; they do not have control over this part of the experiments.
- The very low current status of hydrogen storage capacity (2.2 weight percent materials only) does not bode well for more significant storage. This value is way below all other storage technologies.
- It is not clear that storage is linearly related to fill pressure; that is if double pressure to 10,000 psi will get 4.4 weight percent.
- The potential complexity and cost of the system (with flash lamps uniformly "bathing" materials stored) is in question.
- Need to cool the system and fill at high pressure (e.g., 10,000 psi) for a realistic system.
- The system will not meet volumetric storage targets.
- The length of time needed to perform hydrogen fills (due to transport and scheduling) is unacceptable.
- The amount of data gathered in key areas (weight percent hydrogen storage, ability to cycle hydrogen, rate of hydrogen take up and release) is not commensurate with the length of time this project has been ongoing.

### **Specific recommendations and additions or deletions to the work scope**

- Accelerate discovery of a mechanism for photo-induced hydrogen release – do this in the next year.
- Accelerate development of a working prototype, cut time to two years.
- Off ramp if cannot show at least 6 weight percent hydrogen storage in the next year.

- Develop a strict schedule for getting high pressure hydrogen into spheres at SRNL.
- Develop a plan to study high pressure cycling of hydrogen - this is the key real-world data needed.
- Recommend no-go at the end of Phase II.

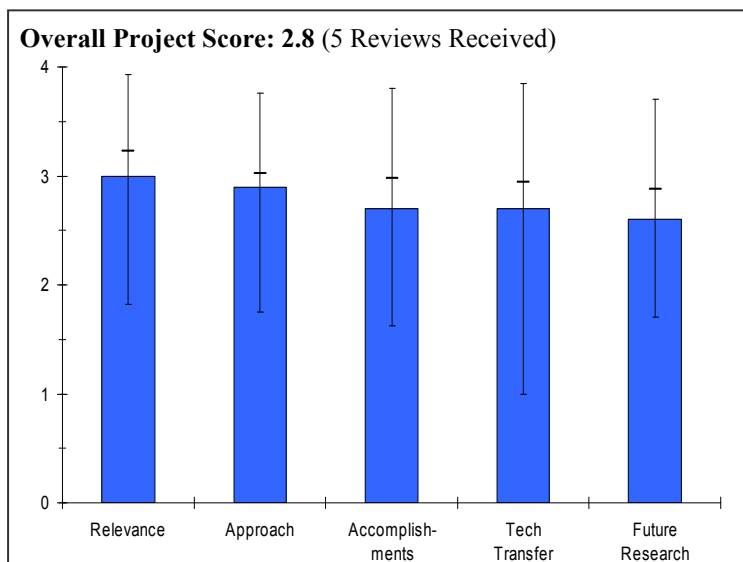
**Project # STP-28: Electron-Charged Graphite-Based Hydrogen Storage Material**

*Chinbay Fan; Gas Technology Institute*

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

The overall objective of the project is to develop a hydrogen storage material and device for hydrogen quick charge and discharge, high wt% and vol% storage capacities, good durability over many cycles, and safe handling and transport. Objectives for 2007 are to 1) select and synthesize carbon-based materials; 2) test and evaluate cycles for hydrogen storage; and 3) test external electron charge effect on hydrogen storage capacities. Objectives for 2008 are to 1) combine internal electron-charge (doping) and external charge to increase hydrogen storage capacities; and 2) investigate performance optimization and prototype container systems.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.0** for its relevance to DOE objectives.

- The project objectives are aligned with Department of Energy research and development objectives.
- Introducing electron charge on sorbent is one of the critical factors to improve the hydrogen uptake.
- The overall program objective is to develop a hydrogen storage material and device for hydrogen to quickly charge and discharge with high weight percent and volume percent storage capacities.
- The program is highly relevant to the President's Hydrogen Fuel Initiative.
- It has been clear for some time that carbon can only adsorb modest amounts of hydrogen compared to the targets for on-board storage. The results now available from this project show that the concept of internal doping and/or external means to result in a surface charge on the carbon can increase the amount of hydrogen adsorbed but the results are still far from the DOE targets. It appears unlikely that this approach can ever meet the DOE targets.
- Good emphasis on room temperature hydrogen storage.
- The project generally addresses DOE target and technical barriers.
- No quantitative discussion is made of volumetric capacity.

**Question 2: Approach to performing the research and development**

This project was rated **2.9** on its approach.

- The principal investigator did not show how much hydrogen uptake is expected through theoretical calculation.
- An optimized experimental design of electron charged sorbent materials should be guided by theory.
- The hydrogen storage is based on hydrogen adsorption with electron shift (physisorption) and electron transfer (chemisorption). The approach uses external electron charge to increase hydrogen adsorption and change hydrogen desorption kinetics. The approach also uses internal electron-rich or poor materials to change carbon-based material surface electron density affects hydrogen storage.
- The technical approaches and concepts are an excellent and novel idea. The carbon materials are very cheap.
- Good science and experimental approaches are utilized in this project to study the impact of electron charging carbon to improve hydrogen adsorption.

- Other researchers have shown 7 weight percent hydrogen at room temperature on a carbon doped with Li, but the system loses its ability to absorb much hydrogen after only a few cycles. Gas Technology Institute (GTI) hopes that doping with a metal in combination with its approach of charging the carbon may yield good results. Based on the GTI data presented in combination with other results from metal hydride and carbon systems, the probability of meeting the DOE storage targets is very low with this approach.
- The system needed to charge the carbon with an external device may prove impractical and/or too costly for on-board storage.
- The project seems a bit weak on the theory of electric field and electrical charge effects on hydrogen storage.
- The approach, namely to control hydrogen physisorption properties of carbon by internal and external electron charges, is not very well explained, a priori. There should be some better physics discussed in order to justify the potential of the approach.
- It is not made clear how the external charge approach, if successful, can be practically applied to vehicle storage. What will the real tank look like and how will it be controlled.
- The concept seems interesting and different, but there seems to be more hand waving than solid physics.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- The principal investigator has demonstrated a modest progress on overcoming the barriers.
- There is not enough data to demonstrate the relationship between surface area, pore size, electron charge, and hydrogen uptake.
- Some of the measured hydrogen uptake improvements (such as 1.185% to 1.476%) are within experimental noise.
- The isotherm of hydrogen uptake should include both adsorption and desorption.
- The hydrogen storage capacity is significantly improved by using charge control agent.
- Partnered with industrial (Superior Graphite Company) and academic (State University of New York at Syracuse and University of Houston) to improve hydrogen capacity with carbon materials.
- Good progress was made. Dopants, different carbons, and external charging were all carefully examined with good repeatable data obtained.
- The project did demonstrate an improvement in hydrogen adsorption with an internal charge control agent and with an external charging approach. However, the improvement still left this system far from the DOE storage targets.
- 1.5 weight percent hydrogen storage demonstrated at room temperature with the charge control agent. But what is the desorption temperature?
- Results with the charge control agent might be indicative of possible interesting capacitive charging effects on hydrogen storage.
- An external electric field appears to have relatively little effect on room temperature hydrogen storage.
- The project is apparently well behind schedule. Although 75 percent of the project time frame has passed, the principal investigator lists it as only 15 percent complete.
- The experimental results so far show only minor improvements, arguably within batch-to-batch and experimental scatter.
- The H-capacity increases shown to date are less than the 50 to 100 percent required to pass the upcoming DOE go/no-go gate.
- Technical details are sometimes withheld, such as the composition of the charge control agent added.
- Based on the results so far, this project offers little hope for meeting DOE targets.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.7** for technology transfer and collaboration.

- The principal investigator did not demonstrate a close coordination with theory group that might play a critical role in this technology.

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- The experimental results need to be verified with large sample size when the higher hydrogen uptake is within experimental noise.
- Cooperation with universities and industries are excellent.
- Carbon materials are supported and modified from partners; the technology is easily transferred to industrial company or universities.
- There appears to be only a very modest amount of collaboration and technology transfer with the State University of New York, ATMI, the University of Houston, and a Japanese company.
- Effective interactions with a Japanese company to identify a charge control agent and with the State University of New York on a high surface area carbon material.
- A few industrial and academic collaborators are listed.
- The exact roles of the collaborations are not very clearly stated.
- The names of two collaborators are kept secret: The charge control agent was "obtained from a Japanese company." "High surface area carbon from a partner."

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.6** for proposed future work.

- The hydrogen uptake measurement based on larger sample size (10-20 g) should be considered in future research plans to address the measurement noise issue.
- The lower-than-room-temperature measurement should be included in future research plans.
- The future work is clearly stated in the slides and directions are excellent.
- Investigate the electron charge effect on different hydrogen storage materials are very important.
- There is nothing in the Future Work Plan nor the data presented that suggests this approach has any reasonable chance of achieving the on-board storage targets.
- The future work seems somewhat vague on strategies to increase the room temperature hydrogen storage capacity.
- Future work plans are vague and rather qualitative.

### **Strengths and weaknesses**

#### Strengths

- The concept is well-aligned with DOE Hydrogen Program objectives and some of the results will help in understanding the relationship between surface charge and improved hydrogen uptake.
- Carbon materials are very cheap and easily prepared compared to most alloyed materials for hydrogen storage.
- The concept and idea are novel.
- Good science and experimental approaches were utilized in this project to study the impact of electron charging carbon to improve hydrogen adsorption.
- Innovative approach. This is an area of hydrogen storage that has not been studied a great deal.
- It offers a different idea that was worth trying.

#### Weaknesses

- Lack of theory guided experimental design.
- It has been clear for some time that carbon can only adsorb modest amounts of hydrogen compared to the targets for on-board storage. The results now available from this project show that the concept of internal doping and/or external means to result in a surface charge on the carbon can increase the amount of hydrogen adsorbed but the results are still far from the DOE targets. It appears unlikely that this approach can ever meet the DOE targets.
- Lack of theoretical guidance.
- The project has not kept to the schedule.
- The physics behind the idea are not clear and convincing.
- The results obtained so far do not look promising.

**Specific recommendations and additions or deletions to the work scope**

- Send samples to independent parties for evaluation.
- This project should be closed out.
- This project would benefit from interactions with the hydrogen storage theoreticians.

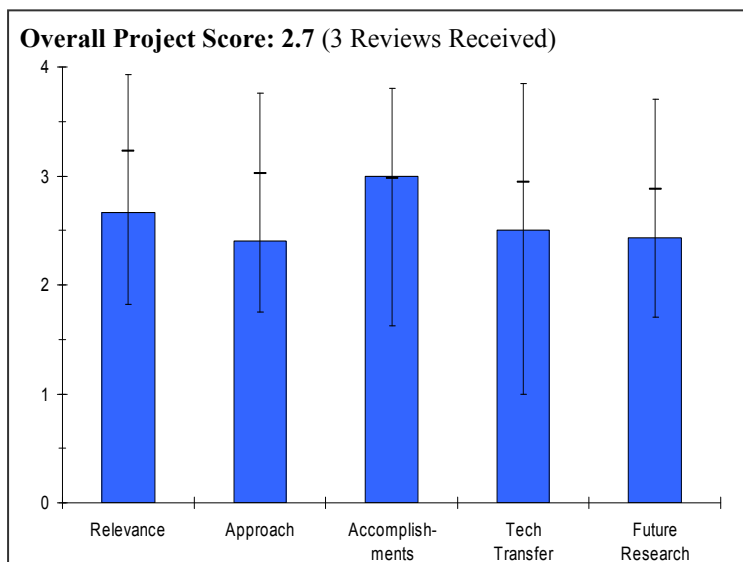


**Project # STP-29: Polymer-Based Activated Carbon Nanostructures for H<sub>2</sub> Storage***Israel Cabasso; State University of New York*

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

The overall objective of the project is to develop and demonstrate reversible nanostructured activated carbon hydrogen storage materials with materials-based volumetric capacity of 50 g H<sub>2</sub>/L, with potential to meet DOE 2010 system-level targets. The objectives for fiscal year 2007-2008 are to 1) develop polymer-based nanostructured carbons with high surface area and high micropore volume; 2) demonstrate reproducibility of 10-gram scale batch production of high surface area carbon; 3) characterize hydrogen storage capacity under various pressure and temperature conditions - target for 2007 >6 wt% and 40 g/L of material-based H<sub>2</sub> capacity; and 4) develop methods for organometallic and multicyclic ligand-doped polymer/carbon.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.7** for its relevance to DOE objectives.

- The project is relevant to the Department of Energy's Hydrogen Program goals.
- Based on a lot of work that has already been done with carbons, it is very doubtful that a carbon system will be capable of meeting the challenging DOE on-board storage targets. The data resulting from this project shows improvement over prior work with carbon, but is still fundamentally very far from the DOE targets.
- Consistent with the goal of arriving at material for an ambient conditions hydrogen reversible adsorption.

**Question 2: Approach to performing the research and development**

This project was rated **2.4** on its approach.

- The approach is quite trivial but efficient.
- The approach taken is to develop carbon substrates with optimized nanopore size and very high surface area for hydrogen sorption by carbonizing and carefully processing polymer precursors. The work will also include incorporating doping with organometallics, metal hydrides and multicyclic ligands. Other prior data available and the data from this project make it appear doubtful that this approach can meet the DOE on-board storage targets. The carbon system has been improved to having 6-7 weight percent hydrogen and good hydrogen volumetric density but only at 77K and under 6 MPa hydrogen pressure. This is still very far from the DOE combination of performance and system cost targets.
- The researchers are using excellent science and laboratory techniques to perform this research.
- The use of polymers as precursors and processing them into carbon sorption systems is a novel approach and results in the capability to control pore size and surface area.
- It is well recognized that for an effective ambient temperatures sorption of hydrogen, a heat of about 20-25 kJ/mol is needed. This is not going to be realized by just optimizing the carbon's pore structure and the use of ill-defined, fundamentally unjustified "dopants."

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Impressive surface areas.
- Good repeatability.
- Good storage capacities at 77K.
- The approach being taken has significantly improved the weight percent and hydrogen volumetric density for carbon-based hydrogen storage materials (e.g. from ~2 weight% to ~6 weight% at 77K).
- The hydrogen weight percent and volumetric density at a cost effective temperature is not shown but from the data provided it is clear that it is very far from the DOE combined performance and cost targets.
- Very good to excellent scientific work on optimizing the nanostructure of carbons. Lacking data on hydrogen heat of adsorption which is the critical determining factor for the development of a useful hydrogen solvent.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.5** for technology transfer and collaboration.

- Very limited collaboration with other members of the Hydrogen Program.
- There appears to be only one partner working with the State University of New York researchers.
- Papers and conference presentations are very limited.
- Coordination on hydrogen isotherm measurements.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.4** for proposed future work.

- Future Work is not well defined.
- Goals are very general.
- The future plan is to continue to pursue the same approach pursued to date and to do more doping research. The data already generated along with other data available on similar approaches with carbon materials makes it doubtful this approach will meet the DOE on-board storage targets.
- Investigators should measure their progress by improvements in the isotonic heat of hydrogen adsorption which needs to heat 20-25 kJ/mole. Need to develop a rationale, an underlying basis for choosing metal and other dopants.

**Strengths and weaknesses****Strengths**

- Very good experimental work.
- Deep understanding of experimental procedures.
- The researchers are using excellent science and laboratory techniques to perform this research.
- The use of polymers as precursors and processing them into carbon sorption systems is a novel approach and results in the capability to control nanopore size and surface area.
- Ability to tailor polymer - derived carbons.

**Weaknesses**

- Strategic planning can be improved.
- Collaboration needs improvement ( include industrial collaboration).
- The approach taken is to develop carbon substrates with optimized nanopore size and very high surface area for hydrogen sorption by carbonizing and carefully processing polymer precursors. The work will also include incorporating doping with organometallics, metal hydrides and multicyclic ligands. Other prior data available and the data from this project make it appear doubtful that this approach can meet the DOE on-board storage targets. The carbon system has been improved to having 6-7 weight percent hydrogen and good hydrogen

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volumetric density but only at 77K and under 6 MPa hydrogen pressure. This is still very far from the DOE combination of performance and system cost targets.

- Lack of credible pathway to a room temperature hydrogen solvent. Could be a good solvent for a 100K application.

### **Specific recommendations and additions or deletions to the work scope**

- This project should be stopped.

**Project # STP-32: An Integrated Approach for Hydrogen Production and Storage in Complex Hydrides of Transitional Elements**

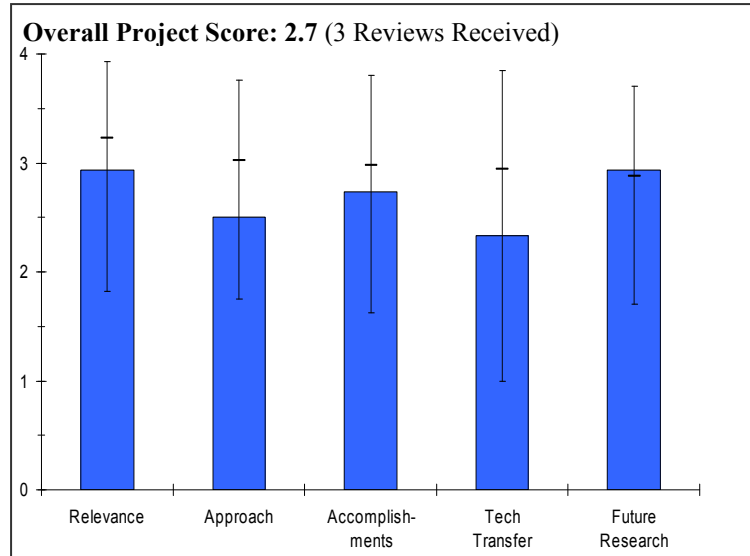
*Abhijit Bhattacharyya; University of Arkansas-Little Rock*

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

The objective for this project is to find complex hydrides of transitional elements for hydrogen storage that meet the following project targets by 2010: 6% weight percent; a pressure of 100 bar, kinetics of 3 min; and a temperature of -30/50°C. Objectives for bulk materials are hydrogen storage characterization and development of materials for hydrogen storage, including 1) increasing reversible hydrogen capacity in complex metal hydrides by developing new systems including hydride phases; 2) developing catalytic compounds to enhance the formation and decomposition of complex metal hydrides; 3) investigating hydrogen storage capacity in metal (Ti and Li)

decorated polymers; and 4) investigation of enhancement of hydrogen storage capacity in metal hydrides dispersed in polymer matrix. Objectives for nanostructures are the: 1) investigation of maximum hydrogen storage capacity and adsorption/desorption kinetics of thin films and nanostructures of magnesium alanate and magnesium borohydride; 2) utilization of glancing angle deposition technique for the growth of nanorod arrays of magnesium as a model system; 3) construction and utilization of new quartz crystal microbalance gas chamber system; and 4) investigation of effect of catalyst on hydrogen adsorption/desorption properties of Mg, magnesium alanate, and magnesium borohydride.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.9** for its relevance to DOE objectives.

- The project objectives relevant to overall materials synthesis is relevant to the Department of Energy targets. The objective of building Sievert-type equipment is not relevant and is recommended to be removed from the overall objectives.
- Testing of theoretical predictions is relevant.
- Mostly working on relevant systems.
- The project is relevant to the overall DOE Hydrogen Program objectives. It attempts to build (at low cost) high performance facilities and find ways to increase considerably the uptake of specific materials at room temperature.

**Question 2: Approach to performing the research and development**

This project was rated **2.5** on its approach.

- Suggested to clarify the approach to increasing the weight percent hydrogen by transition metal polymer decoration, such as using Ti to obtain 4.1 weight percent at RT from current 1.8 weight percent.
- Plan to utilize glancing angle deposition synthesis and quantify using a quartz crystal microbalance is suggested to be revisited due to practicality issues in meeting targets.
- Suggest trying to avoid overlap with other projects.

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- The work on the polymer side seems well addressed and promising. However, the work on the Mg-based compounds (alanate, borohydride) needs to be put into some perspective with regard to other on-going work, conclusions reached elsewhere about these materials (e.g. Mg-alanate irreversibility; different behavior of films compared to bulk materials), and time left till the project end.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- Ti-decorated PANI's formation appears to be preliminary and requires further confirmation. Care should be taken for "Kubas" type hydrogen bonding resulting.
- The purpose behind the inclusion of hydrides in PANI matrix is not clear and effects are not illustrated.
- Much time is spent on experimental and synthesis capabilities establishment.
- Lots of effort devoted to building apparatus (completed?); should now shift focus on doing science.
- Of great value are the facilities developed in-house by the University of Arkansas research group. The results on Ti-decorated PANI look promising and the work in that direction seems interesting. On the nanostructures side, the work done on thin films could provide some ideas about the observed discrepancy between films and bulk materials (e.g. in the case of Mg-based compounds).

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.3** for technology transfer and collaboration.

- Collaboration with other groups working nanohydrides systems is not visible and its suggested to have more interactions.
- No significant collaborations are evident.
- Some collaborations are mentioned but the role of each of the collaborating institutions (especially the Romanian one) should be further clarified.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- Suggest the path forward and the experimental plan to achieve theoretical hydrogen weight percent in polymers per theoretical estimation, such as 4 weight percent at room temperature in decorated PANI systems, should be clarified.
- The practicality could be an issue of using glancing angle deposition and a quartz crystal microbalance for materials synthesis and testing to achieving the DOE targets. A clear plan is suggested to be created on how this would be made possible.
- Looks reasonable.
- The proposed future work on the polymer side is quite interesting and holds promise for useful results. However, the plans on Mg-based materials should account better for work done elsewhere to avoid duplications (given also the limited time left until the end of the project).

### **Strengths and weaknesses**

#### Strengths

- Promising results and approach for Ti-decorated PANI.
- Good, powerful facilities built by the team at very much reduced costs.

#### Weaknesses

- Time spent on building equipment like a Sievert's apparatus which is commercially available.
- Plan to achieve targets using the proposed synthetic routes.
- The project finishes in August 2009. While the percentage of completeness is currently only 45 percent. It is questionable if within the remaining time the project can fulfill its aims.

- Some of the materials addressed have already been found to be irreversible (Mg-alanate) or are studied elsewhere (Mg(BH<sub>4</sub>)<sub>2</sub>).

**Specific recommendations and additions or deletions to the work scope**

- Suggest shifting from glancing angle deposition system synthesis if no materials upscale plan could be devised.
- It should be reconsidered if the work on Mg-alanate and Mg-borohydride is of real interest to the project and the DOE program.
- The work on thin films could possibly be used to provide hints/clues.
- The work on thin films could possibly be used to provide hints/clues on the different behavior observed between films and bulk materials.

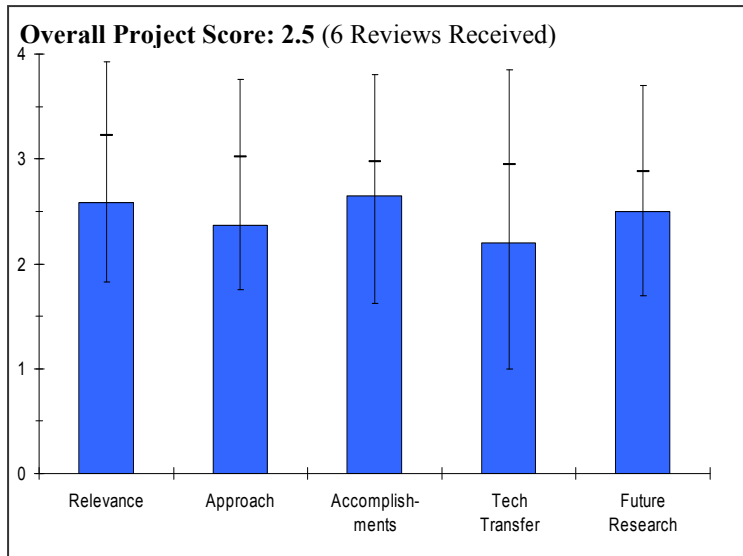
**Project # STP-33: Hydrogen Fuel Cells and Storage Technology Project**

*Clemens Heske; Balakrishnan Naduvalath (Co-PIs); Robert Perret, Project Manager, University of Nevada – Las Vegas (UNLV)*

[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

**Brief Summary of Project**

Objectives for this project are to perform closely-coupled theoretical and experimental investigations of 1) hydrogen adsorption/desorption in various matrices to establish a solid understanding of optimal storage concepts; 2) the electronic and geometric structure of metal hydrides, nanomaterials (C, B, N, transition metals, alloys), metal adatoms, and adsorbed hydrogen molecules/atoms; and 3) fuel cell membranes and catalytic materials; to predict optimized materials and structures for hydrogen storage and fuel cells in the DOE Hydrogen Program. The project will also collaborate closely with external partners.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.6** for its relevance to DOE objectives.

- Addressing relevant barriers and aligned with Department of Energy goals.
- This project consists of three tasks involving hydrogen storage materials and two tasks on materials and catalysts for fuel cell membranes. While major improvements are needed in both areas, the choices selected by this team for study offer little or no greater performance than existing candidates being done elsewhere.
- Neither the metal doped single wall nanotubes (SWNT) nor palladium (Pd) doped aniline polymers (PANI/Pd) are viable storage materials that are likely to meet the DOE hydrogen storage targets.
- The high Pd levels in the polymers would make these materials much too expensive to meet DOE cost levels.
- While assessment of Co/Pt catalysts would provide a greater understanding in their roles within fuel cells, it doesn't seem to be a direct path for developing lower cost alternative catalysts.
- Addressing relevant barriers and aligned with DOE goals.
- This project seeks to elucidate the fundamentals of the mechanisms that influence the kinetics and thermodynamics of hydrogen uptake and release by candidate hydrogen storage material types - metals, carbon forms, etc.
- The nature of the results produced by this project shed light on what limits hydrogen storage capacity and what controls the charging and discharging rates. In this respect, the quality of the science is quite good in that it produces insights that help to define what limits the storage capacity and the delivery characteristics of selected classes of materials currently under investigation at the Hydrogen Storage Centers of Excellence.
- The degree of relevance to the hydrogen vision and DOE research and development objectives is good in most respects.
- Effort seems to be more interested in understanding changes in electronic structure than with developing materials for hydrogen storage.
- The project bears adequate relevance to DOE program objectives. The statement is more valid with regard to the two tasks related to fuel cell research. The three tasks on hydrogen storage offer some insight to specific material issues but lack overall focus.

**Question 2: Approach to performing the research and development**

This project was rated **2.4** on its approach.

- Approach is broad in scope, covering storage and fuel cells – a more focused approach might be more productive.
- Modeling addressing relevant materials issues, but need to be more integrated into Hydrogen Program.
- It is not clear what targets the membrane work is addressing. Are they attempting to reduce cost, achieve high temperature low relative humidity targets? Improve durability?
- Fluorinated sulfonamides have potential, but what benefits over Nafion?
- The project has five independent and non-complementary tasks that do not address common goals.
- Good coordination of theoretical modeling of metal clusters on surfaces and experimental spectroscopies of surfaces for both nanophase storage materials and fuel cell catalysts that do suggest synergistic interactions.
- Thermodynamic assessment of Li-Al-H phases has already been reported in the literature and assessments of very high pressure phase transitions of complex hydrides have little bearing on their reactivity or means to improve hydrogen storage properties.
- The approach is broad in scope, covering storage and fuel cells. A more focused approach might be more productive.
- This project is orchestrated to be multidisciplinary and highly interactive within the University of Nevada, Las Vegas. Theory and experiment are closely connected.
- The program is being stretched beyond its originally intended time span through a no-cost extension. This has allowed the principal investigator to focus the emphasis of the remaining funding on the most productive research tasks that evolved from the dozen or so individual tasks that comprised the project at its inception.
- The project also includes work on membranes and catalysts for fuel cells as an add-on to the original project.
- The project seeks to predict optimized materials/structures/approaches for hydrogen storage.
- There is no apparent connection between theory and experimental efforts.
- Should focus more on direct storage measurements.
- There does not appear to be a clear strategy for focusing efforts on achieving DOE goals.
- The approach regarding Tasks 4 and 5 (fuel cells) seems adequate although the present reviewer does not feel experienced enough in the field to provide detailed judgment. With reference to Tasks 1, 2 and 3 (hydrogen storage), although some interesting results are shown, the overall approach lacks focus and convergence on specific objectives. It looks more like a work program in support of other investigations (i.e., it consists of seemingly unrelated packages of work).

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- Modeling of Ti-Alloy structures is useful.
- Membrane synthesis work has a good start, but should be aligned with DOE high-temperature membrane working group goals and targets.
- The investigators performed a variety of calculations on surfaces and clusters interacting with hydrogen that resulted in published papers.
- X-ray photoemission spectroscopy (XPS) instrumentation was developed to assess clusters and metals on surfaces that allowed evaluation of interactions with hydrogen with single-walled carbon nanotubes (SWNT) and assessment of Co/Pt catalyst particles.
- A number of PANI/Pd composite samples were prepared and relative hydrogen sorption properties were determined, although thorough measurements of their storage capacities were not measured.
- Several sulfonated polymers were prepared and tested for their potential as proton exchange membrane (PEM) materials; however, no assessment was for actual performance in fuel cells.
- Showed how metal doping of titanium modulates the chemisorption energy.
- Resolved issues about differences in the adsorption of molecular and atomic hydrogen on SWNTs with and without Ti and Li doping.



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- Some interesting hydrogen sorption results were obtained for Pd-doped mesoporous polyaniline composite materials.
- Work on partially fluorinated sulfonated co-polyamides showed improved proton conductivity relative to Nafion.
- Studies of Co/Pt clusters are starting to produce some interesting results concerning electronic states and charge transfer within and around the cluster.
- No significant progress.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.2** for technology transfer and collaboration.

- Collaborations with United Technologies Corporation (UTC) should be useful.
- Collaborations with hydrogen storage centers of excellence appear to be lacking.
- Collaboration with the DOE High Temperature Membrane Working Group would be beneficial and appears to be lacking.
- This project showed an active collaboration with UTC on characterization of Pt/Co catalysts for fuel cells where UNLV has developed XPS and other analysis capabilities to compare with theoretical modeling work at UTC.
- While there are also indications of fruitful interactions of the UNLV theory team with some other research groups on carbon and metal clusters, the other tasks seemed to be done mostly in isolation from outside hydrogen research organizations.
- Several other organizations are listed as partners, but it is not completely obvious throughout the slides how each of these partners interacts with or contributes to the project at UNLV.
- The project needs access to hydrogen storage measurement capability at an affordable price to provide a means of testing the impact of their findings on hydrogen storage capacity and hydriding/dehydriding kinetics.
- One gets the sense that this project needs to experience more embracement by the centers of excellence.
- There are no significant external collaborations.
- There exist partners but it is not clear how interaction and collaboration among them takes place and how fruitful it has been.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.5** for proposed future work.

- The proposed activities in Tasks 1, 3, 4 and 5 are all reasonable and within the capabilities of the various investigators.
- The assessment of Pt-Co alloy catalysts using in-situ XPS system looks promising when combined with appropriate electronic structure calculations.
- The proposed synthesis and evaluations of both the PANI/Pd and various sulfonated co-polyamides seems more like fishing expeditions rather than system development of high performance materials.
- The plan for future work emphasizes the most informative and productive aspects of the present program.
- The project generally addresses understanding barriers more than overcoming them.
- The material types chosen for study are ones that can provide beneficial insights into hydrogen storage but are for the most part not likely candidates for meeting DOE storage capacity targets.
- Suggest coordinating efforts with one (or more) of the centers of excellence to guide work in more relevant directions.
- Certain plans are mentioned but the remaining time and resources make their realization questionable. Again these plans (especially for the first three tasks) look incoherent and unfocused.

### **Strengths and weaknesses**

#### Strengths

- Strong modeling component to direct experimental efforts.

- From the description of the scanning tunneling and XPS systems, UNLV has developed a high quality experimental research facility that should be capable of providing valuable in-situ characterizations of surfaces, clusters, etc. that would support strong collaborations in sorption storage materials and fuel cell catalysts.
- The investigators have published a number of research papers in peer reviewed journals that indicate positive contributions.
- Strong modeling component to direct experimental efforts.
- Highly motivated and scholarly principal investigator working with other equally qualified faculty at UNLV.
- Strong peer reviewed publication record and impressive list of presentations is getting their message out.
- Projects like this one produce well educated graduates that will be up to speed in the hydrogen storage field and ready to contribute new approaches and new directions for fuel cell research and development.
- Certain results obtained provide useful data for specific material issues.

#### Weaknesses

- Apparent lack of interaction and feedback from the storage centers (including data for model validations, etc.). Lack of interaction with the DOE High Temperature Membrane Working Group, which would help define targets for membrane work
- Much of the work described in this report is similar to other DOE-funded projects, especially with regard to the theory of clusters and additives to carbon systems.
- Most of the XPS results pertain to SWNT systems, which have little potential as viable hydrogen storage materials.
- While the results obtained on phases transitions of hydrides at high pressure add to the general fundamental knowledge of these materials, they will not directly impact development of storage materials that can meet DOE targets.
- The properties reported by the investigators for either the PANI/Pd or sulfonated co-polyamides do not indicate any significant advantages over candidates being developed and studied by other groups.
- This project needs to be better integrated into one or more of the centers of excellence for hydrogen storage. Perhaps it is the appropriate center of excellence that should make the overtures necessary to build an effective collaborative relationship.
- Now that the UNLV project has moved into membrane and catalyst areas, some collaborations with fuel cell research and development components of the DOE Hydrogen Program seem in order.
- Remaining time for the project barely sufficient to carry out planned work.
- Work carried out seems rather fragmented and without proper focus (especially for tasks 1,2 and 3).

#### Specific recommendations and additions or deletions to the work scope

- Interact with the DOE High Temperature Membrane Working Group.
- Increase interactions with hydrogen storage centers of excellence.
- The capabilities of the UNLV surface spectroscopy instrumentation should be explored in partnership with other teams to investigate sorption hydrogenation reactions of clusters and/or catalysts.
- More obvious connection to partners.
- Closer interaction with the appropriate centers of excellence for hydrogen storage.
- Sustain the impressive publication record.

### Project # STP-34: Modular Storage Systems

Scott Redmond; Limnia (formerly FST)

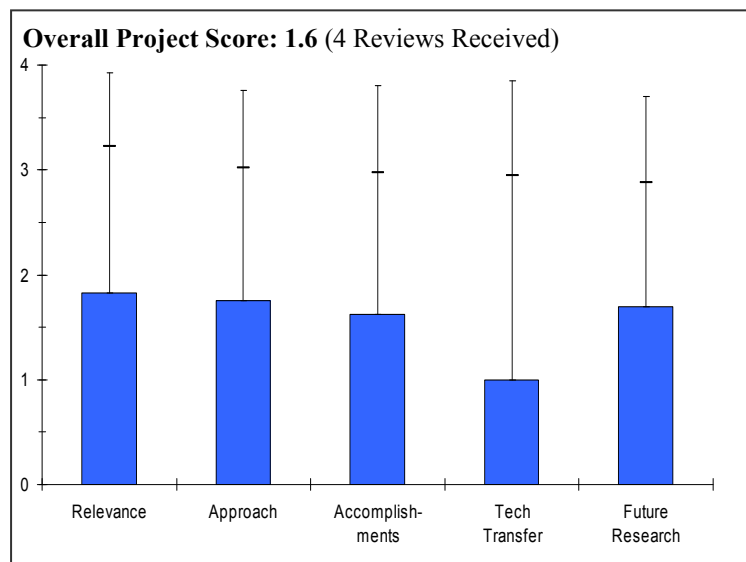
[NOTE: This project is not part of the Centers of Excellence; it is an independent project.]

#### Brief Summary of Project

Objectives for this project are to 1) develop a hardware/software system that stores and releases H<sub>2</sub> at optimum efficiency; 2) implement flexibility that facilitates use of the best available metal hydrides; and 3) provide the following system characteristics: built from readily available materials, scalable for multiple applications, and market adoptable via simple adjustments to existing infrastructure.

#### Question 1: Relevance to overall DOE objectives

This project earned a score of **1.8** for its relevance to DOE objectives.



- The approach is not in line with the Department of Energy hydrogen storage for vehicular applications.
- This project describes a metal hydride storage container that could be interchanged for filling to minimize thermal effects associated with on-board filling of the hydrogen gas.
- The design and construction of these storage vessels do not address most of the DOE hydrogen storage targets or requirements with respect to mass and many other parameters. The only significant attribute would be potential switching of externally charged and depleted storage vessels.
- Relevance is mixed. It is aimed at storing hydrogen, but it is not all that clear how useful the work is so in that sense it is not so relevant.
- There was no presenter for this poster.
- It is not obvious from the slide file that this project is well aligned with many of the hydrogen vision and DOE research and development objectives for on-board hydrogen storage.
- The stated strategy is to develop a hydrogen storage and distribution technology that is safer, modular, adaptive, regenerative, and transportable.

#### Question 2: Approach to performing the research and development

This project was rated **1.8** on its approach.

- There is no novel approach.
- A basic model analysis for heat transfer was presented to rationalize a rather naïve bed design for the hydride material. The predicted performance of this bed was compared to high pressure gas cylinders.
- A number of unspecified and hypothetical hydride sorbents were numerically evaluated to compare sensitivity of heat transfer performance and system mass ratios within the same basic design configuration.
- Relatively incomplete analysis and system is nowhere near the full system required for use. Not very impressive.
- The approach involves modeling, evaluation, design, and testing of a cassette-type storage platform.
- Materials selection, storage capacity, thermodynamics, kinetics, heat transfer, and balance of plant issues are addressed.
- The approach appears to be geared more towards transportable power supplies than to on-board storage of hydrogen for fuel cell powered vehicles.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **1.6** based on accomplishments.

- While a Sieverts type testing station was shown to be constructed for experimental evaluation of both sorbent materials and presumably prototype storage vessels, no test results were presented.
- Fluent modeling results for a conceptual bed design that contains sodium alanate were presented along with some simple mass ratios comparisons to unspecified high pressure gas tanks.
- Essentially built a Sieverts apparatus and did some modeling that replicates well known results from ME/ChemE in heat transfer from finned plates.
- Needed to validate that the system could work, but the system analyzed in the spread sheet is only a portion of the whole system. Results are thus non-instructive for actual application or comparison to goals.
- Parameters selected for hypothetical metal hydride storage material.
- Modeled and compared heat transfer for selected systems.
- Created a "virtual" cassette model and compared to other hydrogen storage methods.
- Designed/constructed "demonstration" cassette system hardware and software to illustrate feature.
- Modified materials and evaluated properties; compared different hydrogen storage systems in cassette test system.
- In the absence of a presenter to clarify what all this means, it is hard to figure out exactly what they really did.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **1.0** for technology transfer and collaboration.

- The Limnia poster does not indicate any interaction, consultation, or technical exchange with any other organization or individuals other than unnamed patent attorneys.
- None apparent
- No collaborators or partners mentioned.
- No evidence of interaction with one of the hydrogen storage centers of excellence.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **1.7** for proposed future work.

- Not applicable as this project is completed and no validation test data was provided in review package.
- Actual plans unclear, areas may be appropriate.
- Evaluate two other storage materials; complete study of carbon doped materials; continue studies of material densification.
- Refine balance of plant; adapt cassette to a "slurry system."
- Improve automation of experiments and systems.
- It's hard to appreciate what all of this means from the slides alone.
- Presumably, at some point we will see actual results of heat transfer measurements and cyclic hydriding/dehydriding tests.

**Strengths and weaknesses****Strengths**

- Modularity for assembly and manufacture.
- Limnia seems to be doing something that is producing both modeling information and testing data; there may be some useful results in this work but without someone to talk me through it, it is hard to appreciate what I'm looking at in the slides.

**Weaknesses**

- There is little of technical merit in this project as simulation results are for an impractical storage vessel.
- This is not a novel approach. Nor is it practical to address infrastructure issues.

## HYDROGEN STORAGE

- The storage material is the key to evaluate the system. However very little is devoted to the actual storage material.
- The proposed system is a variation of many different devices that have already been tried and tested.
- Bed design does not address any of the pressure containment issues or the feasibility of fabricating any demonstration vessel for assessment. The critical issues of heat transfer of the hydride powder within the bed during both desorption and refilling does not appear to have been considered.
- Extended shells of many cassettes plus mass and volume of multiplexer and holder.
- Effort at a much less robust level than needed for breakthrough or real progress.
- Electric heat is unlikely to be a good way to get heat. Remember you automatically double the energy requirement this way.
- There are no collaborations or interactions with the greater fuel cell/hydrogen storage community.
- Slide 4 is not overly informative without someone to talk me through it; also, slides 8 through 10 look rather superficial; looked at the tables on slides 11 and 12 for some time without being really sure I understand what their story is. In slide 15, one begins to get a sense of what is actually being done.
- Why are there no collaborations with the centers of excellence? Projects like this need the oversight of a larger group to make sure they are working up to the standard of the rest of the storage program and are using the most up to date information available.

### Specific recommendations and additions or deletions to the work scope

- This project does not appear to materially support the DOE goals for developing a storage system for vehicular application as such it is recommended to appropriately phase this project out of the portfolio.
- Not applicable as the project is completed.
- Need to go to much greater analysis to actually improve the storage and performance over simple engineering rules. For example, no performance simulations were shown or suggested, only heat transfer. Mass transfer is also a key factor. The use of electric release is highly wasteful because roughly two hydrogen will be consumed in the fuel cell to get the heat equivalent of one hydrogen in electric resistance. This alone will doom the program to failure visa vie the program goals.
- This project should get an oral review. If Limnia has really done something worthwhile here, it should be made clear to DOE.
- Actual performance results from testing of a real cassette would solve most of the problems I have with this project.

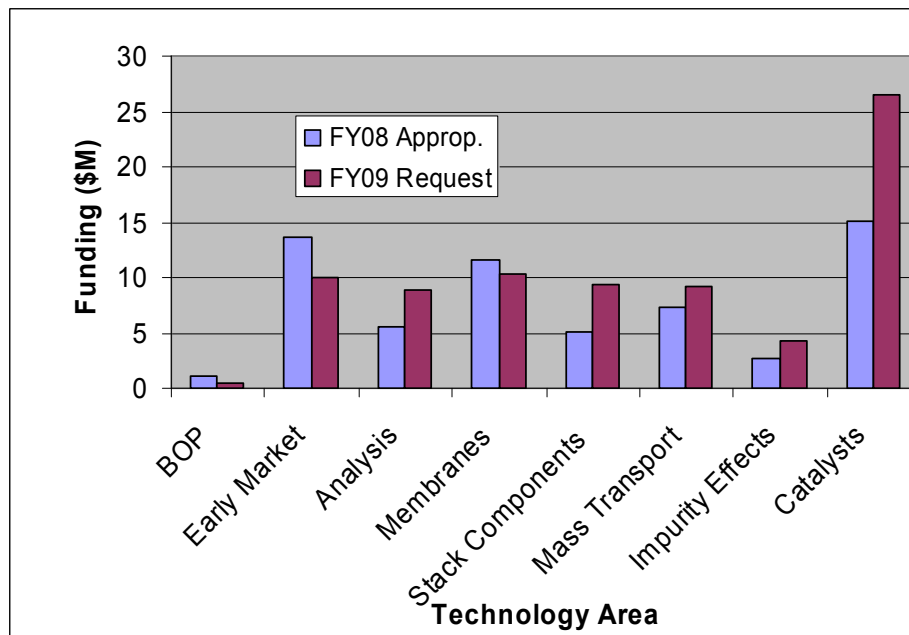
## 2008 Fuel Cells Summary of Annual Merit Review Fuel Cells Subprogram

### Summary of Reviewer Comments on Fuel Cells Subprogram:

Reviewers consider fuel cell development to be a critical enabling technology for the success of the President's Hydrogen Fuel and Advanced Energy Initiatives. Overall, the research and development portfolio was judged to be well managed, appropriately diverse, and focused on addressing technical barriers and meeting performance targets. Progress was considered outstanding. The continuing focus on partnering (industry, national laboratories, universities, etc.) was applauded and reviewers suggested that some projects might benefit from more interaction with industry, developers, and other program projects to establish a stronger and more technically sound research effort with improved outcomes and deliverables. New projects from the 2006 solicitation were kicked off in February 2007 and were reviewed for the first time this year.

### Fuel Cell Funding by Technology:

The Fuel Cell Technology Subprogram continues to concentrate on the critical path technology of stack components (membranes, catalysts, bipolar plates, gas diffusion layers, and analysis and characterization). Cost and durability of stack components continue to be a key focus of the subprogram.



### Majority of Reviewer Comments and Recommendations:

This year 56 fuel cell projects were reviewed of the 64 projects presented. In general, the reviewer scores for the fuel cell projects were average to high, with scores ranging from 3.8 to 1.9 for the highest and lowest scores, respectively. The average score of fuel cell subprogram scores was 3.0. The range of

scores and the average score were higher than those of the 2007 review. The majority of the projects were reviewed by six to seven reviewers each. Project scores reflect the technical progress made over the past year; relevance to the DOE Hydrogen Program; technical approach; extent of technical transfer; and proposed future plans. While reviewers tend to award those projects closer to commercial application with higher scores, their comments reveal that they also appreciate and support more fundamental work attacking key barriers to commercialization. Key recommendations and weaknesses are summarized below. DOE will respond to reviewer recommendations as appropriate for the scope and coherency of the overall fuel cell research effort.

**Catalysts:** The six catalyst projects reviewed received an overall rating of average, but they were rated above average in the categories of relevance to the DOE Hydrogen Program and technical approach. The demonstration of more than 7,300 hour life for a 3M nanostructured thin film electrode on a mechanically-stabilized 3M membrane, with voltage cycling, was particularly notable. This particular project was rated second highest in the entire subprogram. The required total platinum content continues to fall as a result of subprogram research, and Brookhaven National Laboratory has demonstrated ternary alloy catalysts with significantly higher mass activity than conventional platinum catalysts. Reviewers again expressed concern about approaches that replace platinum with other platinum group metals (PGM). Some durability results from the non-precious metal catalyst projects are promising, but performance generally needs to be at least an order-of-magnitude higher before this durability matters. The reviewers commented that these efforts in alternative electrocatalysts, though high risk, represent a potential high pay-off option and should be supported in the future. Reviewers suggest conducting in situ testing on promising materials as soon as practical.

**Membranes:** The fifteen membrane projects reviewed were ranked from below average to well above average. The 3M project ranked the highest among membrane projects, and received the fourth highest score in the subprogram. A membrane based on sulfonated poly(arylene ether sulfone) nanocapillaries in an inert polymer resin from Case Western Reserve University meets the DOE interim proton conductivity milestone and exceeds Nafion performance at the prescribed conditions. A cost of production study of most promising membranes was recommended for many of the projects. Reviewers expressed concern about the ongoing disagreements among membrane researchers about the validity of the proposed standardized conductivity test procedures. In several projects, reviewers commented that membrane principal investigators would benefit from closer collaboration with fuel cell researchers and developers.

**Impurities:** Three projects on the effects of impurities were rated average. Reviewers note the scope of the projects exceeds what can be reasonably accomplished with resources available. Although the researchers are sharing information and working on coordination, several reviewers recommended increased coordination to avoid duplication of effort and to accelerate the development of engineering models for use in standards development. Researchers are encouraged to move to lower, more representative catalyst loadings as soon as practical.

**Water Transport:** Three water transport projects were rated above average, with the Rochester Institute of Technology visualization and characterization project receiving the fourth highest score in the subprogram (along with the 3M project mentioned above). The increasing resolution of neutron imaging is helping to validate water transport computational fluid dynamics models. Reviewers recommend that all transport mechanisms for all pertinent phases and species should be accounted for, and that unsteady and transient effects be included as soon as possible.

**Water Management:** Two projects in water management received average scores. Reviewers questioned the ability of the microchannel humidifier approach to work with realistic automotive fuel cell operating conditions and recommend appropriate transient testing with changing conditions. Reviewers

also note that the Nuvera cold-start tests did not account for the heat introduced into the stack by room temperature reactant gases.

**Recycling:** Two recycling projects were evaluated and each received an overall rating of average. Reviewers generally consider PGM recovery an important aspect of the overall fuel cell life cycle, because it addresses both environmental issues and cost issues that impact the cost of fuel cell systems. BASF has made significant progress toward identification of the most efficient processes to recycle both catalyst-coated membranes and membrane electrode assemblies. Significant progress has been made by Ion Power in economic analysis and prototype process demonstration, including demonstration of performance of recycled ionomer and catalysts in fuel cells.

**Distributed Energy:** The six distributed energy projects reviewed were ranked overall as average, while the Plug Power international stationary fuel cell demonstration received the third highest score in the subprogram. Reviewers suggest that projects should work with U.S.-based home energy suppliers to determine if options exist in the U.S. for the proposed technology. They also suggest that a collaboration with stack component and materials researchers supported by the Program would help resolve issues with the demonstration systems.

**Analysis and Characterization:** The nine projects in this category included both the lowest ranked and highest ranked projects in the fuel cell subprogram, with the overall category score above average. These diverse projects were noted to strongly support the fuel cell program objectives and goals. The National Institute of Standards and Technology Neutron Imaging Project again received the highest score throughout the entire fuel cell subprogram. The Oak Ridge National Laboratory transmission electron microscopy characterization effort again ranked high, with reviewers continuing to comment that correlating the microstructure of membrane electrode assemblies revealed in these images with performance data would increase the value of the effort. Components such as membranes, gas diffusion layers, and catalysts more representative of those being used by stack developers and original equipment manufacturers should be considered for study. The reviewers again encouraged the modelers in the fuel cell program to validate their models with real world data, and to move to transient modeling as soon as practical. Fuel cell manufacturers need to supply more experimental data to the modelers. The cost of an 80-kW automotive polymer electrolyte membrane fuel cell system operating on direct hydrogen and projected to a manufacturing volume of 500,000 units per year continues to fall, currently estimated at \$94/kW. The market opportunity assessment methodology is thought to have merit.

**Portable Power, Auxiliary Power, Special Applications, and Innovative Concepts:** Two portable power projects, one auxiliary power project, one special application project, and one innovative concepts project were reviewed this year. These projects received average scores with the exception of the portable power projects, which ranked below average. Some reviewers question the relevance of the portable power projects to the President's Hydrogen Fuel Initiative. The auxiliary power projects received good scores for the focused applications being investigated and for teaming. The special application project developing a fuel cell-powered golf course maintenance vehicle received mixed reviews based on the lack of end-user involvement and the belief that this type of vehicle is not a particularly robust nor compelling application. The reviewed innovative concept project received good scores for objectives and relevance, but lower scores for approach and progress.

**Bipolar Plates:** Two bipolar plate projects were reviewed in the Annual Merit Review and Peer Evaluation. Both projects received scores of 3.4, which tie for the fourth highest scores in the subprogram. Reviewers suggest increased collaboration with stack developers and investigating remaining issues of concern, including: metal plate joining, further reductions of processing temperature and cost, and the permeability and durability of expanded graphite/resin plates.



**Balance-of-Plant and Integration:** One balance-of-plant project and an integration project were reviewed this year. Both projects reviewed were rated well below average. Collaboration with stack developers and original equipment manufacturers will be important to ensure these projects are focused on systems of interest to those working to commercialize automotive fuel cell technology. The integration project on the development of low-cost, durable seals received good scores.

**Cross Cutting:** The one cross-cutting project from the University of South Carolina received a score well below average. Reviewers generally did not consider the four disparate tasks as a well-defined coordinated project making progress toward targets.

## Project # FC-01: Advanced Cathode Catalysts and Supports for PEM Fuel Cells

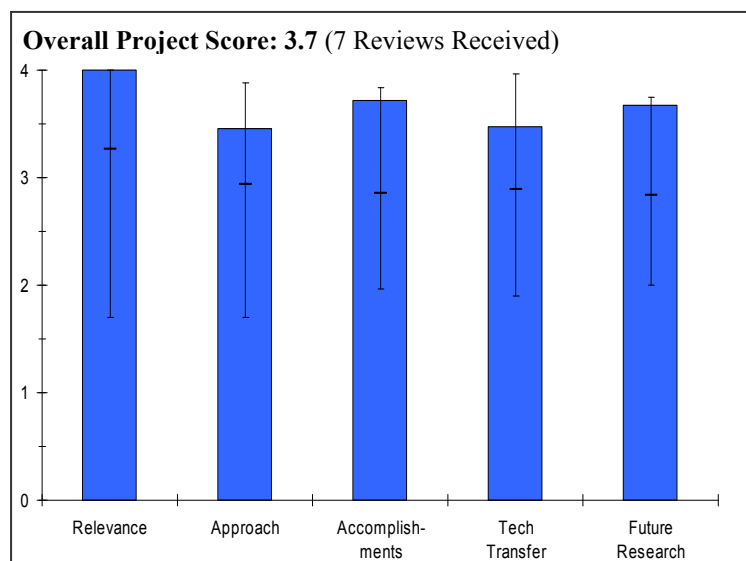
Mark Debe; 3M Company

### Brief Summary of Project

The overall objective is to develop a durable, low cost, high performance cathode electrode (catalyst and support), that is fully integrated into a fuel cell membrane electrode assembly with gas diffusion media, fabricated by high volume capable processes and is able to meet the 2015 DOE targets. The objectives of this project for the past year were to 1) apply DOE specified accelerated durability tests to benchmark the nanostructured thin film catalyst;

2) define and implement multiple strategies for increasing catalyst surface area, activity, and durability with catalyst loadings of  $<0.25 \text{ mg-Pt/cm}^2$  total per membrane electrode assembly;

3) work closely with collaborators to fabricate and screen new electrocatalysts using high throughput characterization methods, for durability and activity gains; 4) conduct fundamental studies of the nanostructured thin film catalyst activities for oxygen reduction reaction; 5) define and implement multiple strategies to optimize the membrane electrode assembly water management; 6) advance the high volume roll-good nanostructured thin film catalyst /membrane integration.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **4.0** for its relevance to DOE objectives.

- This project is fully focused on the DOE research and development objectives.
- Project addresses DOE goals on durability and reducing precious metal loading. Both of these goals are critical to Hydrogen Fuel Initiative.
- This effort is critical as it addresses membranes, electrodes, and manufacturing by a single entity which is known for its technical and manufacturing expertise.
- Addresses key issues of ultimate importance: "durability" and also Pt-reduction.
- Water transport notwithstanding, the 3M nanostructured thin film has demonstrated an extraordinary opportunity to meet catalyst cost and durability targets according to data generated using DOE protocols.
- Because 2015 targets have not yet been met, further work is required to achieve performance and durability targets using 2015 target Pt loadings.
- Further work is also required to understand the robustness of the nanostructured thin film over a range of operating conditions.
- Fuel cell durability is key to the Hydrogen Program and industry fuel cell success, and this project is directly aligned with this goal.
- This project fully supports the objectives in developing an automotive-capable membrane electrode assembly design.

### Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- The technical barriers are addressed in a direct, well-defined approach. As a result, most of the DOE targets are met. The exception is Platinum Mass Activity, which should be significantly improved.

- Technical barriers are clearly identified.
- Approach is well thought and focused on overcoming technical barriers.
- Excellent combination of fundamental and applied research.
- This reviewer feels that the appropriate tests and technical aspects of the problem are being addressed.
- Alternative nanoelectrodes or variations should be evaluated in the event that the 3M electrode does not yield.
- The membrane support activity is leading to new potential successes and needs to be better understood.
- Clearly focused.
- Well led and managed; good bottom-up approach.
- Good risk mitigation.
- Sound testing.
- Because 2015 performance criteria have not yet been met, Task 1 (activity improvements) is necessary.
- Given the passing of DOE durability protocols, Task 2 (durability improvements) should not be as critical as other tasks, particularly Tasks 5.1 and 5.2 (gas diffusion layers and interfacial optimization). Although durability is commonly a concern in DOE projects, in the case of the nanostructured thin film, robustness to a wide range of operating conditions is presently a greater concern. That said, attention to anode starvation is a pleasant surprise.
- Tasks 3, 4, and 5.3 (large single cell, durability of advanced structures, and stack testing) are rightfully put aside early in the project.
- The approach is logically laid out, starting from detailed catalyst work and working up to larger media to incrementally validate the progress of the project.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.7** based on accomplishments.

- Remarkable progress has been made during last year. Performances are outstanding. The cost of platinum should be reexamined in defining further research.
- The principal investigator demonstrated steady progress towards 2010/2015 DOE goals; several barriers are already overcome.
- Although some of the 2015 targets are achieved for 50 cm<sup>2</sup> cells, the results have to be confirmed in stacks.
- Excellent progress towards durability and specific activity.
- Accomplishments are significant and insightful. The neutron imaging will yield additional valuable water dynamics data.
- The Gore support has lead to some interesting results, but these results need to be better understood.
- The fluoride data are perplexing. The unsupported membranes fail early; the supported membranes last many hours; yet why are the early membranes failing early when the 3M electrode is carbon support-free? What is the source of the peroxide?
- The Gore supported membrane needs to be looked at carefully for thickness changes vs. time. Is it the catalyst which is leading to the peroxide? Or the stability of the ternary catalyst elements? Or dissolution of the catalyst data?
- Great achievement with respect to durability.
- Huge amount of convincing test results.
- Promising novel Carbon-free catalyst materials
- Passed DOE catalyst accelerated stress tests at sub-2010 loadings.
- Passed DOE polymer electrolyte membrane chemical accelerated stress test at 0.4 mg Pt/cm<sup>2</sup>.
- Anode starvation test shows progress in modifying the nanostructured thin film. This was a particularly proactive measure given that investigators do not have access to how this test would relate to realistic on-board cell operation.
- Translation between electrochemically active surface area stability from compositional study and mass activity stability was not reported. 3M also did not report the effect of composition on grain size, lattice spacing and other parameters. Conclusions cannot be drawn upon whether progress has been made from this task to control those parameters.
- 3M did not report voltage in cool start test. More detail regarding gas diffusion layer studies should also be reported.

- Outstanding progress in the last year relative to most of the project targets, most importantly the 7300 h durability which may be longer as it is still on the test stand.
- This project has achieved the gold standard for membrane electrode assembly durability of > 7000 h and should satisfy the DOE durability goals. Catalyst loading appears to have room to decrease further as catalyst support "whiskers" are further optimized.

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.5** for technology transfer and collaboration.

- The collaboration with National laboratories and one University is successful.
- Close collaboration with Dalhousie Universities and Argonne National Laboratory.
- Appropriate teaming is in place.
- Excelling consortium.
- The work with Dalhousie is promising in terms of research-level fabrication. More data need to be reported from this activity.
- Results from Argonne National Laboratory appear to suggest competitive alloy compositions. Degree of reproducibility would be good to see.
- Validation of Tafel slope trends from the Jet Propulsion Laboratory cell on conventional rotating disk electrode or from *in situ* fuel cell testing would add to the perceived value of this testing.
- In general, range of collaborators is wide and useful to particular parts of the 3M study.
- Good interactions, not only with the project partners but also with other Federally Funded Research and Development Centers, companies, and system integrators.
- Principal investigator is collaborating with the appropriate national labs and industry partners to develop membrane electrode assemblies. 3M has strong relationships with most original equipment manufacturers and will likely leverage those resources for this project.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.7** for proposed future work.

- Plans are well-defined, realistic and based on previous successful work.
- Future work is focused on significant improvement of a current baseline and sounds very challenging.
- Future plans may need to focus more on fuel cell stack tests.
- Neutron imaging will be helpful.
- Study leaching and catalyst stability earlier rather than later.
- Why is the supported membrane performing as it is?
- Start-stops electrochemical behavior of the membrane electrode assembly?
- Continuation of the project is straightforward, and the future plans are well justified and promising.
- The answer to nanostructured thin film issues with robustness is likely greater than gas diffusion layer optimization; therefore, the brief note about optimizing interfacial characteristics mentioned in the approach slide should be taken to heart.
- 3M indicates that anode starvation studies will continue, as they should.
- Very specific and understandable future proposed research.
- Future research sounds promising toward improving mass activity, improving durability, and improving water management, which are the appropriate areas on which to focus.

#### **Strengths and weaknesses**

##### Strengths

- Project has considerable strengths in the in-house catalysts production, and its scalability, which eliminates a part of the problem of technology transfer.
- Strong management has resulted in significant progress towards durability and activity goals.
- Strong team combines knowledge and experience in technology and fundamental science.

- Willing to work and collaborate in new areas (Gore support).
- Only a few key players with complementary expertise.
- 3M has paid rigorous and disciplined attention to all deficiencies of nanostructured thin film and has developed a plan of action to address them.
- 3M has developed collaborative efforts in areas where it may need help (e.g., combinatorial thin film formulations).
- For *in situ* testing, data are thoroughly reported.
- 3M shows excellent progress on durability using sub-2010 target Pt loadings.
- Attention is given to manufacturing process improvements.
- Pushing the envelope of high tech research in the important application area for fuel cells.
- Absolute clarity (no questions!) about the status of the project relative to targets and where the shortfalls still lie.
- It is nice to have such a concise explanation of the durability tests on the same slide as the results.

### Weaknesses

- Basic insights into the origin of the activity and stability are lacking and these insights would be useful for further projects' plans and for other projects in general.
- Unclear if there is any scientific approach towards making new catalyst composition.
- Project needs greater emphasis on *in situ* operational robustness, particularly with respect to water transport.
- Collaborative efforts should deliver more tangible results.
- More information is needed regarding certain tasks, such as cool start testing and the compositional testing at Dalhousie.
- Iron content in catalyst might be of concern due to Fenton effect of causing peroxide formation.
- No major weaknesses.

### Specific recommendations and additions or deletions to the work scope

- Explore possibilities of reducing Pt loadings.
- Project needs to be more focused on fundamental understanding of oxygen reduction reaction on proposed catalysts.
- Water transport and gas diffusion layer optimization efforts should be prioritized higher.
- In Task 3, the design of the large single cell should be reviewed with DOE. It is unclear whether this work is most appropriate for this project or for eventual nanostructured thin film customers (e.g., original equipment manufacturers) to perform.
- The above comment about cell design should be applied to cool start efforts at stack level.
- Accelerate progress so that this wonderful technology gets into the hands of the system integrators and automotive original equipment manufacturers so that the hydrogen fuel cell automobile can continue to move toward the marketplace!

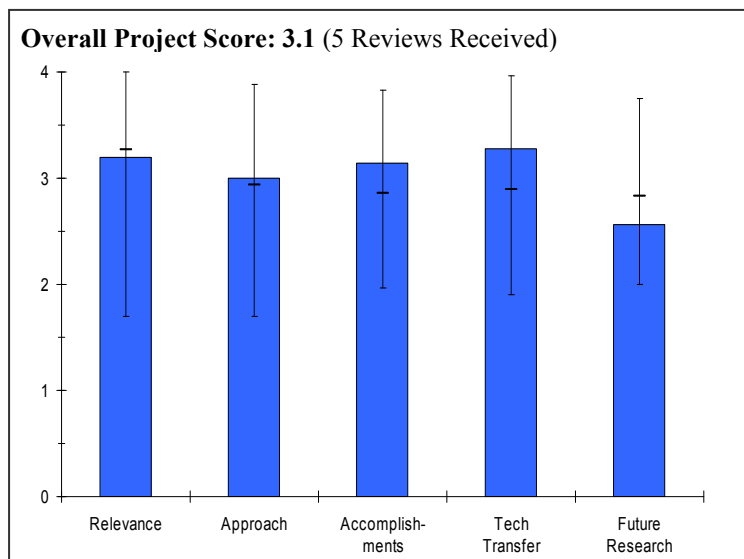
## Project # FC-02: Non-Platinum Bimetallic Cathode Electrocatalysts

Debbie Myers; Argonne National Laboratory

### Brief Summary of Project

The overall objective is to develop a non-platinum cathode electrocatalyst for polymer electrolyte fuel cells to meet Department of Energy targets that 1) promote the direct four-electron oxygen reduction reaction with high electrocatalytic activity; 2) is chemically compatible with the acidic electrolyte and resistant to dissolution; and 3) is low cost. The objective for the past year was to synthesize and evaluate the oxygen reduction activity, stability, and electronic structure of nanoparticles of three palladium alloy systems (PdCu, PdNi, and PdFe).

### Question 1: Relevance to overall DOE objectives



This project earned a score of **3.2** for its relevance to DOE objectives.

- The principal investigator's justifications for how the project addresses durability and performance (technical barriers A and C) with the binary transition metal catalysts are not convincing. The cost barrier addressed by the research is very clear however.
- The project objectives are relevant to the DOE objectives.
- Insofar as the project is set up to address electrocatalyst targets for performance, durability and cost, there are few projects that are more relevant to DOE objectives for the eventual commercialization of fuel cell vehicles.
- Relevance should also be predicated upon the catalyst composition being considered here. Thankfully, this project's compositions are intended to displace PGMs.
- Bimetallic core/shell and alloy compositions can be well-tread ground unless a systematic, thorough approach is taken.
- The project addresses key elements for the replacement of platinum catalyst for the anode.
- Success of this project will further DOE's goals for developing better/cheaper catalysts.

### Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The proposed approach is logical for reducing the amount of Pt and extendable to metal systems other than the Pd-Transition metal binaries currently the focus of the research. The effect on durability in a working fuel cell may not be fully addressed by the project plans since factors other than the oxophilicity of the catalyst can be important for stability of surface area and specific oxygen reduction reaction activity. The cost savings by replacing Pt may not be realized unless the full performance equivalence to Pt is obtained since the added cost of extra cells, bipolar plates, etc. will offset the cost savings of the Pt replacement. The project's research is definitely breaking new ground and appears to be well executed. Using carbon as a support is both limiting in its process methods and fundamental corrosion limitations, but the concepts may be extendable to other process methods and supports.
- Use of Norskov-inspired d-band shift approach helps to prevent an exercise in the random selection of elements. Unclear, however, if this approach directed investigators towards PdNi, PdFe and PdCo the same way it did toward PdCu.
- Possible use of fourth period metals (Cu, Ni, Fe) as cores enable a pathway towards meeting cost targets.

- Approach assumes that the same measures taken to enhance activity will also enhance durability. Given the range of surface reactions possible in oxygen reduction reaction-intended environments, the probability that this will be true is low.
- The project incorporates copper as an alloy with palladium to enhance the oxygen reduction activity. Copper is a poison for the anode reaction and plates out onto the surface of platinum. While the project uses copper in the cathode, the prospects for cross contamination to the anode could be high and lead to failure of the anode.
- The project uses iron as an alloying addition to platinum. The use of Fe can promote the failure of the membrane and iron should be avoided.
- It is not clear what alloy is used in the graph on slide 20. Performance is very low.
- Project shows high relevance to DOE's barriers for durability, cost, and electrode performance.
- Approach lays out very specific means to address these barriers.
- Project includes good mix of theoretical and experimental work.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- Impressive results to date on oxygen reduction reaction activity with PdCu and "tricking" oxygen to think it is Pt. Good progress rather than outstanding just because it is a tremendous challenge to replace Pt and even these impressive results are just a start on a long path. Durability has not really been addressed and probably cannot until fuel cell testing begins in earnest. It is not clear why adequate catalysts were not made for at least a few membrane electrode assembly tests, as getting some insight sooner rather than later as to how the rotating disk electrode activities translate to fuel cell performance could be important for helping direct the project to success. Good use of fundamental modeling, state-of-the art characterization and understanding.
- Progress was made to fabricate a PdCu alloy (by colloidal methods) that in terms of activity and valence band energy approximates Pt. Particle size is still a few nm high.
- Very low activity shown for PdNi and PdFe despite best efforts to change impregnation and fabrication parameters.
- PtCo by strong electrostatic adsorption had low activity; not reported whether other eligible core/shells could be made this way.
- In general, a very thorough job has been done of showing – by rotating disk electrode – that catalyst particles will not directly meet DOE objectives.
- The progress made is impressive. If the progress can be moved toward palladium cobalt alloys then the possibility exists for a replacement of platinum.
- The issue of palladium as a precious metal was discussed at the presentation. It is not clear that palladium price will not escalate should it be a replacement for platinum.
- Colloidal technique appears to be effective mechanism to produce smaller particles in a narrower distribution.
- Achieved Pd-based catalysts similar to that of Pt (40% of the cost for the same activity).

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- Appears to be good in some respects, but could be improved by more focus on fewer material systems and processes.
- Collaboration with others is visible.
- Collaboration with the California Institute of Technology motivated the study of PdCu.
- Collaboration with University of Illinois at Chicago produced PdCo core/shell particles.
- Collaboration with University of Nevada at Las Vegas uncovered the valence band resemblance of PdCu to Pt.
- A larger breadth of collaboration was expected for this project and appears to have been executed.
- A strong team was established for this program. There is a good mix of modeling and experimental effort.
- Appears as though adequate collaborations are in place to move the project forward.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.6** for proposed future work.

- The likelihood of finding a non-Pt core-shell structure having a specific activity 2x better than current state-of-the-art Pt (the target in a working membrane electrode assembly) would seem to be extremely low. So at this time, rather than trying to screen many different binary combinations, the project should focus on trying to obtain a more fundamental understanding of what the source of oxygen reduction reaction is on one material system considered representative of the class.
- Try to determine what the entitlement activity for this model catalyst system would be if it could be made perfectly, and see how close the measurements come to the theoretical values.
- The second focus should be to put the representative catalyst system into a working membrane electrode assembly as soon as possible and determine durability issues (or benefits) again with the objective of determining whether there is any chance of meeting the targets for durability.
- Unless path forward for how PdCu will meet targets is in sight, PdCu computational analysis should be deleted.
- Modeling should be carried out before preparing more model systems. Justification should be provided for Pd/M and M/Pd systems.
- Only the most active Pd alloys should be considered for membrane electrode assembly testing. *Ex situ* stability testing will not provide appropriate fuel cell validation.
- Pd on Pd-containing core work should either be avoided (for high-PGM cost reasons) or should be merged somehow with Los Alamos National Laboratory/UTC Power projects.
- This project has showed that Pd-containing particles do not meet DOE objectives. Remaining tasks must be focused.
- The project emphasizes copper and iron alloys for future work. An immediate test of the stability of these alloys is necessary to demonstrate they will not poison the anode or promote the degradation of the membrane.
- Detailed plans are in place for future computational, modeling, and experimental work.

**Strengths and weaknesses**Strengths

- Experienced and high quality collaborators.
- The principal investigators have done an excellent job experimenting with catalyst synthesis parameters to find whether Pd/M non-Pt catalyst particles can be as active as Pt.
- Investigators applied "apples-to-apples" *ex situ* electrochemical comparisons to find whether synthesized particles could meet DOE objectives.
- Mastery of experimental techniques was evident throughout data presentation.
- Strong list of collaborators were included.
- Systematic approach was followed. No unnecessary durability tests were done.
- The project is developing a strong modeling – predictive understanding of catalysis based on the alloy compositions under test.
- Focused on critical fuel cell barriers.
- Good project team assembled making steady progress.

Weaknesses

- Trying to meet difficult practical targets with a basic research effort.
- Materials synthesized were not as active as Pt and do not meet DOE objectives.
- The principal investigator needs to reconsider whether bimetallic species on conventional supports, in general, will meet DOE objectives. Justifications need to be provided, whether by modeling or through literature, to say that a particular composition has a real chance of achieving 0.44 A/mg PGM, given a conventional particle-on-C-support structure.
- The use of copper and iron as alloying agents needs to be evaluated for their impact on fuel cell stability.

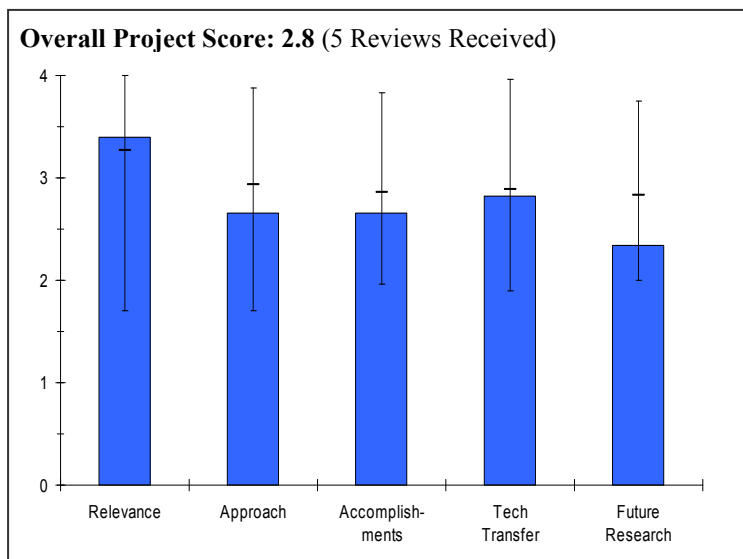


**Specific recommendations and additions or deletions to the work scope**

- Focus on gaining a more in-depth understanding of a model catalyst system representative of their approach, and refrain from trying to screen many materials to see what is obtained.
- Suggest keeping the project.
- If there is no theoretical justification to continue with bimetallic particles, the entire project should refocus on other chemistries. Because catalyst work is critical for the commercialization of fuel cells, academic interest cannot be the reason to continue any of the tasks described in the future work. Future work must have impact.
- Pd on PGM-containing core work should be given to or merged with Los Alamos National Laboratory/UTC Power projects, if carried out at all (latter decision should depend on expected cost, given high use of selected PGM).
- Future work should strongly emphasize improving palladium nickel alloys and cobalt alloys.
- The effort on nanostructures should continue, but not on copper or nickel until their stability is proven.
- Rhodium should only be considered for expanding the understanding of alloy interactions with the oxygen reduction reaction. Rhodium is considered too costly for use in oxygen reduction reaction catalysis.
- Look for opportunities to accelerate sharing of learnings with potential industry partners and systems integrators.

**Project # FC-03: Advanced Cathode Catalysts***Piotr Zelenay; Los Alamos National Laboratory***Brief Summary of Project**

The overall objective is to develop an oxygen reduction reaction catalyst, other than pure platinum, capable of fulfilling cost, performance, and durability requirements established by the Department of Energy for the polymer electrolyte fuel cell cathode. Other objectives of this project are to 1) design, synthesize and characterize new catalyst supports and electrode structures for new-generation oxygen reduction reaction catalysts; 2) determine the oxygen reduction reaction mechanism on newly developed catalysts via extensive physicochemical and electrochemical characterization and fuel cell testing; 3) optimize electrode with new catalysts and structures for maximum performance and catalyst utilization; 4) evaluate catalyst stability and minimize performance loss over time; 5) assure path forward for fabrication and scale-up of viable catalysts.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.4** for its relevance to DOE objectives.

- The project clearly addresses the major technical barrier, C. for cost reduction by replacing Pt with lower cost materials. But it is not clear that any of the approaches solve any of the durability or performance issues facing even state-of-the-art Pt based catalysts today.
- Improvement of the oxygen reduction reaction efficiency is vital.
- Ultra-low loading of Pt is needed.
- Non-Pt catalysts are the ultimate goal.
- All aspects will improve the cost competitiveness of polymer electrolyte membrane and are highly necessary.
- Project goals directly focused on addressing oxygen reduction reaction performance and durability issues while keeping cost considerations in mind.
- The results of this research have the potential for broad impact in the industry for enabling commercialization of fuel cell technologies.
- Cathode catalyst technology is one of the most critical areas for performance, durability, and cost.
- Particularly, lower PGM loading or alternative novel catalyst technology is highly demanded to develop commercially viable fuel cell technology.
- This project is dedicated to meeting DOE objectives for electrocatalysts by synthesizing new materials, which is highly relevant.
- The project is committed to minimizing PGM content.
- The project is committed to looking at novel structures.
- Too much of the ultra-low Pt task uses PGMs to displace Pt. Although high activities are shown, in principle, non-PGMs should be used to displace PGM since all PGM prices will increase at commercialization.

**Question 2: Approach to performing the research and development**

This project was rated **2.7** on its approach.

- The project has many, unrelated approaches, all with significant challenges.
- Approach is strong with excellent team but there are some weaknesses that need to be addressed.
- Fe is a known accelerant for membrane degradation – what will be ultimate price in durability for this cost saving?
- Is Fe in electrodes even a worthwhile material to investigate or is it already a known dead-end?
- *In situ* fuel cell experiments are poorly run and understood.
- Appears to be a 4-year program of parallel efforts, each with their own independent goals. Need to address specific overall project metrics and plans for downselect/direct comparison between different catalyst approaches before the end of the project.
- Individual approaches are generally strong, and in particular, the microemulsion approach is innovative.
- It is good to cover various approaches in a project.
- It is necessary to develop a common set of metrics to screen the technical approaches. It is not appropriate to set different metrics and target criteria between PGM catalyst and non-PGM catalyst.
- A common set of metrics and criteria should be developed from fuel cell requirements.
- The overall sequence of the approach – synthesize, understand oxygen reduction reaction mechanism, durability / membrane electrode assembly testing – is appropriate.
- The motivations for particular materials (e.g., chalcogenides) are not clear (other than to eliminate Pt).
- Go/no-go decisions should be applied for each material even before fuel cell testing. Criteria could include open circuit voltage, %H<sub>2</sub>O<sub>2</sub>, ability to be fabricated into a membrane electrode assembly, thickness of catalyst layer (which should be reported each time a fuel cell test is performed).
- Wide diversity of materials is commendable, since each material has a low probability of succeeding.
- Polarization curves should be broken into kinetic / ohmic / mass transport losses. Particularly for PtAuNi<sub>5</sub>/C.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- The first year's progress has been good in demonstrating or advancing the concepts for several different new catalyst approaches. But none of them show significant progress in overcoming the DOE technical barriers A, B, and C. The highly experienced principal investigator and collaborators' work is excellent but fragmented due to the very broad nature of the project.
- High degree of fundamental electrode preparation and analysis has already been accomplished.
- *In situ* fuel cell experiments, which are the ultimate indicator of feasibility, are poorly run and understood based upon the results shown at this review meeting.
- Scanning Electron Microscope / Transmission Electron Microscope images are vital to understand phenomena and are well used.
- Microemulsion approach is very innovative and will likely lead to significant results in terms of practical catalyst fabrication and performance.
- Good progress being made in each of the parallel catalyst development efforts, with improvements of state-of-the-art demonstrated in most cases.
- Some good performance is shown with core-shell catalyst.
- Potential of Ru replacement with Fe is good but performance is still too low.
- High activity shown for PtAuNi<sub>5</sub>/C, along with compositional confirmation – not stable under fuel cell conditions.
- Throughout ultra-low Pt section, activity numbers need to be re-normalized based on mg PGM, not mg Pt (inconsistency between 1.5 A/mg Pt for PtML/Pd<sub>3</sub>Fe on milestones slides and bar plot showing activity later).
- Need to show actual current densities as well for RuSe/C and better indication of core/shell character than compositional analysis.
- Use of polypyrrole nanotube to improve *ex situ* durability is good. Investigators need to show path towards *in situ* testing, particularly how catalyst layer will interact with polymer electrolyte membrane, gas diffusion media.
- CoFe complexes show low open circuit voltage, which lowers the probability for good performance.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.8** for technology transfer and collaboration.

- The project has all the right kinds of collaborators for effective technology transfer.
- Work between National Labs and Universities is high and clear.
- Unclear what the level of interaction between National Labs/Universities and Cabot.
- Membrane electrode assembly developer / stack developer should be considered to be added to the program to validate feasibility of materials, membrane electrode assembly preparation and fuel cell testing.
- Not really addressed. Doesn't even appear to be much interaction between members of the team, much less other projects/programs.
- Many collaborations.
- Collaboration is with at least two proven institutions (Brookhaven National Laboratory, Los Alamos National Laboratory on fuel cell catalysis).
- Collaboration is perhaps the most wide-ranging in the fuel cell subprogram.
- Collaboration is evident in the presented data, particularly with Brookhaven National Laboratory and University of Illinois Urbana-Champaign.
- Contributions of University of New Mexico, University of California-Riverside and others are not clear at present.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.3** for proposed future work.

- The project still appears to be trying to do too much and cover too much ground.
- For the second year, it would be advised to start downselecting the various approaches to one or two at most and focus on just those for achieving the performance target.
- The next focus should be on taking the best candidate and begin to study the durability issues.
- Fundamental approach is strong and should continue.
- Re-evaluation of Fe-based electrodes is necessary to determine end-use feasibility.
- Improvement of membrane electrode assembly and fuel cell testing is desperately needed and is not addressed sufficiently.
- In some cases, the principal investigator did not show data to support issues identified/future plans (i.e., how do they know there is a need for improved uniformity of Au on Ni core in the PtAuNi<sub>5</sub>/C catalyst?).
- What is approach to prevent Fe dissolution in Pt<sub>3</sub>F<sub>3</sub> catalysts?
- It would be more beneficial to focus on the characterization work. For instance, it would be valuable to identify critical materials/design parameters to synthesize core/shell catalyst, rather than just aiming for better performance by trying various approaches.
- Screening milestone is necessary to sort out approaches. There are too many approaches on-going.
- Open circuit voltage for polyaniline-based and N-free catalysts should be improved before fuel cell testing ("performance") is done.
- System for direct electrochemical detection of H<sub>2</sub>O<sub>2</sub> in polymer electrolyte membrane fuel cells should be mostly developed, or else this could be a considerable task.
- Hierarchical catalyst study should immediately address durability in some form since the probability of an activity / durability tradeoff is very high (high surface area, but low stability).

**Strengths and weaknesses**Strengths

- Excellent and experienced collaborators.
- Core strength of various National Laboratories/Universities for fundamental work is exceptional.
- Strong team with very complementary expertise and clear lead roles in program.
- Variety of technical approaches.
- Diversity of materials.

- Well-executed electrochemical and analytical analyses.
- Challenges for each material clearly identified.
- Novelty of materials.
- Attention given to both support and active species.

### Weaknesses

- Too many diverse approaches.
- Lack of membrane electrode assembly developer / stack developer for research direction and high level fuel cell testing hurts the program and causes unneeded diversions.
- Use of Fe in electrode is known drawback and should be avoided from day 1.
- Lots of parallel approaches here. Would like to know plan for future direct comparison of the catalysts being developed and whether any downselects will be made during the 4-year. Lack of a direct comparison (apples-to-apples) during the program will prevent identification of best catalysts to implement.
- Would benefit from spending more time on a few key highlights in depth in next year's brief rather than trying to cover everything in the program.
- Project management, since this project seems to be just collecting data for each task.
- Project should be conducted with a common set of metric and criteria.
- Reliance upon PGM-containing cores for some of the low-Pt work.
- Even greater attention to "red flags" (e.g., low open circuit voltage) needed in earlier stages of testing.

### Specific recommendations and additions or deletions to the work scope

- Select one or two catalyst approaches and discard the others for next year.
- Reassessment of Fe in electrodes.
- Addition of membrane electrode assembly/stack developer.
- Project could benefit from putting together its own list of criteria that each catalyst / catalyst layer has to achieve. Attributes could include open circuit voltage, mass activity at 0.9 V, thickness of layer (may be dependent upon gas permeability, electrical conductivity, support stability), H<sub>2</sub>O<sub>2</sub> evolution, etc. Although improvements are identified, this process could be more systematic.
- Greater emphasis upon performance loss breakdown when polarization curves are taken.
- More reported detail about catalyst layer ionomers and polymer electrolyte membranes used in testing.

## Project # FC-04: Development of Alternative and Durable High Performance Cathode Supports for PEM Fuel Cells

Yong Wang; Pacific Northwest National Laboratory

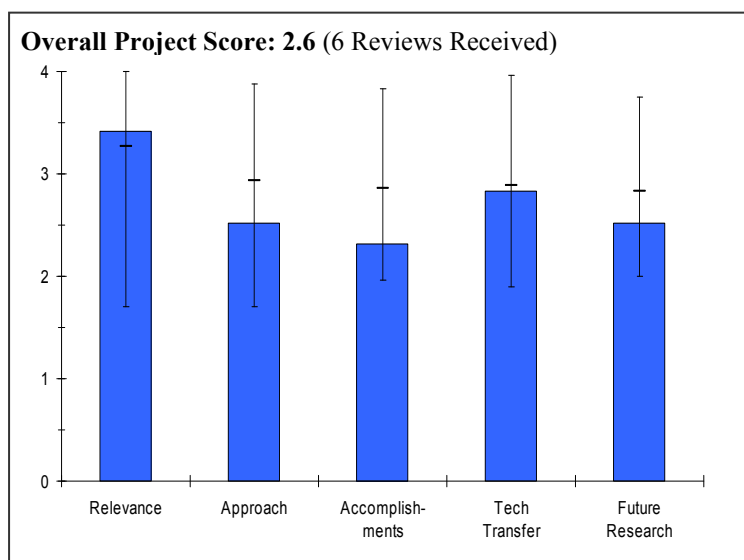
### Brief Summary of Project

The overall object is to develop and evaluate new classes of alternative and durable high-performance cathode supports. The objective for 2008 was to identify leading cathode compositions with better durability than carbon black supported Pt cathode.

### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Improvement of catalyst support is highly needed to meet durability targets.
- Improvement of catalyst utilization is highly needed to meet cost targets.
- Both improvements will aid fuel cell commercialization.
- Project is relevant to DOE objectives.
- The goal of the project – improving durability of the catalyst supports – is critical for the Hydrogen Fuel Initiative.
- Project is relevant to DOE targets although it is not properly focused.
- This project has the potential to yield valuable insight into the stability of the electrode supports leading to new guidance in durable electrodes.
- The testing of new materials as a support is critical to understanding and yielding a new stable electrode composition.
- The project objectives are relevant to the DOE objectives.
- Corrosion of conventional carbon supports is known to be a threat to automotive fuel cell durability targets. This project attempts to make more durable catalyst supports.
- Work that shows loss of Pt on Pt/ highly ordered pyrolytic graphite with electrochemical cycling (and not thermal stress) should be related to realistic *in situ* stresses (if necessary beyond providing answers about Pt deposition). Sulfuric acid anion has an unrepresentative interaction with Pt. The relationship of highly ordered pyrolytic graphite to realistic support in terms of contact angle, strength of Pt anchoring, and surface morphology is not established. This part of the work is not relevant to DOE objectives without all of the above.



### Question 2: Approach to performing the research and development

This project was rated **2.5** on its approach.

- Exploration of new supports is good.
- Unclear why carbon nanotubes are used due to cost.
- Residual Chlorine in catalyst layer will cause significant issues if not completely removed.
- Project management needs improvement.
- In general, approach is effective. However, it can be improved by more careful characterization of synthesized supports.
- Catalyst support projects should focus on un-catalyzed supports and not on supported catalyst.
- Pacific Northwest National Laboratory is not using DOE-defined accelerated test protocols so the data cannot be directly compared to data from other approaches/researchers.

- The protocols being used by Pacific Northwest National Laboratory probably cause multiple degradation effects (i.e., not isolated effects), rendering the data and conclusions suspect.
- Pacific Northwest National Laboratory needs to monitor mass activity as well as electrochemical area.
- An overall sound approach and good use of microscopy and electrochemistry.
- Pacific Northwest National Laboratory should not only evaluate the materials, but also evaluate them in an electrode structure and configuration that might represent what will be utilized in the fuel cell. It is not apparent that the tests included ionomer in the electrode or other components.
- Using E-TEK as a reference is understandable, yet the composition of E-TEK is proprietary; therefore, industry might not use it.
- The Pt/WC system was developed and studied by General Electric in the 1960s and 1970s.
- Good approach of utilizing different catalyst supports. Down selection criteria is suggested to relate to *in situ* testing as well.
- Even though the corrosion of carbon is well-known, the project does not seek to entirely eliminate carbon-containing structures. Catalysts that are entirely supported by alternative structures (e.g., WC, ITO) should be studied.
- Beyond the Pt/WC durability data, quantitative justification for the proposed supports is lacking. It would be interesting to see "downselection criteria" for supports such as electrical conductivity, thermal/hydrolytic stability, strength of Pt interactions, etc.
- Catalyst durability testing should seek to isolate failure modes (e.g., agglomeration and support loss).
- E-TEK should only be used as a baseline if the carbon structure or graphitization level is well-known.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.3** based on accomplishments.

- Accelerated protocol which is different than accepted industry protocol could be providing data which is not useful.
- These protocols make the progress difficult to assess.
- Limited/unclear durability data at this point.
- Going directly to new catalyst support with platinum jumps over the first ideal step of catalyst support durability alone.
- Technical accomplishments are not convincing. Quality of rotating disk electrode data is poor in order to claim higher catalytic activity of the synthesized catalysts compared to Pt/WC.
- The statement on higher surface area on synthesized supports is not supported by experimental surface area measurements.
- The statement on improved activity of Pt-TiO<sub>2</sub>-WC catalyst over E-TEK is not supported by experimental data given on the chart on P.14.
- The inappropriate protocols make the progress difficult to assess.
- It was not made clear that the TiO<sub>2</sub> system is more stable than the XC72 (slide 14).
- WC is as old as the early General Electric work of the 1970s.
- The testing should include negative voltages as well.
- Electrode stability is critical; yet it is the electrode that generates hydrogen peroxide which then destroys the ionomer in the electrode and the membrane. Can the team incorporate a peroxide generation test?
- What is the phase of WC as there are many sub-stoichiometric phases; same question for TiO<sub>2</sub>?
- Will the mesoporous carbon generate peroxide species?
- Pacific Northwest National Laboratory should spend more time on alternative supports and stability.
- The surface area from both Brunauer, Emmett, and Teller theory and electrochemical active Pt sites should be evaluated for each catalyst support system as well as Pt loss following cyclic voltammetry (CV) under both higher and lower potential conditions.
- *In situ* testing is suggested to be included in comparing and down selecting the supports.
- Although it has been observed that Pt/WC is more stable than WC, there is no clear indication why.
- Fundamental understanding of other Pt/support model systems (support = ITO, SnO<sub>2</sub>, TiO<sub>2</sub>, oxycarbides, SiO<sub>2</sub>) has not been shown.
- Scaffold structure has still not been selected, contrary to scheduled deadline in 2007.

- Pt/ ordered mesoporous carbon activity should be shown in comparison to Pt/XC72. Currents should be normalized by area.
- A considerable matrix of materials still needs to be synthesized by the end of 2008. The investigators have not shown the ability to quickly move through a large quantity of experimentation.
- TiO<sub>2</sub>-XC72 stability has not been clearly established over XC72 stability, given limited data set.

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.8** for technology transfer and collaboration.

- Good collaboration with existing partners seems to be appropriate for this program.
- Close collaboration between National Laboratories and the University; presence of industry is not indicated yet.
- The project needs more participation by industrial partners who build and operate stacks.
- Appropriate at this stage.
- Collaboration with others is not visible; Pacific Northwest National Laboratory should clarify the interactions amongst the group.
- There is no evidence of an Automotive Fuel Cell Cooperation contribution thus far.
- Oak Ridge National Laboratory has successfully been used to provide mesoporous carbon materials.
- The role of the University of Delaware is not clear. It is unknown if "model materials" refers to highly ordered pyrolytic graphite.
- Without evidence to the contrary, the project appears to be firmly led by Pacific Northwest National Laboratory with only material inputs from other organizations.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.5** for proposed future work.

- Using different accelerated protocol is a concern and should be reevaluated.
- Analysis of catalyst support alone would be a worthwhile intermediate step.
- In-depth cost analysis of the different catalyst supports would be useful before experiments begin.
- Future work is based on the previous progress.
- Priorities should be shifted towards identification of the reasons for low catalytic activity of the synthesized catalysts.
- Pacific Northwest National Laboratory needs to focus on supports before studying supported catalysts.
- Further work is as planned in the original scope.
- Additional detail on future work would be helpful – more specificity on what is going to be done (i.e., how does the work on interfacial interactions compare with prior work?).
- Better understanding of stability of such systems.
- Regarding the plan to test under potential sweep between 1.4-0.6 V, it is suggested to quantify electrochemically active surface area losses for each support system.
- It is suggested to consider including *in situ* testing following down selection of the support systems.
- Clarify path forward towards obtaining the 2X better stability than carbon black supports.
- Data to justify replacing XC72 with ordered mesoporous carbon and carbon nanotubes in future work has not been shown.
- Both potentiostatic and potentiodynamic testing should be considered for *in situ* future work if different failure modes are to be decoupled.
- Emphasis on *in situ* fuel cell work must be accelerated.
- Process for membrane electrode assembly fabrication will need to be validated, including ink formulation, ink application and gas diffusion layer selection.

#### **Strengths and weaknesses**

##### Strengths

- Analytical work is high.



- *Ex situ* materials characterization clearly demonstrated interaction between Pt and WC.
- Novel approach to synthesize carbon materials.
- Strong synthetic background.
- Solid team that understands the key stability issues.
- Team is not biased with respect to testing of new materials.
- Appropriate testing capability.
- This project is uniquely positioned to address catalyst support corrosion, a failure mode that is critical to meet DOE objectives.
- The project is linked to competent fuel cell research organizations (Pacific Northwest National Laboratory, Oak Ridge National Laboratory, Automotive Fuel Cell Cooperative, and the University of Delaware).
- The researchers demonstrate proficiency with the required test techniques.

### Weaknesses

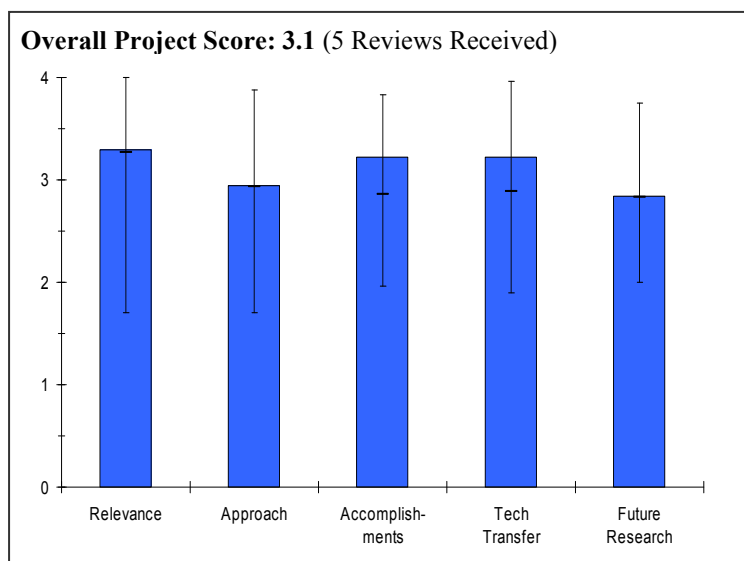
- Use of chlorine is a potential downfall.
- Use of different accelerated protocol.
- Not investigating durability/cost of catalyst support only.
- Project management.
- Quality of rotating disk electrode data needs to be improved starting from Pt/WC as a standard.
- Since the rotating disk electrode curve and mass activity for Pt/WC are not presented on P.14, it is unclear if poor catalytic activity of the synthesized catalysts is due to support of poor quality of rotating disk electrode data.
- In order to demonstrate better catalytic activity/durability, both surface areas and mass activities should be presented in absolute and relative numbers.
- Incorrect focus.
- Incorrect test protocols.
- Would like to see the team evaluate other potential support materials such as mixed metal oxides, sub-stoichiometric oxides, and not just use the same materials such as carbon nanotubes.
- Should understand other degradation issues such as dissolution, agglomeration, as well.
- Collaboration with others not visible.
- Several groups seem to be included; however, roles are not very clear.
- Fabrication of materials has not proceeded quickly enough.
- Researchers have not justified present scope of materials nor have they considered higher risk/reward possibilities that eliminate carbon.
- There has not yet been enough *in situ* fuel cell testing.
- Researchers need to carefully consider parameters used in test techniques, which metrics to report and how data are reported versus baselines.

### Specific recommendations and additions or deletions to the work scope

- Use of accepted accelerated protocol.
- Investigation of durability/cost of catalyst support only.
- Complement rotating disk electrode experiments with fuel cell testing.
- Suggest keeping the project; however suggest testing several types of catalyst-coated membranes other than Pt/Nafion-based and creating mitigation strategies as the effects of each impurity are investigated
- Collaborators, such as Oak Ridge National Laboratory, could be more valuable if involved at a level greater than merely material input.
- Attempt to synthesize Pt/WC or Pt/TiO<sub>2</sub> without carbon nanotubes, ordered mesoporous carbon or XC72.
- Delete *ex situ* testing if it interferes with time needed for more valuable *in situ* testing and post-mortem analyses.

**Project # FC-05: Highly Dispersed Alloy Cathode Catalyst for Durability***Sathya Motupally; UTC Power***Brief Summary of Project**

The objective of this project is to develop a structurally and compositionally advanced cathode catalyst that will meet the Department of Energy 2010 targets for performance and durability. The impact of oxygen on Pt dissolution and structural stability for various core/shell systems has been qualified. A number of elemental and alloy cores have been evaluated; Pd<sub>3</sub>Co and Ir cores lead to the highest improvement in oxygen reduction reaction. Various PtIrX alloys have been synthesized and tested to understand activity and durability trade-off. Objectives for the past year were the bench-scale demonstration of appropriate dispersed alloy catalyst formulations and downselection and verification of a dispersed alloy catalyst.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- Strong rationale for improving performance by 2.5X to achieve lowered catalyst loading while simultaneously focusing on durability to achieve 2010 goals.
- Addresses both fundamental understanding and pathway(s) for scaling catalysts and transitioning to practical systems to address DOE goals.
- Project is relevant to the Hydrogen Fuel Initiative.
- Addresses DOE goals on improved electrocatalytic activity/durability.
- 100 % fit with overall objectives.
- Commercialization of fuel cell vehicles will increase the price of any PGM (spot prices are irrelevant). The catalysts studied in this project all seek to displace Pt with other PGMs. This creates difficulty addressing cost.
- Fundamental knowledge gained from modeling and *ex situ* studies is not applicable toward reducing PGM content.
- There is no plan to investigate compositions that significantly reduce PGM content.
- This project has not addressed the "barriers" sufficiently – little supporting evidence that these catalysts have any advantage over Pt-only.
- COST has not been addressed adequately.
- The systems chosen (Pt-Ir, Pd, Au) do not appear to have any cost, loading, or durability advantages.
- Most of the presentation focused on modeling, but little evidence was presented to justify the investigation of the systems chosen for the research or that supported the fact that a core-shell structure existed.

**Question 2: Approach to performing the research and development**

This project was rated **2.9** on its approach.

- Strong approach with coordinated experiment and theory.
- Team roles and synergies are well defined.
- Strong scientific rationale that leverages best of mass activity and durability catalysts known to date to develop catalysts that exhibit both properties.

- Approach is well designed, but combines only fundamental instruments of catalyst investigation such as thermodynamic modeling and rotating disk electrode experiments.
- Approach can be improved by validating rotating disk electrode experiments with single cell testing.
- Results of modeling also need to be validated.
- Lack of microstructural characterization raises questions about core/shell structures.
- Convincing approach.
- Good use of complementary expertise.
- Use of broad background know-how.
- *Ex situ* cyclic voltammetry cycling does not speak to *in situ* durability. Investigators should develop *in situ* path forward immediately.
- Atomic structures (e.g., slabs) used for modeling may not be sufficient to capture nanoscale phenomena. Geometry not reported.
- So far, no consideration has been given to processes needed to obtain *in situ* data (e.g., ink, ink application).
- Again, a proper approach for reducing cost must seek to use non-PGM materials.
- Rationale for choosing bimetallic cores (Pd<sub>3</sub>Co and Pd<sub>3</sub>Fe) for analysis is unclear.
- There is way too much emphasis on modeling.
- The presenter did not provide sufficient evidence supporting the presence of a core-shell structure, however all modeling efforts assume that the catalysts are core-shell.
- MUST have additional confirmation that the catalyst structure exhibits core-shell (TEM, and X-ray photoelectron spectroscopy (XPS)).

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.2** based on accomplishments.

- Theoretical progress in understanding impact of oxygen on Pt segregation and dissolution is an important finding.
- Significant progress in demonstrating improved catalysts, including attempts to scale the technology.
- Good synergy between experimental and theoretical efforts – they are impacting each other beneficially.
- Principal investigator demonstrated promising results on durability and electrocatalytic activity.
- Progress is measured well.
- Interesting modeling activity; seems to be useful for catalyst development.
- Risk minimized by two parallel routes that might ultimately be combined.
- Reproducibility of mass activity data was not reported.
- The principal investigator did not present analysis to verify core/shell structure of Ir/Pt or Pd<sub>3</sub>Co/Pt samples.
- Activity / durability tradeoff with dispersed alloy materials was not presented with data.
- Effect of particle size or particle size distribution was not reported for any samples.
- For what was planned, bimetallic PtM modeling analysis was comprehensive.
- It is unclear why the catalyst systems listed in presentation (Ir, Au, Pd) have been chosen – these systems will not help reach cost targets or perform any better than Pt-only catalysts.
- Catalyst systems are more like "model" systems than practical fuel cell cathode catalysts.
- There are not enough comparisons with Pt-only catalysts to justify replacement with these alloy/mono-layer catalysts.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.2** for technology transfer and collaboration.

- Individual projects well coordinated, and results from theory and experiment impacting each other and accelerating the catalyst development effort.
- There is close collaboration between academic institutions and industry
- Small consortium with excellent individual expertise results in efficiency and effectiveness.
- The collaborators assembled (UTC Power, Johnson Matthey, Texas A&M University, and Brookhaven National Laboratory) have an impressive amount of experience and capability.

- There is no direct evidence of Brookhaven National Laboratory collaboration.
- Modeling performed by Texas A&M University directly led to core/shell selections.
- Johnson Matthey provided material input but it is unclear whether they provided additional collaboration.
- The collaborators on this project represent some of the best in fuel cell development, but it is unclear as to the role each is playing in the project and what goals have been reached/targeted by each participant.
- The majority of research presented focuses too much on modeling without supporting data on actual catalyst structure.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- Future plans clearly derived from most recent results and focus on further advancing the technological successes while addressing the remaining challenges.
- Future plans are based on previous progress and focused on problems identified during the first year of research.
- Natural straightforward continuation as proposed makes sense.
- Future work is confined to PGM catalysts.
- *In situ* durability tests are regarded as a late-project activity, but should be a primary part of the project.
- The project should place more focus on *in situ* durability to achieve DOE objectives.
- The future work should definitely include additional characterization to verify core-shell structure – otherwise, the modeling effort is not representative of actual catalysts being studied.
- A cost analysis comparing Pt-only catalysts to Pt(Ir,Pd) should be conducted to support additional work in this development effort.
- Present more evidence that shows that these catalysts demonstrate enhanced durability and activity. This should be a major focus.

#### **Strengths and weaknesses**

##### Strengths

- Appreciate honesty about scale-up issues and retaining performance. Good to hear about both successes and challenges going forward.
- Project combines both modeling and experimental parts.
- New modeling approach is developed to predict stability and durability of core/shell catalysts
- Small consortium with excellent individual expertise results in efficiency and effectiveness.
- Results of modeling are applied to limit experimentation.
- Researchers are familiar with experimental techniques and correctly use electrolyte with low interaction with samples.
- High mass activities are shown.
- Collaborators with proven experience are involved.
- Clearly, a strength is the modeling effort, but there is too much modeling without supporting data for the catalyst structure.

##### Weaknesses

- Lack of materials characterization.
- Activities evaluated by a rotating disk electrode technique are not validated with the fuel cell testing.
- Mass activities are not always accompanied by specific activities, raising questions about the origin of improved mass activities.
- Unclear if baseline Pt/C catalyst employs the same support as core/shell catalysts.
- Too many numbers were presented.
- Reliance only on PGM for all catalyst materials (and cores) with no other plans.
- Low derivation, at present, of fundamental knowledge relating activity to catalyst particle parameters or core/shell compositional analysis.
- No *in situ* durability data reported.
- Not enough emphasis on characterization of catalyst structure.

- Not enough information presented to justify investigating the catalyst systems chosen for study.
- Too much modeling, not enough testing.

### **Specific recommendations and additions or deletions to the work scope**

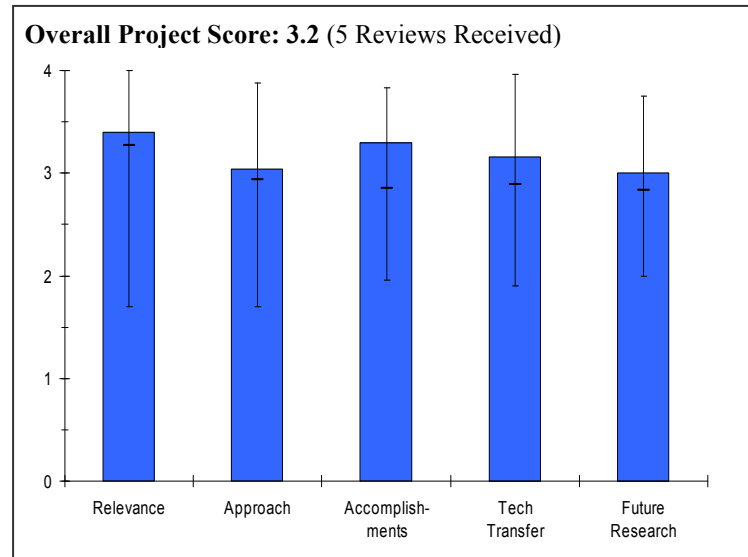
- Complement activities evaluated by rotating disk electrode technique by fuel cell testing.
- Validate results of thermodynamic modeling.
- Project should study catalyst particle cores that are non-PGM.
- Immediately begin to study *in situ* degradation phenomena.
- Directly compare of these catalyst systems to Pt-only catalysts to determine whether worth pursuing further.
- Greater evidence should be placed on activity and necessary loading of these catalyst systems compared with Pt-only.

**Project # FC-06: Fuel Cell Systems Analysis***Rajesh Ahluwalia; Argonne National Laboratory***Brief Summary of Project**

The objective of this project is to develop a validated system model and use it to assess design-point, part-load and dynamic performance of automotive fuel cell systems. This includes supporting the Department of Energy in setting technical targets and directing component development as well as establishing metrics for gauging progress of research and development projects.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.4** for its relevance to DOE objectives.



- Project elaborates valuable modeling tools to support development of fuel cell systems and components.
- Extremely relevant. Not only does competent modeling allow a more comprehensive screening of technology options, it is also clear that none of the current models accurately account for start-stop, part-load, or transient effects on durability. More and better modeling and simulation, especially those which could provide an indication of performance deterioration, are obviously needed.
- Relevance is compromised by use of only elevated temperature and not a complete range of stack operating temperatures.
- Original equipment manufacturers use of distinct fuel cell systems limits project relevance to its ability to describe system componentry to DOE and DOE-funded projects.
- Impurity modeling covers familiar phenomena and does not add to understanding of impurity effects.
- Project addresses design of a pressurized fuel cell system. Industry is reporting performance similar to pressurized systems at reasonable temperatures using atmospheric pressure. The energy losses associated with transients are not fully addressed while the load cycles for automobiles, stationary power plants, and motive power (e.g., forklifts) are based on rapid transients, even with battery hybrid systems.
- The project appears fully centered on compressors, thermal management, and water management technology associated with Honeywell and does not address a broad base of manufacturers.
- This project fully supports the objectives in developing an automotive-capable membrane electrode assembly design-principal investigator was wise to avoid premature discussion of high temperature systems. These models serve to establish trends and suggest efforts to achieve maximal results in the overall system design. Providing Sensitivity analysis is perhaps the most useful function of such models.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- Clear approach resulted in clear results!
- Collaboration with "real world" manufacturers as e.g., Honeywell is beneficial.
- Generally very good.
- Some of the assumptions appear to require more justification than presented.
- There was no evidence of expected accuracy and no real discussion of limitations.
- The effect of operational turndown ratios (pressure, flow rates, temperatures, humidification) and especially stop/start operation has not been sufficiently explored to determine consequences for system component selection.

- Investigators should consult future Directed Technologies, Inc. system assumptions (2010 and 2015). Enthalpy wheel is unlikely at commercialization due to total weight (including auxiliaries) and reliability.
- Analyzing needed Pt loading with changing operating conditions should be unnecessary since automotive operating conditions should already be assumed to be widely varying over a drive cycle.
- Stack operating conditions (100% relative humidity, outlet temperature vs. inlet temperature) should be verified.
- Consideration should be given to transient operation. Software packages (e.g., Simulink) exist to enable this.
- The project's analytical approach is based on GC-Tools. At one time, GC-Tool was a steady-state model and not capable of addressing transients. If this is still the case, the success of the project will be limited.
- Industry groups are using a version of Aspen which was adapted to address transients. Has Argonne National Laboratory considered using Aspen?
- The approach is strongly tied to Honeywell. Since Argonne National Laboratory is addressing the DOE model for fuel cell systems for more than automotive applications it is recommended the program consider other system component manufacturers.
- These models are only as useful as the information inputted in them. Principal investigator must take care to ensure that all the parameters used compliment each other. Principal investigator must avoid picking and choosing the best parameters from multiple systems.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- Important results for deeper understanding of system issues and further optimization of fuel cell systems/components.
- Collaboration with key players is strengthening the effort.
- Very good.
- Especially interesting were the efforts to assist in determination of nozzle area control to improve part-load efficiencies.
- Also very relevant was the inclusion of heat exchanger options to improve overall performance.
- Incorporation of variable area nozzle to facilitate both flow and pressure control is an important new addition to the model.
- Collaborations have allowed progress on modeling air management, water management and thermal management systems, but the deficiencies already mentioned in the "Approach" section prevent this project from delivering results more representative of automotive operation.
- System dynamics and membrane electrode assembly characteristics will have a profound effect on impurity buildup. The impurity calculations are not based upon dynamic assumptions, and therefore, progress here is left without value. Validation will be nearly impossible.
- The discrepancy between the Argonne National Laboratory model and the Japan Automobile Research Institute data appears to be dependent on which isotherm is used in the analysis. The presentation did not provide background information on the Langmuirian isotherm or the Temkin isotherms.
- What is the estimate for 35% high platinum loadings for atmospheric stacks based on? Does the Argonne National Laboratory data predict we have hit a limit for Pt loading? Argonne National Laboratory did not report the platinum utilization in the cell stack, but their prediction would require that information. How did Argonne National Laboratory come to this prediction?
- Rajesh's work is always thorough and provides a good feel for sensitivity of key parameters in the system design. The model could only be improved to a more realistic scenario if proprietary information is supplied. This is unlikely to occur.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.2** for technology transfer and collaboration.

- Dissemination of results and collaboration in various groups is very good.
- Generally appears to be very good.
- Most actual collaboration seems to be with only one or two groups.

- The project has collaborated moderately well with component-level organizations, such as Honeywell, 3M, Emprise, and PermaPure. In this respect, the project has gathered detailed component parameters and injected these parameters into the model.
- The project fails with respect to collaborations that would provide a more realistic set of assumptions for the overall system, in terms of both components and realistic automotive operating conditions. The proper parties are not listed in the presentation and must be sought out.
- Argonne National Laboratory is limited its system work to Honeywell and system components based on Honeywell compressor expander, Emprise, and PermaPure. It is recommended they include other system component manufacturers in their analysis who are operating at constant near-atmospheric pressure.
- Argonne National Laboratory is working with the North American Hydrogen Quality Team but did not mention the team composition or team's objectives.
- Principal investigator is collaborating with the appropriate national labs. Principal investigator could use more guidance from original equipment manufacturers to further narrow component and performance selection.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- Convincing.
- Generally good.
- No mention in presentation of plans for further efforts on start-stop, transients, extreme operating conditions, etc., which seem to have huge "real-world" effects on both fuel cell durability and overall efficiencies.
- At present, the work proposed for the future of the project continues with the same assumptions. Instead of attacking the minutia of humidifier operation, and attempting to learn automotive stack operation from a membrane electrode assembly supplier, the project needs to take a "step back" and reconsider many of the assumptions involved.
- The future work information provided was very broad and did not supply sufficient information regarding tasks Argonne National Laboratory would be working on.
- No statement regarding evaluations of transient systems.
- Continued work on the Honeywell compressor and Pacific Northwest National Laboratory humidifiers is recommended. Principal investigator should exercise caution about modeling a high temperature system until more robust information and results about such systems are provided. Principal investigator runs the risk of using too many unfounded assumptions at this point.

#### **Strengths and weaknesses**

##### Strengths

- Very clear – no confusing details.
- Adds much needed modeling capabilities especially in air management, heat exchangers, and water management. There are also possible benefits in reductions in platinum loadings.
- When given component-level collaborator information, the project aggressively seeks to incorporate it in its models.
- The addition of variable area nozzle for the air management system was a realistic step.
- The acknowledgement of oxygen loss issues in the enthalpy wheel was a needed addition.
- Argonne National Laboratory has developed a background in fuel cell systems that should provide support to DOE.
- Model ability to provide sensitivity analysis and gauge where progress need to be made to achieve maximum value for effort.

##### Weaknesses

- There seemed to be no planned modeling efforts in the areas where it is clear that "real-world" effects are having disastrous consequences relative to projected durabilities and efficiencies. This area should have very high priority.
- The model has not embraced widely varying operating conditions and modes.



- Assumptions regarding static stack operation must be removed unless hybridization is also an assumption (which, at present, it is not).
- The principal investigator has not developed system-level collaboration relationships. In fairness to the investigators, though, it must be acknowledged that many parties that could be helpful to this project have been reluctant to contribute.
- The limited interaction with fuel cell system component companies provides only a narrow view for analysis by Argonne National Laboratory. The incorporation of portable, stationary, and backup power would suggest that other fuel cell system designs will become important in the near term.
- The focus on steady state systems limits the value of the Argonne National Laboratory analysis. Transient systems are real world and need to be addressed.
- Not including transients is a weakness of the Argonne National Laboratory analysis.
- Information in is only as good as the information put in. Principal investigator must be clear about assumptions and clearly state references, etc.

### **Specific recommendations and additions or deletions to the work scope**

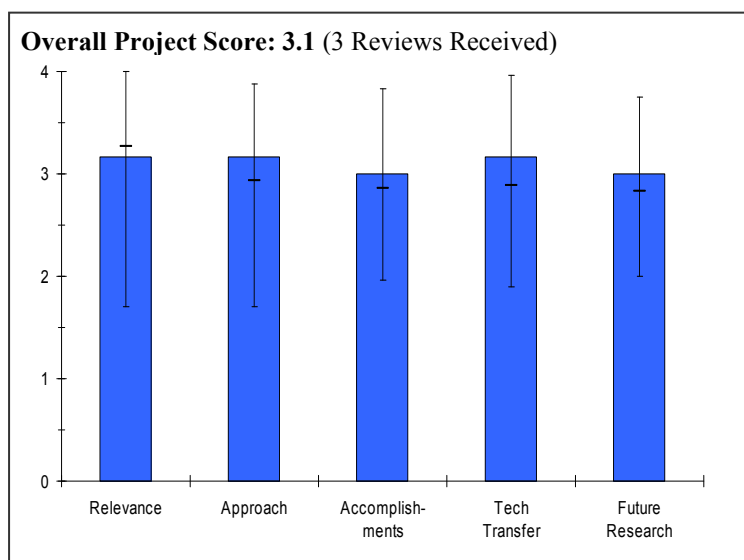
- Expanding from static to dynamic modeling would be great.
- Use composite National Renewable Energy Laboratory data (among other sources) to try to better take into account the various losses and adverse effects associated with repeated starts, idling, short run times, shutdowns, etc. of fuel cell vehicles.
- More emphasis should be placed on planning follow-on modeling and simulation.
- Cultivate relationships with multiple parties that run automotive fuel cell systems. Even though confidential borders exist, there should be some non-confidential means available of providing more realistic operating conditions and component assumptions. The possibility exists that just the operating conditions alone will be able to drive more realistic component assumptions once the operating condition implications are realized.
- Delete the impurity study.
- Ignore any feedback to perform system-level validation. The project is not yet ready.
- Consider transient operation.
- Argonne National Laboratory should include atmospheric fuel cell systems in their analysis using systems that are consistent with backup power, stationary power, portable power, and industrial motive power.
- Argonne National Laboratory should include transient evaluations in their analysis.

## Project # FC-07: Mass Production Cost Estimation for Direct H<sub>2</sub> PEM Fuel Cell System for Automotive Applications

Brian James; Directed Technologies, Inc. (DTI)

### Brief Summary of Project

The objectives of this project are to 1) identify system design and manufacturing methods for an 80-kW<sub>e</sub> direct H<sub>2</sub> automotive polymer electrolyte membrane fuel cell system based on three technology levels (2007 status technology, 2010 projected technology, 2015 projected technology); 2) determine costs for these three technology level systems at five production rates (1,000, 30,000, 80,000, 130,000, and 500,000 vehicles per year); and 3) analyze, quantify, and document the impact of system performance on cost. Some costs were not included (warranty, building costs, sales tax, and non-recurring engineering costs).



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Very good – captures cell stack assembly costs and balance-of-plant.
- The principal investigator demonstrated the relevance of the project to directing projects of technologic importance to meeting the long-term cost targets.
- The principal investigator demonstrated alignment with the major changes in technology metrics for the overall Program.
- Well-aligned with understanding the cost and path forward.
- By design does not address improving technical problems.

### Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- Very good – systematic approach. Balance-of-plant could have been further itemized (like the cell stack assembly) to focus industry as to where to focus development.
- The design for manufacturing and assembly approach provides a good basis for the analysis of the materials and assembly costs.
- Neglecting the building, safety and waste handling costs may have a significant effect especially at the lower volumes.
- Approach seems basically fine, though assumptions such as leaving out mark-up can be debated.
- It would be nice if impacts of excluded systems at some generic level could be an input to see if there are system-wide optimization trade-offs possible.
- Need to expand the sensitivity analysis of assumptions.

### Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Very good. Cell stack assembly component breakdown is detailed.

- The principal investigator demonstrated that the model has been refined from the previous year to reflect technological accomplishments and demonstrate key cost drivers at low and high volume production.
- The principal investigator demonstrated consideration of potential technology drivers that may increase the cost such as bipolar plate coating and stack conditioning.
- Re-evaluated the stack with updated projections. Seems they have gotten closer to a real system.
- Showed very different cost of high vs. low volume.
- Showed power density and Pt loading drive cost with membrane at low volume.
- Work has value but the rate of progress is not high.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.2** for technology transfer and collaboration.

- Estimated to be very good. It is assumed that the values and trends come from industry input and quotes.
- The principal investigator highlighted collaboration efforts to remain current with changes with technological metrics overall strategy.
- Suitable intersection with producers.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- Very good – Agree that balance-of-plant is the weak point.
- The project plans address some key cost assumptions that need further analysis in the model for the stack.
- Any significant cost drivers in the building and facilities management including safety and waste handling should be addressed in the cost drivers for the membrane electrode assembly and membrane processes.
- Suitable, but not aggressive.

### **Strengths and weaknesses**

#### Strengths

- Cell stack assembly cost model.
- Balance-of-plant estimates.
- The project provides some good general direction and confirmation of the future direction for the importance of technical projects.
- The principal investigator seems to have taken into account changing technology metrics for the stack and system design into the evaluation of future cost.

#### Weaknesses

- Platinum cost estimates.
- Balance-of-plant component details.
- The project uses potentially divergent assumptions of the lowest cost manufacturing and the highest performance membrane electrode assemblies, which may lead to divergent results and may need to be taken into account more fully in the sensitivity analysis.
- The cost of the building and infrastructure was not taken into account and may be a major sensitivity especially at the lower volume.

### **Specific recommendations and additions or deletions to the work scope**

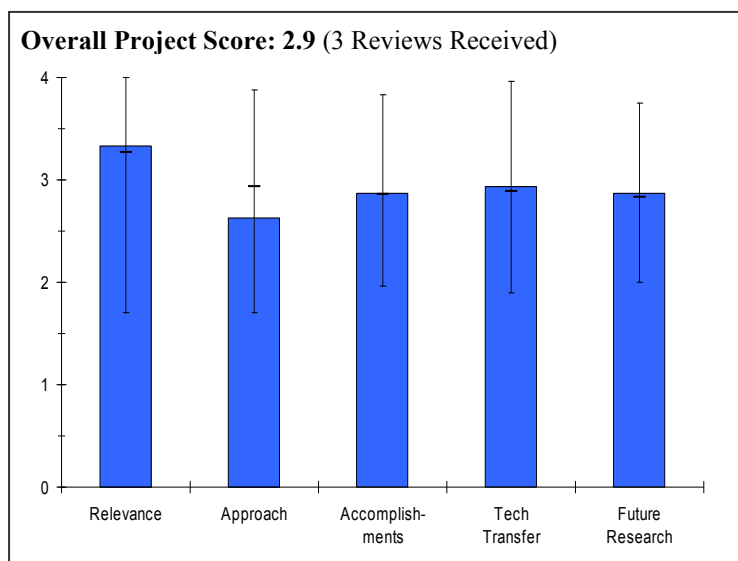
- No mention of synergy between stationary and transportation markets. One area of synergy would be balance-of-plant hardware: regulators, valves, sensors, blowers, etc.

## Project # FC-08: Direct Hydrogen PEMFC Manufacturing Cost Estimation for Automotive Applications

Jayanti Sinha; TIAX

### Brief Summary of Project

The overall objective of this project is a bottom-up manufacturing cost assessment of an 80-kW direct H<sub>2</sub> polymer electrolyte membrane fuel cell system for automotive applications. The objectives for 2007 were to 1) conduct a high volume (500,000 units per year) cost projection of the Argonne National Laboratory 2007 polymer electrolyte membrane fuel cell system configuration assuming a nanostructured thin film-based membrane electrode assembly and a 30 μm membrane; 2) conduct a bottom-up manufacturing cost analysis of balance-of-plant components; 3) perform a sensitivity analysis on stack and system parameters; and 4) economies-of-scale impacts on 2007 balance-of-plant costs. The objectives for 2008-2011 are to provide annual updates of high-volume cost projections.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Cost analysis is important to identify technology path toward commercial viability.
- Allows evaluation of status of cost and sensitivity of cost that are important in making progress in this one metric.
- Analysis of the manufacturing cost of state-of-the-art fuel cell technology is critical to appropriating research and development funds appropriately and should be undertaken annually, or as frequently as the rate of technology development progress justifies.

### Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- Only one technical assumption is used. Various technology assumptions should be analyzed to identify promising technology path.
- Enthalpy wheel is not a very likely component, but may have seemed so once. Otherwise reasonable approach.
- Only one state-of-the-art membrane type was considered; analysis of additional membranes or fuel cell systems would ensure that all of the potentially important manufacturing cost factors are identified.
- Assumptions and approach appear to be appropriate.

### Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- More detailed sensitivity study is required.
- Dedicated balance-of-plant components, such as H<sub>2</sub> blower and turbo compressor, should use bottom-up cost model. Off the shelf components, such as the radiator, should use industry standard.
- Economies-of-Scale analysis is good.
- Detailed breakdown is necessary.

- See that material is 44% of cost for balance-of-plant and labor is 33%.
- New assumptions lower cost significantly but have similar sensitivity.
- Compressor-expander is a high-cost item in the balance-of-plant.
- TIAX has completed its 2007 manufacturing cost estimate using a 3M-like membrane.
- Costs have been analyzed for the stack and the balance-of-plant.
- Sensitivities to various parameters were presented, and the most important ones were identified.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.9** for technology transfer and collaboration.

- Collaborates with Argonne National Laboratory and accesses suppliers' information.
- Proper contact with suppliers and original equipment manufacturers through the FreedomCAR Fuel Cell Technology Team.
- TIAX has coordinated with component developers and vendors to ensure that the appropriate assumptions and inputs are used and has plans to vet the model and results with them as well.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- Future plans are appropriate.
- Analysis of additional membranes/systems should be considered in future years.

### **Strengths and weaknesses**

#### Strengths

- TIAX seems to have strong collaborations with technology developers and vendors to acquire appropriate inputs for their model and to vet the assumptions and results.
- The project strongly supports the DOE research and development program by examining the cost impacts of fuel cell system components and suggesting research priorities.
- The bottom-up approach to cost analysis is appropriate for a state-of-the-art system where some of the parts are not yet manufactured in volume.

#### Weaknesses

- Duplication with the Directed Technologies, Inc. project.
- Analyzing only one state-of-the-art membrane/system may limit the identification of potential manufacturing cost impacts.

### **Specific recommendations and additions or deletions to the work scope**

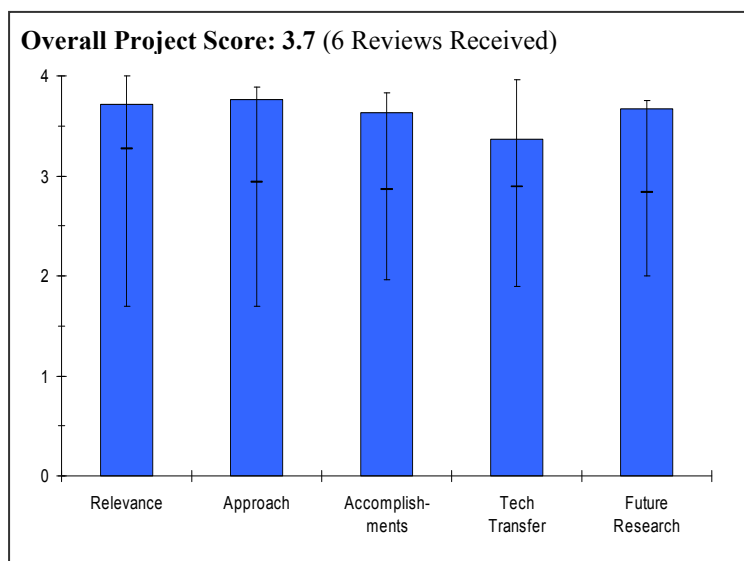
- Consider analyzing multiple fuel cell systems in future manufacturing cost estimates.

## Project # FC-09: Microstructural Characterization of PEM Fuel Cell MEAs

Karren More; Oak Ridge National Laboratory

### Brief Summary of Project

The overall objectives of this project are to 1) identify high resolution imaging and compositional/chemical analysis techniques for characterization of the material constituents comprising polymer electrolyte membrane fuel cell membrane electrode assemblies; 2) apply these analytical and imaging techniques for the evaluation of microstructural and microchemical changes that determine fuel cell stability; and 3) elucidate microstructure-related degradation mechanisms contributing to polymer electrolyte membrane fuel cell performance loss. Collaboration with industry, academia, and national laboratories will be conducted to make these techniques (and expertise) available to correlate structure and composition with membrane electrode assembly processing and life-testing studies.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- Critical program for obtaining fundamental insight into the structural nature of fuel cell materials.
- The study of catalysis and supports is critical to President's Hydrogen Fuel Initiative.
- Microstructural analysis is needed to gain scientific understanding of the effect of structural parameters of fuel cell materials (including changes occurring as a result of specific operating conditions) on their performance and durability.
- Project has provided significant value to DOE program. Insight into structure and durability gained by pictures obtained are invaluable to other researchers.
- Tool development is novel and interesting. Tools can address key aspects of catalyst durability and structure.
- This project is valuable to the overall objective since it provides another analytical tool to observe and measure catalyst activity in fuel cell applications. Full understanding of catalyst activity and distribution is fundamental to achieving loading targets.

### Question 2: Approach to performing the research and development

This project was rated **3.8** on its approach.

- Excellent state-of-the-art facilities and knowledge of how to use them to address the durability and structural aspects of catalysts.
- Very high-resolution microscope down to 0.75 angstroms, probably a unique tool for catalysis imaging.
- 3-D profiling, able to image metals on carbon.
- *In situ* microscopy.
- Advanced Electron Microscopy techniques are very suitable for atomic-scale characterization of structure and composition.
- All tools, know-how, and experience necessary to meet the project milestones are available.
- *In situ* imaging is needed to better understand aging effects in fuel cells. The size scales investigated in this project have not been approached by other techniques.
- Depth profiling has value in non-precious and low loading catalysts.

- Tool development helps others in their development efforts but does not directly address critical barriers.
- Very strong technical tools. Should work to maximize available insight.
- Work should focus on providing high throughput characterization, with associated statistics, of most important catalysts.
- The work would benefit from a much better feel for how common some of the reported effects are. Because of the inherent singular nature of sampling and studying images, one is left with a question (whether justified or not) of how pervasive a given effect is.
- Additional quantitative analysis, provided by modeling coupled to investigations of kinetics of particle growth processes, particle size dependence of processes, etc would be highly desirable.
- The principal investigator is using a very high resolution technique to film catalyst orientation and migration. Currently the technique has not been demonstrated *in situ* in a fuel cell application or in a fuel cell environment (e.g., in an ionomer dispersion). This is the next step required to achieve a representative observation of catalyst activity in a true fuel cell environment.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.6** based on accomplishments.

- The principal investigator and her colleagues have demonstrated a significant amount of progress and output of results for the resources applied to this project. They are pushing the envelope in terms of catalyst structure characterization. This knowledge should translate well to understanding how to overcome the durability or performance targets.
- Acquired new microscope upgrade.
- *In situ* microscopy observed agglomeration of Pt particles on the nm scale.
- Continued excellent evaluation of catalysts.
- *In situ* microstructural characterization of materials in a fuel cell environment is an important accomplishment to accelerate understanding of fuel cell degradation mechanisms.
- Depth sectioning and 3D reconstruction enable a more detailed determination of the structure of catalyst nanoparticles, such as core-shell.
- Visualization of Pt migration across the surface at high temperature can be very valuable to durability issues.
- Depth profiling and single atom resolution have been very impressive.
- There can be no doubt that this work is a tour de force.
- This provides an excellent and unique picture of critical processes occurring on the supported catalyst.
- Automation of the film is the next logical step and principal investigator indicates that that work is in progress.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.4** for technology transfer and collaboration.

- Very good outreach attempts and communication of results.
- Excellent, biggest goal is to collaborate with industry.
- Provides extremely useful characterization to several other DOE contractors.
- The principal investigator works with key members of the fuel cell community and has excellent collaborators.
- The expertise gained by this project hasn't been passed along to other members of the TEM community; the discrepancy between other researcher's TEM quality and this project's TEM is significant. Educating the community to provide higher quality data would be beneficial.
- Strong effort to pull together most major players.
- Given the potentially limitless supply of possible collaborators and sample sources, I would suggest that the principal investigator put together an unbiased advisory group to help to set priorities.
- Principal investigator has just recently demonstrated feasibility of concept and tool and is openly seeking partners to test materials. Success of this technique will depend on successfully collaborating with many catalyst developers using different techniques and materials.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.7** for proposed future work.

- Some aspects of the future work plan should be reconsidered. Trying to solve carbon support degradation mechanisms with TEM may not be sufficient, and in the end, it will not likely be able to eliminate the corrosion that is a fundamental limitation of carbon supports. Increased application to understand better things that work well (e.g., catalyst aspects which give increased activity) may have greater impact than studying things that are destined to fail.
- *In situ* holder for microscopy extended to voltage cycling, liquids, and electrolyte.
- Statistical analysis.
- Collaborations for relevant experiments.
- Further develop 3D technique.
- This is a comprehensive and ambitious plan.
- Tools demonstrated to date will be extremely useful.
- It is unclear that proposed *in situ* tests (humidity, liquid water) will give enough information to be useful.
- With the addition of quantization and statistics, this project could be invaluable.
- Principal investigator will automate system and attempt to view activity of particles in an ionomer dispersion (i.e., fuel cell environment); this is the next key milestone for them.

**Strengths and weaknesses**Strengths

- The experience of the principal investigator and team combined with the great facilities and willingness to apply their tools to others' problems of interest.
- Dedication of extremely powerful imaging techniques to fuel cell relevant catalysts.
- Unique capabilities and expertise to address the need for microstructural visualization of catalysts and membrane electrode assemblies.
- Enables other DOE contractors to improve performance, durability and cost of materials they are developing.
- Widely applicable to other projects. This project alone will not enable fuel cell commercialization. However, it is advancing the state-of-the-art significantly and has a broad collaboration base.
- Some of the most powerful microscopy equipment expertise available.
- Very strong technical leadership.
- Taking advantage of access to advanced and relevant catalysts.
- This technique allows researchers to greatly improve observation of catalyst particle migration which will clearly lead to improved catalyst/ support designs in the future.

Weaknesses

- Need for more *ex situ* synthetic manipulation at Oak Ridge National Laboratory to support project.
- Could use statistics and collaboration with strong modeling.
- Technique might not be suitable for all catalyst alloys – i.e., the principal investigator indicated that the technique does not distinguish well between Pt and Ir in a Pt/Ir alloy.

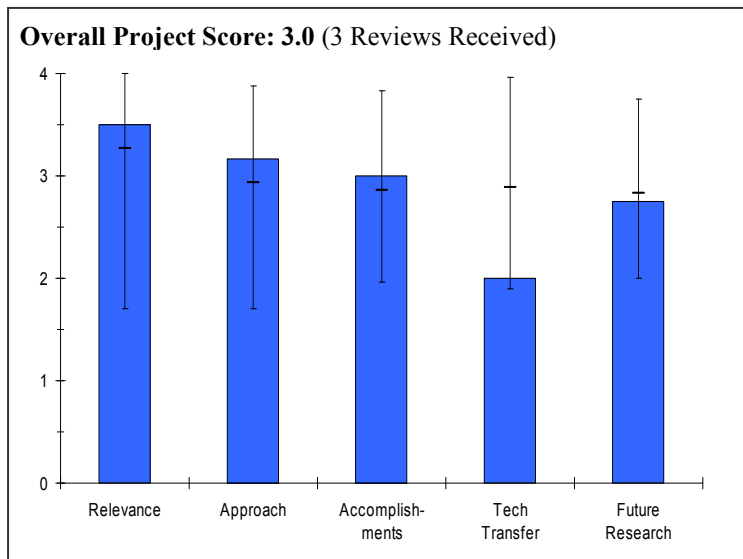
**Specific recommendations and additions or deletions to the work scope**

- Recommend reducing the effort to study carbon corrosion and spend more effort on developing capabilities to reveal surface structure and surface composition of catalysts that determines activity and stability under high voltage.
- Educating the community to provide higher quality data would be beneficial.
- Collaboration with group or groups that model nanocatalysts would be ideal.



**Project # FC-10: Applied Science for Electrode Cost, Performance, and Durability***Christina Johnston; Los Alamos National Laboratory***Brief Summary of Project**

The overall objective of this project is to assist the Department of Energy's Hydrogen, Fuel Cells & Infrastructure Technologies Program in meeting cost, durability and performance targets by addressing issues directly associated with electrodes. In 2008, Los Alamos National Laboratory will explore the effect of catalyst ink composition and processing on utilization and performance. Additionally, Los Alamos National Laboratory will use microscopy and other tools to better understand structure and impact on performance.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- The work reported is interesting but will not yield significant findings to advance the electrode inks that the membrane electrode assembly companies do not already understand.
- Cannot see how this program will yield fundamental knowledge.
- Pt catalyst/electrode is one of the most critical technical areas.
- Comprehensive investigation on Pt catalyst/electrode is valuable to characterize electrode/membrane electrode assembly.
- The project is focused on the major barriers to fuel cell commercialization, namely performance, durability and cost.

**Question 2: Approach to performing the research and development**

This project was rated **3.2** on its approach.

- The approach is not at a high enough level for the talent of the group. Also, the electrodes in these studies may not reflect what are actually used in commercially available membrane electrode assemblies. It is expected the learnings will be utilized by the membrane electrode assembly manufacturers but they should already have these data.
- The ionomer in the electrode and its effectiveness as a proton conductor should be studied in greater detail. In particular, the "architecture" of the electrode.
- Selected methods, like ball milling, are not considered serious fabrication methods as 1) ball milling will break up agglomerates, not nanoparticles, 2) ball milling is well known to introduce impurities which come from the media.
- Should use jet milling.
- It is good to cover various approaches in a project.
- A more detailed explanation of the approach would be helpful.
- How do ink composition and processing affect electrode durability?

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Work reported is not representative of what should be coming out of Los Alamos National Laboratory in particular the role of the ionomer in the electrode (slide 20). This result should be a sign of the role of the ionomer in the structure of the electrode.
- There are other properties of the electrodes which should be looked at to try to correlate performance with such key properties, e.g., pore size distribution, effect of microlayer, ionomer composition and placement, particle (and agglomerate) size, tortuosity – all as a function of processing.
- Good analysis on electrochemically active surface area methodologies.
- Some insight into the catalyst ink processing and effect of ionomer to catalyst ratio was gained.
- More compelling conclusions are needed to help fuel cell developers.
- Properties of "advanced" catalyst should be described in more detail, and an explanation offered why they behave differently than the conventional catalyst.
- Data suggests that half-cell results are not relevant to fuel cell operation.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.0** for technology transfer and collaboration.

- This is satisfactory as there needs to be an environment to report the results openly.
- Should encourage closer ties to membrane electrode assembly companies or companies that supply the inks.
- For the research to be helpful to fuel cell developers, the studies should be applied to common classes of catalysts, which should be described in sufficient detail to allow application of the results to any particular catalyst.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- The role of catalyst layer interactions studied by neutron scattering is highly recommended in addition to the proposed work on solutions.
- Greater emphasis on architecture and the structure and placement of the catalyst particles is suggested to assess electrochemically active surface area.
- It is good to cover ink solution to characterize electrode. Development of water management metric will be necessary.
- It is recommended to extend Pt alloy catalysts for electrode characterization.
- It is recommended to pursue a durability evaluation.
- Correlating composition and processing to aging is extremely important.
- Study of advanced supports has the potential to better integrate this project with other DOE projects focused on developing such catalysts.

**Strengths and weaknesses****Strengths**

- National lab facilities and talent.
- Independent.
- Fundamental studies can be focused on significant details science-wise.
- Project has potential to provide some fundamental understanding of basic ink and electrode parameters.
- Electroanalytical results were correlated to microstructural analysis.

### Weaknesses

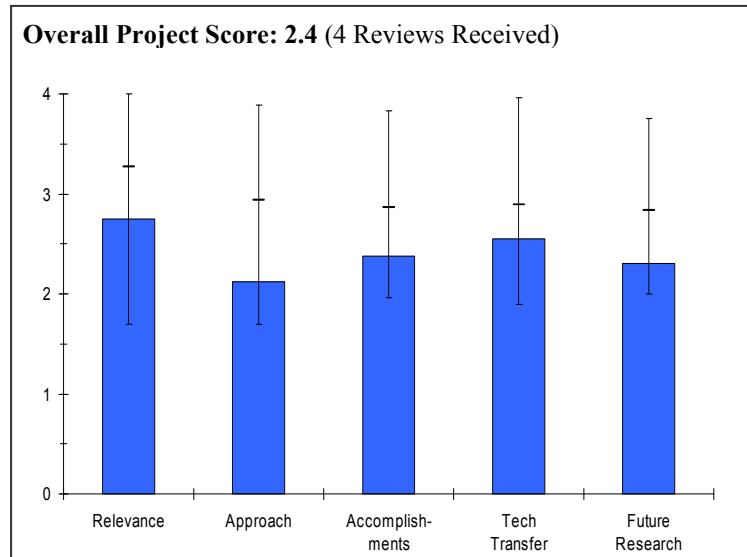
- This is a very difficult topic and one which needs the strength of the national labs but with the ties to a membrane electrode assembly company. The proposed work suggests looking at alternative supports, etc. Stick to the current scope.
- Approach is not well defined.
- Durability has not yet been addressed.

### Specific recommendations and additions or deletions to the work scope

- Take the science to the next level and do not dilute the effort. The learnings here are too valuable and must be representative of real world ink processing. Get the guidance from meetings with the membrane electrode assembly companies.

**Project # FC-11: Low-cost Co-Production of Hydrogen and Electricity***Fred Mitlitsky; Bloom Energy***Brief Summary of Project**

The objectives of this project are to 1) demonstrate cost-effective, efficient, reliable and durable solid oxide fuel cells for stationary applications; 2) determine the economics of hydrogen and electricity co-production for comparison to stand-alone hydrogen production facilities; and 3) determine the feasibility of a delivered cost of hydrogen below \$2.50 per gallon of gasoline equivalent. The rated power of the planar solid oxide fuel cell system, planar solid oxide fuel cell system efficiency, of >45%, and remote monitoring was demonstrated. The hydrogen pump design was validated with a 15-cell prototype connected to the planar solid oxide fuel cell test stand.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.8** for its relevance to DOE objectives.

- This project does not address the barriers in the DOE H<sub>2</sub> Program for polymer electrolyte membrane fuel cell stationary units, as the system is a solid oxide fuel cell.
- Economic analysis of the hydrogen production has not been done yet.
- This project addresses programmatic infrastructure goals through distributed production of hydrogen from natural gas.
- Target of \$2.50 per gallon of gasoline equivalent.
- Stationary power generation using a solid oxide fuel cell.
- Project is highly relevant. High electrochemical efficiency (low power required/kg H<sub>2</sub>) ~\$0.12/kg H<sub>2</sub>@ \$0.10/kWh electrical costs seems compatible with DOE targets.
- It is an excellent idea to build and test a dedicated fuel cell system for using the hydrogen that is not consumed at the anode for some useful purpose. The value of the hydrogen as a fuel or industrial resource could in some niche markets be greater than the value of the electricity. Diverting a reformer for hydrogen production exclusively/primarily could increase the capacity utilization of this device, and therefore its economics.

**Question 2: Approach to performing the research and development**

This project was rated **2.1** on its approach.

- It is uncertain how a small demonstration project like this one can hope to realistically demonstrate the feasibility of a delivered cost of hydrogen below \$2.50 per gallon of gasoline equivalent. The hydrogen is produced and not delivered anywhere outside of the demonstration site. It is not a true delivery scenario.
- Approach is a planar solid oxide fuel cell coupled with H<sub>2</sub> pump.
- Demonstration target is H<sub>2</sub> of sufficient purity to power a polymer electrolyte membrane fuel cell.
- Hydrogen outlet gas constituent compositions are not discussed.
- Technology is based on solid oxide systems. These types of high temperature systems offer the potential for the highest efficiencies but have the most severe materials issues (interfaces, sealing, etc.).
- Co-production of hydrogen and electricity by combining a solid oxide fuel cell with an electrochemical pump.
- System will run on (mostly) natural gas. Future system proposed to run on liquid fuels like ethanol.

- Exhaust gas from the solid oxide fuel cell stack is utilized in the H<sub>2</sub> pump. Essentially the pump removes residual H<sub>2</sub> for transportation polymer electrolyte membrane fuel cell uses. Turn down in solid oxide fuel cell system produces more hydrogen.
- Water gas shift system greatly reduces power needs to operate.
- Bloom has excellent understanding of solid oxide fuel cell barriers and has apparently overcome many at least short-term barrier issues. However, not enough stack data provided.
- The project is too loosely integrated. Other concepts have a more integrated solid oxide fuel cell/electrolyzer that will probably have better efficiency. The electrochemical pump is a subcontracting project and almost an add-on.
- Principal investigator should describe the electrochemical hydrogen separator in more detail, in achieving purity requirements.
- The system uses external reforming (not internal) with good thermal management (slide 6). Slide 6 with the schematic of the system design is excellent.
- Although the project team evaluated pressure swing adsorption vs. electrochemical H<sub>2</sub> pumping vs. partial pressure swing absorption), it could have also considered chemical separation, such as preferential oxidation or methanation. It should state the reasons for downselecting to H<sub>2</sub> pump over these options as well.
- The project team is planning to test the system with which liquid fuel?

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.4** based on accomplishments.

- Hydrogen purity discussed in round about fashion – gas impurities targeted were only CO and CO<sub>2</sub>, how is S in reformed natural gas removed?
- The benefit of a Hydrogen pump is its ability to produce H<sub>2</sub> at high pressures for storage in vessel or delivery to vehicle, otherwise all it is a separation membrane. Why isn't higher pressure H<sub>2</sub> produced?
- Performance degradation not discussed and principal investigator indicated stack technology is off limits for discussion.
- H<sub>2</sub> pump is under construction.
- Operation of planar solid oxide fuel cell at >45% system efficiency.
- H<sub>2</sub> purity analysis concentrated only on CO<sub>2</sub> and CO; need to consider other impurities especially H<sub>2</sub>S.
- Demonstrated 3000 hr of balance-of-plant component testing.
- Demonstration in Alaska in Q3 of 2008 (this has slipped from planned start in Q1).
- The 120-cell hydrogen pump stack was just recently developed. The state of development and testing of the Bloom solid oxide fuel cell system is uncertain.
- Hydrogen pump earlier validated with 15-cell prototype.
- System efficiency of 45% for solid oxide fuel cell claimed. Good but not overly impressive. Apparently over 50% has been demonstrated in the lab.
- No publications or presentations listed.
- There was little data presented. It is difficult to evaluate the electrochemical tradeoff between fuel cell/reformer/electrochemical pump.
- Slide 15 shows a decrease in electric power required per unit of hydrogen when water gas shift reactors are used. The primary reason for this is the increase in hydrogen concentration in the gas stream after the water gas shift reaction, resulting in a lower power requirement per unit volume of hydrogen gas. The increase in hydrogen concentration at the anode might be expected to lead to an increase in electrical power requirements per unit volume of gas due to the lower concentration gradient of hydrogen across the hydrogen pump's electrolyte. Therefore, Slide 15 implicitly shows the trade-off between 1) higher electrical power requirements per unit volume of gas due to a lower H<sub>2</sub> concentration gradient across the electrolyte in the case of water gas shift use and 2) the higher concentration of hydrogen in the water gas shifted reformat leading to more H<sub>2</sub> available for diffusion. However, it would be helpful to clarify Bloom's desired take-aways from this slide.
- Bloom seems to have accomplished good progress considering the funding level.
- 25 kW system tested for > 3000 h, team of operators trained, remote monitoring was set-up, and control systems developed for transient operation.

- Demonstrating above 45% net electrical efficiency (DOE goal) in the lab is quite good. Principal investigator should show these results in the field. Principal investigator should report hydrogen generation efficiency, and overall efficiency (electricity and hydrogen), as a function of hydrogen generation rate.

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.6** for technology transfer and collaboration.

- Collaborations are weak. H<sub>2</sub> Pump is the only collaborator discussed in presentation.
- Partnership between Bloom Energy and H<sub>2</sub> Pump LLC, with each partner concentrating on individual components.
- Collaboration with system component supplier (H<sub>2</sub> Pump LLC) and University of Alaska for demonstration.
- Bloom may or not be the commercializer; however, likely will need a commercialization partner and this is not evident.
- Bloom works well with University of Alaska. Remote monitoring will greatly aid the project.
- Excellent to collaborate with a local university (University of Alaska, Fairbanks). This collaboration brings educational and research opportunities for the university, and is excellent educational outreach.
- Downselect process for Anchorage Airport as installation site is based on having excellent potential commercial customer there. Great partnering.
- Bloom Energy outsources the electrochemical hydrogen separation entirely to third-party supplier (H<sub>2</sub> Pump LLC). This approach is of greater benefit to the DOE, in that other fuel cell system developers also have the opportunity to use this technology in their systems and push technology progress forward more quickly, collectively.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.3** for proposed future work.

- Future work weak. No mention of demonstration. It appears that all work is on H<sub>2</sub> pump, which is not really a pump.
- Remainder of project fabricates H<sub>2</sub> pump, connects to planar solid oxide fuel cell and installs in Alaska.
- As Demo project, there is little in the manner of research.
- Phase II will provide a field demonstration for a 25 kW solid oxide fuel cell system in Alaska. 50% peak net electrical efficiency demonstrated in lab testing in California.
- The hydrogen pump module will be tested in California; plans call for the integrated system to be tested in California. Not clear why the integrated system planned to be tested in Alaska is not to be done although it appears that there have been some slippage in the project plan.
- Project appears to be on schedule to achieve goals.
- Demonstration of the economics of hydrogen co-production is an excellent future task.
- Electrochemical hydrogen separator testing and optimization and integration with solid oxide fuel cell onsite is an excellent future path.
- Principal investigator should show more results similar to slide 15 illustrating the effect of system design changes on H<sub>2</sub> pumping efficiency, system efficiency, H<sub>2</sub> production rate, etc.
- Slide 6 shows a water gas shift reactor orientated at the anode exhaust. While water gas shift reactors have been developed for use between a fuel reformer and the fuel cell stack (in polymer electrolyte membrane and phosphoric acid fuel cell systems), this change in orientation of the water gas shift may be expected to require additional research and development work. For example, water gas shift reactor catalysts tend to work well at relatively low temperatures (around 200°C). To better integrate a water gas shift reactor with a high temperature solid oxide fuel cell, it may be helpful to conduct additional research and development on higher temperature water gas shift reactor catalysts.

#### **Strengths and weaknesses**

##### Strengths

- Demonstration project with novel design.
- Good choice of technology for best efficiency.

- Good plan for demonstration.
- Separates fuel cell from hydrogen generation - does not do what some have proposed by combining solid oxide fuel cell and electrolyzer in one device, which would not be desirable from a materials standpoint.
- Uses reasonable electricity costs to evaluate system efficiency for hydrogen production.
- Good system integration to improve efficiency but timetable to demonstrate this is not clear.
- A strength of the project is successfully designing, building, and testing systems with a high net electrical efficiency.
- Speaker was polite, diligent, and informed in response to reviewer questions, and with clear communication style.
- Bloom seems to have accomplished good progress considering the timeline and funding level.
- Successful collaboration with many parties (such as local utilities).

### Weaknesses

- Principal investigator was evasive, no real information was disclosed.
- H<sub>2</sub> pump should produce usable pressure. There are several electrochemical compressors under development with DOE funding that can deliver 4000 psi today. There are also working H<sub>2</sub> separation membranes that can be purchased off the shelf. The purpose for H<sub>2</sub> pump needs to be defined.
- Very little science discussed.
- Little in-lab long term testing before attempt field demonstration - only 3000 h of testing to date and only on balance-of-plant components. Previous researchers have found this to not be desirable.
- System cycling could present very severe materials issues.
- Overall system costs not clear.
- Bloom Energy appears to view electricity as more valuable than heat recovered for hot water and space heating, and as a result, does not do cogeneration at this site. However, in Alaska, the demand for heat can be great. At certain times and in certain locations (such as at night in a cold climate such as Alaska), heat can be more valuable than electricity. Therefore, some exploration of cogeneration of heat could be useful.
- Although the project team evaluated pressure swing adsorption vs. electrochemical H<sub>2</sub> pumping vs. partial pressure swing absorption, they could have also considered chemical separation, such as preferential oxidation or methanation.
- Bloom should report H<sub>2</sub> production rate as a function of H<sub>2</sub> generation efficiency and overall efficiency (electricity and hydrogen).

### Specific recommendations and additions or deletions to the work scope

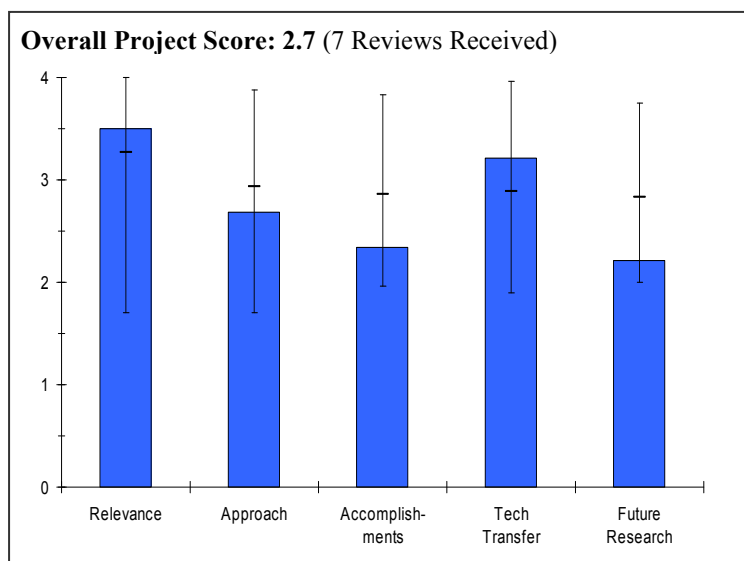
- Analysis of H<sub>2</sub> purity from H<sub>2</sub> pump, concentrating of polymer electrolyte membrane fuel cell poisoning species (H<sub>2</sub>S, S-containing hydrocarbons, CO).
- Need economic analysis of the hydrogen production
- Provide date and evidence for integrated system testing; would have been nice to have done this in Alaska as originally planned.
- Include analysis for system integration parameters/strategy to show optimum overall system efficiency.
- Bloom should work more closely with researchers from Sandia National Laboratories and the National Renewable Energy Laboratory to include accurate representations of similar systems in these laboratories including environmental and financial models of hydrogen co-production.
- Slide 6 shows a water gas shift reactor orientated at the anode exhaust. While water gas shift reactors have been developed for use between a fuel reformer and the fuel cell stack (in polymer electrolyte membrane and phosphoric acid fuel cell systems), this change in orientation of the water gas shift may be expected to require additional research and development work. For example, water gas shift reactor catalysts tend to work well at relatively low temperatures (around 200°C). To better integrate a water gas shift reactor with a high temperature solid oxide fuel cell, it may be helpful to conduct additional research and development on higher temperature water gas shift reactor catalysts. Also, Bloom should investigate and show the results for the benefits/drawbacks of placing the water gas shift reactor 1) between the reformer and stack, or 2) after the stack's outlet at the anode exhaust.
- Bloom should report hydrogen generation efficiency as a function of hydrogen generation rate, hydrogen purity, and overall efficiency (electricity and hydrogen).
- If the system uses precious group metal (PGM) in the catalytic afterburner, it could be useful to investigate reducing reliance on PGMs in this component. The same holds for the electrochemical hydrogen separation.

**Project # FC-12: Improved, Low-Cost, Durable Fuel Cell Membranes**

James Goldbach; Arkema

**Brief Summary of Project**

The objectives of this project are to 1) develop a membrane capable of operating at 80°C at low relative humidity (25-50%); 2) develop a membrane capable of operating at temperatures up to 120°C and ultra-low relative humidity of inlet gases (<1.5 kPa); and 3) elucidate ionomer and membrane failure and degradation mechanisms via *ex situ* and *in situ* accelerated testing. Mitigation strategies will be developed for any identified degradation mechanism. Membrane formulation M41 was shown to have superior durability in accelerated *in situ* testing, and M41 membrane electrode assemblies met the target of 20,000 relative-humidity cycles.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- Addresses relevant DOE goals.
- More durable, broad-operating-range membranes are critical to achieving DOE technical targets.
- Ultimate objective is development of high-temperature, low-relative humidity membranes.
- Quite relevant – new and alternative membranes are required to provide developers with options, as well as equal or better current materials properties.
- New membranes for drier proton conduction/higher durability are critical to President's Hydrogen Fuel Initiative.
- Polymer electrolytes are not the most significant barrier for fuel cell commercialization.

**Question 2: Approach to performing the research and development**

This project was rated **2.7** on its approach.

- Not clear what the strategy or approach is to obtain conductivity under low-relative humidity conditions. What other ionomers are they planning to use? Use of mixed sulfonic - phosphonic acids is one approach- what other ionomer approaches is Arkema using?
- The presentation gives the impression of empiricism and doesn't adequately discuss the rationale for the choice of polyelectrolytes.
- Good approach to develop new membrane materials tailored to high-temperature and low relative humidity.
- This reviewer rates it a "3", because more work needs to be focused only on the membrane. The electrode work is important yet secondary. Would like to see testing take place at the conditions being proposed by the effort and would like to see physical, mechanical, and chemical properties relevant to the fuel cell application, including surface chemistry for electrode interface and improvement development, and the cross-sectional microscopy analyses to determine if thinning due to chemical attack is happening at the inlet areas.
- Decouple proton conductivity from other membrane properties.
- Blend highly sulfonated hydrocarbon-based polyelectrolyte with Kynar.
- Investigating Kynar as a potential cheap/durable polymer is sensible for a company with poly (vinylidene fluoride) experience.
- The use of polymer blends brings up issues of phase stability over longer periods of time.



- Fuel cell testing has been too limited; *ex situ* tests are not addressing key issues of low conductivity particularly at low relative humidity.
- The approach presented to increase low-relative humidity conductivity is unclear in that information was not presented on chemistry or how the approaches planned to go forward would likely lead to increased conductivity.
- Incorporation of phosphonic acid as replacements to sulfonic acids is unlikely to lead to conductivity improvements.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.3** based on accomplishments.

- Mixed acid ionomers had poor conductivity and the sulfonated membrane had poor conductivity compared to Nafion.
- Steady and methodical progress is being made on several fronts – conductivity, mechanical properties, cell performance, and durability.
- Relatively new project – only 20% complete to date. Good start.
- Good performance for new material at higher relative humidity and normal temperature – need to emphasize extension to low relative humidity and 120°C.
- To date, M41 is another high water content sulfonic acid membrane. Reviewer would like to see fluoride release data. Open circuit voltage data is an electrode stability event more than a membrane issue.
- Separate membrane from electrode issues at this stage of the program.
- No apparent voltage vs. time data. It is clear the membrane is conductive; therefore a polarization curve should be a reflection of the electrode. Again focus on the membrane properties (permeability, stability, mechanicals, etc.).
- It is unclear how the conclusion is reached that M41 is a good platform for low-relative humidity membrane (slide 23).
- Improved mechanical strength versus Perfluorinated Sulfonic Acid (PFSA).
- Best conductivity 130 mS/cm at 70°C is only obtained in liquid water.
- Stability of 700 h with no sulfate/fluoride is not very long.
- Performance (membrane electrode assembly and conductivity) presented is below state-of-the-art Nafion. Conductivity is far below targets, and only minor improvements were found by processing differences between M41 and M43. No reason to believe significant improvements should be expected.
- Substitution of sulfonic acid sites with phosphonic acid sites only led to decreases in performance.
- No fuel cell lifetime data was presented. Open circuit voltage tests are function of crossover rates primarily and these are almost always lower in novel ionomers than in PFSAs.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.2** for technology transfer and collaboration.

- Work with partners at Virginia Tech and Oak Ridge National Laboratory should help define structure-property relationships.
- Excellent broad collaborations with universities, industry, and national labs.
- Arkema is leading a strong, well-balanced team with expertise in all areas needed to address project goals and objectives including *in situ* fuel cell performance testing.
- Appropriate teaming is in place.
- Interaction with industry, national labs and universities.
- Several high quality partners are involved in the project. The level of interaction was difficult to assess.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.2** for proposed future work.

- Plans for future are vague. It is not clear what the strategy is to obtain conductivity at low relative humidity; therefore, it is difficult to judge the potential for success.
- Unclear what class of electrolytes will be investigated.
- Vague description of work - how will you investigate structure property relationships? What will you vary, chemical structure of the ionomer or structure of the ionomer/ poly (vinylidene fluoride) blend while keeping the same ionomer as M41? (This would be unlikely to have desired conductivity at high temperature, low relative humidity. Are you varying both?)
- General approach is sound but specific information on candidate electrolytes is lacking.
- Good plan for continued effort addressing project objectives and DOE targets.
- More development and testing of membrane properties to guide further work.
- Improved scaffold.
- Use of phosphonic acid groups to retain water.
- Future directions presented did not include approach to increase low-relative humidity conductivity (information on chemistry or how the approaches planned to go forward would likely lead to increased conductivity).
- Little information has been given on processing conditions and how changes in processing conditions affect performance.
- Incorporation of phosphonic acid groups has only led to decreased performance.

### **Strengths and weaknesses**

#### Strengths

- Team has people with the right experience and knowledge.
- Good approach and plans.
- Strong and knowledgeable team.
- Scaffold.
- Cheap/chemical resistant polymer systems could lower cost of fuel cell ionomers.

#### Weaknesses

- Plans are too vague and do not allow one to gauge the probability of success. Presentation must reveal more information - this can be done while still protecting intellectual property.
- Too dependent on conventional approaches.
- Behaves like a hydrocarbon ionomer, i.e., conductivity falls off rapidly with relative humidity.
- Phosphonic acid groups may not improve conductivity.
- Performance (membrane electrode assembly and conductivity) presented is below state-of-the-art Nafion. Conductivity is far below targets, and only minor improvements were found by processing differences between M41 and M43. There is no reason to believe significant improvements should be expected.
- The approach presented to increase low-relative humidity conductivity is unclear in that information was not presented on chemistry or how the approaches planned to go forward would likely lead to increased conductivity.
- Reviewer expected significantly more progress for a project funded at this level.

### **Specific recommendations and additions or deletions to the work scope**

- Fuel cell testing needs to include H<sub>2</sub>/air rather than H<sub>2</sub>/O<sub>2</sub> in order to provide more useful performance data.
- Needs to focus on better polyelectrolytes.
- The strength here is the scaffold; team should look at PFSA in the scaffold, not hydrocarbons of questionable value.
- Lifetime fuel cell testing (including cyclic testing) to better understand the stability of the polymer blend under operating conditions.

**Project # FC-13: Membranes and MEAs for Dry, Hot Operating Conditions***Steven Hamrock; 3M***Brief Summary of Project**

The objective of this project is to develop a new polymer electrolyte membrane with higher proton conductivity and improved durability under hotter and drier conditions compared to current membranes. 3M Fuel Cell Components is developing new membrane additives for both increased conductivity and improved stability/durability under dry conditions. Experimental and theoretical studies will be conducted of factors controlling proton transport both within the membrane and mechanisms of polymer degradation and membrane durability in a membrane electrode assembly.

**Question 1: Relevance to overall DOE objectives**

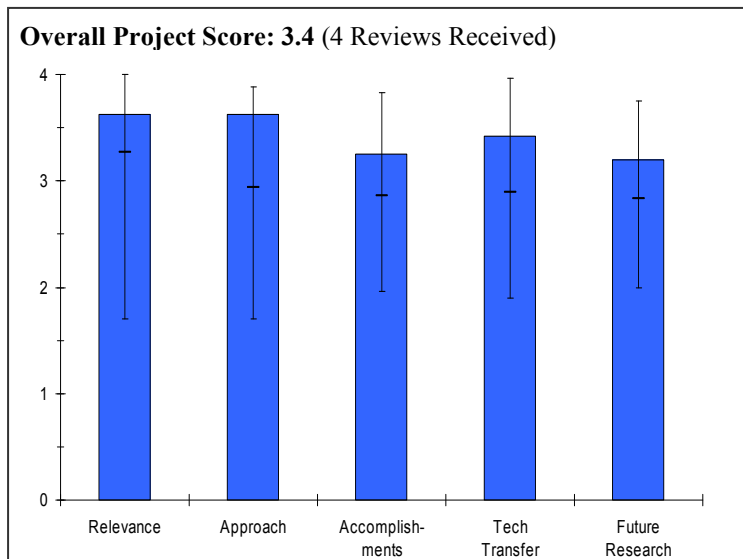
This project earned a score of **3.6** for its relevance to DOE objectives.

- Strong alignment with DOE barriers to performance and durability.
- The goal of developing a new polymer electrolyte membrane with higher proton conductivity and improved durability under hotter and drier conditions compared, to current membranes is of high relevance.
- The development of membranes capable of operating under a wide variety of conditions, especially under low relative humidity and higher temperatures will drastically improve system performance and lower system complexity and cost.
- Project addresses development of membranes that operate at higher temperatures and lower relative humidity which is consistent with automotive requirements.
- Project does not address membranes for stationary or backup power that may not require higher operating temperatures (no radiator size limitation).

**Question 2: Approach to performing the research and development**

This project was rated **3.6** on its approach.

- Good scientific rationale for polymer modification approaches.
- Good combination of experiment and theory.
- Good balance between exploring the fundamentals and demonstrating improvements.
- Excellent approach to evaluate broadly initially, with intent to combine the best of the approaches to achieve the final targets.
- A shotgun approach to improve conductivity and durability is proposed: new polymers, fluoropolymers, non-fluorinated polymers and composite/hybrid systems; new membrane additives; experimental and theoretical studies on proton transport and mechanisms of polymer degradation and membrane durability in a membrane electrode assembly; new membrane fabrication methods; and processes which are scalable to commercial volumes. Tests will be performed in conductivity cells, single fuel cells and short stacks using realistic automotive testing conditions and protocols. This approach appears to be overly ambitious and costly. The work should be redirected so that more milestones and go/no-go decision points eliminate unfruitful paths.



- The approach is extremely broad and should be focused to allow faster progress in what is deemed the approach with the highest probability of success. Focus on 3M's strength in low equivalent weight fluoropolymers; many promising approaches for improving the low-relative humidity conductivity of this material were presented.
- The project systematically addresses multiple approaches to resolving the technical issues associated with higher temperature and lower humidity operating conditions.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- Project on schedule per milestones given in presentation.
- Initial materials results are promising for several approaches. Reasonable progress on the individual approaches.
- Difficult to fully assess progress at this point since still in highly exploratory stage. Progress at next Annual Merit Review & Peer Evaluation will be significant indicator of potential of this project to make a breakthrough since first promising materials sets should be identified by then.
- Good progress in developing and finalizing test conditions for materials testing.
- Project seems to be gaining momentum.
- It is well known that lower equivalent weight perfluorinated sulfonic acid (PFSA) ionomers improve the conductivity, but that their water solubility increases. Work to cross-link is proposed, but it is unclear whether the partners will contribute to this task. It is also unclear what ionomeric materials will be used in the catalyst layer. If the 3M nanocatalyst approach is used, how will the changes in the membrane's physical properties alter the performance of the catalyst? Will additives to the membrane alter the performance of the catalysts? Conductivity of membranes is reported as a function of temperature, not as a function of relative humidity at a fixed temperature. This form of graphical presentation does not make it clear if milestones are met.
- Considering the project is already 25% complete, there are too many tasks remaining in future work and not enough accomplishments.
- Good progress in meeting the interim room temperature conductivity target.
- The technical accomplishments are reasonable based on short period the project has operated.
- The data provided suggest that progress is being made and greater understanding of the composition of the membrane and fabrication of membranes has and will be obtained.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.4** for technology transfer and collaboration.

- Limited interaction between team members so far, but appears to be developing in most areas and specific areas of initiated collaboration identified. It is expected that these collaborations will evolve before next year's Annual Merit Review.
- While there are several partners in this program who are doing good work, it does not appear that the partners will provide a path for success. The presentation bounced around too much and treated the partners as separate projects.
- Good interaction with universities.
- 3M has established a strong team that provides a broad base of technology for membrane development.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- Not covered in presentation (ran out of time), so reviewer is dependent on slides on the compact disk to assess.
- Natural follow-on tasks proposed, and they are consistent with schedule presented.
- Will be telling at next Annual Merit Review whether collaborative projects are beginning to pay off and whether there is a combination of approaches that can be integrated to achieve the DOE targets.
- Better focus and a better path involving interaction from the partners to achieve success are required.
- Future work should be focused on the most promising areas rather than a "shotgun" approach.
- Most of effort is future effort.

**Strengths and weaknesses**

Strengths

- An outstanding team is assembled and many approaches are proposed to achieve success.
- Strength in low equivalent weight fluoropolymers and modifying properties of this material.
- 3M brings a combination of membrane understanding at a molecular level and membrane manufacturing.

Weaknesses

- A shotgun approach will not lead to success. It is not clear how the team members will be used to provide success.
- Approach is too broad.
- It was not clear how the program would address the water solubility of heteropoly acids.

**Specific recommendations and additions or deletions to the work scope**

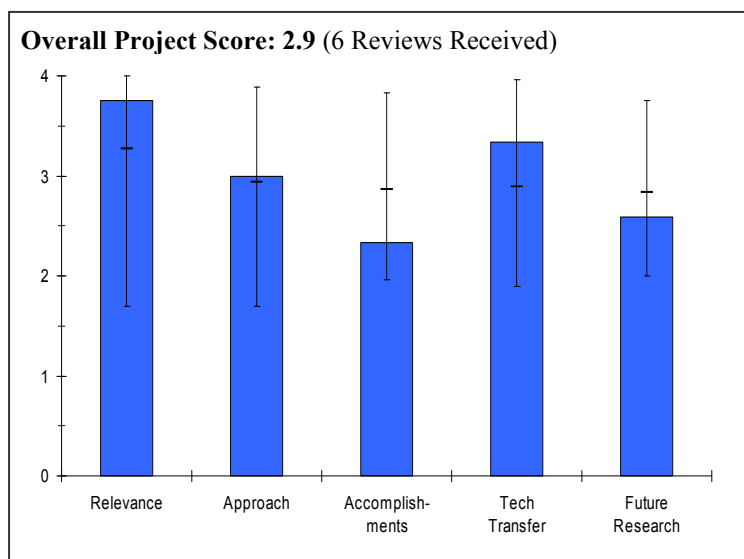
- Go/no-go decision points should be added to eliminate unsuccessful paths.
- Recommend deletion of scope of materials outside of the fluoropolymer approach.

## Project # FC-14: New Polyelectrolyte Materials for High Temperature Fuel Cells

John Kerr; Lawrence Berkeley National Laboratory

### Brief Summary of Project

The objectives of this project are to 1) investigate the feasibility of solid polyelectrolyte proton conductors that do not require water to achieve practical conductivities (0.1 S/cm at 120°C); 2) significantly simplify fuel cell systems (heat and water management and water rejection); and 3) provide car manufacturers with the knowledge of how to prepare the next generation materials. Proton-conducting materials will be prepared and tested based on heterocyclic bases (imidazole) and acids (sulfonates, sulfonylimides, phosphates). Solid polyelectrolytes will be prepared and tested where only the proton moves. Both solvent and acid groups will be tethered.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- The project is relevant to the high-temperature membrane development requirement to meet overall DOE objectives.
- The goals and objectives of the project are designed satisfactorily.
- The multi-year plan is in line with DOE research and development objectives.
- Project outcome and learning are valuable for determining the degree to which current material can be modified or re-engineered to meet the goals. Quite relevant to the long term outcome of the effort, as membrane materials are one of the limiting components in this technology.
- The goal of developing a new polymer electrolyte membrane, with higher proton conductivity and improved durability under hotter and drier conditions compared to current membranes, is of high relevance.
- Developing a membrane that can conduct protons without water would be a significant step towards the commercial viability of fuel cells.
- Membranes for proton conduction under drier conditions are critical to President's Hydrogen Fuel Initiative.
- High-temperature polymer electrolyte membranes are needed for transportation applications (to facilitate thermal management) as well as for stationary applications (higher value heat in combined heat and power and/or CO-tolerance).
- Polymer electrolyte membranes that are highly proton conducting in the absence of water have the potential to significantly simplify polymer electrolyte membrane fuel cell systems.

### Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The project has been designed appropriately to address the technical barriers of low-relative humidity and achieving higher conductivity.
- The approach of the project is good and its outcome will address some of the key technical barriers.
- The technical feasibility of the synthetic route to an oxidatively stable ionomeric polymer is doubtful.
- The oxidative stability of the new polymer should have been considered.
- The modified backbone (slide #21) is expected to be oxidatively degradable under fuel cell operating conditions.

- Interesting approach – as the right questions are being asked and novel ionic groups are being evaluated yet the effort needs to focus on expanding such ionic species – yet it seems like modeling of selected ionic species might yield additional concepts.
- Performing relevant tests at the 120°C and desired relative humidity range, should be stressed, rather than just at room temperature.
- The magnitude of the storage modulus is critical, but why is the glass transition temperature from dynamic mechanical analysis data THAT critical?
- The older General Electric electrode work using hydrophobic electrodes should be investigated for its learning value.
- Preparing and testing proton-conducting materials based on heterocyclic bases (imidazole) and acids (sulfonates, sulfonylimides, phosphates) is not new. Tethering both the solvent and acid groups is new. Unfortunately, all the work presented was on material properties, and the tethering work did not appear until slide 16, and then it appears to be started mostly by the subcontractor Los Alamos National Laboratory.
- The approach of testing ionic liquid conductivity in solution is sound, but if solution phase conductivity is too low, the principal investigator should not spend time and resources making membranes with these ionic liquids.
- The principal investigator should not spend resources studying binders for electrodes until membrane conductivity target is proven.
- Blending ionic liquids with biphenyl sulfone H form should have lower priority than low equivalent weight PFSA/ionic liquid blends.
- Use heterocyclic bases.
- Tether groups to polymer backbone.
- Model anhydrous conduction.
- Control morphology.
- Good selection of materials for synthesis.
- Building on previous experience.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.3** based on accomplishments.

- Since the polymer is chemically modified PFSA material, the cost of the material will be much higher than existing PFSA material.
- The conductivity efficiencies of proposed new polyelectrolyte material are not known.
- If the new polyelectrolyte functions, as proposed by the team, then the benefit would be immense.
- The technical progress had been good and the development plan is satisfactory.
- The screening process has yielded valuable insight and will provide guidance for the next generation membranes.
- Lawrence Berkeley National Laboratory needs additional guidance and then they should perform testing, especially *ex situ* testing, to determine membrane properties.
- A reasonable amount of progress had occurred on characterizing the bases and acids, but little to no progress on the tethering of the materials to the membrane. The presentation highlighted the capabilities of the team members, but most of the work was done on other projects and not this project.
- Limited solution phase data does not show promise towards meeting 0.1 S/cm target.
- No data for membranes was presented.
- The project still has a long way to go to achieve goals.
- Team needs to be better integrated.
- More emphasis should be placed on the novel aspects of the project.
- The presentation showed an interesting comparison of different classes of ion-conducting materials.
- Optimized catalyst loading is too high.
- Complete test conditions, such as relative humidity, temperature, pressure, etc., should be provided for all test data.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- The project has good collaboration for the proposed development work.
- There has been good technical interface and information sharing among the concerned groups.
- The project has an industrial partner as well as another National Laboratory.
- Overall, the project possesses good teamwork.
- The technology transfer appears to be satisfactory at this time.
- The team members are assembled and the synthesis of materials is occurring, but little to no progress was made on the tethering of the materials to the membrane. Work on synthesis of new materials is of no value if the tethering work is not performed!
- Los Alamos National Laboratory focused on sulfonated polymers, which are of lesser value, rather than non-aqueous proton conducting polymers, which would be of greater value.
- Access to 3M low equivalent weight ionomers is beneficial.
- 3M, UCB, and Los Alamos National Laboratory are partners on this project.
- Good collaborations within National Lab system and with industry.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.6** for proposed future work.

- The future research with imidazole end group modification of PFSA polymer will not provide a stable membrane.
- The siloxane modified route to new polyelectrolyte is not expected to give an oxidatively stable polyelectrolyte.
- The reviewer questions whether the current effort will yield results and recommends expanding the species or the approach to determine if other ionic species might yield results.
- Tethering of the materials to the membrane must occur. It is not clear that task this will be performed.
- Principal investigator did not clearly describe the primary path to meet near-term or 2015 DOE conductivity targets.
- The future research plan is well thought out.
- Date and criteria of go/no-go decision are not clear.

**Strengths and weaknesses**Strengths

- Good group with solid knowledge base of fuel cell fundamentals.
- Good interaction between the collaborative groups.
- Good fundamental approach in understanding the major technical barriers of low-relative humidity proton conductivity.
- Solid team.
- Facilities are appropriate.
- Novel ideas generated for tethering ionic liquids to conductive polymers.
- Very strong team.
- Novel approach with potentially high return.
- The team has significant polymer synthesis expertise.

Weaknesses

- No measures have been in place to evaluate the oxidative stability of proposed electrolyte materials.
- The new polyelectrolyte material may be interesting to study, but it is not expected to give long-term stability under fuel cell conditions.
- Difficult to tell how the electrode development should proceed when the membrane and subsequent membrane properties are moving targets at this stage of the program. Focus on the membrane first, then the electrode.
- Lack of progress.



## FUEL CELLS

- No clear direction for meeting targets.
- Modeling efforts focus on system and cell performance rather than conduction mechanism.
- Fundamental model does not show proof of concept.
- Lack of team integration.
- Non-Nafion binder requires significant improvement to reach Nafion's performance levels.

### **Specific recommendations and additions or deletions to the work scope**

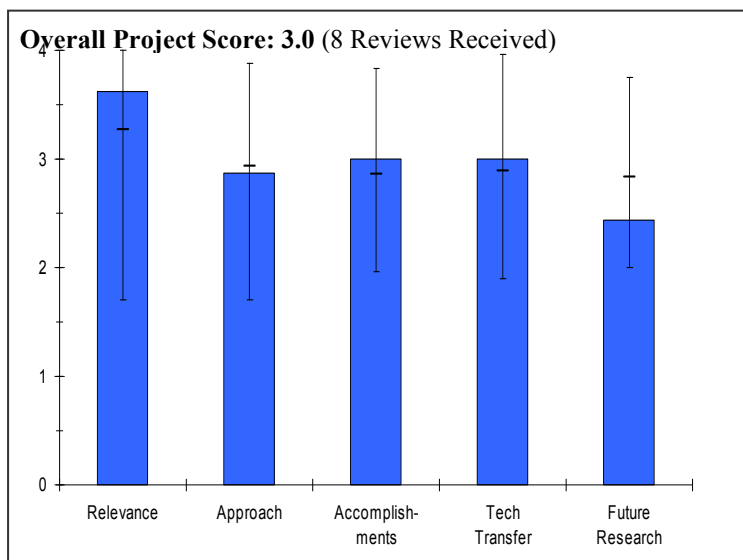
- The principal investigator should consider evaluating the oxidative stability of any new polyelectrolyte material.
- The backbone change to manipulate the polymer morphology should be reconsidered and the approach should be changed to synthesize an oxidatively stable polyelectrolyte.
- Discontinue all new synthesis work and focus on the tethering of the ionic liquids to the membrane.
- Eliminate electrode binder work.
- Eliminate cell performance modeling.
- Concentrate more on the fundamentals at this point.
- Deemphasize PFSA.

## Project # FC-15: Lead Research and Development Activity for DOE's High Temperature, Low Relative Humidity Membrane Program

James Fenton; U of Central Florida

### Brief Summary of Project

The objectives of this project are to 1) investigate new polymeric electrolyte/phosphotungstic acid membranes; 2) develop standardized characterization methodologies, including conductivity, mechanical, mass transport and surface properties of membranes; 3) provide High-Temperature Membrane Working Group members with standardized methodologies; and 4) organize High-Temperature Membrane Working Group biannual meetings. Fuel cell performance will be evaluated and the durability of membranes will be predicted. Membrane electrode assemblies will be fabricated from other high-temperature, low-relative-humidity membrane programs.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- Addresses DOE targets for membranes and is aligned with DOE goals and objectives.
- A coordinated effort to develop fuel cell membranes for operation at elevated temperatures.
- The project is relevant to the Hydrogen Fuel Initiative.
- The goal and objectives fit well with Multi-Year RD&D Plan.
- The focus of the project is aligned with the need of good measurement system and a reliable membrane electrode assembly test protocol.
- Project addresses the development of new membrane materials for polymer electrolyte membrane fuel cells that provide higher conductivity at high temperature and low relative humidity and also have good durability.
- Membranes with improved conductivity at lower relative humidity are important to achieving DOE objectives. Having conductivity as the primary initial focus is a benefit.
- It is imperative to develop a common test protocol and criteria to conduct and screen numbers of technical approaches.
- Addresses DOE targets for membranes and is aligned with DOE goals and objectives.
- This project both leads and participates in the DOE's thrust to develop new and improved fuel cell membranes. This activity has been identified by the Department as a relevant activity.

### Question 2: Approach to performing the research and development

This project was rated **2.9** on its approach.

- Approach as lead of the High-Temperature Membrane Working Group / testing center is addressing the right barriers.
- Membrane durability/degradation testing should use already developed protocols and not develop new protocols.
- Approach for improving membranes is not described well. Not clear what they plan to do to improve their current membranes.
- Effectively addressing the challenge of membrane conductivity and durability at 120°C.

- The approach to the project is good and phosphotungstic acid is well known to have good impact on membrane conductivity.
- The approach is technically feasible and it will address the low-relative humidity proton conductivity issues.
- The testing method development is well integrated with other research groups.
- Project has a bi-directional approach to development of membrane materials (PFSA- phosphotungstic acid and sulfonated poly(ether ether ketone)- phosphotungstic acid. These are alternative materials to Nafion 212 which will not meet desired high-temperature requirements.
- Also has a team approach to characterize membrane electrode assembly performance and standardize testing.
- Eleven team members.
- Sound scientific approach; however, testing protocols that are being developed may not apply to all classes of materials, in particular those that swell or require more equilibration.
- The principal investigator should work with partners on a more individualized basis. These new materials will have very different properties, and it is important to evaluate their potential of meeting DOE targets once they are optimized. This may require a more individualized testing regime done in closer collaboration with each individual partner. This is more work for the principal investigator, but it is important so that promising materials are not overlooked.
- The principal investigator should work with the membrane providers in some cases to assess why certain samples either did not meet the target milestones or did not give the same results as when tested by the membrane providers.
- Proton conductivity is a direct measure but it depends on thickness, which should be determined by other factors, such as hydrogen permeability and membrane electrode assembly durability.
- A normalized process is necessary to compare proton conductivity.
- The activity is structured in a way that this principal investigator both supervises a number of principal investigators that are working competitively, and works on one of those competitive activities.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Have met DOE milestone for relative humidity conductivity.
- Have increased conductivity 50% over Nafion 212 at 120°C, 50% relative humidity.
- Have developed conductivity testing protocols for in-plane and thru-plane conductivity.
- Have completed testing of samples submitted by the other members of the High-Temperature Membrane Working Group.
- Effectively developing standardized test procedures. Individual members are making significant progress in new membrane material discovery.
- Good technical progress has been made so far.
- The cost of the new membrane (Florida Solar Energy Center samples) fabricated by the workgroups is not known.
- It will be nice to know the cost of the new membrane material.
- The benefit of Florida Solar Energy Center samples in low-relative humidity, low-temperature regime is clear. More development is needed for its application in high-temperature, low-relative humidity region.
- Materials from all team members tested at 30, 80, and 120°C.
- Promising new materials Florida Solar Energy Center -3 investigated with better conductivity than Nafion.
- Materials showing much lower fluoride emission rates and better durability than Nafion demonstrated.
- Manufactured membrane electrode assemblies from new Florida Solar Energy Center membrane materials.
- The samples prepared by the principal investigator show good conductivity.
- Simple comparison on proton conductivity is not apples-to-apples. It should be normalized by thickness and other factors.
- Targets for low relative humidity and for high conductivity not met.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.0** for technology transfer and collaboration.

- Have had good collaborations within the High-Temperature Membrane Working Group.
- Could have better coordination with groups which have already developed or are developing durability test protocols such as the US Fuel Cell Council (USFCC).
- Extensive collaborations among the High-Temperature Membrane Working Group participants with support from several independent testing organizations.
- The team is the lead for High-Temperature Membrane Working Group and they are working on the project with many Universities and Industry.
- The project evaluates membrane samples from other industry/institute and universities.
- The team has good network among the lead Fuel Cell research organizations.
- Eleven team members, including industry but not industry that could be involved in commercialization.
- Very interactive in area of development of standardized testing protocols; has web-based interactive service.
- Good interaction with BekkTech and Scribner.
- The program would benefit with a closer, collaborative relationship with membrane providers, not just "screening" membranes. Lead the team technically; don't just test their membranes.
- It is necessary to leverage inputs from membrane electrode assembly research to normalize proton conductivity.
- Have had good collaborations within the High-Temperature Membrane Working Group.
- Collaborations listed are with vendors, which don't count.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.4** for proposed future work.

- Plans for improving conductivity of their current membranes are not clear. Path to achieving 120°C target is not apparent.
- Plans for 8-cell durability test station are good and will allow for durability testing of High-Temperature Membrane Working Group members samples more rapidly and uniformly.
- Plans to use Nafion as catalyst layer ionomer in high-temperature membrane electrode assembly, when Nafion will not perform under the high-temperature, low-relative humidity conditions is questionable - limits of ionomer in the catalyst layer will limit membrane electrode assembly performance and not allow a true measure of the performance of the new membranes in the membrane electrode assembly under high temperature, low-relative humidity conditions.
- Plans for continued high-temperature membrane development are reasonable.
- The proposed research is too broad.
- More details should have been given on the future work plans.
- Focus on the role of particle size and casting procedures in order to improve performance.
- Focus on underlying mechanisms for mechanical decay.
- Not explicitly described in presentation.
- The future research proposed is a list of milestones. How will these be achieved?
- It is good to look at durability and mechanical degradation. However, it is necessary to identify the quality metric (measure) to evaluate membrane durability.
- Test protocols should be verified with Gage R&R (repeatability and reproducibility).

**Strengths and weaknesses****Strengths**

- Testing and involvement of BekkTech and Scribner.
- Good collaboration with different workgroups which will help in obtaining many samples.
- The team has good expertise in conductivity measurements and membrane fabrication.
- The team has extensive knowledge of fuel cell membranes.

- Good correlation method for determining cell performance with membrane conductivity and electrochemically active surface area has been established.
- Good team participation.
- Good go/no-go milestone on materials in Q3 for conductivity - 0.1 S/cm, 50% relative humidity, 120°C.
- Provides good intercomparison between materials from the various team members.
- Good combined synthesis and measurement capability.
- The focus on improving membrane conductivity is a benefit to the program.
- The collaboration with BekkTech and Scribner provides a strong team.
- Testing and involvement of BekkTech and Scribner.
- A testing protocol (using a commercial apparatus) has been scripted that will result in more reliable evaluation of conductivity. Studies in polymer degradation mechanisms are necessary and useful.

### Weaknesses

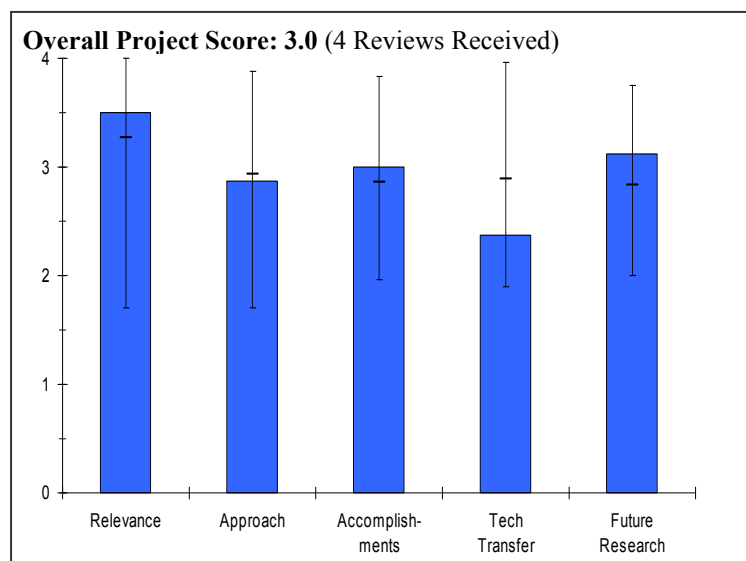
- Interaction with USFCC groups working on durability protocols appears to be lacking.
- Needs to work on different membrane fabrications methods.
- Beside phosphotungsticacid, the team should develop other ideas for making high-temperature membrane.
- Testing protocols may not have universal applicability.
- No industry involvement that could provide direction in terms of ultimate manufacturing potential.
- More collaboration between the principal investigator and the membrane providing partners will benefit this program.
- The part of this project focused on leading the team and the part of this project focused on developing a new membrane should be presented separately.
- Communication with membrane electrode assembly research teams.
- No mention of reproducibility and uniformity of test polymers samples and characterization measurements.

### Specific recommendations and additions or deletions to the work scope

- Must resolve disagreement among participants regarding standardized conductivity measurement.
- The project is on right course and nothing should be deleted.
- Team should start developing more ideas on how to make high-temperature membranes.
- Downplay the development of standardize testing protocols because they may not apply to all materials. Use these only internally for team members. If want to widely disseminate, then DOE must become involved in arbitration/or establishment of a committee to examine the protocols developed.
- Incorporate longer term testing as milestone go/no-go.
- Increase emphasis on understanding mechanism for mechanical decay and develop more solid plan for using this information in follow-on studies.
- There is need to settle the controversy about the validity of the conductivity test protocol document. In addition to the measurement of polymer protonic conductivity, all other evaluation measurements that characterize polymer performance need to have similar proscribed testing protocols. This includes polymer synthesis and subsequent workup. There also needs to be discipline in statistical analysis of testing results that illustrates the reproducibility of the testing and evaluation efforts.

**Project # FC-16: Advanced Materials for Proton Exchange Membranes***James McGrath; Virginia Tech***Brief Summary of Project**

The objectives of this project are to 1) design, identify, and develop the knowledge base to enable polymer electrolyte membrane films and related materials to be utilized in fuel cell applications, particularly for H<sub>2</sub>/air systems at 100-120°C and low relative humidity; 2) develop nanophase separated hydrophilic-hydrophobic thermally stable multi-block copolymers; 3) correlate water diffusion coefficients with proton conductivity under partially hydrated conditions; and 4) relate thermodynamics of nanophase formation to ordered morphology and to conductivity, diffusivity, and novel membrane self assembly.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- Addresses membrane development only, and at the level of new materials synthesis primarily. This is important but therefore limited in its ability to address multiple DOE objectives.
- The objectives of this project are consistent with the Hydrogen Fuel Initiative.
- This membrane development effort clearly addresses the DOE research and development objectives.
- Very relevant work that demonstrates the importance of all aspects of making membranes from scratch all the way to manufacturing methods.
- Perhaps the large emphasis on manufacturing is not so appropriate at this stage and possibly is more suited for the DOE Manufacturing efforts so that more resources are available for the fundamental work.
- It is not clear to this reviewer how these materials could reach a conductivity of 0.1 S/cm at 120°C. The conductivity mechanism is still dependent upon water.

**Question 2: Approach to performing the research and development**

This project was rated **2.9** on its approach.

- Appears to be a potentially effective approach to improve membrane conductivity and cost. It may therefore impact one or more barriers.
- Tailoring morphology to optimizing membrane performance and durability is a very sound approach.
- It is not clear that this approach will enable achievement of 2015 DOE conductivity target.
- More effort should be given to addressing the stability and durability characteristics of these materials.
- The morphology control provided by this block co-polymer approach is an excellent tool in meeting the DOE objectives. The principal investigator is doing an excellent job here.
- The project is well-designed, particularly feasible within its goals and integrated. However, there seems to be no effort at all to reach the high-temperature goal. There is no effort to find a different mechanism of solvation or charge transport. This is a significant weakness that undermines the value of all the fine work that is done. This reviewer is concerned that all the work will finish by producing another Nafion-like material with the same limitations.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Recently achieved values of conductivity the principal investigator reported are very promising. Progress on film casting is also very promising to allow correlation of the end material properties with the processing conditions as well as the material properties.
- Limited progress shown since last year's review towards meeting DOE targets.
- Demonstration of continuous casting process is promising.
- Utilization of hexafluorobenzene linkage group may enable synthesis of polymers with superior properties.
- Benefit of hydroquinone-based hydrophilic oligomers has potential, but still unproven.
- Increasing conductivity and controlling swelling through changing block sizes is an important result.
- Progress towards the 120°C goal is not evident. This is the only, albeit large, weakness.
- The technical accomplishments and progress are terrific. All areas attempted are carried out admirably and the results are extremely valuable. The development of membrane synthesis methods, morphology control and processing methods are very valuable for the DOE program and can be adapted to provide membranes that do not depend on water for conduction.
- The swelling issues are worrying. Cross-linking can help with this but the curing has to be totally uniform else there will be non-uniform current distributions that will accelerate failure.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.4** for technology transfer and collaboration.

- The interactions are fairly limited to the principal investigator's institution. But this is not inappropriate for the nature and status of the project at this time.
- Good collaboration with Giner on data verification.
- Roll of industrial partners (Nissan, Arkema) is unclear.
- The membrane casting work should be done in collaboration with and industrial partner.
- The disagreements with Florida Solar Energy Center contractors over measurement methods should have been resolved privately. This indicates a lack of communication that is disturbing.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Increased emphasis on the film casting is good as it will bring in another dimension to the effort to develop a new membrane material.
- Future research plans should include relative humidity cycling testing to verify mechanical benefit of multi-block structures.
- Polymer synthesis and characterization plans are sound.
- Understanding the chemical stability of these polymers should be a focus.
- Non-open circuit voltage lifetime tests in fuel cells should be performed.
- Future plans have no provision for reaching the 120°C goal.
- Plans are continuation of what has gone before without much attempt to be really radical.

**Strengths and weaknesses****Strengths**

- Knowledge and experience of the principal investigator with these materials.
- Principal investigator has excellent polymer synthesis and processing capabilities.
- Approach has proven that controlled polymer morphology leads to improved conductivity.
- Techniques are proven to enable tailoring of membrane dimensional stability.

- Excellent focus on understanding structure property relationships related to conductivity.
- Very strong on synthesis, morphology, and membrane processing.

#### Weaknesses

- Approach may not be sufficient to achieve DOE performance targets.
- It should be made clearer how the membrane casting work contributes to meeting the objectives of the program. Is the relationship between casting methods or conditions and performance or durability being evaluated? If not, the principal investigator should identify the chemistry and morphology needed to meet the DOE objectives before looking at scale-up.
- No attempt to eliminate water problems and find 120°C solution. This approach will not solve the problems for the fuel cell vehicles. There is a need to collaborate with the more unconventional projects that are trying to replace the water.

#### Specific recommendations and additions or deletions to the work scope

- The principal investigators may want to consult a membrane manufacturing company for input on any constraints to solvents allowable in some industrial film processing plants.
- Principal investigator should conduct relative humidity cycling of most promising membranes.

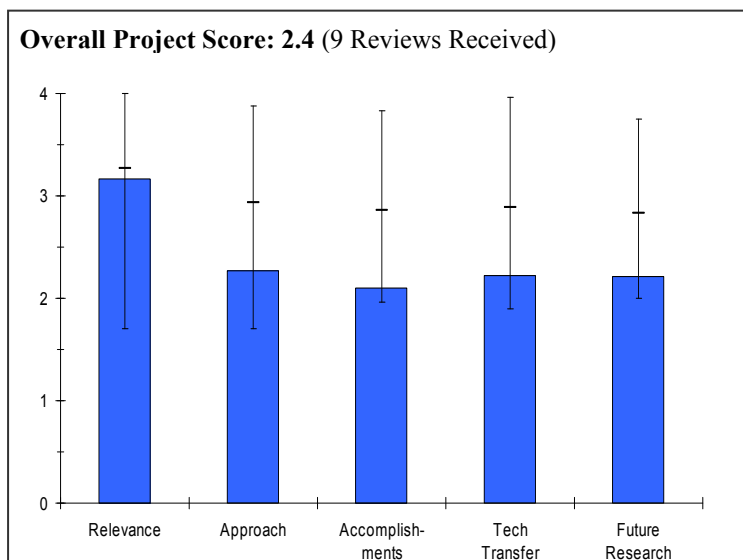


### Project # FC-17: Protic Salt Polymer Membranes: High-Temperature Water-Free Proton-Conducting Membranes

*Dominic Gervasio; Arizona State*

#### **Brief Summary of Project**

The objective of this project is to make proton-conducting solid polymer electrolyte membrane materials having 1) high proton conductivity at high temperature (up to 120°C); 2) effectively no co-transport of molecular species with protons; 3) reduction of fuel cell overvoltage; and 4) good mechanical strength and chemical stability. Polymer electrolyte membranes are being made based on “solvent-free” protic ionic liquid concepts, which can be used to model membranes (stability, conductivity) and to act as plasticizers in membranes. Acid and base moieties and polymers are varied to optimize properties in two kinds of polymer electrolyte membranes. Proton conductivity will be characterized by electrochemical impedance spectroscopy from -20 to 120°C.



#### **Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.

- The objectives of this project are consistent with the President’s Hydrogen Fuel Initiative.
- This membrane development effort addresses the DOE research and development objectives.
- Proton conductivity with no dependence on co-transport of molecular species is leading to dry operation membrane.
- This technology would be an enabler to make balance-of-plant less complex and imperative to achieve system cost target.
- Polymer electrolytes are not the most significant barrier for fuel cell commercialization.
- The project supports the President’s Hydrogen Fuel Initiative.
- This project is part of the DOE’s hydrogen fuel cell technology thrust, working to develop new materials for polymer electrolyte membranes. Membranes for this purpose have been identified as a relevant topic.
- This is an important area for DOE investment.
- This project has significant flaws that impact its relevance. These are not proton conductors.

#### **Question 2: Approach to performing the research and development**

This project was rated **2.3** on its approach.

- Novel approach, focus should shift more to immobilized ionic liquids rather than ionic liquid filled membranes.
- Potential for truly water-free protonic conduction.
- Ionic liquids have fundamental potential to conduct protons without water.
- Significant effort wasted on fuel cell testing of unstable membranes.
- Conductivity of base ionic liquid solutions lower than DOE target – questions whether membranes would ever meet targets.
- Significant efforts wasted on electrode development when membrane performance not yet proven.
- It needs to be demonstrated that the conductivity measured in proton conductivity.

- The polymers shown are aliphatic hydrocarbons. These are known to not survive under fuel cell operating conditions.
- It needs to be demonstrated that the ionic liquids are stable at the electrodes.
- Taking a novel approach (protic ionic liquid concept) which shows good progress for proton conductivity.
- The investigation of protic ionic liquids for proton transport has interesting fundamental aspects for non-aqueous conduction of protons; however it is very unlikely to yield materials suitable for broad commercial applications.
- Conductivities reported, essentially salt solutions, are only marginally more interesting than acid solutions. The typical approach looks like it is replacing protons with ammonium ions that almost certainly act as proton shuttles. This often happens in ammonia-poisoned fuel cells and significantly lowers performance.
- The approach is to form ionic liquids, formed from pure acid-base pairs that could serve as a membrane for fuel cells. This idea depends on finding two suitable compounds, which when mixed, will form an aggregate that results in fast proton transport. This appears difficult because most useful materials are those which are strong acids, and such aggregates just cannot be strong acids. This approach does not seem promising.
- The approach has serious shortcomings. The 'salts' are not proton conductors.
- Conductivity measured does not reflect proton conductivity.
- The project is supposed to focus on membranes but barriers given are for 'Electrode Performance'.
- Creative approach but they really need to get to proton conductivity.
- The project seems doomed to study anomalies in systems that are not viable fuel cell electrolytes because of lack of free protons.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.1** based on accomplishments.

- The membrane electrode assemblies with these membranes have low open circuit voltage and have only achieved fairly low current densities.
- Membranes with non-leachable protic ionic liquid have not been obtained (one example given was unstable and water soluble).
- This is a new area and progress from the starting point has been good, but a long ways to go to catch up to established membranes and longer to meet DOE membrane targets.
- Have achieved conductivity close to the milestone, but with a membrane with leachable ionomer.
- Non-leachable protic salt membranes synthesized.
- Fuel cell tests done, but results are very, very poor.
- The fuel cell performance is very poor. The principal investigator should use conductivity or hydrogen pump measurements to help explain this.
- The principal investigator suggested that Pt oxide will not be formed because this is a "non-aqueous electrolyte". Water is still present, so why is this? What data suggests this?
- Good progress on proton conductivity, however, fuel cell performance is too low.
- It is making sense to focus on gas permeation due to lower open circuit voltage. It is still necessary to explain low current density performance.
- Membrane resistance (*in situ*) is highly temperature-dependent. It may indicate that proton conductivity of this membrane still depends on water transport.
- Further investigation is necessary.
- The researchers have made ionic liquids, put them in membranes, and characterized them using electrochemical and fuel cell testing.
- Fuel cell performance and resistance measured in cells is extremely low and is only presented with liquid electrolytes; acid solutions in the same environment would have given better performance. Immobilizing the ammonia in the membrane resulted in lower performance.
- A path towards useful materials was not shown and would not be expected based on the results presented.
- Results disappointed. The aggregates were only conductive in the presence of water.
- There is no unambiguous evidence that these are proton conductors. Ammonium ions will simply not be a reasonable proton source.

- Electrochemical nuclear magnetic resonance (NMR): the principal investigator carried out Electrophoretic NMR. Electrochemical NMR is different.
- The imidazole-containing polymers provide a possible path forward.
- The polarization curves tell the story: there is little fuel cell activity before a large drop in voltage.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.2** for technology transfer and collaboration.

- Only coordination was with Akron for polymer synthesis.
- This project would benefit from collaboration with someone having more fuel cell experience (Los Alamos National Laboratory?) to clarify the viability of this approach.
- Some collaboration.
- Part of the High-Temperature Membrane Working Group. Samples have been transferred for testing.
- This is not ready for transfer.
- Not responsive to FreedomCAR Fuel Cell Technology Team recommendations.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.2** for proposed future work.

- A large portion of future work focused on leachable protic ionic liquid membranes, not what this project should be directed at.
- Other planned work to look at electrode interactions, while relevant, is really outside the scope of membrane development.
- Working with hpolyphosphazenes is only specific idea for new chemistry approach, but benefit is unclear.
- The principal investigator needs to clarify his plan for moving to materials that have the chemical and oxidative stability for use in a fuel cell.
- It is necessary to pursue further investigation of low fuel cell performance with current materials.
- Proposed research focuses on understanding the system better, but not how conductivity and fuel cell performance can be improved by some systematic approach. Using ammonia as a proton shuttle is unlikely to be stable or lead to improvements over current systems.
- The principal investigator suggested a change in direction, moving to a classical polymer structure that would imbibe the protic liquids.
- A rather significant change in direction is suggested--shifting to an imidazole on a polymer.
- Project seems like it will end up focusing efforts on understanding spurious phenomena unlikely to lead to promising materials.

**Strengths and weaknesses****Strengths**

- Novel idea.
- Potential for water-free conduction over the desired temperature range.
- Protic salts are a unique approach to non-aqueous proton conduction.
- There is value in studying new proton-conducting materials with different conduction pathways.
- Leverage NMR for analysis.
- Creative approach, with lots of synthetic input.

**Weaknesses**

- Not focused on membranes that would be applicable for the automotive application DOE is targeting.
- Unclear from data if principal investigator is measuring proton or salt cation (ammonium) conduction.
- Principal investigator spends too much time on membrane electrode assembly testing of unstable materials with low conductivity.
- More work should be done understanding the stability of these materials.

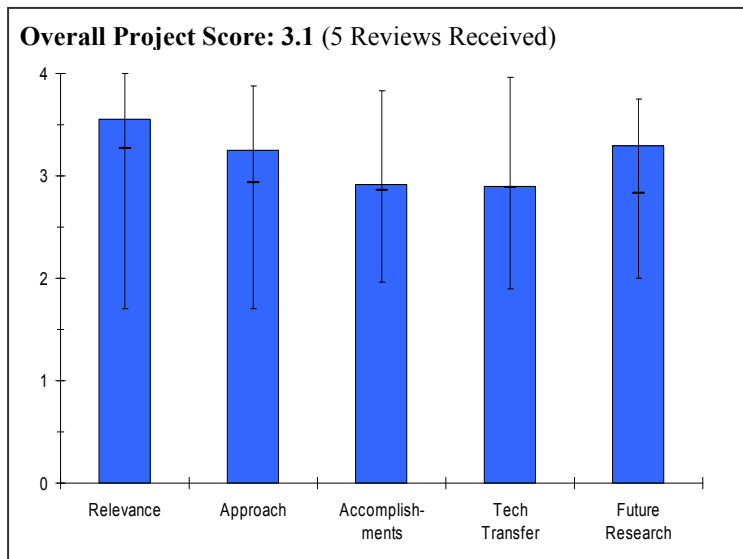
- Show that conductivity is due to proton transport.
- Interaction with collaborators.
- Ammonium ionin fuel cells "reacts" (ammonia/ammonia+proton dynamics are complicated) at the cathode and has the ability to liberate the ammonia. Ammonium ion is likely an order of magnitude slower than protons; hence the large resistance in fuel cells shown. Performance of these materials is abysmal and will only get worse with tethering of functional components.
- Flawed approach: difficult to see that proton conduction will be significant.
- Presenter constantly referred to results shown at Electrochemical Society meeting (3 weeks earlier) that were 'not available' for presentation. It seems unlikely that several significant results emerged in the space of a few weeks.
- Polymer-bound imidazole approach has already been shown to be insufficient due to lack of mobility.

**Specific recommendations and additions or deletions to the work scope**

- Focus on making unleachable membranes and measuring proton conductivity.
- This project needs to be restructured, perhaps with a change in scope.

**Project # FC-18: Fluoroalkyl-phosphonic-acid-based Proton Conductors***Stephen Creager; Clemson***Brief Summary of Project**

The objectives of this project are to 1) synthesize and characterize new proton-conducting electrolytes based on fluoroalkylphosphonic acid functional group; and 2) perform a simulation study of structure and proton conduction in fluoroalkylphosphonic acid-based electrolytes. Tasks were to 1) synthesize and/or purify at least 5 g each of one or more trifluorovinyl-ether (TFVE) fluoroalkylphosphonic acid monomers; 2) complete development and validation of classical force fields for fluoroalkylphosphonic and fluoroalkyl-bis-phosphonic acids and perform MD simulations of these acids as a function of fluoroalkyl chain length; 3) perform density function theory-based Born Oppenheimer Molecular Dynamics simulations; and 4) complete synthesis of TFVE and development and validation of models. Year 2 milestones include testing the membrane for electrolyte conductivity of 0.07 S/cm at 80% RH at ambient temperature and delivering a sample membrane to the Topic 2 Contractor for evaluation.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.6** for its relevance to DOE objectives.

- Durability, cost and performance improvements of membranes are all highly necessary for fuel cell commercialization.
- Project addresses cost, durability, and performance goals in the development of new membrane materials for polymer electrolyte membrane fuel cells. Relative to the standard of Nafion materials, these new materials must provide higher conductivity at high temperature and low relative humidity and also have better durability.
- Good studies of model compounds and modeling of proton transport that addresses the DOE needs to come up with new mechanisms of proton transport.
- Project focus appears to be diverted by better results with water present which is resulting in the development of another Nafion-like material with the same limitations. The amphotericity of the phosphonic and phosphinic acids are the interesting property (Kreuer) and this aspect is not receiving adequate attention.
- Seeks to develop high-temperature membranes with good conductivity at low relative humidity – key DOE goal.
- This is an important area for DOE investment.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- Fundamental look at performance limitations with model compounds and modeling is strong.
- Phosphonated "Nafion" like material has the potential to be a good learning experience but ultimately will not be the goal.
- Project seeks to synthesize and characterize new proton-conducting electrolytes based on the fluoroalkylphosphonic acid functional group. Computational chemistry used to understand order and mechanisms and improve molecular design.
- Excellent end-to-end plan including small molecule analysis, synthesis, characterization, theory/computational method.
- Targets of membrane conductivity greater than 0.1 S/cm at 120° C and water partial pressure of 1.5 kPa.

- Starts from a small molecule approach.
- Logical project plan at least at start.
- The approach of using model compounds combined with modeling in order to guide the polymer synthesis is excellent.
- The project is losing focus due to better results in the presence of water. Should focus on how to get high conductivity with little or no water. This is the barrier that needs to be addressed.
- Methodical approach going from model compounds to ionomers.
- Good balance between theory and experiment.
- Well-organized, comprehensive team.
- Model compounds studies are very revealing.
- Not clear how polymerization will improve the shortcomings revealed by model compound studies.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.9** based on accomplishments.

- Model compound work is high.
- Synthetic approach and results are impressive – characterization of membrane however is weak.
- Computer modeling results are highly interesting and may be of value.
- Quantitative correlation made between acid:water ratios and conductivity; more water up to 1:20 yields higher conductivity for monomers.
- Good study of monomers. Increased fluorocarbon character shows decreased conductivity because lower volume of acid in condensed phase to conduct protons.
- Synthesis of membranes by casting of ionomers.
- Have begun to understand the relationship between number of waters needed to deprotonate the acid group.
- Good progress and accomplishments in model compound studies, modeling and polymer synthesis.
- Needs to consider how to obtain high conductivity without water.
- Good Progress.
- Membranes fall short of milestone but do hold promise.
- Need to get membrane preparation optimized.
- Good definition of 'limits' of approach via model compound study.
- What water content is acceptable for conductivity measurements?
- It is unfortunate for these researchers that they have taken a more basic approach, synthesizing membranes from scratch, as opposed to others who focus on processing existing materials.
- It is important to follow through completely with this project in spite of a somewhat slower 'delivery rate' caused by the high degree of difficulty of getting the synthesis and processing right.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.9** for technology transfer and collaboration.

- Excellent collaboration between Clemson and University of Utah (UT) is evident.
- Possibility to include industrial partner in the future may speed up/focus development.
- All academic involvement; industry only involved in measurement.
- Very good experimental/theory coordination.
- Strong theory effort done at Utah.
- Co-ordination between the two partner institutions is good but need to be talking with Kreuer and others much more.
- Need to collaborate with others to eliminate the water.
- Good integration with modeling effort.
- Appropriate samples have been sent out, in spite of the workers being at a self-professed early stage.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.3** for proposed future work.

- Future work is in the right direction.
- Research on phosphonated, short-side chain, low equivalent weight, and reinforced membrane should be highest priority to achieve state-of-the-art status; otherwise it will just be an academic exercise.
- Concentrate on processing to keep ionomers fully protonated. Need to make sure that the principal investigators use proper annealing procedures and get all cations out to evaluate how the new materials compare to Nafion.
- Focus on understanding barriers to proton transport in membrane structures to improve conductivity. Model domain structures.
- The future plans do look as if the project may well refocus on non-water mechanisms of proton transport. The plans look reasonable for this.
- Recommend that the project be more explicit about looking for non-water based conduction.
- Going to lower equivalent weight is a good idea.
- Why is durability not addressed?
- A clear path forward exists.
- Processing these materials will take much effort.

### **Strengths and weaknesses**

#### Strengths

- Chemical synthesis.
- Computer modeling.
- Excellent experimental/theory coordination.
- Well-defined targets.
- Use of model compounds, modeling and strong synthesis is well-balanced and very appropriate.
- Strong team.
- Good integration between modeling and experiment.
- Methodical approach.
- Organized and systematic.
- Excellent theorist involved.
- Truly unique materials.

#### Weaknesses

- Lack of industrial partner may lead principal investigators down non-fruitful pathways.
- Lack of deep understanding on why water is still needed even in a phosphonic acid polyelectrolyte.
- Lack of thorough membrane characterization.
- No real industry involvement.
- Must avoid looking too much like an Office of Science project, although clear value in doing theory in project.
- Project is being derailed by trying to meet milestones using water. This should not divert attention from the need to come up with non-water conduction mechanisms.
- Durability aspect is lacking.
- May be prone to the same durability issues as PFSA's.
- Slow progress due to high difficulty.

### **Specific recommendations and additions or deletions to the work scope**

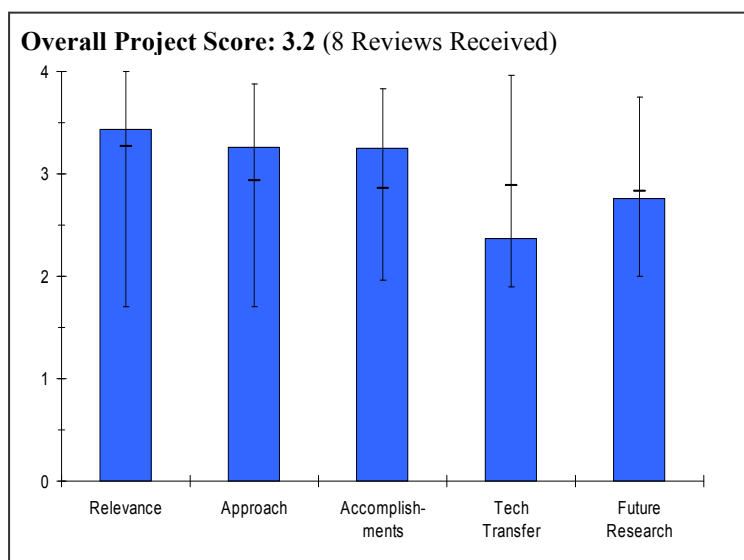
- Add industrial partner.
- Focus strongly on phosphonated, short-side chain, reinforced material.
- Increase membrane characterization.
- Need to develop a stronger membrane evaluation effort so can tell if these efforts will ultimately produce advanced materials that can be used in membrane electrode assemblies. Some concrete go/no-go milestone dates.
- With time must become more applied. This should begin next fiscal year.
- Include at least an estimation of membrane durability under automotive conditions.

## Project # FC-19: Rigid Rod Polyelectrolytes: Effect on Physical Properties Frozen-in Free Volume: High Conductivity at low RH

Morton Litt; Case Western Reserve University

### Brief Summary of Project

The objectives of this project are to 1) synthesize polyelectrolyte membranes that reach or exceed Department of Energy low humidity conductivity requirements; 2) use materials and synthetic methods that could lead to cheap polymer electrolyte membranes; 3) understand structure/property relationships to improve properties; and 4) develop methods to make these materials water-insoluble and dimensionally stable with good mechanical properties. Case Western Reserve University has decided to work with poly(p-phenylenes) with one and two sulfonic acids per ring. These materials have lower equivalent weights and cannot hydrolyze.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Addresses high-temperature membrane performance.
- Project addresses relevant DOE barriers and aligns with DOE objectives.
- The project is relevant to DOE's Multi-Year (RD&D) plan.
- The project directly correlates to the challenges associated with DOE's Hydrogen Program.
- Developing a membrane that can conduct protons at low relative humidity levels would be a significant step towards the commercial viability of fuel cells.
- This membrane development effort clearly addresses the DOE R&D objectives.
- Project addresses relevant DOE barriers and aligns with DOE objectives.
- Polymer electrolytes are not the most significant barrier for fuel cell commercialization.
- The project supports the President's Hydrogen Fuel Initiative.
- This project is part of the Hydrogen Program's effort that explores new fuel cell membranes. The emphasis in that activity is to find materials that perform well at higher temperatures and at low values of water relative humidity.

### Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- Focused on the development of new materials with specialized structures projected to have good performance under high-temperature, low-relative humidity conditions.
- Approach is focused on achieving conductivity targets developed by DOE.
- The choice of material to make cost effective polyelectrolyte has some limitation.
- The Fenton's stability of the polyelectrolyte is doubtful.
- The rigid rod nematic liquid crystal polymers are very robust and strong materials, but they don't make a good membrane-electrode interface.
- The fragile nature of the electrode makes it hard to integrate well to the tough membrane surface created by nematic liquid crystal polymers.



- Development of extremely low equivalent weight ionomers is an excellent approach toward meeting DOE conductivity targets.
- More focus needed on making insoluble membranes.
- The principal investigator has developed a well-designed electrolyte and understands the need to transform it into a stable membrane.
- Approach is focused on achieving conductivity targets developed by DOE.
- Investigating extremely low equivalent weight materials and using rigid rods to freeze in free volume are both interesting approaches to address increasing conductivity at low relative humidity.
- Cross-linking already brittle systems for the purpose of decreasing water uptake/solubility seems likely to only worsen already poor mechanical properties; other approaches addressing mechanical properties are necessary.
- The proposal is to use rigid rod polymers that, when aggregated, will form a structure, that will facilitate proton transport.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- Poly(phenylenedisulfonicacid) material has good conductivity at lower relative humidity and ~80°C and needs to be extended to higher temperature temps.
- Reasonable progress to date with promising new materials.
- Good progress in developing materials with high conductivity, but mechanical stability is lacking.
- New poly(phenylenedisulfonicacid) materials show promise.
- These materials appear to be very anisotropic (see swelling in only the Z direction) and expect conductivity to also be anisotropic and higher in-plane, where water appears to be held. Need thorough-plane conductivity data for these materials to determine if conductivity extends in a direction where water isn't forming a path.
- Modest technical progress has been made so far.
- The problem of layered spacing to accommodate minimum water for proton conduction has been addressed well.
- The conductivity of poly(phenylenedisulfonicacid) is commendable.
- More work is needed to understand the physical property of the membrane material, and to assess the feasibility of fabricating a good membrane electrode assembly interface.
- This is the only membrane project to demonstrate clear path to meet 2015 DOE performance targets.
- Dimensional stability and mechanical durability still a big problem.
- Preferential Z-swell should help with mechanical durability.
- The conductivity shown is outstanding.
- High conductivities of the novel ionomers presented are promising for developing materials with decreased conduction losses.
- Disappointingly few "new results" in this year's presentation compared to prior year presentation.
- Validation of conductivity measurements by another source would lend validity to reported values.
- Considerable numbers of polymer samples have been fabricated and tested.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.4** for technology transfer and collaboration.

- Apparently some internal collaboration, but no significant interactions with outside organizations.
- Collaboration outside of Case Western Reserve University (with original equipment manufacturers if possible) would be helpful.
- The team lacks direct links to National Labs and Industries.
- The team may have National Lab/Industry link through Tom Zawodzinski, but direct link would have been better.
- Future technology transfer for these ionomeric materials is not very clear.
- No external collaboration.
- Modeling the morphology of the hydrated ionomer would be a useful addition to this project.

- The principal investigator should work with BekkTech or others for additional, independent high-temperature conductivity testing.
- Relatively little interactions, however not particularly needed them at this point in time. Validation of conductivity measurements is most important aspect of this criterion.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- Problems have been identified and plans are structured to resolve these problems.
- Plans are to address mechanical property shortcomings
- The proposed research on LCP materials seems to have more academic interest.
- Viability of a practical functional membrane using such LCP is doubtful.
- The research should focus beyond just conductivity enhancements. It should look into the polymer properties that are responsible for making good membrane electrode assembly interfaces.
- Only plan for reducing solubility is chain extension with non-polar biphenols & bi-thiols (they can be oxidized later to sulfones).
- The principal investigator clearly understands the need to couple these molecules with a stable phase or otherwise create a stable, flexible membrane. The path towards this goal should be shown more clearly.
- Plans are to address mechanical property shortcomings
- Cross-linking approach gives additional concerns over already poor mechanical properties.
- Increasing molecular weight may provide improved properties, both in terms of water solubility and mechanical properties.
- Chain extensions may be a mechanism to provide additional improved properties, but other approaches should also be considered.
- The principal investigator proposes moving to complete synthesis and testing with the intent of meeting DOE targets before the December go/no-go decision.

#### **Strengths and weaknesses**

##### Strengths

- Have shown good initial results.
- Good concept to prove the structural advantage of nematic liquid crystal polymers in retaining water at high-temperature and low-relative humidity conditions.
- The project proves the need of minimum water in interlattice spaces of liquid crystal polymers for proton conduction under high-temperature, low-relative humidity conditions.
- Very high conductivity at low relative humidity demonstrated.
- Principal investigator has made very low equivalent weight monomers.
- Poly-p-phenylenes have preferential Z-swelling, which should help with mechanical durability.
- The principal investigator has developed a well-designed electrolyte and understands the need to transform it into a stable membrane.
- Have shown good initial results.
- Extremely high conductivities have been observed, the only example in this program to suggest targets might be able to be far surpassed.
- The principal investigator is an excellent polymer chemist, a very artful, clever, and experienced scientist.

##### Weaknesses

- Must improve mechanical properties.
- Anisotropic nature of the materials means through-plane measurements are necessary.
- Material properties for making membrane electrode assemblies should be assessed.
- Lack of collaboration with researchers who can help improve mechanical stability.
- Reported values have not been validated through verification by other laboratories.
- Mechanical properties are extremely poor, including issues with water solubility.

- This project may have concerns with in-plane versus through-plane conductivity as swelling seems to be a 1-dimensional phenomenon that may make x-y issues different than z direction issues.
- The molecular weight of the subject polymers is perhaps at too low a value to prepare insoluble materials.

### **Specific recommendations and additions or deletions to the work scope**

- The focus of the project should be beyond just conductivity improvement, it should also focus on the material stability under practical fuel cell condition.
- Material surface property study for membrane electrode assembly fabrication should be added.
- Fenton's test study on all the materials should be carried out and it should be added as a part of the project.
- Focus on blocking the poly(p-phenylenes) with hydrophobic units to reduce solubility.
- More collaboration to help solve solubility problem.
- Focus on mechanical properties almost exclusively. Conductivity values are easily high enough; consider trading off conductivity for mechanical property advantages.
- The screening is focused on conductivity, certainly important, but just one of several critical attributes. Durability, low cost, etc. are equally important, but not equally strived for.

## Project # FC-20: NanoCapillary Network Proton Conducting Membranes for High Temperature Hydrogen/Air Fuel Cells

Peter Pintauro; Case Western Reserve University

### Brief Summary of Project

The objective of this project is to fabricate and characterize a new class of NanoCapillary Network proton-conducting membranes for hydrogen/air fuel cells that operate under high temperature, low humidity conditions. The 2007-2008 project goals were to fabricate membranes with the following properties: 1) 0.07 S/cm proton conductivity at 30°C and 80% relative humidity; 2) good mechanical properties; and 3) low gas permeability; and to identify a roadmap to achieve high conductivities at lower humidity and higher temperatures.

### Question 1: Relevance to overall DOE objectives

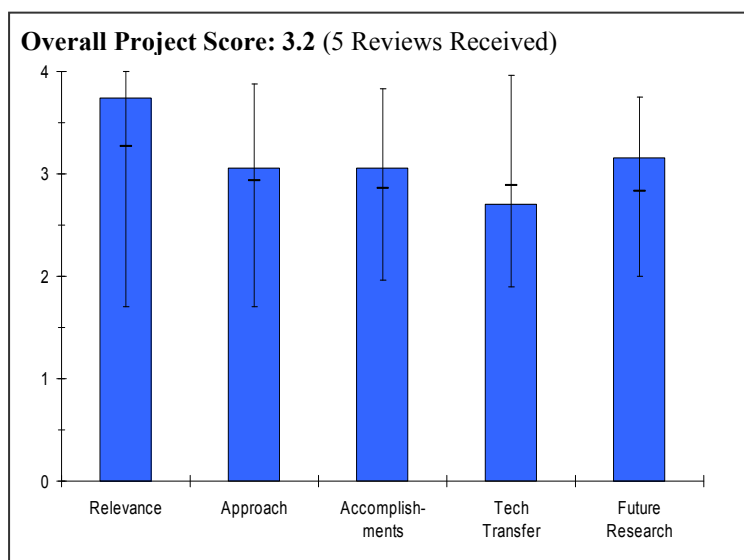
This project earned a score of **3.7** for its relevance to DOE objectives.

- Durability, cost and performance improvements of membranes are all highly necessary for fuel cell commercialization.
- Clearly oriented towards DOE goals.
- The objectives of this project are consistent with the Hydrogen Fuel Initiative.
- Making membranes that conduct protons and separate the gases. This is good and relevant to DOE goals.
- High-temperature polymer electrolyte membranes are needed for transportation applications (to facilitate thermal management) as well as for stationary applications (higher value heat in combined heat and power and/or CO-tolerance).

### Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Very unique approach to improving membrane durability.
- Electrospinning of fibers can provide a lot of flexibility on polyelectrolyte chemistry and geometry.
- Inert matrix also provides a lot of flexibility.
- Polyhedraloligomeric silsesquioxanes material can provide even more benefits for performance.
- Nanofibers are promising novel approach, maybe still high risk, but high potential.
- Convincing strategy to overcome remaining hurdles.
- Use of binder inherently limits conductivity.
- Sulfonated polyhedraloligomeric silsesquioxanes improves conductivity but is still unstable in its current form in the membrane.
- The high-temperature conductivity goals are not being addressed. 0.1 S/cm at 120°C and 50% relative humidity is not practical for a vehicle. How is this going to work at <25% relative humidity?
- Interesting approach to provide ionic conductivity within a network of continuous nanofibers.
- Voids between fibers filled with ionically non-conductive polymer must be minimized for high conductivity.



**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- Has demonstrated materials that meet DOE interim milestones.
- Has proven fiber technology with matrix.
- Understands/identified the newly discovered shortcomings (softness of inert material, sulfonated polyhedraloligomeric silsesquioxanes solubility).
- Good results, but still considerable risk for real high temperature application.
- Status with respect to time-line is okay.
- Met intermediate DOE conductivity target.
- Mechanical durability still unproven and a concern.
- Good progress made in the objectives that are addressed.
- Study of sulfonated polyhedraloligomeric silsesquioxanes loading has shown higher conductivities with greater amounts of sulfonated polyhedraloligomeric silsesquioxanes, providing evidence of the benefit of sulfonated polyhedraloligomeric silsesquioxanes.
- The stability of the sulfonated polyhedraloligomeric silsesquioxanes within the nanofiber composite membrane needs to be verified.
- The room temperature conductivity milestone was met, as verified by BekkTech.
- The conductivity of the sulfonated poly(arylene ether sulfone) /sulfonated polyhedraloligomeric silsesquioxanes nanofiber composite membrane at 120°C and low relative humidity is lower than Nafion's.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.7** for technology transfer and collaboration.

- What is collaboration with Wright State University?
- Pursuing industrial partner that is highly recommended by the reviewer.
- Actually this question is premature for the project.
- The project is worthwhile to be continued
- Outside interaction limited to polyhedraloligomeric silsesquioxanes supplier.
- This could stand improvement.
- The universities appear to collaborate well.
- The role of each party should be more clearly stated.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- Based upon newly identified shortcomings, new approaches will be pursued to overcome them.
- Lining up industrial partner will speed up/help focus development.
- Reasonable strategy for going further.
- Tests of new more thermally stable binder planned.
- No clear path presented to meet 2015 DOE performance and durability targets.
- Future plans should include better collaborations with other groups. Project is now getting into the harder work and it needs help.
- The future work is well focused on increasing the membrane conductivity at higher temperatures and lower relative humidity.

**Strengths and weaknesses****Strengths**

- Unique approach to membrane development.
- Electrospinning technology.

- Good and clear presentation, not lost in details but emphasizing the general route.
- Electrospinning has potential to enable stabilized low equivalent weight ionomers.
- Electrospinning does show promise and real membranes result.
- High mechanical strength (Young's modulus) and low gas permeation has been shown.

#### Weaknesses

- Making no attempt to find a proton conduction mechanism that does not involve water.
- Lack of sufficient membrane characterization (swelling, gas permeability, etc.).
- Lack of industrial partner for the time being.
- Binder inherently lowers conductivity.
- Poly aryl ether sulfones are not highest performing starting ionomers.
- Not addressing water free or water-poor conduction. Need to consider how to do this.
- Higher ionic conductivities at 120°C and low relative humidity have yet to be demonstrated.
- Ability to fabricate a membrane electrode assembly is not known.

#### Specific recommendations and additions or deletions to the work scope

- Improve membrane characterization.
- Add industrial partner.
- Investigate if electrospinning can enable preferential conductivity through plane of membrane instead of isotropic conduction.
- Cost analysis of process warranted to verify if process could be cost effective.
- Use more conductive polymers (such as Professor Litt's poly-p-phenylenes).
- Effect of swelling on epoxy-bonded fiber mats should be investigated to ensure mechanical integrity during automotive drive cycles.

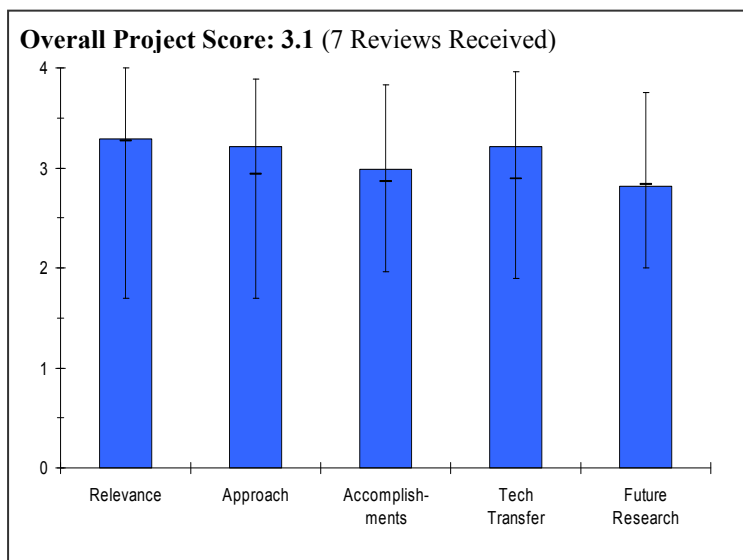
**Project # FC-21: Novel Approaches to Immobilized Heteropoly Acid (HPA) Systems for High Temperature, Low Relative Humidity Polymer-Type Membranes**

*Andrew Herring; Colorado School of Mines*

**Brief Summary of Project**

The overall objective of this project is to fabricate a hybrid HPA polymer from HPA functionalized monomer with  $\sigma > 0.1 \text{ S cm}^{-1}$  at 120°C and 25% relative humidity. The 2008 objective is the synthesis and optimization of hybrid HPA polymers for conductivity from room temperature to 120°C with an understanding of chemistry/morphology conductivity relationships. Materials synthesis will be based on HPA monomers; novel “high and dry” proton conduction pathways will be mediated by organized HPA moieties.

**Question 1: Relevance to overall DOE objectives**



This project earned a score of **3.3** for its relevance to DOE objectives.

- Project is aligned with DOE goals and targets.
- Project addresses requirement for high-temperature, low-relative humidity membranes.
- High-temperature membrane with high conductivity at low relative humidity is needed.
- The project is relevant to the objectives of DOE's Multi-Year RD&D plan.
- The improvement of low-relative humidity, high-temperature membrane conductivity is critical to the success to DOE's Hydrogen Fuel Initiative.
- The goal and initiatives are all aligned with DOE's objectives.
- Project is aligned with DOE goals and targets.
- Polymer electrolytes are not the most significant barrier for fuel cell commercialization.
- The project supports the President's Hydrogen Fuel Initiative.
- This activity is part of the "high-temperature membrane" project, and the relevance is tied to the goals of that activity, the search for a polymer electrolyte membrane that operates under high-temperature and low-relative humidity conditions.

**Question 2: Approach to performing the research and development**

This project was rated **3.2** on its approach.

- Novel approach that has the potential for achieving water-free conduction. A new class of ion-conducting polymer.
- Systematic, well designed experimental plan.
- Approach to work with Si-linked model compounds and model linkers has allowed for faster progress and proof-of-principal type experiments.
- Approach involves systematic and logical exploration of polymers based HPA functionalized with organic monomers design space.
- A different approach than most other membrane projects.
- The approach of making composites using HPA is good.
- HPA does have good conductivity under low-relative humidity, high-temperature conditions.
- Incorporation of HPAs using polystyrene (PS) chains is not good, since PS is known to be vulnerable under fuel cell conditions.

- The approach of using 3M's monomer to anchor HPA is good as PFSA chain will be more stable than PS chain.
- Novel approach that has the potential for achieving water-free conduction. A new class of ion-conducting polymer.
- Systematic, well-designed experimental plan.
- Approach to work with Si-linked model compounds and model linkers has allowed for faster progress and proof-of-principal type experiments.
- HPAs have high conductivity and represent a novel class of materials that merit further study.
- Incorporating HPAs covalently into membranes addresses one of the key problems of these materials, leaching out when not covalently bound.
- The use of a hydrocarbon backbone limits chemical stability, even though HPA may reduce impact of radicals. Even though PFSA's are being proposed as covalently bound hosts, until shown, it is not certain they can be made.
- Lack of a method of externally influencing the distribution of HPAs in the membrane means the only path forward is to increase loading. This is improving performance, but reducing mechanical properties.
- Herring proposes assembly of membranes through the polymerization of monomers that include reactants with organo-metallo moieties. This approach is indeed novel, but not obvious. Vinyl monomers were the initial candidates for membrane fabrications.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Colorado School of Mines has developed a new class of proton-conducting polymers.
- Colorado School of Mines has been successful at immobilizing HPA and preventing HPA leaching.
- Colorado School of Mines has developed and begun initial testing of new membrane materials. To date material performance at lower relative humidity has not been acceptable.
- Good results to date.
- Overall technical progress has been satisfactory.
- Impressive conductivities have been demonstrated by the membrane identified as PolyPOM75.
- The cost of the composite membrane should be addressed to account for the overall system cost.
- There is relative humidity benefit at high temperature, but the water uptake at lower temperature is very high and it can be a problem.
- Colorado School of Mines has reported membranes based on higher HPA loadings have conductivities that are beginning to approach current targets; still, reported values are only 2/3rds of the target.
- Increased conductivity is coming at the price of increased water uptake.
- Mechanical properties and durability are still large concerns yet to be addressed.
- Progress has been made and some samples show acceptable conductivity. However some samples appear to become brittle with aging. So, results are still preliminary.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.2** for technology transfer and collaboration.

- Collaborations in the team (especially with 3M) have been very productive.
- Close collaboration with 3M who is making significant contributions to the project.
- Too early in project to have significant collaboration other than 3M.
- The technical collaborations with industry and National Lab are adequate.
- There is good interaction with other fuel cell research groups.
- The project will help in building good knowledge base at the School of Mines.
- Interactions are limited, but 3M collaboration is yielding significant improvements to the project. At this level further interactions are likely not needed.



**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- Future work is directed towards appropriate barriers, trying to control morphology, and addressing durability.
- Plans adequate to continue material development; however attention must be focused on mechanical stability of developed membrane.
- Proposed research by 3M on anchoring HPA using PFSA monomer seems applicable.
- Si-anchored polymer compound may not be very stable under fuel cell conditions.
- Future work is directed towards appropriate barriers, trying to control morphology, and addressing durability.
- Further increasing loadings of HPAs in polymers could increase conductivity, but likely at the expense of mechanical properties/water uptake that are already likely to limit material usefulness.
- The resulting properties, if incorporation of HPAs into perfluorinated polymers is achievable, will be interesting to see, but resulting structures are not likely to be easily influenced through processing, and chemistry options are limited.
- The suggested future directions were to complete the project, moving along the present pathway.

**Strengths and weaknesses**Strengths

- Novel proton-conducting polymer system.
- Diverse team with the needed expertise, appropriate work breakdown and with good working relationships.
- The project is well thought to use additives for retaining water under high-temperature, low-relative humidity conditions.
- There is a potential to this method of water retention, if HPA is anchored to an oxidatively stable polymer.
- The project demonstrates the flexibility of using HPA with different polymeric systems.
- Novel proton-conducting polymer system.
- Base materials, HPAs, show unusual and compelling conductivity properties. Exploring these materials in covalently bound systems where leaching is not an issue is a worthwhile approach.

Weaknesses

- No clear indication of finding an oxidatively stable polymer for anchoring HPAs.
- High water retention of HPAs under low temperature could be an issue in the system.
- Better HPA with low water uptake properties at lower temperature regime should be explored.
- Lack of morphological control or ability to influence distribution of HPAs in membranes make it uncertain that base properties of HPAs can be taken advantage of in covalently-bound membranes.
- Phosphates in fuel cell systems need to be thought through. Compounds with C-P bonds can be biologically active, and can have some adverse properties, like human toxicity. The indirect methanol fuel cell systems tended to emit methyl phosphate at times. There probably is no problem, but the potential problem needs clarification.

**Specific recommendations and additions or deletions to the work scope**

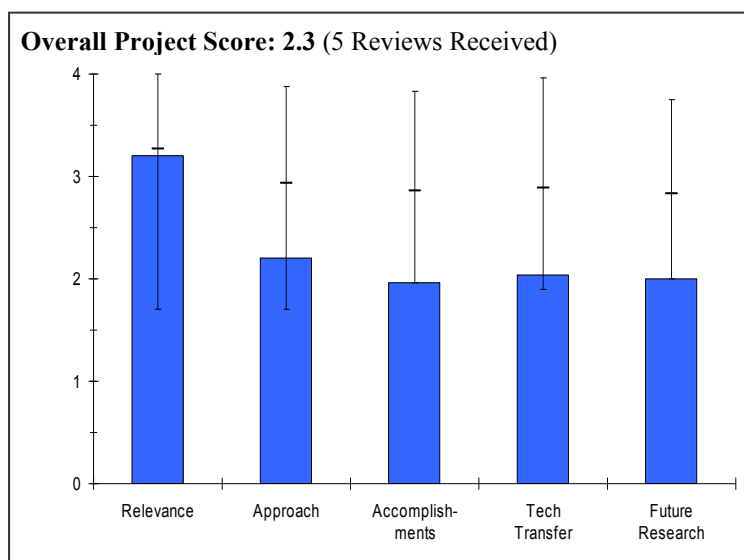
- New HPA with lower water uptake across the fuel cell operational regime should be explored.
- Si-cross-linked method has no practical purpose, since most of the Si polymers are unstable under fuel cell operational conditions. Therefore this part of the project can be deleted.
- Strongest recommendation for this project would be to focus on investigating methods of controlling morphology (distribution of HPAs) in the membrane.

## Project # FC-22: New Proton Conductive Composite Materials with Co-Continuous Phases Using Functionalized and Cross-linkable VDF/CTFE Fluoropolymers

Serguei Lvov; Pennsylvania State University

### Brief Summary of Project

The overall objectives of this project are to 1) contribute to Department of Energy efforts developing high temperature polymer electrolyte membranes for transportation applications; and 2) develop a new composite membrane material with hydrophilic inorganic particles and VDF/CTFE polymer matrix to be used in polymer electrolyte membrane fuel cells at -20-120°C and relative humidity of 25-50%. The year 2 objectives are the 1) scaling up of the supply of inorganic proton-conductive materials and polymers; 2) reaching the milestone of proton conductivity of 0.07 S/Cm at 25°C and 80% relative humidity; and 3) selection of the best membrane based on test results and adjustment of the synthesis procedures.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Durability, cost and performance improvements of membranes are all highly necessary for fuel cell commercialization.
- This membrane development effort addresses the DOE research and development objectives.
- Membranes are being made but probably these membranes are not likely to be stable. Since this presentation does not provide evidence that the work is providing insight into new conduction mechanisms or other novel properties, it appears that the project is becoming irrelevant to the overall DOE objectives. Given that the goal is to provide membranes that allow operation at high temperatures.
- High-temperature polymer electrolyte membranes are desirable for transportation applications (to facilitate thermal management) as well as for stationary applications (higher value heat in combined heat and power and/or CO-tolerance).
- The project is relevant to the DOE high-temperature membrane targets.

### Question 2: Approach to performing the research and development

This project was rated **2.2** on its approach.

- Overall synthetic theory is appealing and has high potential if pursued correctly.
- Sulfonated styrene is well known to desulfonate and should have been avoided even as a "model" compound.
- Sulfonated alumina is well known to dissolve in highly acid environments and should have been avoided even as a "model" compound.
- It is thought by many that polystyrene-containing systems do not have the required durability for long-term fuel cell use. When asked about this, the principal investigator stated that the plan was to replace this with an inorganic proton conductor. It needs to be explained how sPS is a good model for an inorganic proton conductor.
- The approach to performing the research is not very well designed, does not seem to be very feasible and appears to not be well integrated with the needs of the fuel cell. Nothing is mentioned about durability!

- Combining fluoropolymers with proven durability with inorganic proton-conductive materials is quite feasible and has potential to yield good near-term results.
- The approach appears to be unfocused. The first two year's work developed conductivity measurement capability and synthesized membranes that do not appear to have the stability necessary in a fuel cell environment. Better if the approach looked at developing stable systems first even if they are more difficult to synthesize.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.0** based on accomplishments.

- A variety of materials have been prepared; polyelectrolytes and inorganics. Approach, however, was very poor due to chemically weak material selection; the data thus far is not of high value unless new materials with the same properties are found with high chemical durability.
- The addition of hexafluoropropylene to the polymer provided increased dry conductivity. This should be repeated and explained.
- Both this polymer system and these inorganic materials have been studied by others. It needs to be fully explained what is new here in light of past work.
- Progress is modest towards the goals that the project has identified and towards the interim DOE goals. However, there seems to be no thought on how to achieve the ultimate goals and how a durable membrane can be produced that can conduct at 120°C. No thought is given to alternate proton conduction mechanisms; the high temperature performance may be achieved by retention of water by the particles, a strategy which is not really helpful.
- Developed method for *ex situ* measurement of proton conductivity of additives.
- Conductivity improvements at 120°C and low relative humidity have not yet been realized.
- The project has been underway for two years. Progress has been mixed. Pennsylvania State University faced a considerable challenge in obtaining conductivity measurements. Some of their results did not agree with literature values. Pennsylvania State University has developed membranes that meet conductivity targets but are unlikely to be stable in the fuel cell environment. There is also concern that the inorganic additives would leach out of the membranes.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.0** for technology transfer and collaboration.

- Some disagreement in data with sole outside collaborator, BekkTech.
- Should include industrial partner to avoid so many material dead-ends.
- This project would benefit from a collaboration with someone with fuel cell experience (e.g., National Renewable Energy Laboratory or Los Alamos National Laboratory).
- Non-existent!
- The principal investigator collaborates with other professors at Pennsylvania State University.
- BekkTech is essentially providing a conductivity measurement service.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.0** for proposed future work.

- If new materials can be found with improved chemical properties, future work can be of interest.
- The program would benefit if future work were focused on understanding structure-property relationships and using this information to optimize performance through control of factors such as inorganic particle size and distribution, polymer chemistry and morphology, etc. and not focused on "fabricating" or "producing" samples which meet conductivity targets.
- Future plans contain no mention of durability!
- Development of new polymers and inorganic proton conductors appears necessary to improve the chances of meeting the 2009 conductivity milestone.

- The proposed plans are vague. A clear path forward to achieving the DOE targets is not evident in the presentation.

### **Strengths and weaknesses**

#### Strengths

- High material development skills.
- The observation of the effect of added hexafluoropropylene is interesting.

#### Weaknesses

- Use of sulfonated styrene.
- Use of alumina inorganic salts.
- Lack of industrial partner.
- Lack of complete membrane characterization (swelling, gas permeability, etc.).
- There are few "new" materials used here.
- No collaboration.
- The project participants seem to be paying no attention to the needs of fuel cells and appear to be ignoring important needs.
- Requirements for the additives are not clearly defined (size, morphology, proton conductivity etc.).
- The project needs a clearer focus on a path forward to achieve a stable membrane that achieves the DOE targets.
- Several reviewers pointed out that the styrene side chains are not likely to survive in the fuel cell environment.
- Rationale for selecting the polymer candidates for grafting to the backbone and for the inorganic additives is not obvious.

### **Specific recommendations and additions or deletions to the work scope**

- Better selection of materials even if used as "model" compounds.
- Industrial partner to speed up/focus research.
- Since this project appears to make no effort to investigate new conduction mechanisms or the fundamentals of the behavior of the nanoparticles in contact with the polymer, very little of value is appearing. This project should be refocused or terminated.
- The project should consider a layered membrane approach with the inorganic additive contained in the middle layer to prevent the inorganic additives from leaching out of the membrane.
- Other side chains should be considered based on their resistance to oxidative attack.

**Project # FC-23: High Temperature Membrane with Humidification-Independent Cluster Structure***Ludwig Lipp; FuelCell Energy, Inc.***Brief Summary of Project**

FuelCell Energy, Inc. performed three iterations of polymer membranes, examined three types of additives and analyzed the conductivity of over 20 samples. A 20% improvement in conductivity was demonstrated over 2007 and approximately three times higher than Nafion 112 without loss in mechanical properties. Composite membranes show significantly better cell performance at low relative humidity than expected from conductivity tests. Low cell resistance was also achieved.

**Question 1: Relevance to overall DOE objectives**

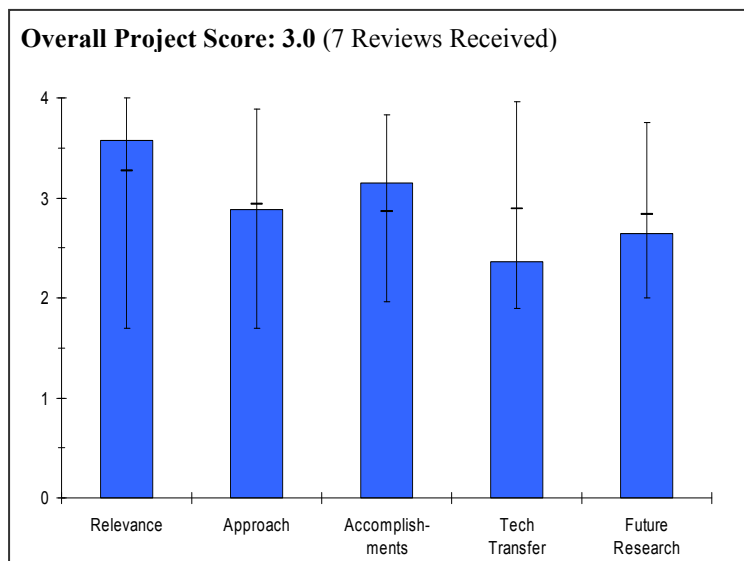
This project earned a score of **3.6** for its relevance to DOE objectives.

- Very relevant to high-temperature, low-relative humidity membrane applications.
- The project fits well with DOE's Multi-Year RD&D plan.
- The goal of developing a new polymer electrolyte membrane with higher proton conductivity and improved durability under hotter and drier conditions compared to current membranes is of high relevance.
- Membranes for proton conduction under drier conditions are critical to the president's hydrogen initiative.
- Project addresses relevant DOE goals and objectives.
- Project fits into the DOE goals of reducing cost and obtaining improved performance of fuel cell materials. Even so, the high temperature part of those targets is now of less importance.
- High temperature membranes are an important area for DOE investment.
- Project addresses relevant DOE goals and objectives.
- Proposed work falls within the expectation of DOE's Hydrogen Fuel Initiative and FCE is in line with the progress of the work.

**Question 2: Approach to performing the research and development**

This project was rated **2.9** on its approach.

- Very innovative and well-thought approach.
- Different additive components for different functionalities are interesting.
- The approach is to combine four elements (co-polymer, support polymer, water additives and conductivity additives) into a membrane. This approach is being addressed by several groups in addition to FuelCell Energy. No information is given about what the four materials are, so evaluation of their interactions is impossible. Is 1+1+1+1 going to be more than 4 or not?
- Supported polymer with additives for water retention and proton conductivity.
- Not particularly novel.
- Composite approach has potential and has several knobs to turn to meet targets.
- The plan was to insert additives into commercial materials, thus improving performance.
- Interesting approach to the problem via empirical equation.
- Not certain that conductivity terms are strictly additive.
- Difficult to judge approach without details on polymer and additives' chemistry.



**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- Initial results look very promising.
- Membrane casting method development needs more work to address processing related issues.
- The cost of the composite membrane has not been addressed.
- Technical challenges to integrate electrodes to this composite membrane should be addressed.
- Membranes have been only fabricated using the co-polymer presumably by the unnamed polymer partner. Work on the additives has not been reported and this work is to be done by the consultants who are not named? If University of Connecticut (investigator not named here either) is doing the cross-over and conductivity work, what is FuelCell Energy doing? Some fuel cell testing work is presented but it is at too high of system pressure (> 20 psig) and no current interrupt measurements were reported so the resistance of the membrane under the conditions of the test (not completely reported) was not presented. What ionomer was used in the catalyst layers?
- Met milestone but not validated by BekkTech.
- Area specific resistance lower at standard conditions.
- Fuel cell tests run.
- Achieved low temperature conductivity milestone (testing at FCE, not with measurements at Florida Solar Energy Center).
- Have achieved ~3x the conductivity of Nafion 212 at 120°C 25% relative humidity.
- Have demonstrated membrane in a membrane electrode assembly at 120°C 25%relative humidity with excellent performance (Pt loading not indicated, so difficult to compare directly without a standard Nafion membrane membrane electrode assembly with same loading and conditions given).
- The short-sidechain PFSA clearly had improved properties following modification by "additives", easily meeting the DOE conductivity target.
- Meeting minimum DOE targets with some samples.
- Good polarization data.
- Seems like there are electrode difficulties.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.4** for technology transfer and collaboration.

- There is good collaboration with different university and testing laboratory.
- Interaction with National Laboratory could have been beneficial.
- As none of the partners are listed by name, it is impossible to judge the interaction or coordination.
- No National Laboratory, but collaboration with original equipment manufacturer planned.
- Collaborations would look better if we knew who the polymer partner was.
- No significant collaborations discussed.
- Electrode performance suggests need for collaborator in this area.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.6** for proposed future work.

- Work should be dedicated to develop better membrane electrode assembly interfaces with these novel composite membranes.
- The proposed future work is so general that will be impossible to benchmark success.
- Improve everything, but approach not necessarily validated yet.
- Without knowing a bit more about the ionomer and additives, it is difficult to judge the future plans. A little more information would be very useful in judging the prospects for success and to determine how much this project overlaps others in the area.

- Essentially, FuelCell Energy announced plans to wrap-up this activity, with additional activities that would continue onward on the "additive" route.
- Future work is a straightforward continuation of ongoing work.
- Difficult to project what is to be expected with higher additive loadings.

### **Strengths and weaknesses**

#### Strengths

- Well thought out concept, seems to be low cost membrane alternative.
- Good initial data; seems to be promising material.
- The approach is a good one, unfortunately it is not unique.
- Well-conceived empirical approach.

#### Weaknesses

- Membrane manufacturing processes should be fine tuned to demonstrate fabrication of consistent quality material.
- Membrane electrode assembly interfaces with these composite membranes should be addressed.
- No technical information is provided to benchmark success. Interactions with unknown partners also make benchmarking impossible.
- More details need to be provided regarding the membrane. More information regarding the ionomer identity, the types of additives, etc. are necessary so we can judge the potential for success as well as the overlap of this project with others in the membrane area.
- Poor electrode performance.
- Additive chemistry is often difficult to integrate into electrodes.

### **Specific recommendations and additions or deletions to the work scope**

- Development of membrane electrode assembly interface work should be explored for this new membrane material.
- If project will not disclose the chemistry of the materials, this program cannot be properly evaluated, hence it is not clear why this project should continue to receive funding.
- What goes into polymers can also come out—there is need to demonstrate that the additives adhere into the polymers and do not result in accelerated polymer degradation.
- Advisable to collaborate with some electrode production expertise.

**Project # FC-24: Dimensionally Stable Membranes***Cortney Mittelsteadt; Giner***Brief Summary of Project**

The ultimate goal of the project is to meet performance targets with film that can be generated in roll at DOE cost targets. The year 2 milestones were achieved and interim conductivity targets have been met. Improvements in fuel cell performance have been shown, including electrode improvements. A realistic pathway for meeting cost targets can be seen for both 2- and 3-dimensionally stable membrane paths. To reach the ultimate DOE goals, Giner might consider incorporating the low equivalent weight materials that have been developed at State University of New York-Syracuse.

**Question 1: Relevance to overall DOE objectives**

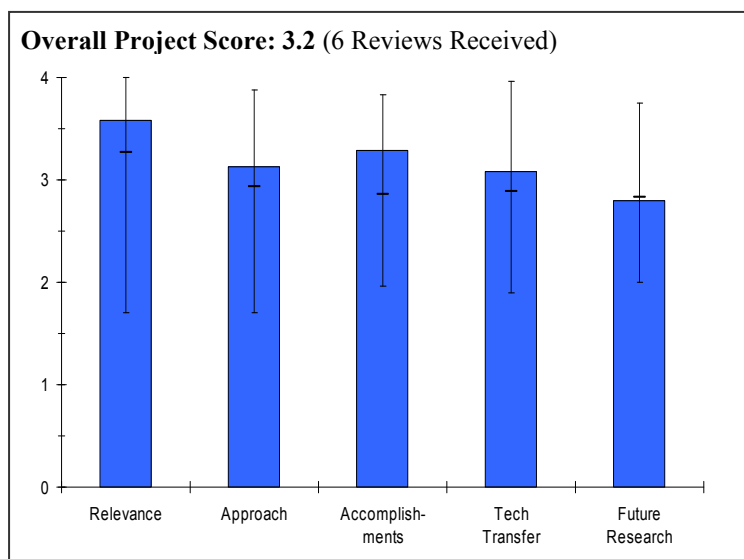
This project earned a score of **3.6** for its relevance to DOE objectives.

- Durability, cost and performance improvements of membranes are all highly necessary for fuel cell commercialization.
- The project objectives are relevant to DOE's RD&D plan.
- The project addresses the fundamentals of low-relative humidity proton transport issues.
- Membranes for proton conduction under drier conditions are critical to the President's Hydrogen Fuel Initiative.
- Good program, focused on providing membrane materials that not only meet the immediate milestone but also shows progress towards the final goal.
- The project is highly relevant to the DOE high-temperature (HT) membrane goals.
- High temperature membranes are an important area for DOE investment.
- Particularly relevant approach because of focus on dimensional stability.
- Good to see electrode preparation directly integrated into project.

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- Reinforcement technology and modification is highly unique but of high cost.
- New reinforcement layer is less novel but could meet cost targets.
- In-depth analysis of existing polyelectrolytes was performed.
- Catalyst-coated membrane vision is also of high value.
- The approach seems to be technically not feasible.
- The dimensionally stable membrane material possesses low void area and membrane impedance will be very high.
- The material research of dimensionally stable membranes seems to be interesting, but it may be associated with prohibitive cost.
- Very low equivalent weight PFSA, but this is water-soluble.
- 2D-reinforced support.
- Will there be membrane electrode assembly testing?
- 3D support (commercially available), but how is this different than Gore's approach?





- Excellent approach, addressing the barriers, looks to be very technically feasible and is integrated. However, not enough detail given on the new polymers made at State University of New York. Cannot make a judgment. Also would like data on durability. Is there a weak spot where the ionomer meets the support?
- The approach is very good. Rather than develop a completely new membrane that has the required physical characteristics and durability under fuel cell operating conditions, Giner is attempting to use dimensionally stable membranes that can retain an imbibed electrolyte under fuel cell operating conditions.
- Very solid and elegant approach.
- The investigators are using fairly conventional materials with the main innovation coming in the processing approach.
- Approach provides an opportunity to readily introduce materials from other projects into a processable membrane.
- Small quibbles with a few details: in question and answer session, commented that water permeation is fast so equilibration will be fast; however, uptake of water is often surface-driven.
- It is not clear how improvements will be realized given the nature of the conducting materials.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- Met DOE milestone target.
- Low equivalent weight material from partner shows promising results but no chemical information was shared so difficult to judge.
- Analytical characterization is top-level.
- The practical demonstration of dimensionally stable membrane concept had been done well.
- More work is needed with commercial ionomeric materials to validate the concept.
- The cost and efficiency of these substrate materials should be addressed using commonly available ionomers.
- Very close to Go/No-Go at 50% relative humidity.
- Homopolymer in 3D support.
- Good progress demonstrated towards DOE goals. However, durability needs to be highlighted.
- Giner has met the 2007 DOE interim goal of 70 mS/cm conductivity. Achieved 0.8 S/cm at 30°C and 80% relative humidity.
- Nearing DOE 2010 target; have demonstrated 0.08 S/cm at 80°C and 30% relative humidity.
- Membranes developed so far exceed the mechanical properties of the Gore-reinforced membrane.
- State University of New York-Syracuse has successfully synthesized several new low-EW ionomer candidates to meet performance targets.
- Good progress toward real membranes and membrane electrode assemblies.
- Substantial progress toward technical goals.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- Difficult to judge because no real information was shared, however, transferred polyelectrolyte material did meet DOE targets.
- General Motors' interest in Giner will ensure good research direction and focus.
- The project has good academic and industrial partner.
- The project seems to have good interaction with academic and industrial communities.
- University, original equipment manufacturer industry partnership.
- Not very clear how this goes beyond the State University of New York-Syracuse partnership. The role of General Motors is unclear.
- General Motors and State University of New York-Syracuse are collaborators. General Motors provides automotive requirements to ensure performance metrics are met.
- Solid collaboration.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- Future work on both reinforcement layer and polyelectrolyte is good.
- Cost considerations are being taken into account and attacked.
- More work should be done with commercially available ionomeric materials.
- Membrane electrode assembly interface issues with these membranes should be addressed.
- The high cost and large membrane impedance issues should be addressed.
- Should concentrate on ionomer development before scale-up.
- Future plans seem a bit vague.
- Exactly what durability studies will be done?
- The cross-linking strategy is dangerous. This can lead to major current density distribution issues.
- Not sure which approach, 2D or 3D, membrane support will work. So Giner pursuing both--the molded 2D support shows promise as well as the 3D membrane.
- Realistic pathways appear to be able to meet the DOE cost and durability targets.
- Looking to State University of New York for a new lower equivalent weight ionomers to reach the DOE conductivity goals of 0.1 S/cm at 120°C and 50% relative humidity.
- Emphasis on very thin membranes is appropriate.
- Durability tests are reasonable.
- Very good approach to attack all barriers to get to a usable membrane.

**Strengths and weaknesses**Strengths

- Unique reinforcement layer.
- Good analytical abilities.
- Polyelectrolyte potential (hard to judge).
- Well-thought out concept.
- Good alternative approach to expanded poly(tetrafluoroethylene) (Gore-Select) approach.
- Very strong electrochemical capabilities as would be expected from this company.
- The project is close to meeting the 2010 HT membrane targets.
- The project has clearly described a viable path forward to meeting the DOE targets.
- Near-term approach to membrane preparation.
- Broadly applicable.
- Includes electrode optimization.

Weaknesses

- Lack of transparency on polyelectrolyte development.
- The cost issue with substrate fabrication should be addressed.
- More commercial ionomer should be integrated to this substrate.
- Commercial supports too thick.
- Homopolymer water-soluble.
- Not enough chemistry background in the team.
- Not clear how the final goal will be met. This company should know that 25% relative humidity at 120°C is the upper limit. They should be well aware that water is a big problem yet they are making no effort to find a new mechanism of proton conduction. The project is incremental and this represents a major weakness that needs to be addressed.
- Nothing fundamental to deliver better materials for low relative humidity.

**Specific recommendations and additions or deletions to the work scope**

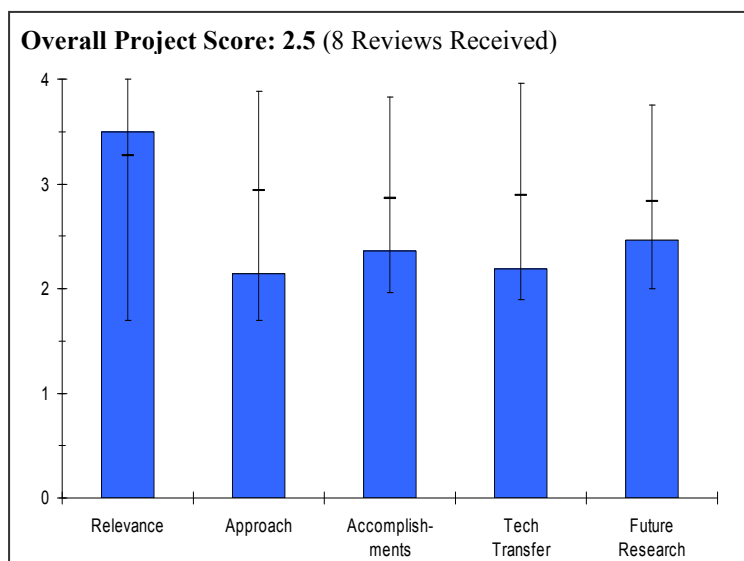
- Continued hard work down this path.
- More serious evaluation of capillary effect especially in light of recent literature results.

## FUEL CELLS

- More commercial ionomers should be used to evaluate the performance with dimensionally stable membrane substrate.
- New dimensionally stable membrane fabrication should be evaluated to reduce the cost.
- More fundamental studies of PFSA polymer.
- How about making some effort to get rid of water and find a new mechanism of proton transport?
- Continue the two-path approach to determine if each can produce a membrane meeting all targets. Then focus development effort on the path that has the lowest cost potential.
- Collaborate with more innovative polymer makers.

**Project # FC-25: Poly(cyclohexadiene)-Based Polymer Electrolyte Membranes for Fuel Cell Applications***Jimmy Mays; University of Tennessee***Brief Summary of Project**

The objective of the project is to synthesize and characterize novel neat and inorganically modified fuel cell membranes based on poly(1,3-cyclohexadiene) (PCHD). To achieve this objective, a range of materials incorporating PCHD will be synthesized, derivatized, and characterized. Successful completion of this project will result in the development of novel potentially inexpensive polymer electrolyte membranes engineered to have high conductivity at elevated temperatures and low relative humidity.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- Project addresses relevant DOE targets and barriers.
- The project is relevant to the Multi-Year RD&D Plan of DOE.
- The project is focused to address low-relative humidity, high-temperature membrane issues.
- The objectives of this project are consistent with the President's Hydrogen Fuel Initiative.
- This membrane development effort addresses the DOE research and development objectives.
- Project addresses relevant DOE targets and barriers.
- Polymer electrolytes are not the most significant barrier for fuel cell commercialization.
- The project supports the President's Hydrogen Fuel Initiative.
- Professor Mays added the two critical targets, cost and durability, to the new polymer list, very welcome additions.
- High temperature membranes are an important area for DOE investment.

**Question 2: Approach to performing the research and development**

This project was rated **2.1** on its approach.

- Not clear how they intend to get conductivity at high temperature, low relative humidity (the target conditions). What is the inorganic additive that will provide good conductivity at low relative humidity?
- Durability of non-aromaticized systems in a fuel cell environment is suspect, as is the durability of S-S linked systems.
- A large portion of the work is being performed on mechanical testing and characterization, which may be premature since conductivity in these materials has yet to meet targets.
- The chemical approach to membrane development is not robust.
- The material, especially the crosslink, is vulnerable to the oxidative condition, especially to Fenton's condition.
- The material may not be stable to fuel cell operational condition.
- Poly(cyclohexadiene) polymers cross-linked via Cl bonds are unlikely to be thermally & chemically stable in a fuel cell environment.
- Focus on thermal analysis provides little insight into relevant performance and durability properties.
- It needs to be made clear how these materials provide a path to membranes with the durability to survive in a fuel cell. Aliphatic hydrocarbons are known to have unacceptable durability in polymer electrolyte membrane fuel cells. Also, while random, sulfonated hydrocarbon polymers are known to have high proton conductivity at

high levels of hydration, the conductivity is very low at low humidification. Why are these expected to be better?

- The pursuit of poly(cyclohexadiene) as an ionomer material is limited because the backbone will have poor durability in fuel cell environments. The pursuit of these materials is unlikely to help achieve DOE targets particularly in the area of durability.
- Anionic polymerization control has some interest in creating polymers of controlled morphology.
- Focus on thermomechanical analysis, dynamic mechanical analysis, and thermogravimetric analysis are the wrong focus for this project. The extent of work in this area reflects the expertise of the co-principal investigator more than what is required to move these materials forward.
- The University of Tennessee chemical synthesis work is first rate. The chemistry seems likely to result in very low cost materials.
- Certainly one of the more original approaches.
- Highly desirable combination of strong synthesis capability with a well-known polymer physical chemist.
- Good level of control of properties. The ability to develop the trade-off between swelling and conductivity is important.
- Very difficult to see these materials achieving even modest durability.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.4** based on accomplishments.

- No work performed on inorganic modification that is intended to provide good conductivity at high temperature, low relative humidity yet.
- Conductivity at low temperature, high relative humidity have not met milestone 2.5.
- The mechanical issues of the membrane are well-addressed.
- No work has been done to address the chemical stability of this polymeric material.
- No fuel cell testing data to see whether the membrane material is functional under fuel cell conditions.
- Principal investigator made films with good wet conductivity – but no data shown at lower relative humidity.
- It needs to be made clear how the thermogravimetric analysis data shown is relevant to fuel cell use.
- The transport properties and chemical stability of these materials need to be evaluated.
- The project has demonstrated materials with reasonable conductivities although reaching target conductivities under target conditions will be difficult.
- Results centering on thermomechanical analysis, thermogravimetric analysis, and dynamic mechanical analysis have little relevance to the limited conductivity data. *In situ* durability data and data related to hydrolytic, oxidative or radical-induced degradation are more important.
- Good progress was evident in the development of low cost materials. Most likely the polymers are good enough, although the DOE target for conductivity was not demonstrated.
- A number of membranes exhibit high enough conductivity for first level milestones.
- Durability not tested and is highly questionable.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.2** for technology transfer and collaboration.

- Little collaboration apparent to date. Collaboration/interactions with experts in fuel cell membrane area would help choices of cross-linkers, etc. that would be more stable in a fuel cell environment.
- No industry partner to give good feedback on the membrane.
- More interactions with Fuel Cell labs and centers are needed to get honest feedback on this material.
- There was no evidence of any external collaboration of future plans for it.
- This project would benefit from a collaboration with someone with Fuel Cell experience (e.g., National Renewable Energy Laboratory or Los Alamos National Laboratory).
- The team has 2 primary participants. The connection between these two participants and how they synergistically benefit each other is unclear.
- Perspective from outside investigators on all requirements of a fuel cell membrane seems almost essential.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.5** for proposed future work.

- Need more focus on membranes that would be stable under fuel cell conditions (aromatic, with stable cross-linkers).
- Need more work on inorganic additives and strategies to provide high-temperature, low-relative humidity conductivity.
- Proposed future research will address some of the durability issues.
- *In situ* chemical stability data should be obtained.
- All the most important tests they have not been conducting are planned for the future (conductivity vs. relative humidity, relative humidity cycling, open circuit voltage).
- No promising plans for improving stability of materials.
- The *ex situ* (Fenton's test) and *in situ* (open circuit voltage) tests proposed are important at this stage and should be done ASAP.
- Future work looks like a laundry list with some items of little relevance. The focus on degradation studies is certainly important, oxygen permeability and dielectric studies will give limited value and seem to be included simply because they are equipment available to the project.
- The future work mentioned was completion of the project, just doing more work, and achieving better performance and lifetime.
- A definite path forward with preparation of inorganic composites, in the lab of highly experienced practitioner planned.
- The investigators clearly understand the issues (durability, further increases in conductivity).

**Strengths and weaknesses**Strengths

- Low-cost option.
- New polymer development and thinking outside the box.
- Lots of cross-linking chemistry has been developed, which could teach other groups on cross-link-mediated membrane stabilization methods.
- None.
- The synthetic chemistry is first rate.
- Strong synthesis capabilities.
- Original approach.

Weaknesses

- Durability concerns with polymer structures currently being studied.
- No industrial partner to give right feedback on the requirements of membrane properties.
- No chemical stability work has been conducted with the present polymeric system to assess its use under fuel cell conditions.
- Too much focus on thermal analysis.
- No data reported on conductivity at low relative humidity.
- No swelling or mechanical data presented.
- Materials being studied are inherently unstable in fuel cell environment.
- This class of materials may not be suitable for fuel cell applications.
- No collaborations.
- Durability concerns with polymer structures currently being studied.
- Too much focus given to mechanical properties. Not enough chemistry development, durability studies, or conductivity data to suggest these materials offer promise. Based on chemistries presented stability and durability are almost certainly poor, and conductivity reported to date is not compelling.
- Fuel cell membrane electrode assembly fabrication and testing should be done in conjunction with DOE partners who excel in those tasks.
- Large questions re: durability.

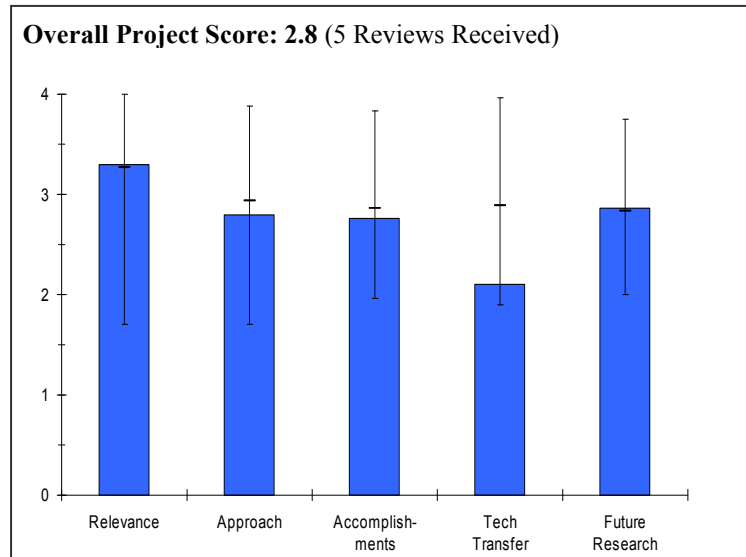
**Specific recommendations and additions or deletions to the work scope**

- Fuel cell testing of the material should be included.
- Chemical degradation work, such as Fenton's decay, should be done.
- The polymer stability should be assessed before proceeding to next phase of the work.
- Membrane electrode assembly development process to generate good membrane electrode assembly interface should be carried out.
- Eliminate Cl cross-linkers.
- Increased focus on aromatic membranes.
- Eliminate mechanical property studies; focus on degradation studies and conductivity studies.
- Modify materials set to a set of materials that has some chance of being fuel cell stable.
- The tests with Fenton's reagent should be avoided, since those conditions are just too aggressive. It is important to test to see how long the membrane materials will perform, rather how quickly they can be destroyed!
- These investigators could really use an infusion of experience with membrane requirements for fuel cell operation.

**Project # FC-26: PEM Fuel Cell Durability**  
 Rod Borup; Los Alamos National Laboratory

**Brief Summary of Project**

The overall objective of this project is to quantify and improve polymer electrolyte membrane fuel cell durability to 5,000 hours (with cycling). The objectives of this project are to 1) define degradation mechanisms; 2) design materials with improved durability; 3) identify and quantify factors that limit polymer electrolyte membrane fuel cell durability; and 4) improve durability. Property changes in fuel cell components during life testing will be measured (membrane-electrode durability, electrocatalyst activity and stability, electrocatalyst and gas diffusion layer carbon corrosion, gas diffusion layer hydrophobicity, bipolar plate materials and corrosion products).



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- Deeper understanding of durability mechanisms are needed to meet automotive fuel cell targets.
- Very good – durability is a major issue. Identifying causes of decay is important. Accelerated tests, as noted, may not have adequate fidelity.
- The overall objective of the project addresses a key barrier, durability. It is not clear from the work described how it addresses performance and cost as claimed.
- Original equipment manufacturers carry out in-house durability testing, so project relevance is predicated upon 1) ability to discover new test protocols for uncovering failure modes, and 2) informing DOE on the durability status of relevant materials in relevant cell designs. Further testing is needed to determine whether #1 will be accomplished. #2 has not occurred.
- Goals align well with DOE technical target of 5000 hours durability.

**Question 2: Approach to performing the research and development**

This project was rated **2.8** on its approach.

- Research objectives have changed over time which creates more issues.
- Segmented cell analysis is unique and interesting.
- Very good – Activity appears to be using the synergy of previous projects.
- The approach is highly experimentally focused and somewhat split between accelerated test method evaluation and their application to membrane electrode assembly materials.
- It is not clear if the approach should be more focused in one way or the other.
- A project that is seeking to look at stack durability should do *in situ* testing followed by failure analysis, which matches this project's approach.
- Challenges involved in doing such a project include 1) validation of test stand (representative system volume, speed of mass flow controllers, reference electrodes to quantify half-cell voltage), 2) selection of relevant materials, 3) selection of relevant cell design, 4) failure mode isolation with protocol, 5) selection of relevant operating conditions, and 6) reporting correct metrics. Project has reported a focus on #4, but #1-3 and 5 are not reported. Before and after performance should be reported to enhance #6.



- Proposed accelerated testing studies appear sound.
- Most of work focused on accelerated testing studies.
- Not much discussion regarding identification of factors limiting durability, mechanisms for degradation of material, or design to improve durability.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- A lot of superficial work was shown due to vastness of program.
- Some results/experiments are not well-controlled or analyzed (step vs. ramp voltage cycling). Some results/experiments, however, do show high value preliminary results (gas diffusion layer degradation).
- Good – Accomplishments and progress appear to be at the expected level due to the complexity of the issues.
- A lot of good work was accomplished since the recent restart, but spread over application of multiple types of accelerated durability tests applied to undefined types of membrane electrode assemblies. It is good to demonstrate the suite of different tests, but as a result, the progress can only be considered modest in overcoming barriers. It is not clear what was learned specifically about materials issues.
- Start-stop phenomena observed (SU/SD CO<sub>2</sub> loss at different temperatures, purge) need to be put in perspective of half-cell voltage, performance data (e.g., mass activity), and failure analysis.
- Gas diffusion layer degradation phenomena study shows good progress. The next step is to test electrochemical/*in situ* stressors and then do single fiber / sessile drop tests again. Chemical analysis should confirm distinction between exposed carbon fiber and degradation that could have occurred to hydrophobic agent.
- On segmentation, *in situ* work should show whether performances losses were recoverable or were the result of low polymer electrolyte membrane humidification, removable catalyst surface oxide/hydroxide.
- H<sub>2</sub>O<sub>2</sub> formation could be higher at 100% relative humidity – validation required. Polymer electrolyte membrane material parameters unknown.
- What is being expected is tough to accomplish, so the efforts thus far should be applauded in spite of low ability to directly apply to automotive realities.
- Have identified certain operational issues important to durability, such as relative humidity and temperature.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.1** for technology transfer and collaboration.

- No official partners hurts the overall program.
- Good/Fair – It would have been cost-effective to leverage the technical activities of Fuel Cell Commercialization Conference of Japan (FCCJ), US Fuel Cell Council (USFCC), and the other academic labs. Consideration should be given in sharing raw data on a Non-Disclosure basis with the other researchers.
- The principal investigator's presentation states there are no formal partners. The stop and recent restart history of the project may be partially responsible for the lack of significant coordination or technology transfer.
- According to the presentation, there are no formal partners, although certain organizations are leveraged for analysis and material inputs.
- Materials sets need to be reported. Membrane electrode assembly composition (gas diffusion layer product code, catalyst loading, polymer electrolyte membrane thickness, etc.) is unknown.
- Materials obtained from other institutions.
- Some analyses performed by others institutions.
- One 2007 and no 2008 publications.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- All proposed research topics are of high value and interest if done properly with the needed resource and scientific depth.
- Good – Plans are rational, but do not appear to leverage other external activities.
- Proposed focus on four major areas may spread the resources too thinly. Accelerated durability measurements/protocol evaluation and trying to correlate durability with the accelerated tests may be a full time project. Or component-interface durability and correlation with property measurements may be a full time project. But combining them may be too much for the resources available.
- The list of expectations is extraordinary, including accelerated stress testing and correlations with *in situ* durability.
- Fundamental validation of test equipment needs to be reported so that investigators know that realistic stressors are being applied. This needs to be the most immediate focus.
- Continuation of gas diffusion layer component durability work is needed, but needs to be related to *in situ* stressors.
- Fundamental mechanistic studies are proposed.
- Good to correlate accelerated testing with durability.

### **Strengths and weaknesses**

#### Strengths

- In-depth background knowledge of fuel cells.
- Ability to do a variety of in-house experiments.
- Addressing a complex and timely issue.
- Experience and reputation of the principal investigator and his facilities.
- Investigators involved are greatly experienced and are experts with conventional fuel cell failure mode knowledge and test capability.
- The correct failure modes are being attacked.
- Thorough reporting of *in situ* metrics for polymer electrolyte membrane fuel cell work.
- Proposed accelerated testing studies appear sound.
- Goals aligned well with DOE technical target of 5000 hours durability.
- Have identified certain operational issues important to durability, such as relative humidity and temperature.
- Fundamental mechanistic studies are proposed for future work.

#### Weaknesses

- Too many research topics.
- No official partners.
- Segmented cell experiments while interesting may not be applicable due to unique cell designs.
- Lack of synergy and collaboration with other researchers doing similar research.
- Lack of closer interactions with key fuel cell system integrators or stack developers for guidance on accelerated tests.
- Relationships with realistic *in situ* stress must be established for all testing.
- Test stand validation needs to be reported (reference electrodes, system volume, etc.).
- Reporting of material set parameters needs to be improved.
- Expectations are extremely high. A direct focus on a failure mode and demonstrating a realistic isolation of that failure mode *in situ* would yield greater benefit.
- Thorough reporting of *in situ* metrics needed for work other than polymer electrolyte membrane fuel cell work.
- No discussion regarding cost barrier.
- Discussion regarding identification of factors limiting durability, mechanisms for degradation of material design to improve durability is limited.
- Progress on the fundamental understanding of decay mechanisms is limited.

### **Specific recommendations and additions or deletions to the work scope**

- Focus on 1-2 key topics.
- Add official partners to program; possibly original equipment manufacturers to help in understanding.

## FUEL CELLS

- More collaboration and a willingness to share raw data with other researchers.
- Reconsider the scope of the future work plan to allow accomplishing more and faster progress on just the top one or two most critical aspects of durability.
- Delete chemical hydride work until a validated means of hydrogen storage is known.
- Focus on linking one particular failure mode to realistic stack operation. Once this is accomplished, a similar methodology could be applied to other failure modes. For example, this project could just devote itself to start/stop phenomena, or to gas diffusion layer degradation, and deliver greater results than what it has done so far.
- May want to also suggest fundamental mechanisms for experimental observations.

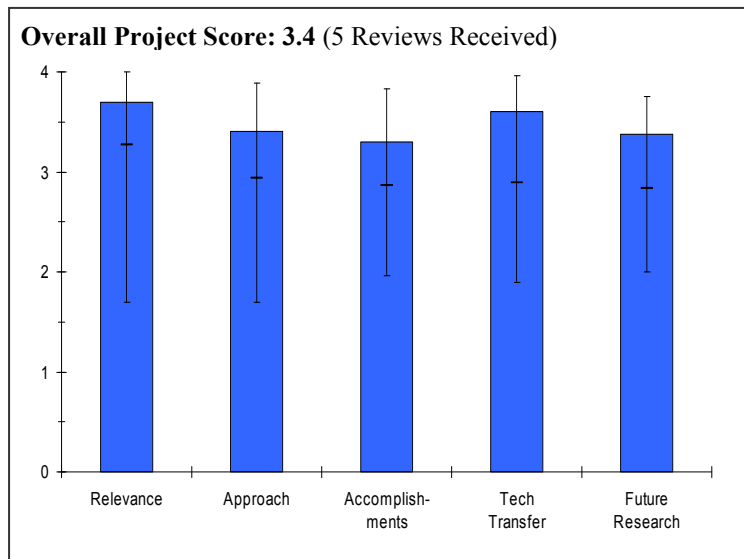
## Project # FC-27: Nitrided Metallic Bipolar Plates

Peter Tortorelli; Oak Ridge National Laboratory

### Brief Summary of Project

The overall objective of this project is to demonstrate potential for metallic bipolar plates to meet automotive durability goals at a cost of <\$5/kW. Ferritic and duplex compositions amenable to both stamping and nitriding have been identified. An alloy and nitriding envelope capable of imparting low interfacial contact resistance and high corrosion resistance at potentially acceptable nitriding cost has been identified (all in the range of Department of Energy targets). Stamped alloy foils without embrittlement and with little warping were also demonstrated.

### Question 1: Relevance to overall DOE objectives



This project earned a score of **3.7** for its relevance to DOE objectives.

- Metal bipolar plates with a low cost, low thickness, and high durability are needed to meet fuel cell commercialization requirements.
- The project is relevant toward meeting bipolar plate cost targets.
- Cheap mass production of metal bipolar plates is critical to the President's Hydrogen Fuel Initiative.
- This task is strongly relevant to the Hydrogen Fuel Initiative and goals and objectives of the Multi-Year RD&D Plan.
- Durable, cost-effective bipolar plates that meet targets for conductivity and corrosion resistance are essential to the commercial viability of automotive polymer electrolyte membrane fuel cells.
- Nitrided metallic plates – corrosion resistance of metallic plates is key to successful implementation in automotive systems.

### Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- Overall approach and concept are high level.
- It is unclear why two model materials were needed to validate the concept – time and money were wasted.
- Nitriding of metal plates is a unique approach to enable use of low-cost alloys without the addition of conductive coatings.
- Corrosion and durability show potential but more work is required.
- Nitrided bipolar plates and their characterization/mechanical properties.
- Scale-up to single cell, then scale-up to stack.
- The approach is very well laid out and delineated with clear go/no-go milestones.
- Resistivity, corrosion, and cost goals are clearly and methodically being addressed.
- Results to date indicate the approach is technically feasible and reasonably well integrated with other research via the diverse team Oak Ridge National Laboratory has organized.
- Nitriding is a well-developed technology in other industries and should be explored for use in bipolar plates. The principal investigator has a thorough understanding of the materials interaction and coating technologies.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- Good progress was shown with materials, however, two model materials slowed down overall progress unnecessarily.
- Durability studies showed good results, however, are the durability conditions valid and worthwhile for automotive conditions?
- The pathway was developed to meet performance and durability targets with low-cost Ferritic plates.
- The principal investigator claims (no data shown) that nitriding can be done without embrittlement and with little warping.
- The project met its first milestone.
- Vary Cr/Ni/V to optimize the plate.
- The corrosion test was passed.
- Ferritic foil was developed.
- The project has achieved the first of three significant go/no-go milestones and is progressing toward the second.
- It appears promising that the second go/no-go milestone will be achieved given that targets for contact and corrosion resistance have largely been achieved.
- Cost estimates indicate that cost targets are potentially within reach. High volume, cost-effective nitriding techniques will have to be further explored to achieve delta of \$0.75/kW.
- When looking at level of Nickel addition to alloy, it is a balancing act between stampability, nitride protection, and cost.
- Significant accomplishments have been achieved metallurgically.
- Overall, significant progress has been achieved and clear pathways for further progression are evident.
- Excellent effort in identifying cheaper metals - final step in joining two stamped plates to form the bipolar plate hasn't been demonstrated.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.6** for technology transfer and collaboration.

- Very high level/clear interaction with all of the players.
- All of the key players (minus original equipment manufacturer) are involved and interactive.
- The principal investigator showed good collaborative effort with metal sheet supplier and labs for testing.
- Valuable input from Directed Technologies, Inc. on nitriding cost analysis.
- Good industrial collaborations.
- Continued cost analysis.
- Oak Ridge National Laboratory has built a solid and appropriate team for the task including a commercial alloy foil manufacturer, commercial bipolar plate company, and laboratory/university fuel cell testing entities. All the major bases are covered.
- Teaming arrangement with Allegheny Ludlum and GenCell will provide the basis for future commercialization of the nitrided stainless steel bipolar plates.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.4** for proposed future work.

- Proposed research work is well-planned.
- Milestones with go/no-go decisions are wise and well thought-out.
- Detailed characterization of corrosion and electrical properties is planned.
- Planned stack testing will be critical to prove the technology.
- Additional effort should be taken to reduce nitriding process cost by reducing time and temperature or alternating nitriding methods.
- Detailed characterization of corrosion.

- Proposed future research is right on target for achieving the correct balance between stampability, cost, and corrosion protection.
- Oak Ridge National Laboratory has identified several options for achieving low-cost nitriding that will be pursued in collaboration with a commercial company in fiscal year 2009.
- There is little discussion of other options should low cost, nitriding processes not achieved or if an appropriate balance of elements, including addition of Nickel, cannot be achieved.
- Questions were raised during the presentation with respect to the effect of welding or other joining techniques on the durability of the nitride layer. This may be an open issue that should be explored.

### **Strengths and weaknesses**

#### Strengths

- Key players are all involved.
- Unique surface technology.
- Understanding of cost targets.
- Ability to tailor hydrophobicity of nitride layer.
- Ability to implement lower cost (Ferritic) thin metal plates.
- Excellent project clearly targeted to the needs of bipolar plates for polymer electrolyte membrane fuel cells and the Hydrogen Fuel Initiative.
- Very deep, well rounded team.
- Demonstrating steady, consistent technical progress with strong potential to achieve all targets for bipolar plates.
- The principal investigator identified a reasonable pathway to use cheaper metals and maintain conductivity.

#### Weaknesses

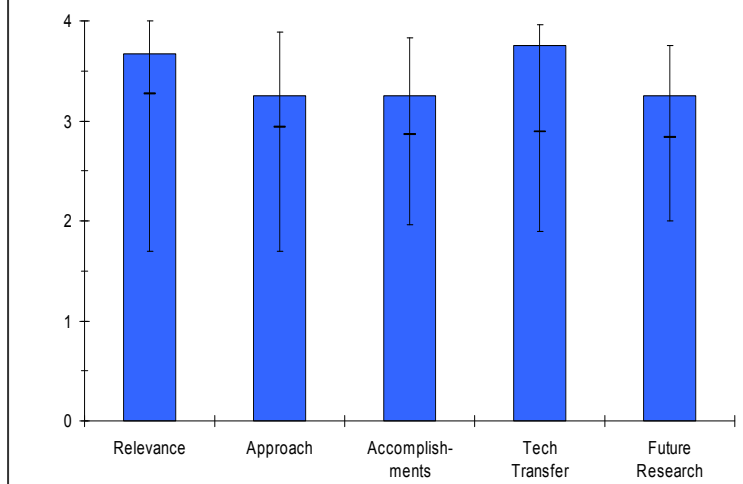
- Lack of original equipment manufacturer input specifically on durability.
- High temperature, relatively long nitriding process may be cost-prohibitive.
- No significant apparent weaknesses.

### **Specific recommendations and additions or deletions to the work scope**

- Perhaps the addition of original equipment manufacturers to help with targets.
- The principal investigator needs to figure out the last step of joining the plates and preventing scratches and damage of coated plates in shipping, assembly, etc.
- More focus on joining of unipolar plates including welding.
- Look into lower nitriding temperatures and plasma nitriding processing.
- Explore possible effects of fuel cell joining techniques on durability of the nitriding layer.
- Consider other options for squeezing a little more cost out of the alloy and stamping phases, should nitriding prove a little more costly than expected.

**Project # FC-28: Next Generation Bipolar Plates for Automotive PEM Fuel Cells***Orest Andrianowycz; GrafTech International, Ltd.***Brief Summary of Project**

The overall objective of this project is to develop the next-generation automotive bipolar plates based on an engineered composite of expanded graphite and resin capable of operation at 120°C. The goals for year 1 are to 1) develop a graphite/polymer composite to meet the 120°C fuel cell operating temperature; and 2) demonstrate manufacturing capability of new materials to a reduced bipolar plate thickness of 1.6 mm. The year 2 goals are to 1) manufacture high-temperature flow field plates for full scale testing; 2) validate performance of new plates under automotive condition using a short (10-cell) stack; and 3) show viability of published cost target through the use of low-cost materials amenable to high-volume manufacturing.

**Overall Project Score: 3.4 (6 Reviews Received)****Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.7** for its relevance to DOE objectives.

- Low cost, thin, highly durable bipolar plates are necessary for fuel cell commercialization.
- Cost and durability at extreme operating conditions are critical. This project addresses both issues for the bipolar plate.
- Project focused on the development of manufacturable, lower-cost bipolar plates.
- The development of a low cost bipolar plate is critical to meeting the targets for the automotive application of polymer electrolyte membrane fuel cells.
- Developing durable, cost effective plates is important to the Hydrogen Fuel Initiative. Currently, no plate technology meets all the DOE bipolar plate targets – particularly for high temperature systems.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- Technical approach for graphite plates is strong – world experts. However, calculation/proof of power density needed for original equipment manufacturers based upon their thinnest bipolar plate design, is imperative.
- Methodical approach to materials selection and processing into plates.
- Project includes testing in full-area stacks.
- Approach has focused on a comprehensive selection of materials over a very large design space to structure graphite-based plates with high-temperature capability and high-volume manufacture.
- Approach is to develop polymer composite material for operation at 120°C.
- Approach is to demonstrate plates in a stack.
- Evaluation and down-selection of graphite and resin.
- The project has a systematic approach to the development of bipolar plates.
- Modifying existing technology to incorporate more stable resins for the higher temperatures is a logical approach for this foil-type technology. Approach, however, does not improve on all the weaknesses of this plate technology – particularly power density.
- Principal investigator needs to also evaluate effects of resin technology on plate porosity, strength, etc.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- Based on principal investigator's criteria, progress is very strong and targets are being reached. However, hydrogen permeability has not been tested yet – there is only an assumption based on nitrogen permeability.
- Potential to meet thickness requirements needed for original equipment manufacturers has not been accomplished.
- Project is on track and has met critical interim technical milestones to date.
- Good progress has been made in material component selection and initial formulation of composite material for plate fabrication. Initial testing of chosen material has been conducted along with preliminary *in situ* fuel cell testing.
- Bipolar plates survived shock tests.
- Plate has operated for 700 h at 120°C (actually 1000 h of operation).
- The project has completed the objectives of Task 2, 3, & 4. G made in Task 1.
- Very good progress made in fabrication and manufacturing tasks. Proof that materials will meet high temperature goals has not been demonstrated and could be a weakness.
- More effort on porosity work is required.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.8** for technology transfer and collaboration.

- High level, clear collaboration between the various partners.
- Ballard might not be considered an original equipment manufacturer now that they have sold off their automotive section.
- Excellent vertical team including raw materials supplier to polymer electrolyte membrane stack manufacturer.
- A strong partnership has been formed and is actively bringing testing, additive, and design expertise to complement GrafTech's capabilities.
- Good selection of original equipment manufacturers and a university.
- Project has good mix of industry and academic researchers.
- Principal investigator is collaborating with a major stack developer. Ballard, who is a major proponent of GRAFOIL technology and will identify appropriate applications for this type of plate (even if it may not be suitable for automotive use in the end).

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.3** for proposed future work.

- Future research is well described and logical, but needs the calculation of power density based on their thinnest plate design.
- Next steps are logical and follow the original project plan.
- Good plans to continue this project with a focus on manufacturability and cost.
- Future plans include finalized design of plate.
- Future plans include short stack test of full size plates.
- Future plans include economic assessment.
- GrafTech did not identify completion of Tasks 1 and 5 as part of future effort.
- Principal investigator needs to continuously incorporate new plates into stack systems to evaluate performance – such activities are appropriately covered in their future work plan.

**Strengths and weaknesses****Strengths**

- Key players are world experts in this area.



## FUEL CELLS

- Fabrication methodology appears very solid.
- Excellent corrosion resistance.
- Good thermal and electrical conductivity.
- Good flexibility and weight.

### Weaknesses

- Lack data to show viable original equipment manufacturer specifications for commercialization.
- High temperature durability is critical to achieving the DOE goals, and fuel cell testing is lagging the rest of the project.
- The project is moving rapidly toward a finished product without key durability and materials stability data. These data are usually obtained early on in a project. It is of little value to develop a process for a material that will not achieve durability and stability values.
- Plates will always remain bulky volumetrically.
- Porosity issues will be difficult to resolve.
- Poor channel formability might create problems for certain stack designs and/or create high contact resistance or poor fit if tolerances of the plates aren't well controlled.

### Specific recommendations and additions or deletions to the work scope

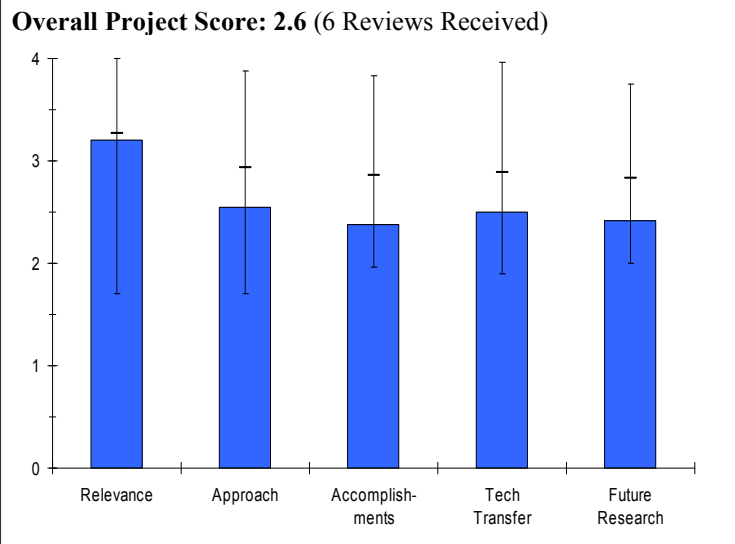
- Hydrogen permeability studies.
- Cost calculations based on plate thickness as soon as possible.
- Accelerate durability testing of the materials.

## Project # FC-29: Effects of Impurities on Fuel Cell Performance and Durability

James Goodwin; Clemson University

### Brief Summary of Project

The overall objectives of this project are to 1) investigate in detail the effects of impurities in the hydrogen fuel and oxygen streams on the operation and durability of fuel cells (CO, CO<sub>2</sub>, NH<sub>3</sub>, H<sub>2</sub>O, HC, O<sub>2</sub>, inert gases, and H<sub>2</sub>S); 2) determine mechanisms of impurity effects; and 3) suggest ways to overcome impurity effects. The year 1 objectives are to 1) obtain and characterize components of the membrane electrode assembly to be used (20% Pt/C, 30% Nafion/C, Nafion-Pt/C, Nafion membrane); 2) design and set-up measurements of impact of impurities on membrane electrode assembly components; 3) install fuel cell test station; 4) calibrate fuel cell test station measurements in “round robin” test of standard membrane electrode assembly with other Department of Energy contractors; and 5) start characterization of effects of CO and NH<sub>3</sub>.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Very good – the compounds listed match the industry concerns. The data on tetrachloroethylene at a concentration of 150 ppm was a very pleasant surprise.
- The project is a mixture of technique development, establishing capabilities and understanding of how to apply those techniques while using some reference impurities. The project is not yet ready to have any significant impact on the durability barrier.
- The project objectives are relevant to the DOE objectives.
- This activity supports DOE’s fuel cell development and speaks to fuel purity issues.
- In general, the study of impurities contributes directly to the DOE objective to meet 5,000 h lifetime over a realistic automotive drive cycle.
- Project relevance is weak versus other projects due to heavy amount of work on the most studied impurity in the literature, carbon monoxide
- A project that mostly focuses on carbon monoxide will likely not be useful since most stack original equipment manufacturers already have a strategy for avoiding the ill effects of CO.

### Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- Very good – the approach to the testing is basically conventional. The benchmarking to the DOE round robin demonstrated that the data is repeatable (multiple runs in the stand) and reproducible (the same results as seen at other labs involved in the round robin).
- The biggest issue appears to be that the objectives are too broad for the available resources and experience of the principal investigator and team members. For example, the principal investigator's experience with fuel cell testing and characterization is just beginning.
- The approach defined in slide 5 could only be carried out well by a much larger and more experienced team. All four boxes in slide 5 are large endeavors on their own.

- Good approach, however recommend testing of impurity effects using membranes other than Nafion.
- Concerns about duplication with other related projects within the group.
- Development of standard durability testing per impurity needs to be considered.
- The project places too much emphasis on fundamental understanding of the interactions of impurities on the surface of Pt, mainly CO. The fuel cell developers are interested in data that would allow them to develop engineering models that can be used to predict performance loss when using fuel grade hydrogen.
- The approach needs to address longer-term testing to understand the effect of impurities on fuel cell durability.
- The plan is to not only document the effect of contaminants on performance, but to develop an understanding of the chemistry of the performance loss—seeking answers about the actual chemical dynamic changes.
- Proposed model mechanism is missing steps (e.g., diffusion of O<sub>2</sub> across catalyst layer ionomer to the Pt surface as a function of relative humidity).
- Relative significance of tetrachloroethylene is suspect as a system contaminant. University of Connecticut project will also study halogenated compounds and these efforts should be coordinated.
- Round robin testing based only on polarization curves at high dew points. Most round robin tests fail when low dew points are needed, or when stoichiometry sensitivity tests are done (especially with gas blending). H<sub>2</sub>/N<sub>2</sub> blending on the anode would help to demonstrate an organization's competency to blend inlet gases.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.4** based on accomplishments.

- Outstanding – starting from scratch, developing test methodologies, getting test facilities online, validating the facilities and methodologies, and generating meaningful data in a year is excellent.
- The project has made progress toward some of its objectives, and shows some interesting new analytical results, but could not claim to have made any real progress toward overcoming the DOE barriers at this time.
- The emphasis on CO is rehashing a much-studied system, going back to the years of membrane electrode assembly development for reformat. Except for training the investigators, this is not likely to provide any new information.
- The electrochemical impedance spectroscopy results should be looked at carefully. The high frequency intercept on the x(real)-axis for the baseline curve cannot be correct since an impedance of 0.5 ohm-cm<sup>2</sup> would imply a voltage loss of 500 mV at 1 A/cm<sup>2</sup> just due to current resistance losses, which can't be true as their round robin polarization curves show.
- Technical results were overall repeated from literature, i.e., NH<sub>3</sub> and H<sub>2</sub>S on similar membranes, so more focus should be given to devising mitigation strategies rather than duplicating previous literature.
- Progress in getting started, set-up and calibration of equipment in this project has been reasonable.
- Clemson University has found some evidence of resistance increase in the ionomer and membrane with NH<sub>3</sub> poisoning but there is some question as to the validity of the impedance spectroscopy data.
- Their results appear to be consistent with those from other round robin test participants.
- Much of the information discussed was not that unique. Others have arrived at much the same conclusions earlier. However, what was shown was a series of useful and intelligent diagnostic tools that explore fuel cell electrochemistry. The fuel cell community has invested considerable resources into the South Carolina economy; it makes sense to build strong technical competence to back that investment. That competence was demonstrated.
- High frequency resistance measurements in the NH<sub>3</sub> study show a baseline (with no NH<sub>3</sub>) >500 mohm-cm<sup>2</sup>. For any standard membrane electrode assembly, like the one used, this number should be between about 20 to 150 mohm-cm<sup>2</sup>, even with 50% inlet relative humidity. There is something wrong either with the alternating current impedance measurement or with the cell assembly. This issue is where further collaboration would help.
- NH<sub>4</sub><sup>+</sup> contamination of polymer electrolyte membrane and ionomer is known.
- Recovery from CO poisoning due to surface restructuring is unlikely. Investigators should check O<sub>2</sub> content in gas inlets.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.5** for technology transfer and collaboration.

- Very good – the formal collaboration appears to be as expected. The current level of collaboration with Los Alamos National Laboratory, Hawaii Natural Energy Institute, University of South Carolina, University of Connecticut, and Argonne National Laboratory is a very pleasant surprise.
- The presentation did not make clear what the various contributions were from each collaborator. It appeared that most of the work was done by Clemson University.
- Appears too early yet to expect any technology transfer.
- Collaboration with others, Los Alamos National Laboratory and University of Connecticut, is highly recommended and seems to be lacking.
- Collaborations are evident in the US Fuel Cell Council round robin testing.
- Savannah River National Laboratory and Greenway Energy are partners with University of South Carolina.
- Other than the University of South Carolina, the collaborators involved do not have a rich history in fuel cell research. This is evident in much of the work, some of which appears to be motivated more by a desire to get familiar with fuel cell research than a desire to add to what is known.
- There is no evidence in the presentation of deep involvement by the University of South Carolina, except for the modeling task.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.4** for proposed future work.

- Very good – though research on low levels of CO<sub>2</sub>, ethylene and ethane may not be cost effective.
- Future focus on halogenated compounds might arise from H<sub>2</sub> from chlor-alkali processes, heat transfer fluid leaks, or cleaning solvents and may be of more immediate support of DOE goals.
- The proposed research is too ambitious for the resources and time to complete the work.
- The work plan should be significantly focused to allow greater in-depth and higher quality results to be extracted.
- Suggest having a clear direction on mitigating strategies and testing several kinds of membranes, i.e., Pt alloy and membranes other than Nafion.
- Provide a plan clarifying the modeling efforts timeline and impurities down-selection.
- Too much emphasis on developing first principles kinetics and rate expressions.
- The way that this diagnostic tool will be deployed to support fuel cell progress was not obvious.
- CO work needs to be cut.
- Plans to study CO<sub>2</sub>, NH<sub>3</sub>, and ethylene are reasonable as long as they do not overlap with other projects.
- Given the familiarity of CO<sub>2</sub> and NH<sub>3</sub>, and the expected low contamination by ethylene, the project could use some higher impact impurities to study.
- Ethane is not expected to be a highly detrimental contaminant.

#### **Strengths and weaknesses**

##### Strengths

- Current collaboration with other investigators.
- They have demonstrated some interesting new analytical techniques.
- Modeling potentials.
- The investigators are part of the round robin single cell testing being sponsored by the US Fuel Cell Council and have matched the results of the other organizations, which is an indication that their results can contribute to the understanding of impurities effects in fuel cells and the setting of standard fuel specifications.
- Project has responded to feedback to use lower Pt loaded membrane electrode assemblies.
- Project has approached tasks with thoroughness in step-by-step evaluations (Nafion/C vs. Nafion/Pt/C and so forth).
- Project has attempted to make use of less familiar analysis techniques.

Weaknesses

- A potential weakness might be the lack of willingness to share preliminary or unpublished data with other investigators. If the DOE target deadlines are to be met with quality results, researchers will need to be less parochial with the data.
- The project is trying to accomplish too much for the available resources and experience level of the investigators.
- Collaboration with others within the center to avoid duplication.
- The project places too much emphasis on the fundamental understanding of the interaction of CO on Pt surfaces. This has been studied extensively in the catalysis literature.
- The levels of CO (10 and 25 ppm) are almost an order-of-magnitude higher than are specified in the international fuel quality standards that are being developed.
- There is little apparent recognition of the large amount of data that exist on the impurities effects on fuel cells.
- Need to refine high frequency resistance measurements.
- Need to look at less-studied impurities.
- Need to collaborate with experienced partners.
- Need to refine modeling algorithm.
- Need to work on more challenging round robin protocols.
- Need to recheck CO recovery to find if there is an experimental artifact.

Specific recommendations and additions or deletions to the work scope

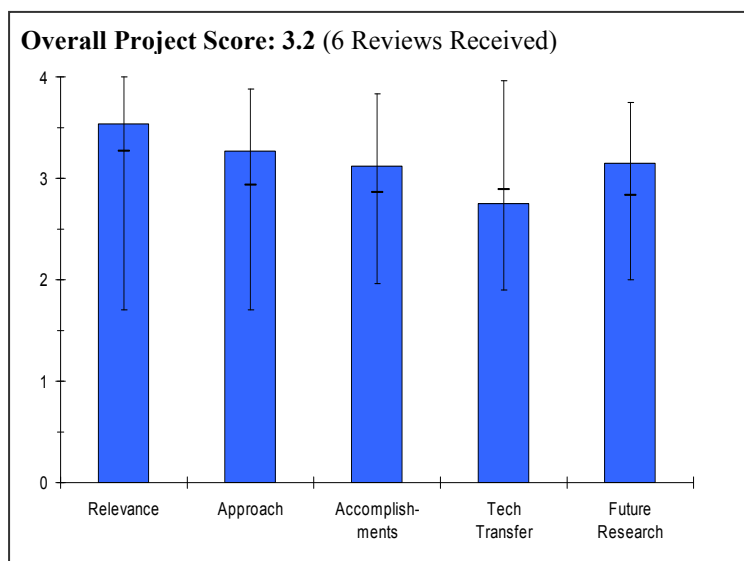
- CO, CO<sub>2</sub>, NH<sub>3</sub>, hydrocarbons (including C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, H<sub>2</sub>CO, HCOOH), Cl<sub>2</sub>, and H<sub>2</sub>S support industry activities.
- Data on non-reactive gases such as He, N<sub>2</sub>, and Ar are not needed or cost effective.
- Testing on O<sub>2</sub> only appears to make sense if the decay mechanism with "air bleed" (CO removal) is being investigated.
- Focus on just one of the three main activities and execute it with more in-depth understanding of one class of impurities, or take just one impurity only (but not the old CO) and try to develop a solid understanding of how it impacts the membrane electrode assembly components in depth.
- Suggest keeping the project; however, focus should be redirected for testing several types of catalyst-coated membranes and for mitigation strategies.
- Redirect the project to deemphasize the H<sub>2</sub>-D<sub>2</sub> exchange work.
- Use much lower levels of impurities for future work.
- The modeling activity needs to be clearly focused. Fundamental understanding is good but will delay getting more empirical data for use in engineering models that are of interest to the fuel cell developers.
- Coordination between the various organizations involved in impurity research should be stressed to accelerate data collection for impurities of most interest to the organizations involved in drafting fuel quality standards.
- Clemson University should review the existing work on impurities effects—primarily from Los Alamos National Laboratory.
- Delete CO work (except for that which can address loose ends of prior work).
- Consider deleting ethane work if initial experiments do not show a detrimental effect on catalyst/ionomer.
- Add more influential impurities, other than NH<sub>3</sub>.
- Add a major collaborator with deep fuel cell experience.

## Project # FC-30: Effects of Fuel and Air Impurities on PEM Fuel Cell Performance

*Fernando Garzon; Los Alamos National Laboratory*

### Brief Summary of Project

The overall objective of this project is to contribute to the scientific understanding of the effects of fuel and air impurities on fuel cell performance and how it affects Department of Energy fuel cell cost and performance targets. The specific objectives are to 1) investigate the effects of impurities on catalysts and other fuel cell components; 2) understand the effect of catalyst loadings on impurity tolerance; 3) investigate the impacts of impurities on catalyst durability; 4) develop methods to mitigate negative effects of impurities; 5) develop models of fuel cell impurity interactions; and 6) collaborate with the US Fuel Cell Council (USFCC), the FreedomCAR Fuel Cell Technology Team, industry, and other national laboratories to foster a better understanding of impurity effects.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Very good – the focus on completing sulfur contamination should be followed through.
- Fits only indirectly.
- It is very important to understand effects of both fuel and air impurities to reduce fuel cell system complexity and meet DOE cost and durability targets.
- The project objectives are relevant to the DOE targets.
- Important topic, however, one must examine if some of the impurities can be eliminated using filters/traps.
- Understanding impurity effects on the fuel cell is crucial in learning to develop more robust systems that meet DOE targets.
- Extremely relevant project fully supporting the President's Hydrogen Fuel Initiative and goals and objectives of the Multi-Year RD&D Plan.
- This project is filling a significant need to better understand the effect of fuel and air impurities on polymer electrolyte membrane fuel cells and their impacts on fuel cell durability and cost.
- Project is examining a number of areas previously not studied (such as co-adsorption of CO and H<sub>2</sub>S) including poisoning at different temperatures and relative humidity levels, and recovery mechanisms.

### Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- Very good – the approach to the testing is basically conventional. The benchmarking to the DOE round robin, glossed over on slide 5, demonstrated that the data is repeatable (multiple runs in the stand) and reproducible (the same results as seen at other labs involved in the round robin). This means data sets for the various labs can be merged to expedite this activity.
- A lot of tests (all, what is available?) to investigate the effects of a few impurities.
- Good approach for analysis and modeling of results.
- Considers effect of impurities on gas diffusion layer.
- Considers all important parameters (electrode kinetics, ionic and mass transport).

- Important to study crossover of contaminants through the membrane.
- Approach is similar to other members working on impurities effects. A collaboration between the impurity working groups is suggested.
- Good, methodical approach combining theory and experiment.
- One concern is that several of the results may be specific to the membrane electrode assembly studied.
- Project is very clearly addressing key fuel cell technical barriers including impurity tolerance and durability of electrocatalysts and membranes to a number of contaminants including H<sub>2</sub>S, CO, CO<sub>2</sub>, and alkali cations.
- Technical approach includes testing under steady state and cycling conditions, supporting experiments to measure fundamental parameters required for modeling, and analyzing and modeling data. Solid balance between empirical and modeling components within the approach.
- An appropriate approach is the project's intent to determine the limits of impurity tolerance within the bounds of the technical targets for electrocatalyst PGM loading.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- Good – the sulfur results while interesting have not been completed. There is mention of completing low catalyst loading tests, but the data were not included.
- The start on combining impurities effects is interesting. Data other than an electrochemically active surface area would have been interesting.
- A huge amount of data.
- Increased knowledge, but no solutions or recommendation to prevent degradation.
- Good experimental and mechanistic study of the effect of H<sub>2</sub>S.
- Co-adsorption of CO and H<sub>2</sub>S results confirm expectations.
- Interesting study of effects of cations on electrodes.
- Effect of catalyst loading not presented.
- *In situ* characterization of H<sub>2</sub>S and its crossover is good however quantifying the amounts chemisorbed as function of H<sub>2</sub>S exposure time and concentrations is suggested.
- Determination of cationic contamination for *in situ* conditions is suggested.
- Good progress towards stated goals.
- Project is geared towards studying the effects of poisoning and hence it is inappropriate to consider the extent to which project improves performance. However, the information gathered in this study will help design mitigation strategies.
- A number of technical accomplishments have been achieved including determination of performance degradation due to H<sub>2</sub>S anode poisoning as a function of catalyst loading; modeling and validation of impurity effects in polymer electrolyte membrane fuel cells including effects of alkali cations; and assessment of combined CO and H<sub>2</sub>S contamination.
- Technical accomplishments encompass balanced empirical and modeling results with a solid pace of results given the project started in October, 2006.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.8** for technology transfer and collaboration.

- Good – the formal collaboration appears to be as expected. The current level of collaboration with Savannah River National Laboratory/Clemson University, Hawaii Natural Energy Institute, University of South Carolina, University of Connecticut, and Argonne National Laboratory is a very pleasant surprise.
- Apart from dissemination in some groups/teams, no indication of transfer.
- Collaboration with Case Western Reserve University appears to be fruitful.
- Collaboration with other groups working on impurities is recommended and does not seem visible.
- Center is somewhat limited partner wise—they don't have a major stack original equipment manufacturer or automotive original equipment manufacturer as a partner to help them determine reasonable impurity sources

for the system. However, Los Alamos National Laboratory is very open with the information they share and consistently seek feedback from the original equipment manufacturers.

- Presentation early on mentions as a specific objective collaboration with the USFCC, the FreedomCAR Fuel Cell Technology Team, industry and other labs to foster a better understanding of impurity effects. However, with the exception of Case Western Reserve University, this objective was not really elaborated on and leaves some question as to the extent in which this is taking place with other entities.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Very good – the question is can we close the story on H<sub>2</sub>S by the end of this year?
- Somehow straightforward but not really clear.
- Hydrocarbon and particulate impurities are important, maybe also SO<sub>2</sub>.
- It is important to identify the lowest level of any particular impurity or combination of impurities that can be tolerated without significant impact on cell life.
- Gas diffusion layer studies mentioned in the approach are not included in the future work.
- Suggest collaboration with groups modeling the impurities effect on fuel cell performance.
- It is suggested that fuel cell performance degradation due to anode and crossover be quantified to predict fuel cell degradation under prolonged exposure to low concentration impurity in real life scenarios.
- Future plan proposed is logical.
- The project provides a very clear sense of proposed future work including continuation of some existing activities such as continued contaminant crossover studies and the effects of divalent cations, as well as new studies looking at air contaminants including hydrocarbons and particulates.
- Presentation does not provide a clear sense of how partnerships with other entities will be used in the future to leverage Los Alamos National Laboratory activities.

### **Strengths and weaknesses**

#### Strengths

- Current collaboration with other investigators.
- Good fundamental understanding of H<sub>2</sub>S poisoning.
- Study of co-adsorption of two impurities (CO and H<sub>2</sub>S).
- Systematic approach.
- Good integration between theory and experiment.
- Focus on fundamentals is encouraging.
- Extremely relevant project with regards to effects of contaminants on fuel cell durability and cost encompassing a strong approach balancing empirical and modeling activities and results.
- Solid pace of technical accomplishments and plan for future work.

#### Weaknesses

- A potential weakness might be the lack of willingness to share preliminary or unpublished data with other investigators. If the DOE target deadlines are to be met with quality results, researchers will need to be less parochial with the data.
- No life studies carried out to date.
- Collaboration with others is not visible.
- Suggest proposing mitigation techniques as the effects are investigated.
- Unclear if model includes forming parameters, and if so, if a sensitivity analysis has been performed.
- Unclear as to full extent of collaboration with other industrial, lab, and university organizations.

### **Specific recommendations and additions or deletions to the work scope**

- Complete the story on H<sub>2</sub>S so that the effects based on pressure, temperature, relative humidity, current density or cell voltage and catalyst loading can be predicted.



## FUEL CELLS

- Study effect of catalyst loading.
- Encourage further studies of combined effect of two or more impurities.
- Suggest keeping the project; however, collaboration with others working on impurities is suggested to avoid duplication.
- May benefit from a modest increase in overt collaboration with other research and industrial entities to leverage activities and maximize impact of results at commercialization interfaces.

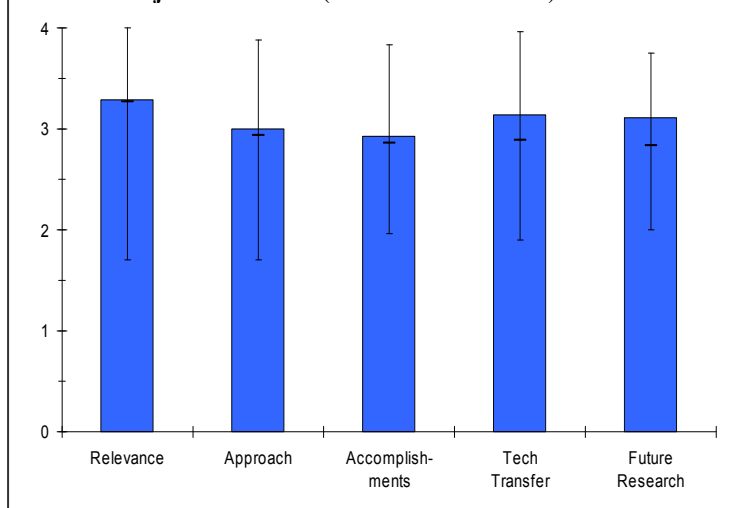
## Project # FC-31: The Effects of Impurities on Fuel Cell Performance and Durability

Trent Molter; University of Connecticut

### Brief Summary of Project

The overall objective of this project is to develop an understanding of the effects of various contaminants on fuel cell performance and durability. The specific objectives are to 1) identify specific contaminants and contaminant families present in both fuel and oxidant streams; 2) develop analytical methods to study contaminants; 3) conduct experimental design of analytical studies; 4) create novel *in situ* detection methods; 5) develop contaminant analytical models to explain effects; 6) establish an understanding of the major contamination controlled mechanisms that cause material degradation in polymer electrolyte membrane fuel cells and stacks under equilibrium and especially dynamic loading conditions; 7) construct material state change models that quantify that material degradation as a foundation for multiphysics modeling; 8) establish the relationship between those mechanisms and models and the loss of polymer electrolyte membrane performance, especially voltage decay; 9) validate contaminant models through single cell experimentation using standardized test protocols; 10) develop and validate novel technologies for mitigating the effects of contamination on fuel cell performance; and 11) conduct outreach activities to disseminate critical data, findings, models, and relationships that describe the effects of certain contaminants on polymer electrolyte membrane fuel cell performance.

Overall Project Score: 3.1 (7 Reviews Received)



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Effect of impurities on polymer electrolyte membrane fuel cell performance is critical to defining H<sub>2</sub> quality and fuel cell durability.
- Focus on fuel impurities.
- Very good – the compounds listed match the industry concerns. The data on methane and ethane at high concentrations combined with the Japan Automobile Research Institute data at low concentrations puts these compounds to bed.
- The selected impurities and overall objectives are relevant to the fuel cell application.
- Supports one barrier only, but is well focused on it.
- Project addresses DOE goal of increasing the durability of fuel cells by investigating the effects of impurities on performance.
- The project objectives are relevant to the DOE objectives.
- Contaminant effects can be a true barrier to fuel cell deployment and must be studied to understand levels, effects and mitigation.

### Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Literature search, analytical method, contaminant experimental studies, contaminant modeling is good valid approach.
- Very good – the approach to the testing is basically conventional. The benchmarking to the USFCC round robin demonstrated that the data is repeatable (multiple runs in the stand) and reproducible (the same results as seen at other labs involved in the round robin). It is surprising that this was not mentioned as it demonstrates a sound approach and a willingness to collaborate.

- Logical approach, but concern that it may be too broad to be fully accomplished by the available resources and time available.
- The choice of membrane electrode assembly loadings and membrane thickness are important for obtaining meaningful results for automotive fuel cells, but this project appears to have been ill-advised on the catalyst loadings and membrane thicknesses chosen.
- Evaluate effects of organic (methane, ethane, ethylene, aldehydes, organic acids, glycols) and cations on fuel cell performance degradation using conventional materials and catalyst loading (however, higher Pt loading on anode is unusual). Also low temperatures (80°C).
- Evaluation is integrated with model development.
- Focused only on membrane properties.
- Metal contaminants focus on automotive alloys.
- Concerns about duplication with other related projects within the group. It is suggested that the 3 groups working on impurities closely communicate to select the impurities to avoid duplication.
- Development of standard durability testing per impurity needs to be considered.
- Good approach to use prior work to define the contaminants of interest.
- Starting with methane and ethane may not have been the best choice since the effects are expected to be limited or zero, but this did serve to get the project started.
- It may have been better to use a known industry protocol, or at least a published testing protocol.
- Testing for contaminants just prior to the cell is a good refinement of a general approach.
- Cation testing based on metallic alloy constituents is a good starting point.
- Work to characterize the mechanical membrane properties is interesting.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.9** based on accomplishments.

- Measured CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, and cation impurity effects on mechanical properties of membranes.
- Apparently literature search was not completed well, because the fact that CH<sub>4</sub> is a non-adsorbing impurity at polymer electrolyte membrane temperatures was missed.
- Spent significant time on impurities that were previously already known not to be detrimental.
- Outstanding – starting from scratch, developing test methodologies, getting test facilities on line, validating the facilities and methodologies and generating meaningful data in a year is excellent.
- The start-high-and-dilute is a good approach to look at the effects of the organic impurities and the team appreciated that there needs to be a reasonable and practical upper bound.
- The high loading and membrane electrode assembly configuration may distort the results especially related to the maximum concentration that can be observed.
- For the metal ions, the measurements of key properties are well targeted, but the use of Nafion 117 and complete metal ion contamination could provide erroneous data.
- Fuel cell relevant conditions for the measurements were not examined.
- Very good results and progress to date toward their objectives.
- The data showing the impact of the cations on the nitrogen permeability are very significant.
- This project appears on track to have a significant impact on overcoming the impurity aspects of the durability barrier.
- Established testing system and protocols.
- Evaluated effects of methane and ethane and ethylene (no effect).
- Established cations decrease membrane water content (expected) plus make membrane more brittle.
- It suggested to test catalyst coated membranes not only with Pt/Nafion but also other types of membranes and catalysts.
- Development of standard durability testing per impurity needs to be considered.
- Good results and good analytics on the contaminants studied.
- Good progress, although the project has far to go.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- Partners include FC Energy, and UT Hamilton Sundstrand.
- Participate in impurity working groups and publish results.
- Very good – the formal collaboration appears to be as expected. The current level of collaboration with Los Alamos National Laboratory, Hawaii Natural Energy Institute, University of South Carolina, Savannah River National Laboratory/Clemson University and Argonne National Laboratory is a very pleasant surprise.
- The team has the appropriate skill sets to address the impurity issues.
- The proposal team is interacting with industry groups to understand the priority items, but should ensure the levels and membrane electrode assembly construction meets industry direction and standards.
- Few but strong partners, and good collaboration indicated.
- Universities and industry involved (with industry providing data and test supports). However, no original equipment manufacturers are involved.
- Several universities are involved in characterization and modeling.
- Collaboration with others, Los Alamos National Laboratory and Clemson University, is highly recommended and seems to be lacking.
- Good team experience with industry and university participants.
- Good use of prior work by other stakeholders.
- A more extensive list of contaminants might have been chosen based on published hydrogen purity specifications and testing by others. If this is a coordinated effort with others, it would have been helpful to make everyone aware of that fact and why the contaminants were chosen.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Contaminant Studies on chart proceeds for only 5 quarters – this should be extended and ongoing.
- Excellent – the focus on compounds and cations likely to be encountered in practical application is a demonstration of applied science and this directly supports the DOE effort to commercialize this technology.
- The proposed direction addresses the program objectives and they have the resources to address the topics.
- The team should ensure the impurity levels, and membrane electrode assembly materials and operating humidity are compatible with industry standards to prevent distortion of the effects of the various impurities and ensure the relevance of the work.
- Focus on key organic species is excellent, but selected organics should be chosen carefully. The choice of their standard membrane electrode assembly on which to carry out the impurity effect studies should be revised. The impurity modeling could be a tour de force and result in a very valuable utility for the fuel cell community.
- Complete industry assigned generic list including halogenated organics.
- Complete cation studies.
- Characterize ammonia and H<sub>2</sub>S.
- Begin modeling efforts.
- Suggest having a clear direction on mitigating strategies and testing several kinds of membranes, i.e., Pt alloy and membranes other than Nafion.
- Provide a plan clarifying the modeling efforts timeline and impurities downselection to avoid duplication with Savannah River National Laboratory/Clemson University.
- It is suggested to consider having *in situ* testing of cationic impurity effects on the performance of the fuel cell.
- Moving into modeling is a good transition towards full understanding of the contaminant effects on a micro level.
- The next set of contaminants will be important.

#### **Strengths and weaknesses**

##### Strengths

- Good approach with literature review, experimental, modeling, model validation.
- Current collaboration with other investigators.
- Strength and experience of the collaborators.
- Good definition of roles in the project.
- Input from industry regarding most useful contaminants to investigate.

- Gets hydrogen purity working group input.
- Good integration with model development.
- Good overall project plan and logical flow of development.
- Good outreach plan.
- Fuel cell testing capabilities.
- Builds on prior work.
- Good steady progress.
- Cation work based on metallic alloy contaminant possibilities.

### Weaknesses

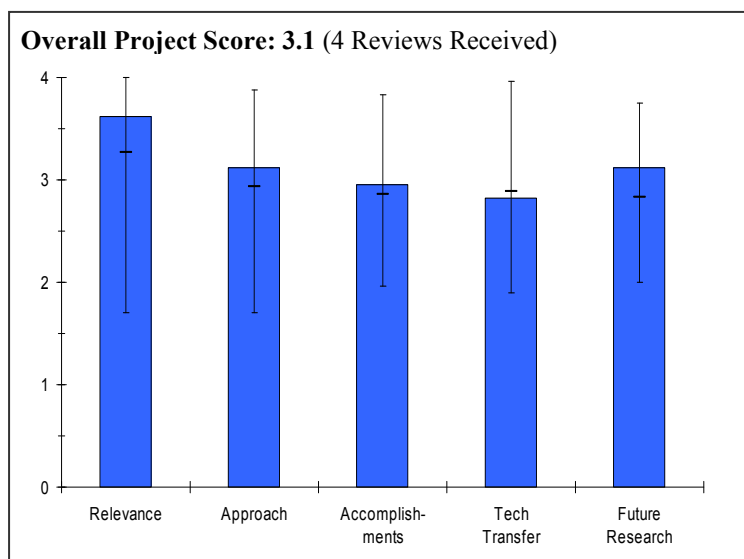
- Publication record to date is weak. There are no peer-reviewed publications, and most are presentations at workshops/meetings. Possibly early in project for significant publications.
- Significant work on CH<sub>4</sub> as impurity, but CH<sub>4</sub> effect on fuel cell performance has been well known by natural gas / polymer electrolyte membrane stationary fuel cell developers for a long time.
- Using too high of a catalyst loading on the anode.
- A potential weakness might be the lack of willingness to share preliminary or unpublished data with other investigators. If the DOE target deadlines are to be met with quality results, researchers will need to be less parochial with the data.
- Fuel cell measurements of the effect of organic impurities are performed with a membrane electrode assembly configuration that may significantly distort the results and behavior.
- Metals effect on the membrane looks at complete exchange and much thicker membrane than the current industry direction. This could distort the effects measured and provide a potentially erroneous direction for the impurity modeling.
- Mechanical measurements should be made under fuel cell type environments and reasonable upper bounds for the metal ion contamination.
- Limited material under investigation - conventional material for membrane only.
- Only lower temperature investigated. If higher temperature membrane materials are developed, this could diminish value of this study.
- No electrochemical characterization.
- Maybe not focused on most important contaminants.
- No publication.
- Collaboration with others within the center to avoid duplication.
- Cation loading may be higher than ever will be seen in use. A lower level, or lower levels, might be better to show the threshold of contaminant effects.
- No degradation seen yet with the gaseous contaminants used. It might have been better to try something with a higher rate of degradation to allow the team to hone their skills.

### Specific recommendations and additions or deletions to the work scope

- Should publish results in more detail and in peer-reviewed journals.
- Impurity review should include more than UT Hamilton Sundstrand's database on electrolyzer contaminants.
- Continue as the program is planned out.
- The effects of relative humidity on the performance with various contaminants should be considered in the degradation reactions.
- The membrane electrode assembly characteristics on which they will base their impurity studies should be revised to better reflect state-of-the-art automotive membrane electrode assemblies. Suggest anode loadings of 0.05 mg-Pt/cm<sup>2</sup> and cathode loadings of 0.15 mg/cm<sup>2</sup>, and membrane thicknesses of 20 microns since that will be more realistic as well as give greater sensitivity to the impurities.
- Should add additional materials.
- Look at higher temperatures and higher temperature membrane materials.
- Should look at lower contaminant level (more realistic).
- Suggest keeping the project; however, suggest testing several types of catalyst coated membranes other than Pt/Nafion based and creating mitigation strategies as the effects of each impurity are investigated.
- Continue the effort coordinated with the other contaminant research.

**Project # FC-32: Subfreezing Start/Stop Protocol for an Advanced Metallic Open-Flowfield Fuel Cell Stack***James Cross; Nuvera Fuel Cells***Brief Summary of Project**

The overall objective of this project is to demonstrate a polymer electrolyte membrane fuel cell stack meeting the Department of Energy 2010 cold start targets. The specific goals are 1) achieving -20°C cold start target respecting the energy budget; and 2) identifying electrochemical material freeze cycle aging models. The energy budget target of 5 MJ is currently exceeded by 12% but will be met with further optimization. The next generation 2010 material sets are in active development and are to be informed by forthcoming post-test analysis.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.6** for its relevance to DOE objectives.

- Project is well focused on issues related to cold start and operation of fuel cells to meet DOE targets.
- Water transport within a polymer electrolyte membrane fuel cell stack is required for optimal fuel cell performance (and thus cost, durability, power density, etc.).
- Extensive work on freeze/thaw, cold start-up.
- An important area, but apparently already being pursued by all major fuel cell manufacturers.
- Demonstration of rapid start-up at freeze conditions is a critical performance parameter for automotive performance. The freeze start-up time may not be as critical for backup power, stationary power, or industrial motive power applications.

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- Baseline system and performance and project metrics/goals (including quantitative where appropriate) clearly defined.
- Strong combination of theory and experiment.
- Stack design modification, testing and modeling for low temperature stack start-up.
- Energy budget optimization discussed, but hard to evaluate approach with information presented.
- Generally reasonable but several serious limitations.
- Inlet flows of air and fuel are at laboratory room temperature, which is not appropriate.
- Hydrogen flow heating value is not included in starting energy as it should be.
- The modeling approach also seems to have limitations associated with level of sophistication.
- Approach appears systematic but has a significant experimental weakness -- the reactants are introduced at ambient temperature. This is a major experimental error because the cell stack is artificially heated by the ambient reactants, and the humidity of the reactant gases will be very different at ambient temperatures than at subzero temperatures.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Significant progress made.
- Have already demonstrated 2010 -20°C start-up goal.
- Significant progress was made in achieving start/stop energy goal with path to achieve the final goal.
- 50% rated power in 30 s from -25°C is an excellent accomplishment.
- While progress has clearly been made, it is of questionable value due to limitations in approach.
- Test results apparently are not yet reliably repeatable.
- The presentation stated that the project claims met the 2010 start-up target of 50% power in 30 seconds, but this target is not demonstrated since the testing used ambient reactants.
- The energy accounting did not take into account the use of ambient temperature reactants, and the value presented is not representative of the test system. The summary makes claims that are not consistent with a thorough research evaluation.
- The reviewer questioned the development of new stack technology with high performance, but that was not an objective identified by DOE in chart 3 and does not appear to be an objective of the program.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.8** for technology transfer and collaboration.

- Other team members appear to be engaged in materials characterization (based on presentation, roles did not come across clearly in printed slides).
- Degree of interaction between team members appears to be very limited. It is not clear how data from materials studies is impacting cell and stack studies and development.
- Strong collaboration between fuel cell stack original equipment manufacturer, membrane electrode assembly / gas diffusion layer component suppliers and academics.
- Interactions seem to be fairly limited.
- The program has several collaborators but the application is restricted to the design of the Nuvera fuel cell stack. The design-specific solution to rapid start-up of freeze does not benefit the complete fuel cell community but is a specific benefit to Nuvera.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Proposed work should require more interaction between team members and results at next Annual Merit Review should demonstrate the impact of materials studies at the system level, particularly if progress made in understanding decay modes.
- Improved materials, installation of environment chamber, and development of 2D model are all needed for project success.
- Addition of controlled inlet flows will add much to the value of test results.
- Removal of mass, associated with higher operating design voltage, should help meet all goals.
- Several topics for proposed research will provide information to the fuel cell community. The development of an advanced stack does not appear to be consistent with the objectives of DOE. The advanced fuel cell stack will benefit Nuvera's business and will not be available to the fuel cell community.

**Strengths and weaknesses**

Strengths

- Freeze/start-up modeling already being correlated to stack start-up experimental measurements.
- Good technical capabilities.
- Good experience with similar experimental work.

Weaknesses

- Unclear how materials development will impact the project; little was stated about materials development approach.
- Too many limitations on results the way the program is currently being conducted.
- Experimental procedures used have yielded results that are inconsistent with real world operating conditions; the project principal investigator acknowledged the limitations of the experimental approach.

Specific recommendations and additions or deletions to the work scope

- Need to add an environmental chamber into stack testing.
- Carefully control inlet flows.
- Insert minimum repeatability into criteria before accepting test results as valid.
- Refocus program to meet DOE objectives at true, real freeze conditions.
- Delete new stack development activities that are not in the project objectives or include new stack in objectives.

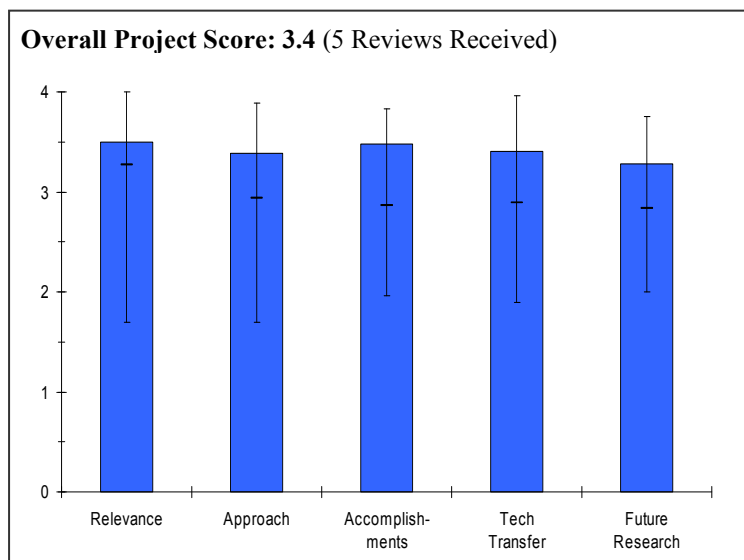


### Project # FC-33: Visualization of Fuel Cell Water Transport and Performance Characterization Under Freezing Conditions

Satish Kandlikar; Rochester Institute of Technology

#### Brief Summary of Project

The overall objectives of this project are to 1) gain a fundamental understanding of the water transport processes in the polymer electrolyte membrane fuel cell stack components; and 2) minimize fuel cell water accumulation while suppressing regions of dehumidification by an optimized combination of new gas diffusion layer material and design, new bipolar plate design and surface treatment, and anode/cathode flow conditions. The phase 1 goal is to establish a baseline system performance. This includes 1) a performance matrix for *ex situ* multi-channel and *in situ* fuel cell experiments; 2) freeze effects on performance and durability; and 3) microscopic study and models for water transport in the gas diffusion layer and parallel channels.



#### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Water transport within a polymer electrolyte membrane fuel cell stack is required for optimal fuel cell performance (and thus cost, durability, power density, etc.).
- The overall objective is to understand and also gain fundamental information on the water transport and performance characterization in the polymer electrolyte membrane fuel cell stack under freezing conditions.
- The program is highly relevant to President's Hydrogen Fuel Initiative.
- Water management in the cell/stack is important to fill gaps of performance, freeze start-up capability, reliability.
- Work is highly relevant toward understanding many automotive fuel cell stack failure modes that relate to water management, including freeze start, and low cells during nominal conditions due to gas diffusion layer intrusion, transition region deficiencies and non-uniform plate features.
- Project attempts to derive fundamental knowledge that can be widely applied, regardless of material sets, cell design and operating conditions.
- Water flow characteristics in flow channels are important parameters to understand the design of fuel cell operating characteristics. Plugging of channels is a known cause of performance degradation that can become permanent. Much of this work is already in the open literature. The development of a model for water and gas transport in gas diffusion layers could be beneficial.

#### Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- Parametric studies could be very valuable.
- Well thought-out approach that gradually moved from parametric studies to *in situ* performance with water distribution.

- The technical approach is to use *in situ* combinatorial water distribution and current density measurement for water transportation. Neutron radiography technology is also used to study water transportation in the polymer electrolyte membrane fuel cell stack. The membrane is Gore membrane.
- Water management is one of the key problems for the polymer electrolyte membrane fuel cell stack performance. The project addresses this issue.
- Cell/stack water management depends on flowfield design configuration. It is not clear whether this characterization includes implications on flowfield design or excludes them. If it includes flowfield design implications, it is unclear how to optimize flowfield configuration.
- Approach seeks to find what "worst case" conditions are upon shutdown.
- Studies incorporate the contribution of gas diffusion layer mechanics and the manufacturing variations that can lead to plate non-uniformity.
- The use of a small channel width (with carbon-based plate style features) will limit application of results for some customers.
- Correlation of pressure drop characteristics to different types of two-phase flow is valuable. According to question responses, this can be adjusted for operation when water is being generated.
- Good use of visual techniques on channel phenomena.
- The approach is systematic and should develop a better understanding of water transport in the flowfields.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.5** based on accomplishments.

- Significant amounts of work shown on flow visualization under many operating parameters.
- Flowfield design with cross-channels (11 degree offset) good for separation of anode/cathode water content during neutron imaging measurements.
- Flow maldistribution measurements and modeling due to gas diffusion layer intrusion are good.
- The technical accomplishments from two universities are excellent.
- It is necessary to explain correlation between gas diffusion layer materials property and water management in the cell/stack.
- Project is in process of completing baseline evaluation, including flow maldistribution, two-phase flow mapping, and shutdown conditions that most stress freeze start.
- Some items still need to be studied, including the relationship of transition region features to pressure drop and flow maldistribution.
- Discussions with investigators revealed that flow maldistribution and gas diffusion layer intrusion have been researched with respect to plate/gas diffusion layer compression.
- Although capillary flow of water is covered, unclear whether gas permeation/diffusion is covered or whether water vapor diffusion is addressed.
- Good progress.
- Intrusion of the gas diffusion layer into the flowfield is commonly known as "tenting" and was resolved with more rigid gas diffusion layer structures by several researchers. The researchers appear surprised by this phenomenon. Researchers would benefit from expanded contacts.
- Slug flow characteristics are well understood by fuel cell industry and previously reported by Los Alamos National Laboratory. It is not clear what is new in the work reported at this review except for the very interesting neutron imaging data.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.4** for technology transfer and collaboration.

- This project has a close collaboration between an automotive original equipment manufacturer and universities.
- Addition of component supplier interactions might help.
- Good publication record to date.
- The joint team includes Rochester Institute of Technology, General Motors Corporation, and Michigan Technological University.

- The technology transfer and cooperation is very good between Rochester Institute of Technology and Michigan Technological University.
- List of collaborators is short, but each collaborator has made a solid contribution.
- Michigan Technological University is contributing capillary flow models; General Motors is contributing cell design, gas diffusion layer coating and knowledge base.
- Collaborators are clearly not limited to mere material and analytical inputs. Many other projects use "collaborators" in this sense and then those collaborators do not contribute to the direction of the research. That has been avoided here.
- Mix of industry and academics, but it is not clear what the fuel cell component experience is.
- Program would benefit from expanding contacts with fuel cell companies.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated 3.3 for proposed future work.

- Spatial variation and current density measurements would be valuable in a real original equipment manufacturer flowfield design.
- The future work is clearly stated in the slides, future work plan and directions are excellent.
- For gas diffusion layer characterization, it is not adequate to look at only contact angle and capillary number. Other considered parameters, such as mechanical properties, permeation/diffusion, etc. should be evaluated.
- Future work is consistent with what is stated in the approach.
- The problem here lies with the metric(s) for qualifying that a gas diffusion layer/plate design is "improved." A possible scenario is that the "worst case" condition for stack shutdown becomes worse, but the overall regime of mist flow increases. In such a case, is the design improved? There should be some way of clearly saying what an improvement constitutes if the familiar tradeoffs involved in water management are realized.
- The future plans are consistent with the program objectives.

### **Strengths and weaknesses**

#### Strengths

- Automotive original equipment manufacturer provides access to most materials and significant amounts of beam time at the National Institute of Standards and Technology.
- The technology cooperation between two universities is good.
- Collaboration with strong industry partners.
- Use of imaging techniques to examine channel phenomena.
- Careful attention to and respect for true automotive ranges of operating conditions and modes.
- Realistic accounting for the way in which manufacturing variations and cell design influence water transport.
- Delivery of useful parameters for wide use (e.g., two-phase flow mapping and shutdown conditions that most severely challenge freeze start).

#### Weaknesses

- Flowfield design might not be applicable to all developers.
- Unclear what the working interaction between the project partners is, and appears most of the work presented was done by General Motors as a subcontractor.
- What is the role of General Motors in the project?
- Modeling capability, e.g., computational fluid dynamics.
- Thorough accounting for all transport mechanisms for all fluids was not fully realized in the presentation shown.
- Some ambiguity exists at the future decision points.
- Context limited by small channel width.
- Interesting testing using the neutron imaging.

**Specific recommendations and additions or deletions to the work scope**

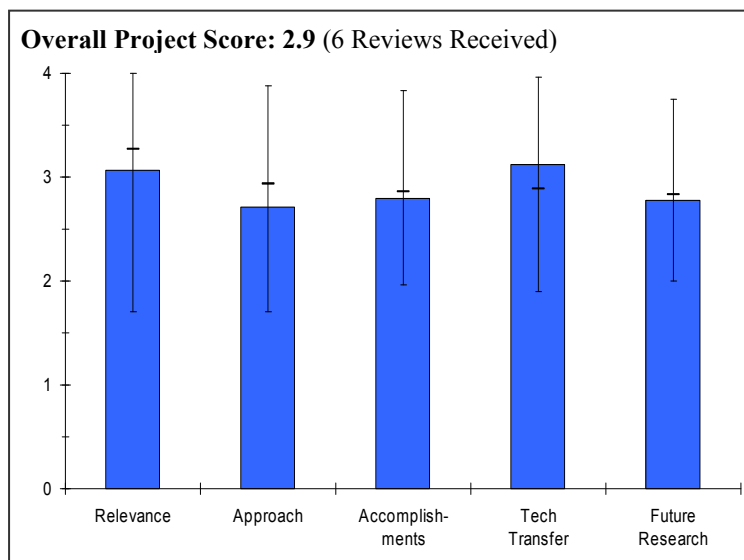
- The project started in March 2007 – we should give the principal investigator and Co-principal investigator more time and then make additions or deletions.
- All transport processes (diffusion, permeation, capillary motion) should be accounted for in all pertinent phases and species. If any are missing, they should be added. It is impossible from this review to determine if there is more research that has already covered this.
- Unless investigators wish to examine wider channel widths, any suggestion of adding the measurement of gas diffusion layer thermal conductivity should be ignored. If wider channel widths are of interest, then, yes, thermal conductivity should be added.

## Project # FC-34: Water Transport in PEM Fuel Cells: Advanced Modeling, Material Selection, Testing, and Design Optimization

Vernon Cole; CFD Research Corp

### Brief Summary of Project

The overall objectives of this project are to 1) develop advanced physical models and conduct material and cell characterization experiments; 2) improve understanding of the effect of various cell component properties and structure on the gas and water transport in a polymer electrolyte membrane fuel cell; 3) demonstrate improvement in water management in cells and short stacks; and 4) encapsulate the developed models in a commercial modeling and analysis tool. The fiscal year 2007 and 2008 objectives are to 1) perform baseline characterization for gas diffusion layer materials; 2) develop procedures for and begin gathering cell and stack-level diagnostic data; and 3) down-select model formulations and implement and test improved models for transport in gas diffusion layers, channels and across interfaces.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- Water transport within a polymer electrolyte membrane fuel cell stack is required for optimal fuel cell performance (and thus cost, durability, power density, etc.).
- Addresses a critical aspect of fuel cell operation and is using relevant cell designs for the modeling.
- The program is quite relevant to the DOE program objectives. Water transport is an important issue in fuel cells.
- Relevant, but likely that all major fuel cell manufacturers have their own approaches and solutions.
- Their work has limitations that somewhat limits the relevance.
- Water transport and management is extremely important to DOE, but Lattice-Boltzmann modeling is not necessarily the best approach.

### Question 2: Approach to performing the research and development

This project was rated **2.7** on its approach.

- Experimental measurements, extensive characterization to be correlated with strong modeling component.
- Combining *in situ* and *ex situ* experimental measurement techniques.
- Use of current interrupt to measure resistance and predict flooding.
- The approach to gathering the data and modeling is based on relevant industrial designs for the cell configuration and is looking at multiple operating conditions.
- The project objectives are well designed for moving forward with obtaining the fundamental characterization of the materials under realistic conditions to develop the model.
- The approach is good; it combines modeling at different length scales to formulate descriptions of the various components with experimental data to produce validated models that can describe water transport in operating fuel cells.

- The combination of modeling along with experimental results for calibration is good. However, significant limitations.
- All work seems to be for steady flow while major problems are also associated with transients.
- Apparently, there is no multi-dimensional capability except within a specific flow channel.
- Results seem to be very configuration-specific.
- Principal investigator is trying to do too much with available funding.
- Principal investigator should focus effort on fewer subjects – would impedance testing be more useful than the current interrupt tests? Are internal resistance tests likely reflecting poor cell setup causing high contact resistance and thus providing erroneous results – more relative humidity range is desirable in testing.
- Tests have been primarily steady state – they will need to be transient in order to be useful.
- The freeze-thaw experiments need more work and should wait on preliminary modeling data.
- Much of the data presented has been well documented by others previously – not much new (innovative) data presented.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- Characterization of gas diffusion layer materials, model development.
- The team is making good progress against their objectives of characterizing the materials and developing baseline data.
- It is not clear if some of the information is an artifact of the cell design to propose flooding.
- Project has spent the first year setting up platforms for model development.
- Good understanding of the need to fully characterize the microstructure in the model formulations.
- Model development for water transport through the gas diffusion layer is ahead of schedule.
- The work is interesting but does not seem to be particularly useful. It is not likely to add much to the basic understanding of water distribution issues.
- Internal resistance use to infer water flooding not accurate since it is an indication of a poorly designed cell (could be an artifact of that).
- Current interrupt technique – only focuses on one frequency – impedance might be a better technique.
- Transport equations – he is only getting permeation but not accounting for diffusion – sounds like they are looking at it.
- What electrochemical model are they aligning with the flow model?
- How many different relative humidity ranges are covered?
- Much of the characterization work has been well documented by other researchers, so isn't a lot of this data already in the literature and can be applied to the models discussed in this program?
- Too much effort devoted to preliminary characterization and "extravagant" imaging techniques that do not provide much additional information to what is already known about gas diffusion layer materials.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- Currently no publications.
- Strong team with fuel cell original equipment manufacturer, component suppliers, academics.
- The team has good participants that should be able to provide industry relevant data and expertise.
- There are numerous collaborators involved in the project including a major fuel cell developer to guide the modeling effort using real world data and assumptions.
- Several good partners but little indication of interaction with other than one or two.
- The list of partners is extensive, but it is not clear what each of the partners is contributing to the project (other than Ballard).
- Cell and stack diagnostics should be the focus (rather than so much effort in unnecessary elaborate characterization).

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- Unclear how modeling results will be verified.
- Little information presented on proposed future work.
- The future work is well directed at addressing the program objectives and moving the understanding forward.
- The presentation indicated that the future work includes studies of transient operation.
- Not clear that future work will add much to understanding.
- Don't focus on freeze-thaw early in the program – get baseline models established first (don't jump ahead of the game) then move onto different fuel cell operation.
- Lessen focus on extensive characterization and utilize existing data to establish baseline models.
- Why isn't some of this research being coupled with imaging observations (such as those done at the National Institute of Standards and Technology)?

**Strengths and weaknesses****Strengths**

- Experimental measurements, extensive characterization to be correlated with strong modeling component.
- Good use of analytical modeling and testing with relevant cell designs to understand the water management.
- Good team working on an important problem.
- Good presentation.
- Partners have excellent combined capabilities.

**Weaknesses**

- Small amount of results shown to date.
- Modeling not yet correlated to experimental results, and unclear exactly how this will be done.
- Use of current interrupt technique is inferior to a complete-frequency alternating current impedance spectroscopy measurement.
- Too many limitations to be very useful and probably duplication of efforts by other groups.
- Too much effort on unnecessary characterization.

**Specific recommendations and additions or deletions to the work scope**

- Incorporate high frequency resistance /alternating current impedance measurements.
- Assess potential value of project as formulated.
- If project continues, add unsteady as well as multi-dimensional efforts – at least experimentally but also analytically if practical.
- Coordinate models and diagnostics with imaging techniques available at the National Institute of Standards and Technology.

## Project # FC-35: Water Transport Exploratory Studies

Rod Borup; Los Alamos National Laboratory

### Brief Summary of Project

The overall objective of this project is to develop an understanding of water transport in polymer electrolyte membrane fuel cells. The specific objectives are to 1) evaluate structural and surface properties of materials affecting water transport and performance; 2) develop new components and operating methods; 3) accurately model water transport within the fuel cell; 4) develop a better understanding of the effects of freeze/thaw cycles and operation; 5) develop models which accurately predict cell water content and water distributions; 6) work with developers to better the state-of-art; and 7) present and publish results.

### Question 1: Relevance to overall DOE objectives

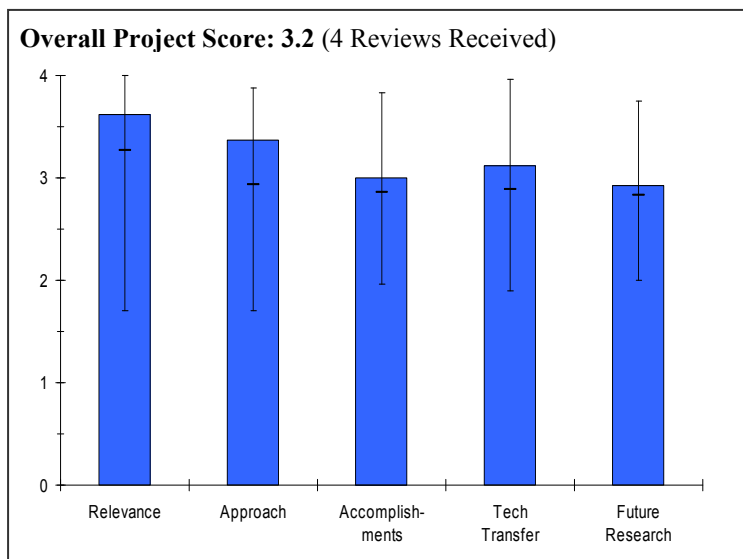
This project earned a score of **3.6** for its relevance to DOE objectives.

- The project is highly relevant to the President's Hydrogen Fuel Initiative.
- The overall objective is to understand water transport in polymer electrolyte membrane fuel cells.
- Very good – the issue of the hydrophobicity of components changing with time has the potential to be a major durability issue.
- Good orientation towards overall goals.
- This project is relevant to the DOE objectives regarding performance, durability and unassisted start from freeze.
- Project seeks to provide original equipment manufacturers with fundamental knowledge regarding water presence in relevant material sets, using relevant operating conditions and standard cell designs.

### Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- Neutron imaging, high frequency resistance, and alternating current impedance technologies are used to study water transport in the polymer electrolyte membrane fuel cell stack.
- The description of the technical approaches is excellent.
- Fair/good – I would expect that Teflon migration due to water transport, carbon oxidation changing the water contact angle and potentially pore structure changes due to freezing would be explored. I don't see this lower hanging fruit being discussed.
- Excellent consortium, in particular key industry partners.
- Solid measurements.
- As with any proper water transport project, this project seeks to link *in situ* phenomena with *ex situ* material characteristics.
- Modeling to be used for those aspects that are difficult to routinely address with experiments (e.g., water movement through gas diffusion layer).
- Operational stresses addressed (e.g., freeze).





- Lack of attention given to cell assembly and channel dimension effects. In a water transport project where mechanical, electrical, and – in some designs – thermal interactions between gas diffusion layer and plates/catalyst layers are important, these parameters must be known.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- The project started in 2007, the technical accomplishments are excellent.
- Fair/good – the modeling of droplet formation and separation is interesting. It is unclear how this actually addresses the issues.
- Good results and insights on water distribution and ice formation. Improvement of empirical understanding. However, transfer of methods/technologies missing.
- General trends should be elaborated.
- A considerable amount of work has been done with neutron imaging, but parameters such as gas diffusion layer type and compression have been left out, therefore making comparisons difficult if not impossible.
- Because contemporary rollable gas diffusion layers now have wide ranges of compressibility, compressing all gas diffusion layers to the same percent thickness will not lead to the same compression. Wide performance and water transport variations will result.
- Freeze study contains some trends that could be of use to developers with knowledge of gas diffusion layer parameters.
- CFD study could be more valuable if parameters were shared that were used to match experimental data (e.g., gas diffusion layer or catalyst layer flow resistance).

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- The technology cooperation among the principal investigator and co-principal investigators is good.
- Good – the list of collaborators is representative of the supply chain.
- Interaction with industry seems to have room for improvement.
- Wide, commendable range of collaborators among national laboratories, universities and membrane electrode assembly component suppliers.
- What is missing from collaborations is the dedicated assistance of a stack assembly original equipment manufacturer. The role of Nuvera is stated to be limited to assistance with the low-temperature conductivity testing. Either a greater role for Nuvera or the entry of a stack assembly collaborator should be sought.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- The future work plan and directions are excellent.
- Good/fair – the proposed work appears to be a rational follow on to the work to date. Consideration of some of the items noted in part 2 may be more relevant.
- Target orientation of future work not clear.
- Transient work utility will depend on ability to replicate the same relative speed of flow increases/decreases versus load up/downturns.
- Work that has already been done should still be related to cell assembly parameters, as well as gas diffusion layer characteristics.
- Assumption has been that neutron imaging shows ice when temperature is below freezing. In polymer electrolyte membrane, this can be debatable. Another technique that can distinguish water from ice would be helpful (e.g., MRI).

**Strengths and weaknesses**Strengths

- The attempt to understand and potentially address a legitimate durability issue.
- Wide range of analytical access and experience.
- Wide range of collaborations with universities, component supplies and other National Laboratories.
- Experiments designed with relevance to the major stressors involved in fuel cell water management.

Weaknesses

- Too many subcontractors, the work and duties are not well-defined.
- It is unclear if the researchers are focusing on the probable physics of the problem.
- Attention to cell assembly information.
- Collaboration with stack original equipment manufacturers.
- Delivery of modeling parameters to possible customers.

**Specific recommendations and additions or deletions to the work scope**

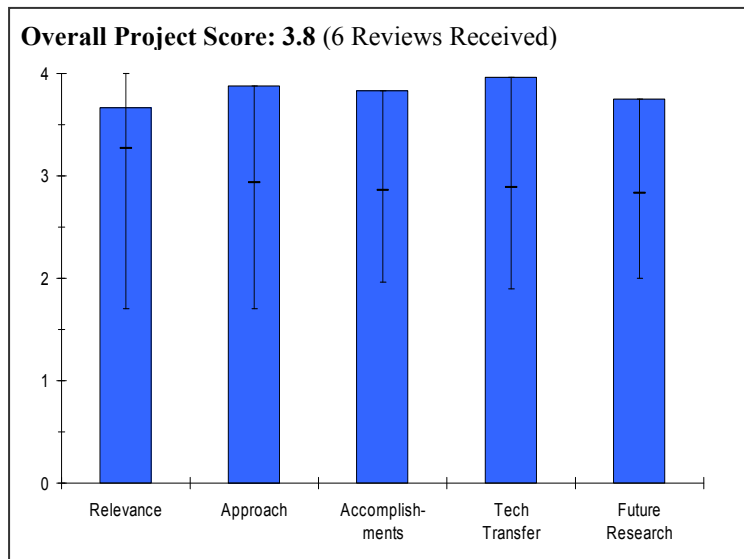
- Should delete a couple of subcontractors.
- I would suggest considering doing some research on the items in part 2.
- Consideration should be given to more advanced hardware selection, similar to that used in the Rochester Institute of Technology project. This would help provide more realistic heat transport in freeze experiments.
- Reporting of gas diffusion layer type and cell compression for every experiment.

**Project # FC-36: Neutron Imaging Study of the Water Transport in Operating Fuel Cells**

David Jacobson; NIST

**Brief Summary of Project**

This project aims to develop and employ an effective neutron imaging based, non-destructive diagnostics tool to characterize water transport in polymer electrolyte membrane fuel cells. The objectives of this project are to 1) form collaborations with industry, national laboratories and academic researchers; 2) provide research and testing infrastructure to enable the fuel cell/hydrogen storage industry to design, test and optimize prototype to commercial grade fuel cells and hydrogen storage devices; 3) make research data available for beneficial use by the fuel cell community; 4) provide secure facility for proprietary research by industry; 5) transfer data interpretation and analysis algorithms techniques to industry to enable them to use research information more effectively and independently; and 6) continually develop methods and technology to accommodate rapidly changing industry/academia need.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.7** for its relevance to DOE objectives.

- Water and thermal management are important problems aligned with the program goals, though not the most critical questions facing the program.
- Very useful facility.
- Analytical instruments like this are critical to fundamental understanding of water management.
- Neutron imaging is an important tool for monitoring the distribution of water in a polymer electrolyte membrane fuel cell. The technique provides a window into the operation and stability of cell components.
- Although not "critical" to hydrogen economy, this project is highly relevant to water transport in fuel cells.
- Neutron imaging is a unique tool for studying water transport *in situ*.
- Project is extremely relevant to DOE objectives as it supports the water management projects and research at many institutions – the National Institute of Standards and Technology is developing the techniques allowing for direct water transport imaging in operating fuel cells, a critical issue for DOE.

**Question 2: Approach to performing the research and development**

This project was rated **3.9** on its approach.

- Uniquely well-poised to look at water management at the micro scale. Very good team to do the work with the special tools and the neutron source.
- Excellent user model – provides unprecedented opportunities.
- Very good.
- The approach combines experimental and modeling methods to better understand the distribution of water in the fuel cell. The development of test cells that permit the location of water within a cell is an important function.
- The facility is well-equipped and well-suited for water imaging in fuel cells.
- The National Institute of Standards and Technology appears to be committed to constantly improving their neutron imaging capabilities, which is a big plus.

- The developmental work during the past year has been great and the addition of high resolution imaging capability is very exciting and extremely relevant.
- Collaborative work is outstanding – since the facility is part of a user center, many fuel cell water management researchers have access to the capabilities at National Institute of Standards and Technology provided they can justify need in a proposal.
- DOE covers cost of the research and development necessary for fuel cell activities related to water management and access to the facilities is open to all organizations involved in fuel cell research. This is a very useful mechanism by which to conduct the research rather than limiting to only a few institutions/collaborators.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.8** based on accomplishments.

- Excellent method development, though in truth most of this is not from the last year.
- Able to discriminate the water to ice ratio in freeze tests.
- Confirmed purge effectiveness in repeated tests and gas effects on water transport.
- Validation of models helps theory groups.
- Lot of excellent work done by university groups.
- Good progress with enhancing facilities.
- This program is leading edge technology!
- The project is developing interesting data. The observation of water collection in the "lands" reveals the complexity of the internal operation of the cell. Data and model prediction provide insights into the design of future cells.
- Progress is not easy to assess as one is dealing with a tool rather than focused research and development task; in the future, projects such as this should be evaluated according to a different set of criteria, specific to a service facility (center), not a research and development entity.
- The service rendered by the National Institute of Standards and Technology to numerous customers appears to have been fully satisfactory.
- More data interpretation would be welcome.
- The addition of an environmental chamber is extremely beneficial for freeze/thaw studies.
- High resolution imaging of water transport is a tremendously useful development for nearly all fuel cell researchers already utilizing the facility at the National Institute of Standards and Technology.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **4.0** for technology transfer and collaboration.

- Working with very many groups and most all the key players. Would be hard to do better in this area.
- Very user-friendly procedure to get beam time
- Could use a few more international participants.
- Excellent and expanding list of collaborations
- An impressive list of collaborators (hardly surprising for a service center).
- Outstanding use of DOE funds for research and development and developing the necessary collaborations within the fuel cell community. Nearly all the fuel cell organizations conducting water transport research have made valuable use of this facility.
- The facility is an extremely important tool for water management studies and should continue to be funded as a baseline program that will benefit all researchers in the fuel cell community.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.8** for proposed future work.

- Looks suitable.
- Would like to see temperature-dependent measurements if possible.

- Very pertinent.
- Very nice work!
- It is not obvious that impedance measurements will distinguish between flooding of pores in gas diffusion layer, microporous layer or electrode. The sensitivity of the neutron imaging is on the order of 10 microns while a catalyst layer is typically less than 10 microns thick. This may be a difficult experiment.
- Planned addition of neutron detector(s) with even higher resolution, implementation of impedance spectroscopy and expansion of research onto hydrogen storage are all good ideas.
- With an advent of even better image resolution, the use of neutron imaging for mapping water in catalytic layers and membranes should also be considered.
- What additional improvements can be made after 10 micron resolution goal is met? This is very impressive, but it is unclear what the next goal will be.
- Little justification given for advantages of coupling impedance spectroscopy with water transport measurements.
- Continue emphasis on establishing collaborations with fuel cell community.

### **Strengths and weaknesses**

#### Strengths

- Non-invasive water visualization. Great partnering at a rare facility.
- Most aspects.
- Develop leading edge analytical tools for fuel cell development.
- Creative application of neutron imaging.
- This is generally a strong and needed project.
- Extensive collaborations with numerous fuel cell researchers – this is important for the dissemination of critical observations in water management.
- The use of DOE funds to develop improved techniques is justified in that the National Institute of Standards and Technology facility is open to all researchers specifically for water transport studies related to fuel cells.
- The high resolution imaging of water transport is critical and thus demonstration of this capability should be a priority.

#### Weaknesses

- None.
- Limited access since there are too many users.
- Rather limited involvement of the National Institute of Standards and Technology in the "pre-neutron" and "post-neutron" phases of projects may be a weakness.
- None!

### **Specific recommendations and additions or deletions to the work scope**

- Keep it up. Look for ways to measure temperature too.
- All in all, an outstanding project.
- Now that the resolution is good (10 microns), can the speed be increased to measure transients?
- Very limited interaction with the fuel cell industry. Program could benefit from industry inputs.
- Expansion of neutron imaging beyond "water transport" into, for example, catalytic layers and membranes, should also be considered.
- The authors should get more involved in the data interpretation and tie their catchy images to it.

## Project # FC-37: Development of Thermal and Water Management System for PEM Fuel Cells

Zia Mirza; Honeywell

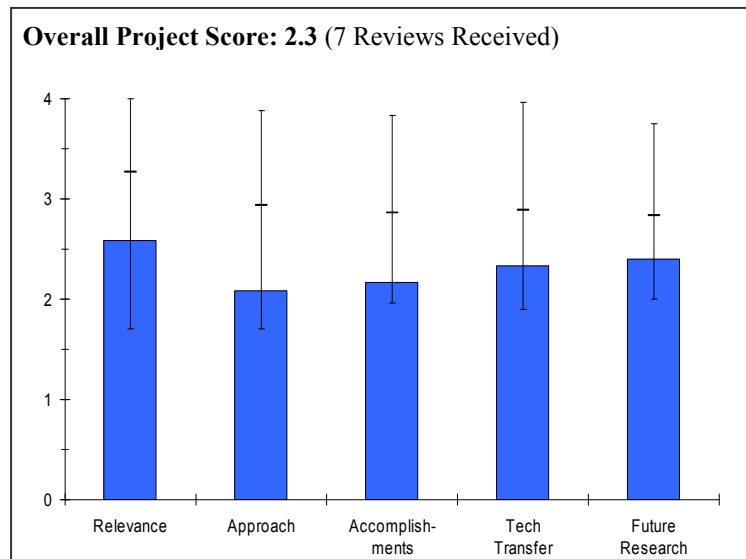
### Brief Summary of Project

The objectives of this project are to 1) validate the performance of full-scale humidification devices sized for 80 kW fuel cells; and 2) design a full-size radiator to meet the 80 kW fuel cell cooling requirements. The Emprise enthalpy wheel and Perma Pure membrane module will be tested.

### Question 1: Relevance to overall DOE objectives

This project earned a score of **2.6** for its relevance to DOE objectives.

- The relevance of this project has to be questioned if it could be delayed (or paused) for two years.
- The overall objective is development of thermal and water management systems for polymer electrolyte membrane fuel cells.
- The program is highly relevant to the President's Hydrogen Fuel Initiative.
- Units being tested are not being incorporated in current or future automotive fuel cell systems.
- Information generated provides no useful insight to original equipment manufacturers.
- Water management is critical to the President's Hydrogen Fuel Initiative.
- Technical gap of thermal and water management is cost, not performance.
- Stack technology is trying to decrease dependency on external thermal and water management (trying to eliminate external humidifier).
- A steady humidity of the input air is important for Nafion-based fuel cells.



### Question 2: Approach to performing the research and development

This project was rated **2.1** on its approach.

- The approach proposed for this project appears to be sound, however the selection approach has to be questioned since neither of the two humidification systems operated satisfactorily and will have to be modified.
- Two system approaches, enthalpy wheel and membrane module are reasonable and good.
- The project is more toward development work.
- Novel technology is not being developed to overcome technical barriers.
- Comparative analysis of overall systems was not included.
- Design humidification system and radiator for 80 kW fuel cell stack use of an enthalpy wheel.
- It is unclear of technology downselection process.
- Down-selected components are not meeting cost targets.
- Two advanced humidity control systems are being studied.

### Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.2** based on accomplishments.

- Granted it is very difficult to stop and restart a technical project such as this one, however the progress since the restart appears to be quite slow. Apparently since the restart no effort has been made on the radiator and the

initial effort in this area will be to revisit the past selection process. It seems that prototype equipment should already have been procured.

- Technical accomplishments are good.
- Testing was conducted on Emprise wheels and a Permapure membrane unit.
- Identified leakage in full-scale units.
- The limited data shown on Emprise wheel was suspect.
- No comparative analysis was shown between the two devices.
- Testing 80% complete, but enthalpy wheel leaks and needs a pre-cooler.
- Testing for design verification done.
- Limitations of both the enthalpy wheel and the membrane systems were identified and characterized.
- Which of these two systems is considered to be the best?

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.3** for technology transfer and collaboration.

- There appears to be little or no collaboration by outside organizations in this project. Clearly interactions with credible polymer electrolyte membrane fuel cell suppliers could benefit from humidification and heat rejection hardware.
- Partnered with Argonne National Laboratory, but no Argonne work in the presentation.
- DOE is a funding agency, what is meant to partner with DOE?
- Principal investigator does collaborate with component suppliers to solve component flaws.
- Better collaboration with original equipment manufacturers would be required.
- Argonne National Laboratory and FreedomCAR Fuel Cell Tech Team; no university or specific company.
- Collaboration indicated with Argonne National Laboratory.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.4** for proposed future work.

- Future plans are adequate, but appear to be drawn out and could be accelerated.
- The future work and plan are excellent.
- Future work includes evaluation of microchannel heat exchanger.
- Re-test humidification device. Radiator optimization.
- Radiator is not technical gap, it is design gap (packaging). Conventional radiator is the baseline.
- Future emphasis will be on the development of a full-scale radiator for an 80 kW polymer electrolyte membrane fuel cell system.
- Studies of advanced radiator technologies have been done.

#### **Strengths and weaknesses**

##### Strengths

- None.
- Project has a good focus.

##### Weaknesses

- Doesn't have fuel cell system developers or fuel cell companies involved in the project.
- Limited data presented.
- No system analysis presented.
- The technology is not state-of-the-art.
- No cost analysis done.
- Enthalpy wheel sealing.
- Project justification.
- Not much indication as to how the shortcomings of the humidity control systems will be overcome.

**Specific recommendations and additions or deletions to the work scope**

- Completion of this project should be accelerated as much as possible and completed in a timely manner in order to make the results of this study available as quickly as possible for the project to have any benefit at all.
- Need to work closely with fuel cell system developers or fuel cell manufacturing companies.
- I recommend discontinuation of this project.
- Enthalpy wheel needs a strong go/no-go decision point based on whether or not it can be sealed.

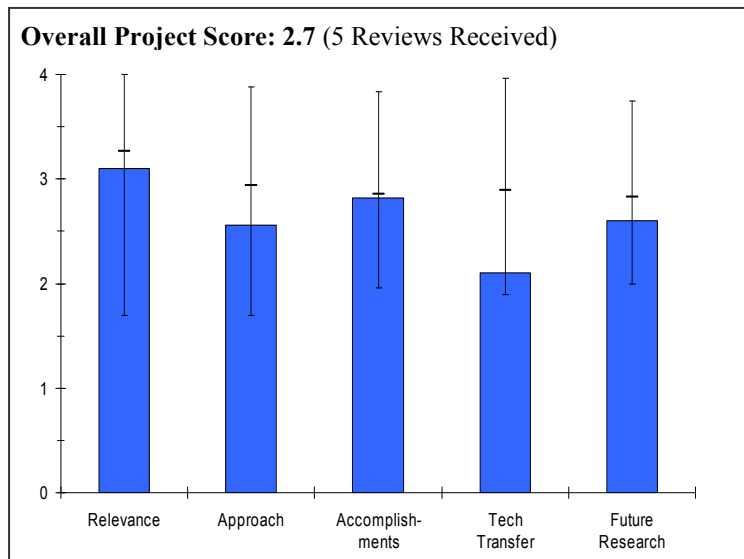


**Project # FC-38: Low-Cost Manufacturable Microchannel Systems for Passive PEM Water Management***Ward TeGrotenhuis; Pacific Northwest National Laboratory***Brief Summary of Project**

The overall objective of this project is to create a low cost, passive technology for water management in polymer electrolyte membrane systems. A 1-kW<sub>e</sub> device has been designed and built at 22-kW<sub>e</sub>/L power density and 4.2-kW<sub>e</sub>/kg specific power. Testing is in progress. The primary cost driver for the device is powder rolled and annealed sheet. Current results indicate the powder rolled sheet will work and, therefore, cost projections will be met.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.1** for its relevance to DOE objectives.



- Low-cost passive water management systems for polymer electrolyte membrane fuel cells are needed.
- Low cost materials for water and heat management are very relevant to the program.
- The project addresses the cost and manufacturability but needs to ensure the applicability to fuel cells.
- The project addresses an important issue.
- Because an anhydrous membrane is not likely, humidifiers will remain in fuel cell systems, and, therefore, this project maintains relevance.
- This project appears to be a design for manufacturing project. Humidification using porous media is well-established for fuel cells and the subject of several patents; therefore, the reviewer questions why this project is included in the DOE's fuel cell research and development activity.

**Question 2: Approach to performing the research and development**

This project was rated **2.6** on its approach.

- Passive low cost approach is good.
- Approach which requires saturated stack gas streams needs to be verified as an applicable approach.
- The design approach for cost and thermal and water management are appropriate.
- The team does not seem to have addressed in its approach possible issues with contaminant generation and transfer to the fuel cell as part of the overall approach.
- This innovative approach should yield promising results.
- Analysis to date has assumed that the exit stream from the stack cathode will be 100% relative humidity. However, throughout many operational modes on-board a vehicle, this assumption will not be true. For example, if someone drives two miles through the neighborhood to the store, there will not be enough water generated to reach 100% relative humidity. In this situation, the humidifier will likely dry.
- The low differential pressure required between two sides of the humidifier (< 102 mbar) dictates against placement downstream of compressor due to low stack pressure drop demand.
- Stack cathode exit stream (humidifier hot side inlet) will have to be expanded to near-ambient pressure, which will lower temperature and therefore, lower water transport.
- The approach follows several similar approaches in the literature and patents. The program did not discuss the solubility of reactants and inert gases in water. The approach should test the potential for crossover in the humidification device.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- Testing of single channel device with saturated gas streams does not verify that this is an applicable approach.
- The team has achieved several accomplishments in reducing the cost and improving the performance of the passive water management technology and in addressing the key barriers as they were identified.
- Progress is good and demonstrates feasibility.
- Good reporting of cost and weight for device.
- With tensile testing, a measure of durability against freeze/thaw has been shown.
- Strategy for manufacturing has been considered.
- Powder rolled material has improved bubble point, although not enough to avoid severe differential pressure limitations.
- A system-level cost analysis, perhaps using parts of TIAX or DTI reports, would have been helpful to compare a system with the humidifier to a system without it.
- Progress is consistent with objectives.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.1** for technology transfer and collaboration.

- Partners include Pacific Northwest National Laboratory, ADMA Products, Argonne National Laboratory.
- This project would benefit from interactions from a fuel cell original equipment manufacturer.
- The team would benefit from more integration with fuel cell testing and fuel cell requirements for the implementation of the device.
- PNNL did not clearly present the technology transfer and collaboration on the project.
- Lack of collaboration is hurting this project and collaboration is needed to provide experience and knowledge in automotive fuel cell systems.
- It is not clear what technology will be transferred if patents exist.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.6** for proposed future work.

- Future plans need to include use of sub-saturated gases.
- The possibility and analyses of potential contamination transfer to the fuel cell should be examined to demonstrate the applicability of the device, in particular under real operating conditions where impurities could further enhance the corrosion of the steel materials.
- The principal investigator indicated that the device could potentially introduce droplets of water into the fuel cell that could contain metal ion impurities.
- The cost implications of any mitigation strategies for impurity problems should be examined.
- Future plans are logical and should advance the project.
- It is good that the investigators are interested in pursuing robustness to various operating conditions.
- Investigators should move quickly towards demonstration of the device in an automotive fuel cell system with realistic transient operation, to drive the project immediately to acknowledge problems implied with the cross-pressure limitation.
- Future work should be expanded to include non-automotive fuel cell applications.

**Strengths and weaknesses****Strengths**

- Good development of a material that could achieve the cost, manufacturability and performance targets.
- Focus on durability (freeze, etc.) is a good idea.
- Project is not just device-based, but has sought to improve a system component with a material improvement.

- Project has been responsive to feedback concerning cost/weight reporting and plans to eventually test a wide range of conditions.
- Strong experience in microchannel devices.

### Weaknesses

- Water flow by capillary action limits the usefulness of this approach, as it requires a saturated fuel cell outlet.
- For transportation applications, outlet/inlet gas flows are not expected to be fully saturated; gas bypass is likely with realistic gas humidification – that amount of water on-board a vehicle is typically not available for saturated gas streams.
- Start-up time may prevent this technology from being used for transportation applications.
- Not enough consideration of the secondary effects of materials selection on the fuel cell nor of the potential issues that could increase the cost or limit the applicability of the solution.
- Model appears overly simplistic.
- The device has inherent limitations that will dictate against its use in an automotive fuel cell system.
- Assumptions regarding operation of an automotive fuel cell system need to be refined.
- Collaborations need to be developed with those who have system test benches and who know representative operating conditions.

### Specific recommendations and additions or deletions to the work scope

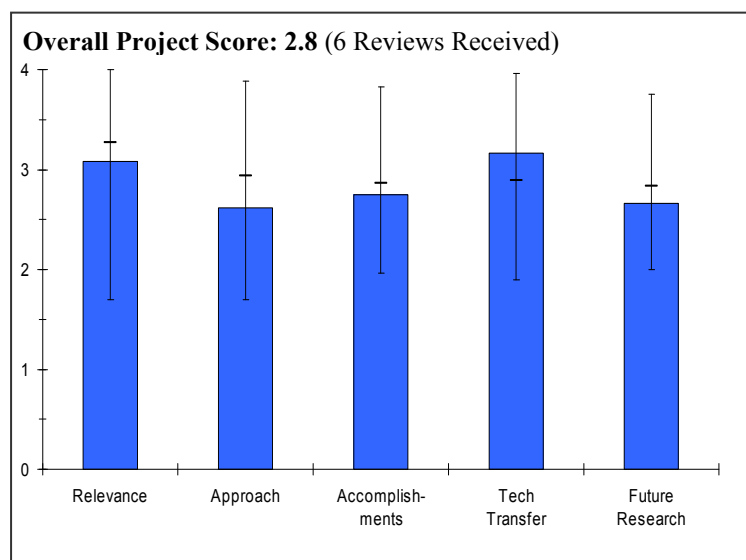
- Need to demonstrate applicability for humidification with streams that are sub-saturated.
- Testing in conjunction with a fuel cell.
- Testing in the presence of fuel cell impurities that may affect the corrosion of the device both in the inlet and the outlet stream.
- Project should seek to immediately do system-level testing with transient conditions.
- If the device is not capable of withstanding realistic system-level environment, it should no longer address DOE automotive fuel cell targets.
- Researchers should research patent literature, particularly under the name Grasso.

## Project # FC-39: Development and Demonstration of a New Generation High-Efficiency 1-10 kW Stationary PEM Fuel Cell Power System

*Durai Swamy; Intelligent Energy*

### Brief Summary of Project

The overall objective of this project is to develop and demonstrate a polymer electrolyte membrane fuel cell based stationary power system that provides a foundation for commercial, mass produced units that address identified technical barriers. The technical objectives are 1) 40% electrical efficiency (fuel to electric energy conversion); 2) 70% overall efficiency (fuel to electric energy plus usable waste heat energy conversion); 3) the potential for 40,000-hour life; and 4) the potential for \$450/kW. Intelligent Energy will engage international partners and enter a demonstration phase with an International Partnership for the Hydrogen Economy country other than the U.S.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- The project certainly addresses its defined objectives.
- Project will provide important information and possibly an important product if they are successful in integrating an ethanol reformer and polymer electrolyte membrane fuel cell power system.
- The use of liquid feedstocks limits the applicability of this system though it would address some market niches.
- Although stationary systems can contribute to advancements in technology, the goals of this project may not be high enough to contribute significant advancements to stationary fuel cell performance.
- Actual accomplishments appear to exceed the goals and might contribute to advancements, if the accomplishments continue to progress.
- System has high potential and technical merit with many fuels. Work appears to meet/exceed stationary targets in efficiency and cost.
- Project team understands and is addressing appropriate barriers.

### Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- Approach seems to result in significant progress, but it is difficult to evaluate on scientific merit with so little revealed information.
- Numerous cell, stack and system changes were implemented between "Baseline" and new version, yet the principal investigator did not present, or show an understanding of how the results were partitioned; so no understanding of the benefits of any particular change were learned.
- Sorbent-enhanced reforming has been tried by others (Air Products and Chemicals, for example) and large challenges on catalyst recovery and other issues surfaced. Principal investigator's modeling and experiment may fall short of predicting actual behavior of catalyst and sorbent in a full system under realistic cycling.
- It is not clear how the project is going to address durability and cost barriers, nor has total efficiency pathway (heat recovery) been discussed.

- The plan to test all combinations of stack design and fuel processing options seems unnecessary; the project should be capable of reducing the number combinations to save schedule and budget.
- General approach, to improve stack efficiency, reformer efficiency, power conditioning efficiency and reduce parasitic losses is a generally sound approach.
- Approach is sound and logical. The isolation of the fuel from the reformer with pressure swing adsorption and H<sub>2</sub> storage appears novel and could result in high purity H<sub>2</sub> at fuel cell inlet with elimination of costly CO/CO<sub>2</sub> cleanup processes. Is pressure swing adsorption impacted by reformer gas composition? Is a H<sub>2</sub> storage device necessary, and if so, what would it be?
- The principal investigator understands what is necessary to achieve the efficiency goals and the incremental improvements required to get there.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- Project seems to be on pace to reach specified targets.
- Principal investigator showed good improvement from their "Benchmark" fuel cell polarization, but it is not obvious how well the "Benchmark" unit was designed so it could be a representative state-of-the-art benchmark.
- The goal of a go/no-go decision by July 2008 is probably overly ambitious for the complexity of this integrated system project, where developments of reformer, fuel cell stack and power electronics are required.
- It appears that the bulk of the work to date has been related to fuel processing. The apparent lack of stack and system testing increases the risk of not initiating the demonstration in a timely manner and not achieving the project's goals.
- The work presented to date does not seem sufficient to support a system design finalization by January 2009.
- The project is meeting or exceeding its stack goals, but is not meeting its reformer goals.
- The project does not appear to be meeting its overall efficiency goals, although future gains may improve this situation.
- Intelligent Energy has made good progress. Meso Reformer may not be a major technical challenge. Fuel cell development appears to be an improvement and under control. Adsorption enhanced reformer achieved proof of concept. Data for polymer electrolyte membrane fuel cell performance showed no fuel composition, temperature or fuel utilization. It is difficult to assess real performance. Pressure swing adsorption unit has not been operated.
- Reasonable progress toward efficiency goal has been made, but definitely not there yet.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.2** for technology transfer and collaboration.

- Planning for future installations outside U.S., etc., and the number of engaged collaborators demonstrates significant integration with the fuel cell community at large.
- Collaborating partners are appropriate.
- The additional no-cost effort by Sandia National Laboratories to model six configurations is a plus.
- The project appears to be making good use of its partners to date.
- University / industry partnership.
- More input from users might be an improvement.
- Although electric utilities are being considered as partners, other industry user stakeholders, such as data center and office building developers, might be a valuable addition.
- Collaboration, including University of South Carolina, California State Polytechnic University, Pomona, and Sandia National Laboratories should be strong and effective.
- Working with Sandia National Laboratories and two universities is reasonable.
- Planning to demonstrate in an International Partnership for the Hydrogen Economy partner country.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.7** for proposed future work.

- As often with industrial presentations, technical evaluation is difficult, but progress has been made toward stated goals and so the success in the future can be inferred.
- The identified issues regarding the potential abandonment of the heat recovery portion of the system and the possible switch to natural gas from liquid fuel are significant scope changes and represent appreciable schedule risk areas.
- The project does not appear to be meeting their current goals, but assumes that the decision to move ahead will be made.
- Good logical plans for future work: six combinations are being considered. Intelligent Energy is downselecting technologies within team and then engineer, test and demonstrate a new generation polymer electrolyte membrane fuel cell power system.
- Inclusion of go/no-go decision point is outstanding.

**Strengths and weaknesses**Strengths

- Good single cell performance demonstrated; goals within reach for efficiency.
- Good fuel cell stack performance.
- Good group of collaborators with potential to eventually meet key project objectives.
- Solid approach to achieving gains.

Weaknesses

- Little information provided for meaningful technical evaluation.
- Too complex a scope for the schedule.
- The project seems to be lacking a rigorous approach to technology development and screening.
- The project does not address cost issues at all, and the presenter was unable to answer any questions regarding cost reduction approaches.
- Project goals do not appear to be a significant advancement over current fuel cell technology.
- The project does not appear to be meeting its overall goals.

**Specific recommendations and additions or deletions to the work scope**

- If principal investigator has not already done so, look into the DOE funded sorbent enhanced reforming done by Air Products and Chemicals in the late 1990s.
- If the project continues past the go/no-go decision point, emphasis should shift to the durability targets.

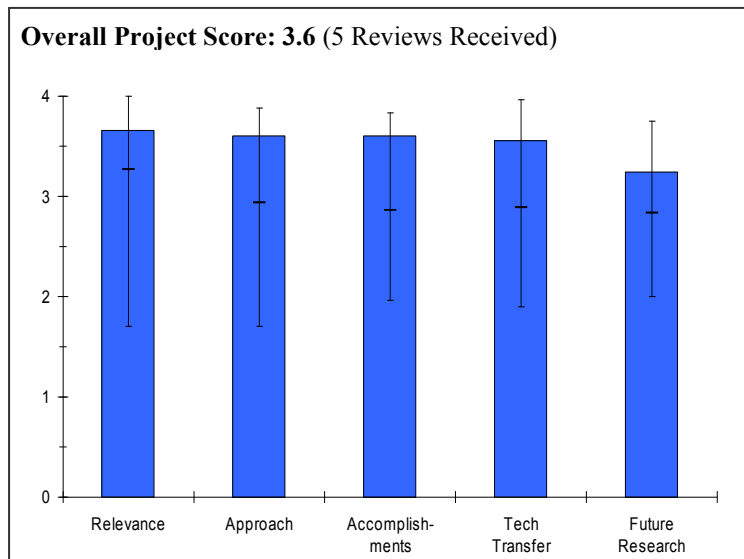
**Project # FC-40: International Stationary Fuel Cell Demonstration**

*John Vogel; Plug Power Inc.*

**Brief Summary of Project**

The overall objective of this project is to develop, test, and validate a high temperature polymer electrolyte membrane, stationary reformat-based, combined heat and power, fuel cell system as the first demonstration of a modular, scalable design for a worldwide market. The technical objectives are 1) total system cost of less than \$750 / kW in production volumes; 2)  $\eta_{\text{electric}} = 35\%$  (line of sight to 40%) and  $\eta_{\text{overall}} = 85\%$ ; 3) system life of 40,000 hours; and 4) modular and scalable system and combined heat and power hydraulics concepts.

**Question 1: Relevance to overall DOE objectives**



This project earned a score of **3.7** for its relevance to DOE objectives.

- The program is well directed at the program objectives.
- Very relevant to the DOE program though not relevant to transportation.
- Supports DOE: total system cost of <\$750/kW in production volumes;  $\eta_{\text{electric}} = 35\%$  (line of sight to 40%);  $\eta_{\text{overall}} = 85\%$ ; System life = 40,000 hours.
- Very well aligned with DOE's stationary fuel cell activities.
- This project is highly relevant to the President's Hydrogen Fuel Initiative and the objectives of the Multi-Year RD&D Plan.
- It is very important that a commercial "win" be achieved in the not to distant future, to help sustain the supplier base and maintain momentum and support for fuel cells in stationary and more challenging applications such as transportation.
- This project is relevant to the Hydrogen Fuel Initiative and the Multi-Year RD&D Plan as it targets a number of key barriers to the successful application of stationary polymer electrolyte membrane fuel cells utilizing different fueling scenarios.
- The basic project building block is the 5-kW fuel cell module. From here, a system can ostensibly be scaled up for a variety of applications including backup power, peak shaving, and prime generation.
- The project includes at least two potential fueling options- electrolyzer and natural gas reformation.
- The project is also evaluating the interconnection of the 5 kW power plants with the electric grid and opportunities for utilization of waste heat from the polymer electrolyte membrane fuel cell.

**Question 2: Approach to performing the research and development**

This project was rated **3.6** on its approach.

- The approach to the technology validation seems well directed to making a commercially acceptable device that can meet residential needs for combined heat and power.
- The team is addressing the major technological barriers that will limit consumer adoption of the fuel cell in a realistic consumer environment.
- The project approach is clearly focused on delivering a 5 kW combined heat and power unit.
- Approach is well-documented; milestones are detailed and appropriate and aggressive.
- Not only are they addressing the technical targets, but also commercialization issues.

- The overarching approach is sound, spreading the developmental cost between the U.S. and EU, private and government sectors, and targeting specific residential combined heat and power applications as a drop-in solution.
- The presentation was somewhat vague and not comprehensive on how each of the technical barriers (durability, cost, and performance) is specifically being addressed.
- Little discussion is provided of alternative technical approaches should current avenues not prove out.
- This project overtly addresses key technical barriers of durability, reliability, electrical and combined heat and power energy efficiency, and cost.
- Project incorporates a completely passive natural water management system mode.
- The project is broad emphasizing a number of areas, but lacks a sharp focus on any one particular technical barrier and does not focus on a specific market niche.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.6** based on accomplishments.

- The team is making good technical progress against the objectives of the program.
- The major technical objectives of durability with the new materials in a fuel cell system need to be demonstrated.
- Three units have been built and are ready to ship to the delivery sites.
- Good progress. A high temperature polymer electrolyte membrane, stationary, reformat-based, combined heat and power fuel cell system has been developed based on commercial requirements.
  - Enabling membrane electrode assembly, stack, reforming and power electronics technologies have been explored, down-selected and developed.
  - Progress has been made toward achieving DOE technical targets; especially performance and system durability.
- Technical improvements are headed in the right direction to achieve efficiency and life.
- Higher efficiency inverters are being developed through the DOE Vehicle Technologies Program.
- There appears to be solid technical advancements with the cathode and inverter but otherwise technical accomplishments seem a little sparse at this point in the project (80% completed). Specifically, with regards to the stack, it appears only limited progress has been made.
- No hard data is provided on specific technical accomplishments vis-a-vis DOE durability, cost, and performance targets.
- No accounting is provided of technical accomplishments on the EU side.
- Clearly, technical progress is being made with regards to efficiency (42% without power conditioning). IR, open circuit voltage, falloff time, and conductivity have exceeded program requirements for unitized electrode assemblies and performance at 1 A/cm<sup>2</sup> is close to minimum criteria.
- There is insufficient information to determine progress towards durability, combined heat and power efficiency, and cost targets.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.6** for technology transfer and collaboration.

- The team has the skills to build and put in place the test units.
- The team is well coordinated with integration of the materials test, integration and build within a reasonable project plan to meet the demonstration objectives.
- Major collaborations with the EU, which is providing funds.
- BASF provides high temperature membrane and new cathode catalyst formulations.
- First of a kind collaboration between the DOE and the EU. Goal to develop “high-temperature” (PBI-based) fuel cell heating appliances for residential use worldwide. Executed through a U.S./EU consortium: Plug Power (U.S.)/(Netherlands), BASF E-TEK (U.S.), BASF (Germany), Vaillant (Germany), Domel (Slovenia), Bulgarian Academy of Sciences (Bulgaria), Gaia (Sweden), Imperial College (United Kingdom).
- Impressed with the consortium that has been assembled for this project.



- Broad collaboration especially on the European side with several different companies and academic institutions.
- Collaboration is narrow on the U.S. side with a notable absence being DOE laboratories.
- It is not clear as to the exact role of each of the participants. For example, which entity is going to help crack the barriers to entry in the boiler market (Vaillant)?
- No discussion of how intellectual property rights would be allocated and shared to protect each entity's achievements but still expedite commercialization.
- The project only has a minimal amount of partners for testing, power conversion / electronics, and refueling options (electrolyzer). There are no other fuel cell industry, laboratory, or university partners. As a result, it is unlikely that significant technology transfer will occur.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated 3.2 for proposed future work.

- The future work is well-designed to meet the remaining engineering tasks to necessary to put the three demonstration units into place and monitor their progress.
- The system will be tested for 6 months in Europe by the end of the first quarter of 2009.
- Well-conceived management milestones.
- Planned work is consistent with goal of completing demo next year.
- Limited discussion is provided as to other commercialization avenues should the residential boiler replacement market not pan out.
- No discussion is provided as to other potential technical paths should further progress toward the technical goals not be achieved under the current strategy.
- It is indicated the technology is modular and "scalable" but little discussion was provided on specifically how it may make the technology amenable to other potential applications.
- The broad scope of the project inherently permits significant flexibility to adjust to future market opportunities. For example, to use the basic 5 kW fuel cell building block to scale up to different applications and accommodate different fueling options. However, the broad scope also hinders strongly focusing on a specific market application that could be achieved in the near term and lead to a commercial foothold.

### **Strengths and weaknesses**

#### Strengths

- Good project team to do the integration and put the systems into place.
- Worked on one of the key materials degradation processes in the catalyst corrosion.
- Addresses a market that could be ready for near-term deployment.
- Overall consortium strategy with EU is interesting and refreshing.
- Project appears strongly focused on commercial applications.
- Focusing on a 5-kW building block that provides inherent commercial flexibility.
- Broad scope of project looking at variety of key technical barriers and fueling options.

#### Weaknesses

- The longer-term durability of the components, in particular the new catalyst and support was not shown.
- Technical progress to date is somewhat limited.
- There is no collaboration with DOE national laboratories, universities, and only one other U.S.-based company.
- The project does not provide a solid discussion of contingencies should the current technical and business approach not be entirely successful.
- No specific near term commercial application is targeted.
- Limited number of project partners especially with regards to the fuel cell system itself.

### **Specific recommendations and additions or deletions to the work scope**

- Is a longer testing period for the demonstration units need to really demonstrate the applicability of the units?
- Involve National Laboratories to help resolve durability issues.

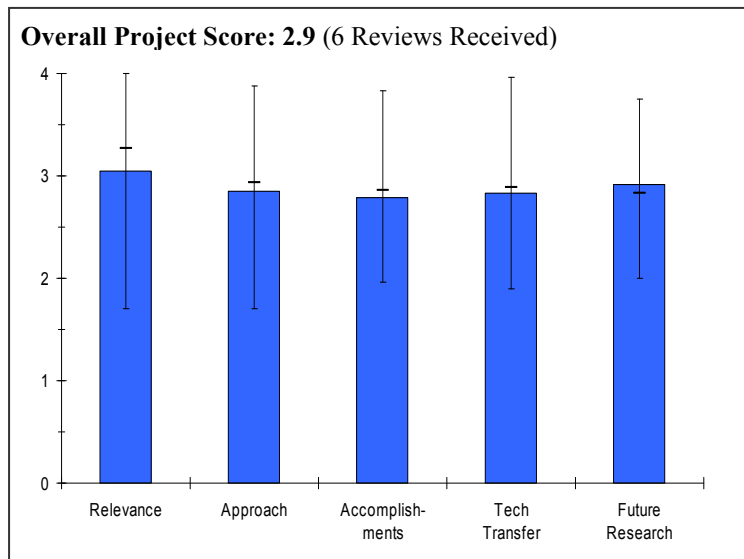
- Clearly delineate intellectual property agreements (if they haven't been already) to enhance commercialization prospects.
- Work with U.S.-based home energy suppliers to determine if options exist in the U.S. for the proposed technology.
- Establish collaboration with the National Lab(s) or universities to help solve most difficult membrane/electrode issues.
- Conduct downselection process to identify and have focus on a specific near term market opportunity such as a backup power. Develop partnership with commercial entities that can facilitate breaking into this market.

**Project # FC-41: Intergovernmental Stationary Fuel Cell System Demonstration**

*Rhonda Staudt; Plug Power Inc.*

**Brief Summary of Project**

The objective of this project is to design and produce an advanced prototype polymer electrolyte membrane fuel cell system with the following features 1) 5-kW net electrical output; 2) flex-fuel capable (liquefied petroleum gas, natural gas, ethanol); 3) reduce material and production cost while increasing durability; 4) increase electrical efficiency over the current alpha design; and 5) increase total efficiency by incorporating combined heat and power. Plug Power will also show a path to meet long-term Department of Energy objectives, including 1) 40% system electrical efficiency; 2) 40,000-hour system/fuel cell stack life; and 3) \$750/kW integrated system cost (with reformer).



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.1** for its relevance to DOE objectives.

- Stationary systems that are flex-fueled are reasonably aligned with the Hydrogen vision.
- A meaningful demonstration of implementation of fuel technology is very relevant. It should encourage other potential first users to pursue deployment of this important technology.
- The overall objective is to design and produce an advanced prototype polymer electrolyte membrane fuel cell system with many different functions such as flexible fuels.
- The program is highly relevant to the President's Hydrogen Fuel Initiative.
- Not to be judged from the presentation.
- Shows a path to meet long-term DOE objectives.
  - 40% system electrical efficiency
  - 40,000 hour system / fuel cell stack life
  - \$750/kW integrated system cost (w/ reformer).
- Pursuing path to efficiency and durability as established by DOE targets.

**Question 2: Approach to performing the research and development**

This project was rated **2.9** on its approach.

- Approach thus far appears to be well-planned, which is necessary for a small company.
- Clear and well-defined steps to approach targets have been established.
- Breakdown of various components is well understood and mapped out.
- Unclear why ethanol was chosen as a fuel.
- The proposed approach appears to be sound and when successfully completed should achieve the desired DOE objectives. The proposed tasks are reasonable and well-defined.
- The project is not research and development; it is primarily system development and integration. The approaches are excellent.
- Only vague general statements.

- Approach may be too ambitious. Flex-fuel capability – liquefied petroleum gas, natural gas, ethanol may be difficult but possible with an autothermal reformer. What about guaranteed output power no matter the fuel? Can fuel switch be done quickly without major modifications?
- Good work plan for a fuel flexible system.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- Despite short funding period, quite a few accomplishments have been met.
- Stationary community has finally recognized issues of start/stop on stack durability.
- Interesting cost analysis has been performed.
- This is a fairly new project.
- Completion of the first task indicates good progress being made.
- The program started August 2007, so far, the accomplishments are good.
- Nothing substantial.
- Modest progress. Completed mostly only conceptual efforts. However, a realistic direct manufacturing cost reduction plan was apparently obtained.
- Determined that continuous operation is financially advantageous.
- Significant analysis and thought has gone into conceptualization of the design.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.8** for technology transfer and collaboration.

- Collaborations exist but at this time it is premature to judge relationships fully.
- Based on work to date, it appears to be sufficient.
- Appropriate partners for this project have been identified and are in the process of being brought onboard.
- Partnered with Ballard and Army's Construction Engineering Research Laboratory, excellent cooperation. The system may be used for the Department of Defense facilities.
- Unclear.
- Collaboration is strong and effective. Ballard and the Construction Engineering Research Laboratory bring excellent test and technical strengths.
- Collaborations are really limited to the demonstration sights. Additional, diversified subcontractors might help accelerate improvements.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- Future research is well described and logical.
- Depends on some criteria coming together so some risks exist.
- A good plan for future work is in place in sufficient detail.
- The future work and plan are clearly stated in the slides and also excellent.
- Unclear.
- Plug Power planned future work is well conceived, but ambitious.
- Go/no-go decision next year.

### **Strengths and weaknesses**

#### Strengths

- Key player in this area.
- Strong Team.
- Good Plan.

Weaknesses

- Inclusion of ethanol seems to be an unnecessary step – perhaps liquefied petroleum gas is sufficient as primary first step.

**Specific recommendations and additions or deletions to the work scope**

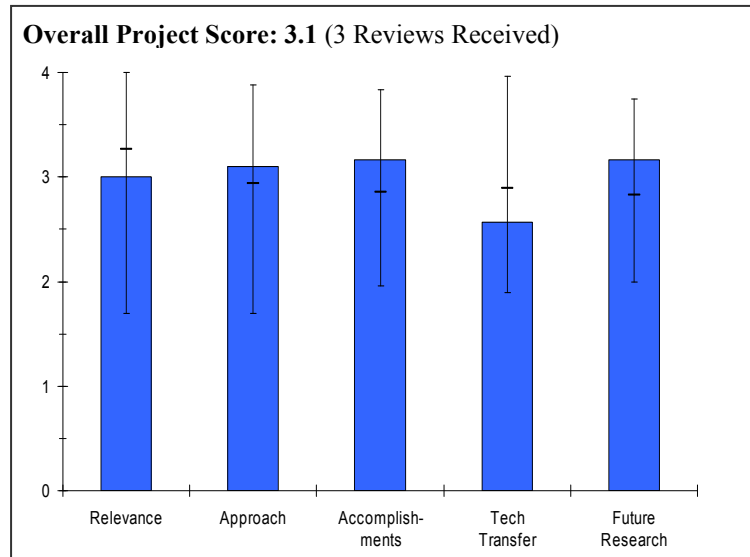
- Consideration of focusing solely on liquefied petroleum gas.
- The project started August 2007, wait for the next year review to decide recommendations.
- Generate and present clear results.

## Project # FC-42: Stationary PEM Fuel Cell Power Plant Verification

*Eric Strayer; UTC Power*

### Brief Summary of Project

The objectives of this project are to 1) evaluate the operation of a 150 kW natural gas-fueled polymer electrolyte membrane fuel cell; 2) assess the market and opportunity for utilization of waste heat from a polymer electrolyte membrane fuel cell; 3) verify the durability and reliability of low cost polymer electrolyte membrane fuel cell stack components; 4) design and validate an advanced 5 kW polymer electrolyte membrane fuel cell system; 5) conduct demonstrations of polymer electrolyte membrane technology with various fueling scenarios; and 6) evaluate the interconnection of the demonstration 5 kW power plants with the electric grid.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- Project addresses the evaluation and advancement of stationary polymer electrolyte membrane fuel cells.
- Relevant to the DOE program objectives though not necessarily relevant to transportation.
- Durability is a critical characteristic for base load stationary power applications.
- The project is also addressing cyclic performance for backup and intermittent power implementations.

### Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Approach seems to move project towards stated targets.
- The approach is clearly focused on developing a commercially viable fuel cell generator.
- UTC Power performance targets are well documented.
- While the approach appears to be working towards addressing the identified barriers, there needs to be a clearer presentation of the linkages between project activities.
- There was very little discussion regarding approaches for reducing cost.

### Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- Goals have been achieved on schedule for evaluating the technology.
- Progress appears to be good in the three enabling fundamental technologies – a low cost membrane electrode assembly, evaporative cooling, and a strategy to mitigate the effects of O<sub>2</sub> in the anode chamber on startup after a shutdown.
- The advanced stack with the above features is under test.
- Progress against targets is well-documented.
- Progress is being made in most areas, though there are a few open issues that need to be addressed, most notably end-cell degradation effects.
- UTC presented little technical information beyond final performance (which is typical of presentations from industry.)

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.6** for technology transfer and collaboration.

- It is unclear whether collaborators provide more than simply pre-built components.
- Key suppliers/developers and independent test organization are identified that contribute to the project.
- It could be inferred how the project partners participated in a meaningful manner, but the project presentation does not clearly identify the partners' activities and contributions.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- Project seems to be well-planned and there are paths for improvement.
- After the test program and data are evaluated, the final design iteration will be completed.
- It is unclear which technology set (baseline or advanced) is being incorporated into which future demonstration.
- As with the project approach, there needs to be a clearer presentation of the linkages between future project activities.

**Strengths and weaknesses**

Strengths

- Shows progress and makes the technology look more promising.
- Clear market-driven focus.
- UTC Power has the system development experience to complete the work and is focusing on important issues.

Weaknesses

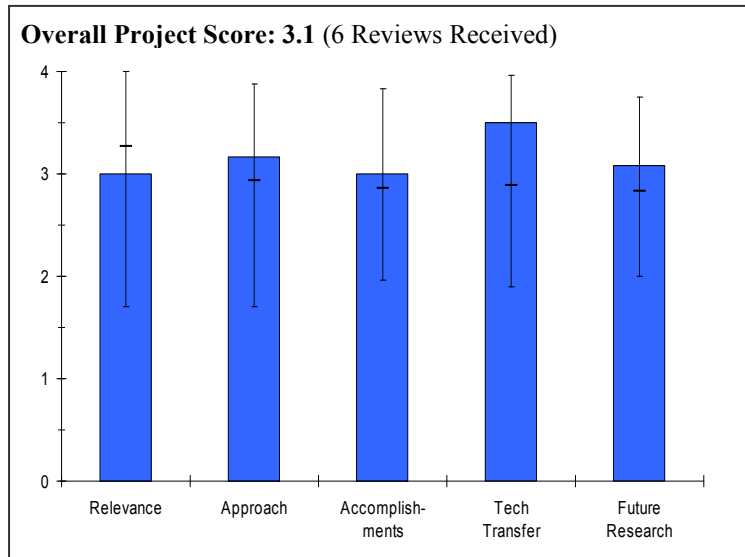
- Unclear if durability issues will prevail against the technology.
- There was no presentation of approaches and progress relative to cost reduction.

**Specific recommendations and additions or deletions to the work scope**

(None provided by reviewers.)

**Project # FC-43: Diesel Fueled SOFC System for Class 7/Class 8 On-Highway Truck Auxiliary Power***Dan Norrick; Cummins***Brief Summary of Project**

The objectives of this project are to 1) demonstrate on-vehicle and evaluate a solid oxide fuel cell (SOFC) auxiliary power unit with integrated on-board reformation of diesel fuel; 2) develop a transparent method of water management for diesel fuel reformation; 3) develop controls to seamlessly start, operate, and shutdown the solid oxide fuel cell auxiliary power unit; 4) evaluate hardening the solid oxide fuel cell auxiliary power unit to enable it to operate reliably in the on-highway environment; and 5) develop the overall system for performance, size, cost, and reliability targets.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.0** for its relevance to DOE objectives.

- Addresses auxiliary power unit application.
- Highly relevant to DOE mission.
- The development of solid oxide fuel cell-based auxiliary power units is critical to reducing the environmental impact of auxiliary power units.
- The project appears well designed to address most substantial issues related to heavy-duty vehicle auxiliary power unit development.
- There is not sufficient focus on durability aside from shock and vibration tolerance.
- Shows path to reducing truck emissions in prospect of anti-idling laws. Also auxiliary power units will lead to lower diesel fuel consumption. Project will become more important as price of diesel continues to increase.

**Question 2: Approach to performing the research and development**

This project was rated **3.2** on its approach.

- Standard approach of analysis and design/sub-system test and development/laboratory testing/on-vehicle evaluation.
- Very good approach matrix to develop the auxiliary power unit.
- Good approach to use existing packaging design and size.
- Tightly integrated packaging of reformer and solid oxide fuel cell.
- Approach is rational and properly staged.
- Use of existing engine-based commercial auxiliary power unit platform/constraints is helpful for integration into vehicle.
- It is not clear how the project is going to address cost reduction or thermal cycling performance.
- Excellent understanding of barriers.
  - Waterless reforming of ultra low sulfur diesel fuel.
  - Transient operation of solid oxide fuel cell system.
  - Power density, specific power (W/L, W/kg).
  - Shock and vibration tolerance.



**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- 17% net efficiency does not come close to the DOE 2010 target of 35%.
- Catalytic partial oxidation improvements appear to sacrifice efficiency.
- Good results for system design, fuel cell components and balance-of-plant.
- No indication how Cummins will harden system for improved sulfur tolerance.
- Good progress on opening operating region for catalytic partial oxidation, but a wider range of conditions is still needed.
- Little progress on anything but reformer development.
- The project team has addressed system demand and packaging issues.
- More information regarding transient performance, solid oxide fuel cell sulfur tolerance, and power density are required.
- Approach is well-organized. Selection of current collection approach is very critical for this solid oxide fuel cell design. Could be costly and ineffective if not correctly done. Tube power density needs to be increased as much as possible. Dry catalytic partial oxidation is best reforming approach but system efficiency of 17% is low. Only 500 h catalytic partial oxidation testing to-date. Transfer switch to shore power is good feature.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.5** for technology transfer and collaboration.

- Partnership between Cummins, Protonex and International Truck and Engine.
- Collaborations utilize all partners' strengths to advance the technology.
- Excellent team covering all aspects of system development and demonstration.
- The project team encompasses and has engaged all pertinent participants.
- Collaboration is excellent. Excellent team skills/subsystems. Cummins Power Generation (project lead), Protonex, LLC (solid oxide fuel cell power module), International Truck and Engine (vehicle and installation). Cummins is already in truck auxiliary power unit business.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Future work shows how system will be finished, integrated and tested.
- No path apparent to reach DOE efficiency targets.
- Future work weak. No mention of demonstration. It appears that all work is on H<sub>2</sub> pump, which is not really a pump.
- There remains much to be done in this project, but the proposed future work should address all issues.
- Future work is largely appropriate relative to the work to date and overall objectives.
- Planned future work is well-conceived: fabricate and test hot zones – build single modules and 4-module sets – test modules in furnace and in insulation packages – optimize bundle performance.

**Strengths and weaknesses****Strengths**

- Operation on diesel with no water makes for simplified system infrastructure requirements.
- Tightly integrated team.
- Cummins is well-positioned given their experience with engine-based commercial auxiliary power unit products to understand the technical and functional requirements of a solid oxide fuel cell-based auxiliary power unit.

**Weaknesses**

- System efficiency limits the application of this project to small niche markets.

- Overall system gross efficiency is not much better than IC engine. How will this concept ever gain acceptance!
- System could be designed to improve fuel utilization and stack efficiency to more than 60% on diesel with redesign. Advanced concepts have been overlooked or neglected to improve system efficiency.
- Somewhat slow progress to date.
- A clearer understanding of how the project is addressing issues related durability and performing relative to DOE power density targets is required.

**Specific recommendations and additions or deletions to the work scope**

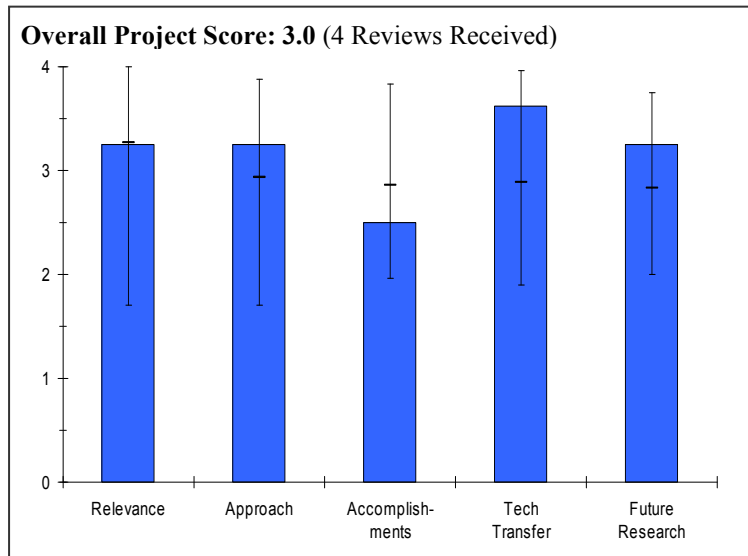
- Need to explore methods to improve catalytic partial oxidation and system efficiency.
- Add wider range of operating conditions to testing of catalytic partial oxidation reformer, including the effect of higher concentrations of sulfur in diesel fuel on performance and durability of catalytic partial oxidation reformer and solid oxide fuel cell stack.

**Project # FC-44: Solid Oxide Fuel Cell System Development for Auxiliary Power in Heavy Duty Vehicle Applications**

*Gary Blake; Delphi*

**Brief Summary of Project**

The objectives of this project are to 1) develop auxiliary power unit system requirements and concepts with major truck original equipment manufacturers; 2) design, develop, and test the needed subsystems for the approved concept; and 3) build and demonstrate a diesel-fueled truck auxiliary power unit system. Delphi is preparing the on-truck installation using a modified natural gas auxiliary power unit in an integration enclosure. Delphi is on target for meeting timing and budget and is committed to introducing solid oxide fuel cell diesel technology in full-scale production for heavy-duty truck applications.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- The project is relevant, but the payoff in terms of fuel and emissions reductions is not quantified.
- The development of solid oxide fuel cell based auxiliary power units is critical to reducing the environmental impact of tractor trailers and the reliance of tractor trailers on carbon-based fuels.
- The project, in principle, can address issues related to heavy-duty vehicle auxiliary power unit development, but project objectives are very high level and lack clarity.
- Shows path to reducing truck emissions in prospect of anti-idling laws. Also auxiliary power units will lead to lower diesel fuel consumption. Project will become more important as price of diesel continues to increase. Fuel cell genset should be lower cost than diesel genset no matter the driver/truck behavior/use pattern.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- This is a typical design, build, test project.
- Good plan to include thermal cycling effects on system performance and durability.
- Excellent understanding and description of requirements.
- The approach lacks specifics regarding how the project will address development issues.
- The lack of a road test represents a risk area.
- Excellent understanding of barriers.
  - Sulfur remediation.
  - Reformer operation.
  - Stack sensitivity – carbon issues.
  - Catalyst plugging.
  - System pre-combustion / combustion.
  - System integrated electrical efficiency could be 30-35%.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.5** based on accomplishments.

- On target for schedule and budget.
- No performance data were presented, just "projected" efficiency data.
- Nice demonstration of projected efficiency of future Delphi solid oxide fuel cell.
- Though the presentation stated that the project is 50% complete, it appears that a large majority of the tasks were not yet complete.
- There was insufficient discussion regarding how the project is progressing against required system characteristics.
- The switch from a catalytic partial oxidation reformer to an “endothermic” reformer represents an appreciable change to system architecture and a program risk that was not adequately discussed.
- Progress has been slow/delayed. Delphi is developing one of highest performing solid oxide fuel cells in world developed under Solid State Energy Conversion Alliance program. Delphi is developing reforming technology for Diesel/JP-8 solid oxide fuel cell applications for the Department of Defense. In solid oxide fuel cells, the water is created on the anode side that is where it is needed – ideal fuel cell for fuel reforming applications to produce H<sub>2</sub>.

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.6** for technology transfer and collaboration.

- Excellent support from the ultimate customer, truck original equipment manufacturers.
- Excellent team covering all aspects of system development and demonstration.
- The project is largely an in-house effort, but appropriate system requirements have flowed down from end users.
- Collaboration is excellent. Excellent team skills/subsystems: Delphi, Paccar, Volvo Truck, and Electricore, Inc. Delphi is already in automotive business. Excellent market understanding and presence.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.3** for proposed future work.

- Logical and according to plan.
- Good plan, but with little time remaining.
- There appears to be a substantial amount of work remaining, but it is appropriately structured.
- Planned future work indicates complete understanding of how to complete this project successfully.
- Finalize the Subsystem Requirements Document and Development Plan.
  - Complete the solid oxide fuel cell auxiliary power unit hardware design and build.
  - Design subsystem test fixture.
  - Begin subsystem testing and development iterations.
  - Build a system for DOE.

#### **Strengths and weaknesses**

##### Strengths

- The team.
- Integrated team.
- Understanding of system issues.
- Delphi is an experienced solid oxide fuel cell developer who understands what is required to develop a system.

##### Weaknesses

- Project started with focus on partial oxidation reforming, but has switched to a vastly different design utilizing steam reforming at a very late stage in the project.
- Lack of progress, with the exception of paper studies.
- The approach and discussion of progress lack specifics.

#### **Specific recommendations and additions or deletions to the work scope**

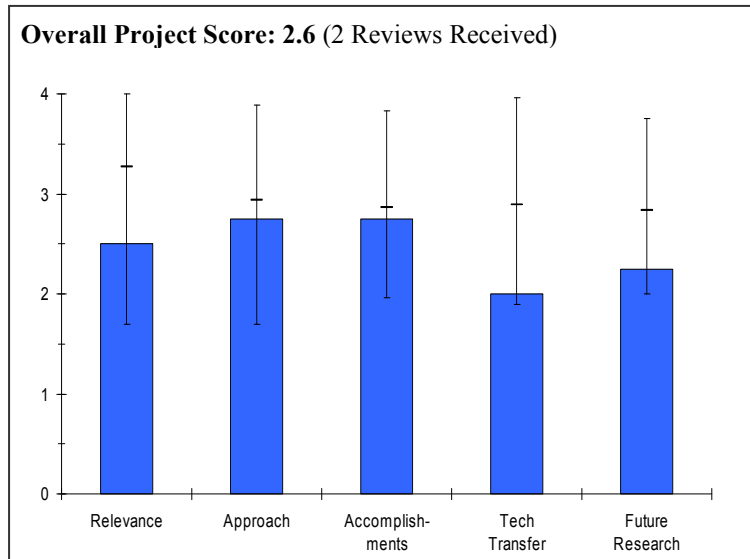
(None provided by reviewers.)

**Project # FC-45: DMFC Prototype Demonstration for Consumer Electronic Applications**

*Chuck Carlstrom; MTI Micro Fuel Cells*

**Brief Summary of Project**

The objectives of this project are to 1) benchmark energy density of 600 Wh/L; 2) demonstrate prototypes; 3) develop pathways to low cost for initial market entry; 4) demonstrate continual operation of 1,000 h; and 5) accelerate codes, standards, and regulations to allow shipping and airline passenger cabin usage. Prototype energy density was demonstrated to be on path to system targets. There was also success on the regulatory road map.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.5** for its relevance to DOE objectives.

- Portable power systems will not directly support the Hydrogen Fuel Initiative; the project has some aspects that could support the advancement of fuel cells thereby providing tangential value to advancing the Hydrogen Fuel Initiative.
- Relevant.

**Question 2: Approach to performing the research and development**

This project was rated **2.8** on its approach.

- Mobion technology has been developed for very low power, portable applications.
- The mostly passive Mobion technology has advantages regarding balance-of-plant issues (fewer components, less system complexity, etc.).
- The energy density produced is not significantly higher than lithium batteries. The project primarily represents an engineering approach to a system that is not likely to be commercially competitive. Significant increases in energy density would make this project more compelling.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- The reported performances were only modestly compelling compared to lithium batteries. The next generation of Mobion technology is a little more interesting, but still not demonstrated. The arbitrary choice of several refills/cartridges in projecting an energy density makes the true performance versus weight characteristics impossible to completely evaluate.
- Good progress towards stated goals.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.0** for technology transfer and collaboration.

- Really not particularly relevant. The community gains little in terms of understanding or scientific advancement for a publicly funded project.

- Not very clear.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.3** for proposed future work.

- It is very hard to judge what the substance behind the future plans is. The demonstration of the next generation system with higher energy density and cartridges is obviously a step forward.
- Difficult to assess.

**Strengths and weaknesses**

Strengths

(None provided by reviewers.)

Weaknesses

(None provided by reviewers.)

**Specific recommendations and additions or deletions to the work scope**

(None provided by reviewers.)

**Project # FC-46: DMFC Power Supply for All-Day True-Wireless Mobile Computing***Brian Wells; Polyfuel Inc.***Brief Summary of Project**

The objectives of this project are to 1) build a direct methanol fuel cell laptop power supply with a significant advantage over lithium ion batteries; and 2) fully integrate this power supply into a laptop computer. A radical departure from conventional active systems is required to realize competitive power density. PolyFuel's intention is to license any arising intellectual property to electronics original equipment manufacturers. PolyFuel has identified a novel method of membrane electrode assemble construction with a new membrane and gas diffusion layer structure.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.9** for its relevance to DOE objectives.

- The main objective of the project is to build a direct methanol fuel cell system for a laptop computer application.
- The cost for a direct methanol fuel cell system is too high to be used for a laptop computer application.
- The project is indirectly relevant to the President's Hydrogen Fuel Initiative.
- Fuel cell introduction into the electronics portable power market is an excellent way for the public to increase its familiarity with and acceptance of fuel cell systems in other markets, such as vehicular.
- Portable power systems won't directly support the Hydrogen Fuel Initiative, but the project has some aspects that could support the advancement of fuel cells thereby providing tangential value to advancing fuel cells.
- Relevant.

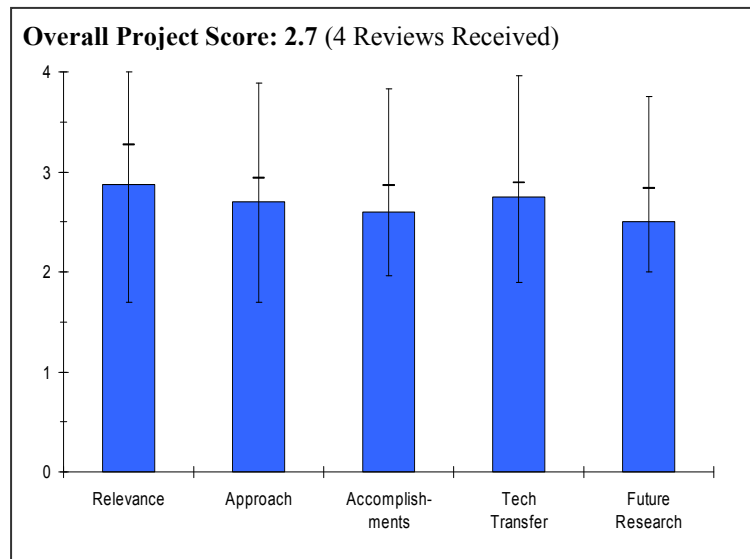
**Question 2: Approach to performing the research and development**

This project was rated **2.7** on its approach.

- PolyFuel is a research and development company for membrane electrolytes while the project involves system integration and manufacturing.
- The power density and energy density are key issues for electronic portable power. These are being aggressively addressed through innovative approaches.
- Development of a direct methanol fuel cell system without active water recovery is beneficial for balance-of-plant issues. Engineering of membranes and gas diffusion layers to remove water is a reasonable approach. The control system strategy seems logical although a deep level of detail is not possible in such a review. An analysis comparing active water recovery systems that can operate at higher temperatures and have higher cell efficiency (although increased balance-of-plant losses and a larger footprint) would have been useful.
- The energy density is not significantly higher than lithium batteries. The project primarily represents an engineering approach to a system that is not likely to be commercially competitive. Significant increases in energy density are necessary to make this project more compelling.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.6** based on accomplishments.



- The single cell performance is not good as Nafion 117 single cell performance. The direct methanol fuel cell system problem is balance-of-plant. The project focuses on single cell research and development.
- The water recovery approach appears to be producing excellent results in terms of fuel cell power density, stability, and operational lifetime.
- Differences in single cell and stack performance suggest that significant issues remain to be solved.
- Performances reported are not compelling for laptop applications because of other advantages of lithium batteries over fuel cells in these applications.
- Substantial shortcomings in terms of implementing technology effectively in the platform considering the funding level.
- Good progress.

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.8** for technology transfer and collaboration.

- The project may not be able to transfer technology.
- The collaborations with others on the project with regard to membrane electrode assembly development appear to be quite effective.
- PolyFuel indicates its intention to license its intellectual property to electronics original equipment manufacturers.
- Reasonable team for commercial development of these systems. However, little is learned by the community from these highly proprietary projects.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.5** for proposed future work.

- Find a system integration and manufacturing company to support the project. The direct methanol fuel cell is too expensive to be used for a laptop computer application.
- The future work is targeted at the remaining issues with the system.
- Not clear how future objectives will be met (i.e., presentation does not have any details).

#### **Strengths and weaknesses**

##### Strengths

- Innovative approaches.
- No active water recovery needed.

##### Weaknesses

- PolyFuel does not have the necessary experience for system integration and balance-of-plant for a direct methanol fuel cell system.
- Energy densities not compelling; no route was presented toward achieving compelling energy densities.

#### **Specific recommendations and additions or deletions to the work scope**

- Find a system integration and manufacturing company to support the project.



**Project # FC-47: Fuel Cell Research at the University of South Carolina***John Van Zee; University of South Carolina***Brief Summary of Project**

The objectives of this project are to 1) develop novel materials (e.g., Nb-doped) for improved corrosion resistance and improved fuel cell components; 2) develop a fundamental understanding of performance and durability loss induced by fuel contaminants; 3) develop a fundamental understanding of the degradation mechanisms of existing gaskets and the performance of improved materials; 4) develop a fundamental understanding of acid loss and acid transport mechanisms in polybenzimidazole systems, and predict performance and lifetime as a function of load cycle.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.8** for its relevance to DOE objectives.

- Project works to develop components and/or make measurements to support modeling.
- Project covers many topics, but none are addressed with the proper methodology.
- Improved fuel cell durability, cost, and performance are relevant goals.

**Question 2: Approach to performing the research and development**

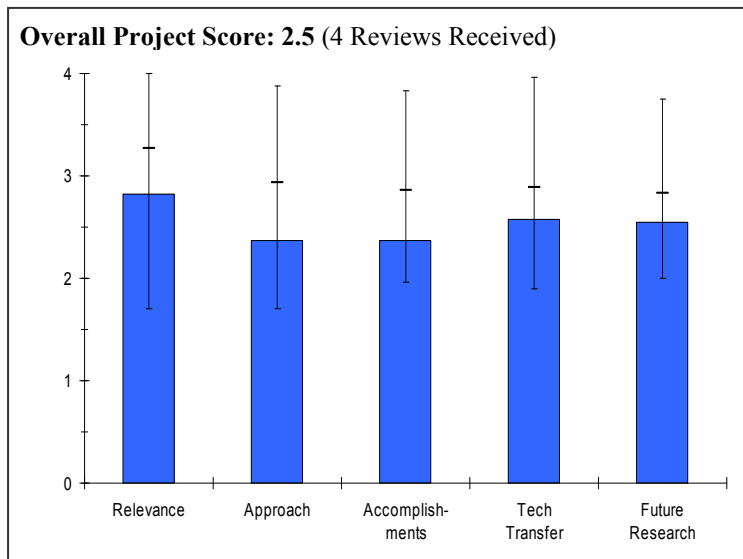
This project was rated **2.4** on its approach.

- Project consists of 4 different/separate approaches.
- Unclear why project is developing non-carbon electrocatalyst supports for direct methanol fuel cell anodes.
- Probably don't need to evaluate silicon gaskets for polymer electrolyte membrane environment as most developers have eliminated those from consideration.
- Polybenzimidazole work supports limited number of applications and developers.
- CO impurity work supports other modeling work that has been requested.
- Catalysis work is improperly benchmarked, both rotating disk electrode and direct methanol fuel cell data.
- Impurity work seems to be repetitive with other DOE projects and with previous literature.
- If the gasket work is focused on so few materials, then *in situ* testing would be appropriate at an earlier point.
- Projects tend to cover well-studied areas. Difficult to see progress toward defined targets.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.4** based on accomplishments.

- Significant data produced for H<sub>2</sub> quality team.
- Possible good progress with non-carbon supports.
- Evaluation of silicon and ethylene propylene diene methylene terpolymer (EPDM) gasket materials already accomplished by industry.
- Project needs to re-evaluate the first two topics with serious attention to what has already been done. Benchmarks must be more accurate.



- Gasket topic includes many simplistic leaching experiments so far, and provides little insight.
- Work on Ti catalyst supports interesting, somewhat novel. Many small projects underway, which were covered with little detail. Hard to see any focus.

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.6** for technology transfer and collaboration.

- Unclear what collaborations exist other than H<sub>2</sub> quality team.
- The gasket topic involves many companies.
- Other topics have no obvious involvement from others, only the intention.
- Principal collaboration is with the University of South Carolina National Science Foundation project, which is the same organization. Things are just beginning, so that may be changing.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.6** for proposed future work.

- Solid extension of approach on impurity work.
- Developing accelerated durability tests for gasket materials and predictive modeling of degradation is a good path.
- Future work not discussed for task 1 and task 4.
- Future work not stated specifically enough in all the topics.
- Durability of catalyst supports was not addressed at all, but should be.
- The future presented was an extension of the past.

#### **Strengths and weaknesses**

##### Strengths

- Topic areas selected are of interest to the hydrogen fuel cell community.
- Some principal investigators have relevant expertise.

##### Weaknesses

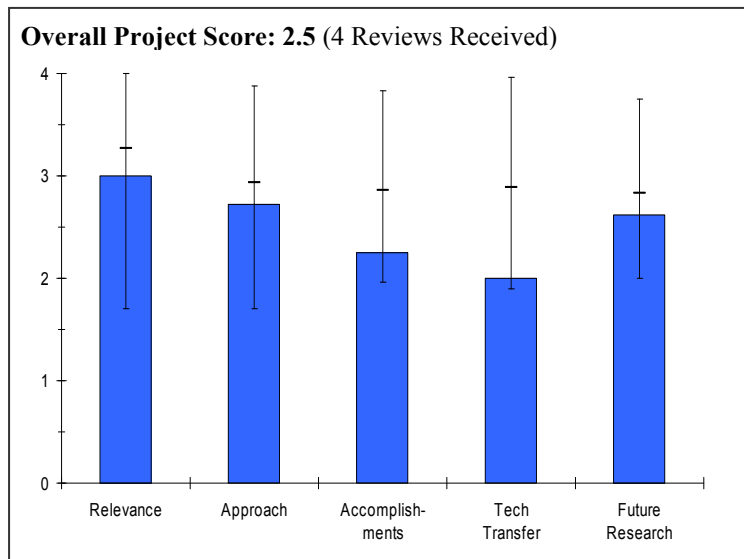
- Four largely unrelated projects with no interconnection.
- Evaluation of materials seems incomplete compared to literature standards, including poor benchmarking.
- The funding level is high enough at a university that the amount of data generated is less than expected in each topic.

#### **Specific recommendations and additions or deletions to the work scope**

- Need to evaluate non-carbon supports for the oxygen reduction reaction on the cathode where carbon corrosion problem exists.
- Perhaps the scope should be narrowed from four to two topics that show the most success. I am not sure yet what those would be. It would be better to evaluate such disparate topics separately.
- The DOE might consider that future funds focus on one or two well-defined tasks that explore alternatives to existing technology. An example might be instead of redoing the very extensive literature on effects of fuel impurities on fuel cell performance, explore sensible approaches that allow fuel cells to live in a "dirty" world. "Fuel filters" come to mind.

**Project # FC-48: Novel PEMFC Stack Using Patterned Aligned Carbon Nanotubes as Electrodes in MEA***Di-Jia Liu; Argonne National Laboratory***Brief Summary of Project**

The objective of this project is to develop a novel aligned carbon nanotube-based membrane electrode assembly and fuel cell with 1) improved efficiency; 2) reduced Pt usage; and 3) simplified stack design. Argonne National Laboratory prepared and characterized the structure and activity of two transition metal-functionalized and one Pt-decorated aligned carbon nanotube samples as electrode catalysts. A transfer method to apply the aligned carbon nanotube layer to the membrane electrolyte with nanotube orientation intact was also developed. The catalyzed aligned carbon nanotube-based membrane electrode assembly with intact carbon nanotube alignment was fabricated.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.0** for its relevance to DOE objectives.

- The approach does not appear to offer a solution to carbon corrosion or Pt nanoparticle dissolution, the two main electrode durability issues.
- Methods of manufacturing and catalyzing the carbon nanotubes will prevent reduction of cost significantly.
- The project appears to be focused on meeting the DOE targets for electrocatalyst platinum loading and durability using a novel aligned carbon nanotube-based membrane electrode assembly.
- Durable, low cost, high performance fuel cell membrane electrode assemblies address many relevant targets.
- If the project works, there will be a contribution to the DOE objectives on cost, since plate forming should be reduced and the gas diffusion layer eliminated.
- Considerable development is likely needed before DOE objectives on performance and durability are achieved.

**Question 2: Approach to performing the research and development**

This project was rated **2.7** on its approach.

- Approach has many or all the disadvantages of carbon black supports.
- There is no expected advantage of surface area or specific activity over standard Pt/C supports.
- The concept of using oriented nanotube supports to improve mass transport is incorrect. The alignment is secondary by far to the length and spacing of the support rods. The porosity of the layer is what matters and that does not require alignment of the rods to make high porosity.
- Improved conductivity of the supports is not required for improved fuel cell performance.
- The high temperature and chemical vapor deposition processes for growing and catalyzing the aligned carbon nanotubes will be very difficult to scale up cost-effectively for anything other than small batch samples.
- The high surface area of the aligned carbon nanotubes is wasted since the catalyst particles are isolated far from one another.
- The approach is adequate to accomplish the project's objectives.
- Figuring how to utilize carbon nanotubes in fuel cell electrodes is a worthy effort.
- The original approach to eliminate gas diffusion layers and allow a flat plate was promising, but this has been somewhat foiled by cell architecture issues. Tests are now run with gas diffusion layers and flow fields.

- Investigators have been diligent in developing various methods of creating Pt/aligned carbon nanotube materials. It would be interesting to see if a more "3M-like" technique could be attempted, but it would be understandable if the hydrophobicity of the aligned carbon nanotubes was a problem.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.3** based on accomplishments.

- Principal investigator has spent its efforts on developing methods for growing and catalyzing the aligned carbon nanotubes, and has not had time yet to seriously evaluate whether the approach can help overcome the DOE barriers A, B, and C it claims to address.
- The benchmark membrane electrode assemblies used to compare their performance are very sub-standard and not representative of state-of-the-art performance.
- The investigators should be trying to make fundamental measurements of the catalyst surface area and specific activity under H<sub>2</sub>/O<sub>2</sub> at 900 mV using the DOE/General Motors recommended protocols.
- Trying to make membrane electrode assemblies is premature until they can show even one single kinetic improvement or durability improvement of their catalysts.
- The project team has made good progress toward achieving its objectives.
- Growing carbon nanotubes is a well-known process. Some success in making electrodes was apparent. However, there was no demonstrated performance improvement. Other attributes would have been lower cost or enhanced durability. However no data was presented to support those goals.
- Performance test with 0.6 mg Pt/cm<sup>2</sup> loading has shown a similar IR-corrected result to a BASF benchmark.
- More appropriate benchmark would aid the presentation of the work.
- Considerable progress has been made in optimizing dispersion and testing different means of fabrication. Further optimization could be considered in terms of placing more Pt near the triple-phase boundary.
- Mass activities are an order-of-magnitude lower than DOE objectives.
- Non-Pt work demonstrates low open-circuit voltages.
- Investigators' pursuit of single cell test was an excellent response to prior feedback.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.0** for technology transfer and collaboration.

- What collaboration has been identified is attributed to helping train the sponsoring organization investigators.
- A technology transfer process has not been enumerated, and there are no industrial collaborators.
- This is a carbon nanotube activity, and there are many experts in this area who could add real value.
- Low amount of collaboration indicated, besides initial consulting with Plug Power and training by Los Alamos National Laboratory.
- Lack of collaboration has not caused egregious mistakes, however, collaboration with a partner like 3M would help explore if there is any possibility of increasing at least the specific activity via vacuum techniques (other than those already attempted here), or increasing the electrochemically active area, which is low.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.6** for proposed future work.

- The investigators should focus more on making fundamental rotating disk electrode measurements, getting advice from Nenad Markovic's team on how to do this, before trying to make and test membrane electrode assemblies. If they cannot achieve the expected gains in activity or durability under potentiostat cyclic-voltammetry cycling, they should not go on.
- The proposed future work is likely to be effective in improving the technology.
- Need for further optimization of catalyst synthesis.
- Need for further optimization of cell design.
- No mention is made of non-Pt work.
- Project needs to get back to investigating whether the gas diffusion layer can be eliminated.

**Strengths and weaknesses****Strengths**

- Strength and experience of the Argonne National Laboratory staff.
- A novel approach is pursued to improve electrocatalyst durability and platinum loading.
- Significant progress has been made toward meeting the DOE targets.
- Of innovative stack concepts that DOE has funded, this concept has the best chance to be amenable to automotive operation.
- Original premise could create considerable cost benefits if realized.
- Good approach to catalyst synthesis and optimization.

**Weaknesses**

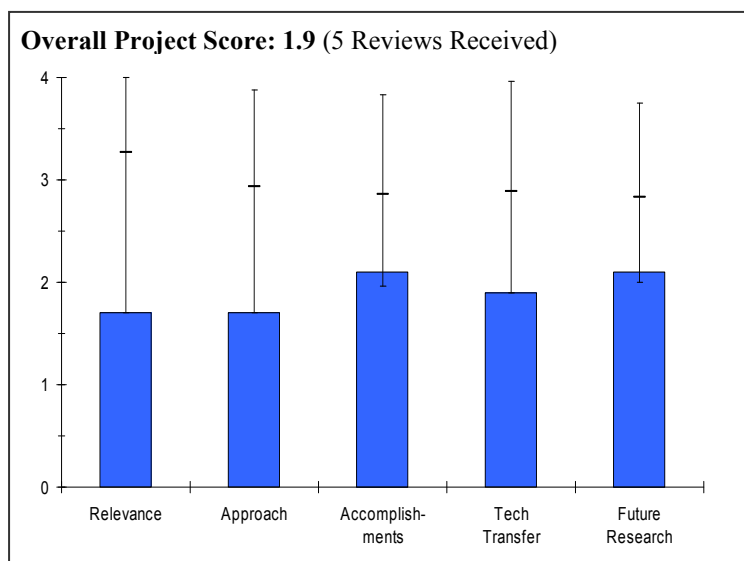
- Concept is flawed that this approach will help overcome any of the three barriers claimed.
- Well-known now to original equipment manufacturers that graphitic-type carbons do not have adequate corrosion resistance.
- There are no industrial collaborators to facilitate technology transfer.
- Much of the activity to date was test sample preparation. There also needs to be considerable focus on sample testing, because it is likely that procedures for "standard" membrane electrode assembly might miss details when testing this new form of electrode. For example, if durability is the real goal, then accelerated durability testing needs to be done, with less regard for voltage performance. Argonne National Laboratory needs to think about how to reach their goals.
- Compromise forced on gas diffusion layer and flowfield presence to facilitate testing, leaving issues about pressure drop and flow fields embedded in the nanotubes largely unexplored.
- More comparable benchmark membrane electrode assembly should be shown.
- Low mass activity and low electrochemically active area.
- Catalyst utilization is likely low.

**Specific recommendations and additions or deletions to the work scope**

- The Argonne National Laboratory investigators' time and resources would be better spent working on some other fundamentally critical problem.
- Involve one or more industrial collaborators to facilitate easier technology transfer.
- The testing procedures for new fuel cell membrane electrode assemblies need to be written and enforced. We need to get away from showing just one or two "best" results but show results from a group of carefully controlled duplicated samples, and then talk about statistical data analysis before comparisons are made.
- Non-Pt work is not successful and distracts from the main goals of this project. It should be deleted.
- Attempts to test without gas diffusion layers or flow fields should be given higher priority. Given that cost objectives will not likely be realized through catalyst reduction, these kinds of tasks may still be able to deliver towards DOE cost objectives.

**Project # FC-49: Detection of Trace Platinum Group Metal Element Particulates with Laser Spectroscopy***Stuart Snyder; Montana State***Brief Summary of Project**

The objectives of this project are to 1) develop laser-induced breakdown spectroscopy to detect and quantify the presence of PGM nanoparticles in very dilute aqueous suspensions; and 2) apply laser-induced breakdown spectroscopy to determine the presence and mass concentration of PGM in water reformed in the stack of polymer electrolyte membrane fuel cells. The presence of nanoparticles of PGMs in this water is an indication of polymer electrolyte membrane fuel cell degradation. This work supports the polymer electrolyte membrane fuel cell field trials conducted at Montana State University-Billings to test and characterize the durability of polymer electrolyte membranes.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **1.7** for its relevance to DOE objectives.

- There is a need to understand degradation in polymer electrolyte membrane fuel cells, however, there is no indication that Pt is dissolving and leaving the fuel cell.
- It could be useful for researchers to know whether Pt nanoparticles are being emitted by the cell as opposed to Pt in solution.
- Relevance is not clear from the presentation.
- Detecting nanoparticles in stack product water does not help enable the President's Hydrogen Fuel Initiative – this has not been seen as a problem.
- Not clear how this technique contributes further to understanding degradation in fuel cells. Metal species are detected, but with little additional insight to previous effluent analyses.
- This program could be potentially relevant to overall DOE objectives if only pure precious metals will be used as cathode/anode catalysts in polymer electrolyte membrane fuel cell. Giving that the activity of pure noble metals is not high enough to meet the DOE activity goals on the cathode side ( $720 \mu\text{A}/\text{cm}^2$  and  $0.44 \text{ A}/\text{mg Pt}$ ) and that bi/multi-metallic systems have much more potential to be used as cathode materials, it would be desirable to develop methodology how to detect both precious and non-precious metals.

**Question 2: Approach to performing the research and development**

This project was rated **1.7** on its approach.

- The approach as stated is misguided. Pt does undergo dissolution in an operating polymer electrolyte membrane fuel cell. However, it re-precipitates within the cell or stack. This process is local (i.e., within the membrane electrode assembly) and the Pt never leaves that environment. There is no opportunity to see Pt in the produced fuel cell water. Even if Pt were in the water it would be in the ppb range.
- Work to date for nearly 2 years has focused on palladium.
- If the issue is platinum in the cathode exit water, then project should be refocused to establish platinum detection.

- The presentation does not adequately discuss the correlation between amount of PGM detected in the cathode exhaust water and membrane electrode assembly degradation.
- The approach seems reasonable enough if you accept the premise that measuring trace PGM levels in water is of value.
- This project adds no unique capability to fuel cell degradation analyses.
- The program should be improved to have impact on the DOE mission. It is surprising that a calibration method is developed first for Pd, which most likely will never be used as the oxygen reduction catalyst.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.1** based on accomplishments.

- Work to date is on Pd. Palladium is not a typical catalyst in a polymer electrolyte membrane fuel cell. Studies should be one Pt and Pt-metal binaries only.
- Individual tests are not as important as long-term continuous testing to see the impact of duty cycle on dissolution of Pt and/or to see if the catalyst ions are in the water all the time.
- The technique has been demonstrated with palladium.
- Work with platinum does not seem to have been done yet.
- The principal investigator has shown that Pd can be detected with this technique.
- Project succeeds in detecting palladium, but there is no demonstrated added value over previous analytical techniques.
- The authors demonstrated that the laser-induced breakdown spectroscopy method is capable for *in situ* monitoring a relatively small amount of Pd and that provides on-site support of polymer electrolyte membrane fuel cell field degradation studies.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **1.9** for technology transfer and collaboration.

- Collaborations should be expanded to other fuel cell original equipment manufacturers and tests should be run on automotive duty cycles.
- Plug Power is a team member, but its role is not clear.
- Technique has been applied on Plug Power unit.
- Connection to partner goals not effectively demonstrated.
- This is a weak part of this program and the authors must have much closer contact with the groups that are focusing on the design stable and active catalysts.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.1** for proposed future work.

- Appears to be one-year project.
- Future work limited.
- Beginning work with platinum is long overdue.
- Principal investigator plans to calibrate device for Pt detection too.
- There does not seem to be a path forward to make the process viable.
- Much more effort should be on detecting Pt during extended operation. The program must focus on the development of detection of trace amount of alloying components (usually 3d elements).

### **Strengths and weaknesses**

#### Strengths

- Novel in-field technique could be feasible.
- Detection of palladium was accomplished.

- This is an innovative method that might be useful in replacing classical analytical tools for detecting small amounts of metals in very dilute aqueous suspensions. Even more importantly, an *in situ* method can provide valuable information in real-time operation.

#### Weaknesses

- Project very limited in scope.
- Project evaluating incorrect fuel cell electrocatalysts.
- Project has not proven that Pt can be detected or that Pt passes out of the fuel cell during operation.
- There is no evidence this technique is needed for fuel cell systems or explanation how the results for the analysis would be used.
- Technique is not truly an in-line test, samples must be taken from system.
- No specific advantage was demonstrated.
- The project is providing only partial information about total degradation of cathode/anode materials (a lot of materials can be trapped in the membrane); and as such it is difficult to justify how relevant the program is.

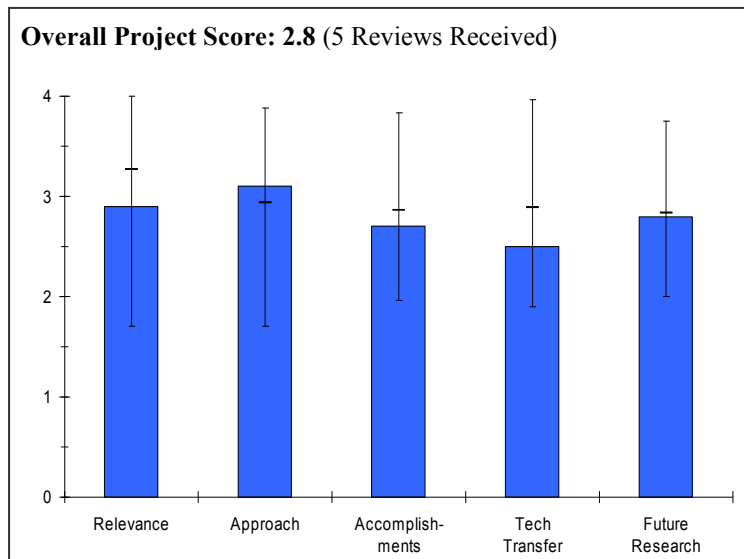
#### Specific recommendations and additions or deletions to the work scope

- Project could use expanded collaborations with catalyst developers.
- Project should also evaluate effect of automotive duty cycle on catalyst dissolution.
- Need to prove that Pd/Pt loss to fuel cell water is a problem before continuing project.
- Not clear where project fits in with fuel cell research needs.
- The program should be extended, and the method must be applicable or the detection of non-noble metals as well.



**Project # FCP-01: Light-Weight, Low Cost PEM Fuel Cell Stacks***Jesse Wainright; Case Western Reserve University***Brief Summary of Project**

The objectives of this project are to 1) demonstrate edge collected stack design capable of >1 kW/kg (system level); 2) develop low cost, injection molded stack components; 3) verify stack performance under adiabatic conditions; and 4) accelerate stack development by incorporation of multiple cell level sensors within the stack coupled with computation fluid dynamics modeling. A combination of molded plastic components and direct fabrication via printing will be used to yield a stack with a very low parts count.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.9** for its relevance to DOE objectives.

- This project addresses a fuel cell design approach with potential for portable power-type applications.
- Very good – this is a novel cell design. This would certainly work with low power, low voltage applications. Has any thought gone into scale up for large stack power/voltage applications?
- New stack concepts are relevant and although some advances are interesting, the potential to displace current configurations is low.
- The value in the program is in the new concepts that will emerge coupled with the modeling results for edge collection.
- New polymer electrolyte membrane fuel cell/stack designs that increase stack power density and decrease part counts can potentially enable this technology. This particular design has issues with achieving the same areal power densities observed with conventional designs.
- The proposed cell/stack design has several issues that make it not applicable to the automotive application, which is the main thrust of the DOE program.
- Innovative cell stack designs might lead to lower costs and higher performance.

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- Approach based on a unique design that should be low-cost and amenable to high-volume, straightforward manufacturing.
- The primary technical challenge is to obtain performance comparable to conventional designs. Early single-cell testing is marginal, however design refinements and improvements may result in enhanced performance.
- Very good – this approach appears to leverage the printed circuit board industry technology. It unclear how reactants are supplied.
- The actual approach is good, especially the modeling. The team needs to continue in the mode to assess fluid dynamics and thermal management.
- The overall approach, which includes modeling, cell and "stack" part development, and testing is a good approach.
- This innovative end-connected design could result in lower costs and higher performance, but the results remain to be seen.

- The approach is both innovative and methodical, encouraging that the prototype will be indicative of an implemented design.
- Stack design appears to be something that can be manufactured and fabricated – no show-stoppers.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- Progress has been relatively slow due, in part, to staffing problem, which the principal investigator stated are now resolved.
- There is much work left to be done and the ultimate success of this project is still in the balance.
- Very good – performance is reasonable compared to conventional polymer electrolyte membrane units.
- The results are interesting and may yield direction towards new cell designs, in particular the in-plane thermal and electrical mechanisms as a function of current density, connectivity, area, and gas fluid dynamics (all relating to performance and fuel utilization).
- Due to difficulties with staffing, this project has been significantly delayed.
- Little progress in the first year and a half of this project, but a no-cost extension has been requested.
- Some prototype components have been fabricated as exemplars.
- No stack has been assembled, as yet.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.5** for technology transfer and collaboration.

- Good collaboration with Endura Plastics to make the molded plastic parts.
- Specific contributions of plastics molding firm were not identified (may just be a supplier).
- Good – collaboration is limited for applied science, but adequate for basic science. Collaborating partners would suggest applications.
- Appropriate for this stage of the program.
- Need an interaction with a cell / stack developer.
- This partnership is an industry / university collaboration.
- More stakeholder collaboration could be an improvement.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- Future plans are not specifically identified, but the task statement indicates the work remaining to be done.
- Very good – future research includes scale-up.
- This reviewer feels the engineering elements of the concept should be focused on more than the actual success of the stack builds. The principal investigator should work on very small systems of a couple to a few cells, and then assess and evaluate the key attributes of such cells.
- There are significant remaining barriers in increasing the achievable current density with this design.
- Without knowing the source of the very low current densities resulting from the use of diagnostic techniques, it is difficult to know what path to pursue toward improving the current densities.
- Stack assembly and testing is yet to come and is needed to illustrate the value of the design.

### **Strengths and weaknesses**

#### Strengths

- Unique design approach.
- Investigator appears to be thinking outside of the box.
- The principal investigator is a solid contributor.
- Uniqueness.

## FUEL CELLS

- Innovative approach.
- Good engineering.
- Methodical progress.

### Weaknesses

- High risk project, but potential high payoff if successful.
- Unclear as to the final power class ( $x < 1$  kW,  $1 < x < 20$  kW, or  $x > 20$  kW).
- Unclear as to the voltage class (i.e., target number of cells in a stack).
- No mention of durability testing.
- Very academic in approach from a practical applied engineering perspective.
- The principal investigator did not present a clear vision on how to achieve the necessary current densities.
- No stack or sub-stack as yet – single cell only.

### Specific recommendations and additions or deletions to the work scope

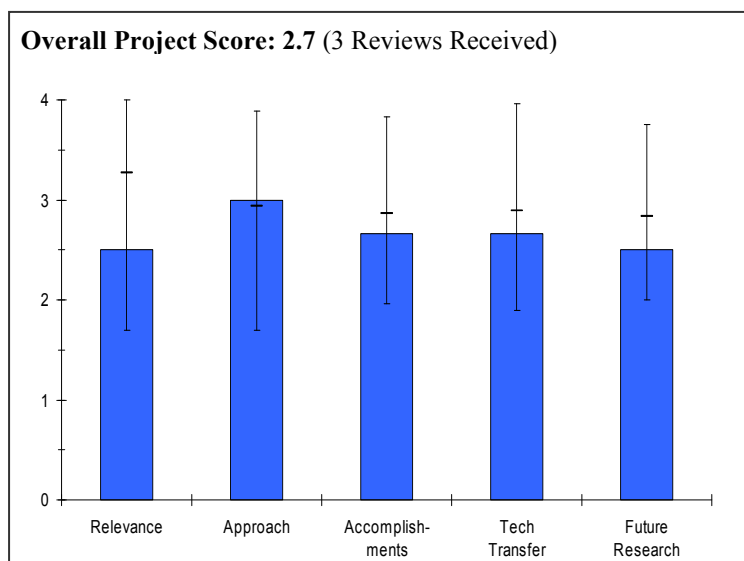
- If weaknesses are addressed a fuel cell manufacturer might have serious interest in the resulting technology.
- Additional research team members might accelerate the project.

## Project # FCP-02: Platinum Group Metal Recycling Technology Development

Larry Shore; BASF

### Brief Summary of Project

The objectives of this project are to 1) determine commercial practicality of cryo-grinding membrane electrode assemblies and the utility of the process for varied membrane electrode assembly architecture and materials; 2) define unit operations for Pt recovery from membrane electrode assemblies, integrate them into a process flow diagram, and estimate process economics; 3) identify apparatus/materials of construction for a pilot plant (1 kg/day) and full-size (1,000 tonne/year) operation; and 4) develop a rapid process control method to determine Pt remaining in leached membrane electrode assembly residues. Pt recovery of >98% is achievable from milled membrane electrode assemblies using an oxidative leaching process. The process has been shown to work with all types of membrane electrode assemblies and electrocatalyst compositions.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **2.5** for its relevance to DOE objectives.

- Platinum recovery from a variety of fuel cell types will be necessary to ensure economical supply.
- Recycling of the precious metals is very important, but the reviewer questions whether it needs government funding.
- Pt recycling has already been demonstrated to be economically viable – DOE should reduce funding effort on these projects because the industry will drive higher yields and efficiencies once the market becomes a large enough player.

### Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Approach avoids solvents and has little waste. The method is applicable to many types of catalyst coated membrane and diffusion media catalysts. Slide 15 presents some issues with larger batch sizes, and it is unclear why the ratio of surfactant to sample was changed.
- Approach appears very viable and should prove to be financially attractive.
- It is doubtful that cryogenic approaches will ever be cost-effective.
- It is doubtful that the principal investigator will combine many of the washing/ leaching, etc., steps into one unit and still achieve high yields and efficiencies.

### Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- Procedure has been developed to a high level of Pt recovery. Cost analysis should be presented in some form, even though the details are proprietary.
- Accomplishments are impressive; however, the expenditure required to get there seems high.

- It is highly doubtful that BASF will achieve a single apparatus for leaching, filtering, washing, neutralization and solids drying to simplify the process.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.7** for technology transfer and collaboration.

- Samples were obtained from many sources, although the work seems to be in-house.
- Collaborations are limited due to proprietary issues.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.5** for proposed future work.

- Goals are reasonable for a project that is ending in March 2009; cost models should be released.
- Priority should be given to the cost analysis, which is on the list of future work.

**Strengths and weaknesses**

Strengths

- Platinum is recovered with high yield, and the process produces little waste.
- Research has been successful.

Weaknesses

- Economic viability was not specifically demonstrated.

**Specific recommendations and additions or deletions to the work scope**

- Complete the cost analysis and document the results.

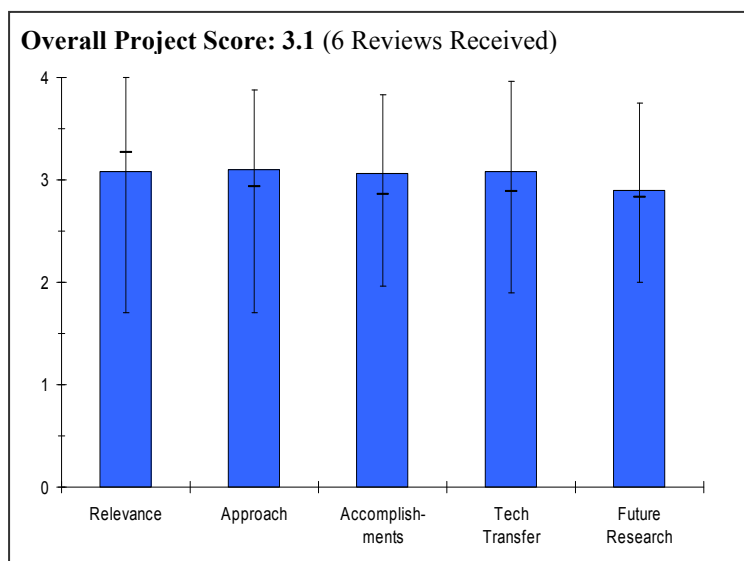
### Project # FCP-03: Platinum Recycling Technology Development

*Stephen Grot; Ion Power, Inc.*

#### **Brief Summary of Project**

The objectives of this project are to 1) assist the Department of Energy to demonstrate a cost effective and environmentally friendly recovery and re-use technology for PGM containing materials used in fuel cell systems; and 2) use new processes that can also separate and recover valuable ionomer materials. Recovery and separation work at scale-up has been demonstrated and good recovery rates are being achieved. The recovered polymer can be remanufactured into fuel cell membranes. The effective removal of trace amounts of PGM from diffusion media needs more development.

#### **Question 1: Relevance to overall DOE objectives**



This project earned a score of **3.1** for its relevance to DOE objectives.

- Recycling addresses issues with cost and availability of Pt.
- 100% fit to general goals.
- Catalyst recycling will be driven by the economic interests of the recycler. Funding this work may not have an impact on that.
- The ability to recycle Pt and ionomer, as well as the ability to fabricate stacks with recycled materials, will be market-driven and should not be a topic for government research.
- There are no clear DOE objectives regarding how much cost savings should be realized with recycling.
- Platinum recovery is key to the future of polymer electrolyte fuel cells.

#### **Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- Approach to recycle Nafion as well as the Pt is a good idea and will reduce impact of fuel cells on the environment and improve economics.
- Good approach; however, reference membrane electrode assembly tests are not up to date: 300 mA/cm<sup>2</sup> @ 0.7 Volts is not the correct measure.
- The principal investigator needs to show that use of the recovered, degraded membrane does not compromise durability through lifetime tests and fluoride release rate measurements.
- Approach to recycle Nafion as well as the Pt is a good idea and will reduce impact of fuel cells on the environment and improve economics.
- Methodology for cost analysis for recycling process was not shown. Directed Technologies, Inc and TIAX use rigorous analyses for their cost estimates. The same discipline should be applied here.
- Given project assignment, approach to fabricate stack from recycled materials is interesting. Good comparison to look at recycled catalyst and ionomer individually.
- Good thought to compare oxygen reduction reaction for fresh catalyst to recycled catalyst.
- Process seems to be relatively inexpensive.
- Ionomer recovery in parallel to platinum is attractive.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- Demonstrated recycled Nafion quality by making a refurbished membrane electrode assembly with it and showed good performance and durability of the membrane electrode assembly.
- Demonstrated remanufactured membrane electrode assemblies in a 5-kW stack, remanufactured membrane with new catalysts that perform as well as a new membrane and catalyst – recycled catalysts have lower activity.
- Need more work to recover Pt from gas diffusion layer.
- Cost analysis completed.
- Good results with a good portion of common sense, i.e., simply recover the noble metal but not the catalyst and use the electrolyte elsewhere.
- In addition to recovering Pt and ionomer, catalyst support is recovered and reused. This degraded material may be the reason for the observed low performance and may not be a viable approach. What about just recovering the PGM?
- Oxygen reduction reaction curves are very different from those presented in catalyst projects. Protocol not described as to whether the current/voltage sweep was done *in situ* or *ex situ*, or if *ex situ*, whether it involved a rotating disk electrode. Experiments should have been done by those familiar with electrocatalytic techniques.
- Reasons not shown for decreased performance for recycled catalyst in the GENCORE stack. No failure analysis reported.
- Previously reported Pt recovery of 96% requires batch operations and, therefore, some labor intensity.
- Procedure works well for recovering Nafion.
- Precise analysis of PGM recovery is not provided.
- Evaluation of Pt activity is confusing as the mass activity is stated to be "good," but the performance per surface area looks poor and the cells made with the recovered catalyst perform poorly.
- Additional processing of Pt appears necessary.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- Plug Power participation was key to the project.
- Convincing consortium.
- It is a benefit that the program involves membrane electrode assembly manufacturers and system integrators.
- Long list of competent collaborators assembled.
- Degree of coordination unknown.
- Plug Power task is clear. Other collaborator contributions are unclear, besides those that are material inputs.
- Role of external partners unclear; work seems to focus on Ion Power technology alone.
- Oxygen reduction reaction activity data from the university partner are low quality.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- Project is scheduled to be completed in August.
- The project is 90% complete, but rather than focusing the remaining time on recovering the PGMs from the diffusion media, the principal investigator should try to show that the recovered catalyst can be used without performance loss.
- Short note given on removing Pt from diffusion media.
- Despite short remaining duration of project, no notes were provided as to what could be done to enhance recycling process to decrease cost / increase volume.
- No plan was given to address how recycled Pt activity could be improved.
- The goal of increasing PGM recovery from diffusion media is reasonable for project that is ending in August 2008.

**Strengths and weaknesses**Strengths

- During the past year, a clear approach was adopted to fabricate a stack from recycled components and test it.
- Appropriate comparisons were made in the course of assembling recycled test articles.
- Ionomer is recovered completely and can be used in a fuel cell.
- Process is cheap relative to the PGM cost.

Weaknesses

- Cost analysis given without detail.
- Failure analysis for low catalyst activity in both *ex situ* and GENCORE was not performed.
- Original recycling process does not appear applicable to high volume.
- In general, low amount of information shown for the different tasks in the project.
- Topic matter will be addressed by market economy.
- PGM recovery process seems incomplete.
- Cost analysis for ionomer recovery versus production needs to be addressed.

**Specific recommendations and additions or deletions to the work scope**

- Pt recycling efforts from DOE should be suspended due to Pt prices and expectation of market-driven incentives to recycle Pt.
- Deeper disclosure of experimental information and parameters.
- Greater focus on improving recycling process and cost analysis.
- Low oxygen reduction reaction activity of recovered Pt should be elucidated.

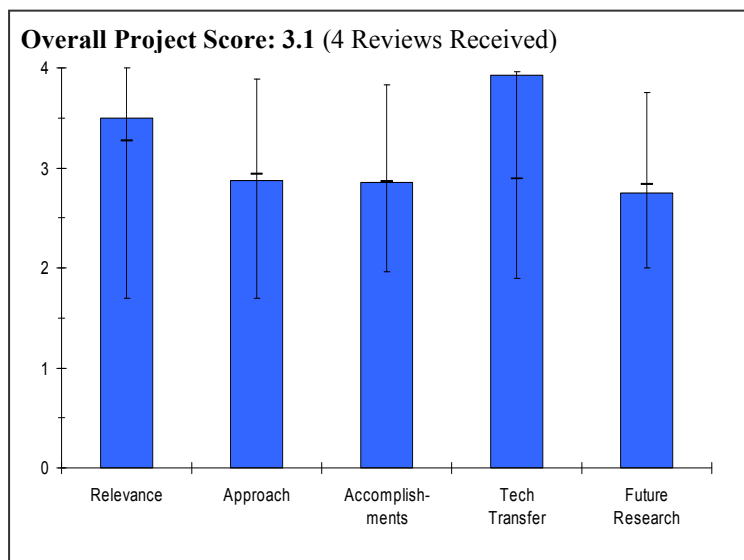


**Project # FCP-04: Component Benchmarking Subtask Reported: USFCC Durability Protocols and Technically-Assisted Industrial and University Partners**

*Tommy Rockward; Los Alamos National Laboratory*

**Brief Summary of Project**

This project provides Los Alamos National Laboratory technical assistance to fuel cell component and system developers as directed by the Department of Energy (DOE). This project is expected to include testing of materials and participation in the further development and validation of single-cell test protocols with the U.S. Fuel Cell Council. This project also covers technical assistance to the U.S. Council for Automotive Research (USCAR) and the USCAR/DOE Freedom Cooperative Automotive Research (FreedomCAR) Fuel Cell Technology Team. This latter assistance includes making technical experts available as questions arise, focused single cell testing to support the development of targets and test protocols, and regular participation in working and review meetings.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- Component Benchmarking is important.
- Component benchmarking critical to the President's Hydrogen Fuel Initiative.
- Important to understanding of water transport and freezing in membrane. Understanding the relative protocol results is also valuable though has less impact on actual progress.
- Project provides assistance to other highly relevant projects for DOE objectives.
- Examples such as water transport studies on 3M's nanostructured thin film electrode, conductivity measurements under freeze conditions, and capability to conduct the FreedomCAR durability protocols all prove relevance.

**Question 2: Approach to performing the research and development**

This project was rated **2.9** on its approach.

- Sharing technical assistance is of importance, but there is no focus on the approach.
- Develop standard testing protocols.
- OK though not highly precise in isolating water content in membrane or certain in identifying meaning and source of changes in conduction of protons to membrane temperature.
- Approach is to assist fuel cell component developers, to establish baselines for durability protocols, to compare durability protocols from other international organizations, and to determine whether US Fuel Cell Council protocols are appropriate, all of which are needed.
- Limited space for presenting data here, so questions remain as to how water content was evaluated in conductivity under freeze studies, or to what extent alternating current impedance or other techniques could have been used to break down voltage losses during protocol comparisons.
- Unknown if study of Cabot supports is with reference to alloy catalyst. If so, that can be valuable.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.9** based on accomplishments.

- If interactions are the figure of merit, then a lot has occurred. Evaluating how much technology transfer has occurred is difficult.
- Developed a number of useful testing protocols.
- Moderate progress. What is done is valuable but relative to budget, progress as presented seemed fair but not exceptional.
- Water results are in good agreement with others results, but not ground-breaking.
- Correlation of protocols is useful.
- For this project, a considerable amount of work likely happens that cannot be reported here.
- Slides show that the project is likely helpful to developers. It is impossible from what is shown here to evaluate whether the 3M water transport assistance has been thorough in looking at different cell configurations, sensitivity to cell thermal characteristics, sensitivity to different gas diffusion layer parameters, or sensitivity to cell design (channel width, transition regions, etc.).
- The work done to critically examine the US Fuel Cell Council cycling protocol is excellent. This is the kind of feedback required to be sure the correct protocols are written.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.9** for technology transfer and collaboration.

- Since the subtask reported, US Fuel Cell Council Durability Protocols and Technical-Assistance to Industrial and University Partners, is one of tech transfer and collaborations, a high score is merited.
- Excellent interactions with all major players.
- Excellent by design.
- This project is entirely built on collaborative efforts.
- Collaborations exist with membrane electrode assembly suppliers, such as 3M, as well as other government entities.
- Los Alamos National Laboratory is being useful in facilitating National Institute of Standards and Technology neutron imaging studies on behalf of developers.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- There is no proposed future research?
- Not clear what will be done in future, however task should continue.
- Probably flexible and that may be as it should be.
- Although not clearly stated in the same manner as other projects, the future work does appear to be appropriate.
- Project is intent on continuing support of industrial collaborators.
- Project is focused on continuing critical examination of established durability protocols, and for those protocols that are valid, establishing baselines for known material sets.

**Strengths and weaknesses****Strengths**

- Assistance is being provided.
- Connectivity to other groups, dissemination of information.
- Utility in providing assistance to developers.
- Examination of protocols. Investigators do not make the assumption that US Fuel Cell Council protocols or those from other sources are appropriate.

- Ability to set baselines assists most projects funded by the DOE by providing a comparison at the membrane-electrode assembly level.
- Safety standards are set that can be useful to other laboratories, even those with experience with hydrogen.

### Weaknesses

- Difficult to evaluate how effective is the assistance.
- Cost effectiveness and depth of analysis.
- In the specifics of some of the collaborations, it is difficult to assess whether experimental techniques are thorough. Most of the work is likely represented in reports from other projects.

### **Specific recommendations and additions or deletions to the work scope**

- This category is difficult to evaluate for this project, since the resource allocation between tasks is not clearly represented.
- Without knowing the weighting of different budget items, perhaps more resources should go towards evaluating protocols and serving as a common experimental source for FreedomCAR durability testing than towards the hosting of workshops. Again, though, without knowing how much is devoted to each task, it is unfair to comment further.

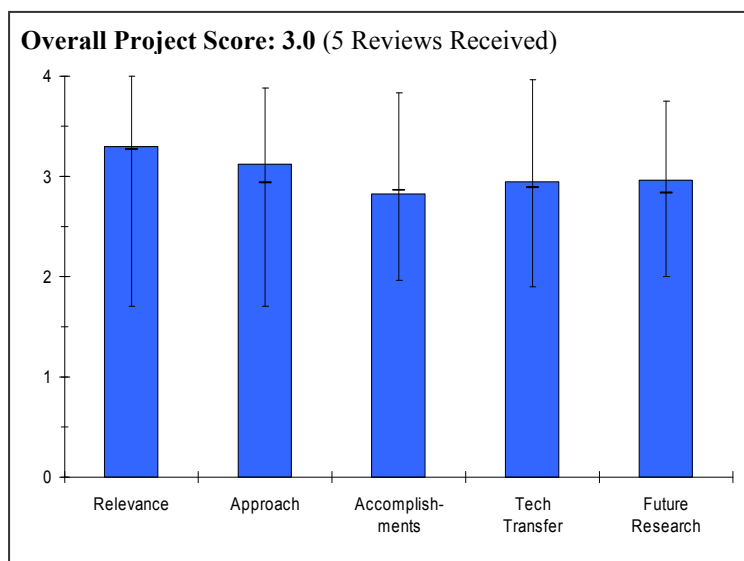
## Project # FCP-05: Low Cost, Durable Seals For PEM Fuel Cells

Jason Parsons; UTC Power

### Brief Summary of Project

The objective of this project is to develop advanced, low cost, durable seal materials and sealing techniques amenable to high volume manufacture of polymer electrolyte membrane stacks. The project goals are to 1) improve mechanical and chemical stability of seals to achieve 40,000 hours of useful operating life; and 2) obtain a material cost equivalent to or less than the cost of high performance silicones in common use. Material properties meet most ultimate program goals – FCS2 is expected to meet all program goals.

### Question 1: Relevance to overall DOE objectives



This project earned a score of **3.3** for its relevance to DOE objectives.

- Supports DOE targets, goals, and objectives.
- Durability – Improve mechanical and chemical stability of seals to achieve 40,000 h of useful operating life (stationary fuel cell target; 5000 hrs with cycling is transportation target).
- Low cost, efficient and durable seals are important to the overall objectives of commercializing fuel cells.
- Funding level may be excessive for narrow scope of topic.
- Very few materials seem to have been considered.
- Very relevant project.
- Seal materials are a long neglected part of the DOE fuel cell subprogram.
- Seals contribute directly to fuel cell durability, both with respect to the durability of seals themselves, but also in how they interact with other components, particularly membranes.
- Although the seal design itself may fall into the domain of original equipment manufacturer development, there is very necessary materials development that needs to be done since silicone seals have known failure modes.

### Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Approach is sound and logical to complete objectives.
- The fundamental materials approach and testing methods developed for the program are well suited for the evaluation of the seal materials for applicability to the fuel cell.
- Some addition of longer-term fuel cell testing and testing of the seals in conjunction with fuel cell membranes may be needed.
- Given the limited number of materials tested, it seems that the testing should have been advanced to the in-cell level within a year.
- Approach is very good. All the engineering steps that are needed are being taken. The weakness of the project is that the supplier of the seals is not sharing the chemical details of what is in the seal material. This makes it hard to do durability studies. This issue should be resolved.
- The *ex situ* testing accounts for tensile strength, compression set, and rupture under different environments (air and humidity).
- In general, looking for more durable materials, but with the same manufacturing ease as silicone, is the right idea.

- It would be preferable for a test looking for migration of organics to have different levels of humidity.
- Work should include *in situ* testing that seeks to examine failure of the seal under reductive / oxidative conditions, as well as failure of the membrane as a consequence of interaction with seal.
- Resistance test would also be useful. This can be done by molding the seal onto a gas diffusion layer / polymer electrolyte membrane / gas diffusion layer sandwich and then checking that resistance is sufficiently high.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- Good progress has been made.
- Initial data from short-term aging and testing is encouraging. Both FCS0 and FCS1 meet or exceed all minimum program goals. Both also meet or exceed most of the ultimate program goals. FCS1 shows notable improvements in elongation and cure temperature.
- The seal materials address the key barriers.
- Additional testing in fuel cell environment with wet/dry cycling and polymer electrolyte membrane materials would be beneficial to ensure the applicability of the materials.
- The team has addressed key concerns of leaching of impurities, reaction or changes in the materials in contact with various fuel cell impurities.
- Long-term degradation tests have not yet been performed incorporating all aspects of operating fuel cell stacks. Such tests should be completed as soon as possible to validate the material downselection. The progress would be easier to evaluate if data were presented versus the original materials used.
- Very good progress but lifetime predictions are a worry. Pinhole failure or tearing is a big issue.
- Of the three materials of interest to the program, results have been reported for only one – FCS0.
- FCS0 results only cover a part of the *ex situ* battery of tests.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.9** for technology transfer and collaboration.

- Collaboration is strong and effective. UTC Power is a leader in research and collaboration.
- The team has the skills necessary to develop and characterize the seals for fuel cell environments.
- The team has participants who can commercialize the technology.
- Interactions with other institutions not specifically highlighted.
- The fact that the supplier is not sharing the formulation details with the customer is unacceptable for such a program.
- Collaboration scheme is rigorously thought out.
- Each collaborator has a definite set role in the project.
- Of all projects at the review, the collaboration strategy is best mapped out in this presentation.
- The proprietary nature of Henkel's material formulations is a disadvantage.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- Excellent. FCS2 expected to meet all program goals. First full-size parts expected by end of Q1FY09.
- The future plans for continued testing and validation of the material are appropriate next steps.
- The authors indicate the need for in-cell testing, and that should be the main goal for such a limited-term project at the halfway point.
- Future plans include accelerated durability testing. The need for formulation details is critical here.
- There should be more *in situ* testing.
- Any *in situ* testing would be welcome, whether a large cell or a small cell.
- There is not enough time to go beyond standard seal testing to genuinely capture the effects of fuel cell environments and membrane electrode assembly interactions.

**Strengths and weaknesses****Strengths**

- Strong team with good expertise in fuel cells and adhesive and seal materials.
- Candidates for the seals seem to have been identified.
- Excellent engineering/testing results in good progress.
- Clear motivation from the start: a seal that processes like silicone, but is more durable than silicone. This is one of the few projects that can be clearly stated in one sentence.
- Well-organized collaboration.
- Good sense of which *ex situ* measurements to use.
- It is the only project in the DOE fuel cell subprogram that is investigating a very critical area.

**Weaknesses**

- Some more fuel cell testing of the materials to ensure applicability would be useful.
- The number of materials screened is limited, and either there should have been more materials investigated or more progress on the few investigated.
- The lack of information on the seal material formulation is unacceptable because accelerated durability testing cannot be performed without this information.
- Need a chemist on the program.
- Lack of *in situ* experimentation.
- Some time appeared to have been spent developing techniques, which probably should have mostly existed before beginning the program.
- Time is now running short for going beyond what was planned.
- Original test plan may not have accounted for resistance failures and seal interaction with polymer electrolyte membrane/gas diffusion layer failures.

**Specific recommendations and additions or deletions to the work scope**

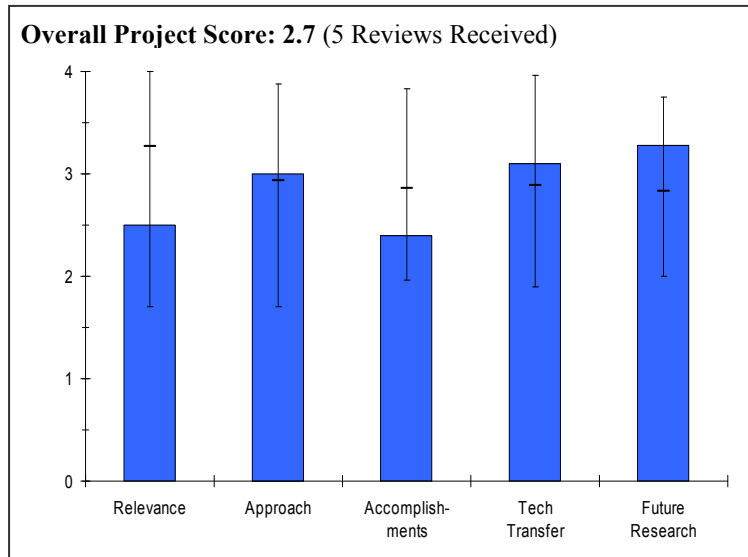
- Funding level seems high for so few materials examined, especially since the materials are based on existing formulations.
- *In situ* testing for polymer electrolyte membrane failure due to interactions as well as failure of the seal itself.
- Resistance testing with gas diffusion layer / polymer electrolyte membrane / gas diffusion layer sandwich.

**Project # FCP-08: Research & Development for Off-Road Fuel Cell Applications**

*Richard Lawrence; Idatech*

**Brief Summary of Project**

The objectives of this project are to 1) have Toro measure loads and report vehicle modifications and specifications; 2) report on shock and vibration profiles and lifetime; 3) complete shock and vibration of fuel cell system; 4) have Donaldson measure contaminants and develop air filter; 5) install a polymer electrolyte membrane liquid fueled system in a golf course maintenance vehicle. The critical assumptions for this project are that the fuel cell system can 1) physically fit into the vehicle; 2) can provide the required energy during field testing and 3) function under applications' shock and vibration loads. Potential solutions include 1) modifying the vehicle; 2) improving controls and response; and 3) incorporating shock and vibration test results.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.5** for its relevance to DOE objectives.

- The value in this effort – especially taking an electric vehicle and converting it to a fuel cell-powered one, will facilitate how such technology will be practical for such mobile devices, especially with liquid fuels.
- Funding is appropriate, but should not be at the expense of other critical technical issues.
- Demonstration of fuel cell stacks in a near-term application allow assessment of readiness levels and can potentially provide important feedback to the materials development projects within DOE.
- This project addresses air filtration and shock and vibration issues of fuel cells operating in off road applications.
- Golf carts are not the most robust off road application possible. It is unclear that the lessons learned on the golf carts will be adequate to address the more robust applications.
- The project relates to DOE objectives, however fits more under the Technology Validation subprogram.
- Good niche market.
- Although the DOE program has moved away from liquid fuel reforming, in a niche market this may be a better fit, and stack experience can support the program.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- The approach is practical and simple so as to minimize complexity.
- The team appears to be using standard off-the shelf components – but with their integration engineering.
- Practical application with respect to the mode of transportation and the fact that real units will be built and tested.
- The principal investigator is well established as one who can develop such practical applications.
- Quantifiable goals for the air quality and shock and vibration barriers would help in the progress assessment.
- The dynamometer and shock and vibration testing will provide valuable data on real-world operation of small-scale (2-3 kW) fuel cells for small off-road vehicle applications.

- Use of the fuel cell vehicle in a real-world golf course maintenance application could produce users that are comfortable with fuel cells, which may translate to an expanded early adopter market for fuel cell highway transportation vehicles.
- Good engineering.
- Good project plan.
- Good coordination with vehicle manufacturer.
- Better coordination with users might be helpful.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.4** based on accomplishments.

- It looks as if good progress has been made even with the limited funding – this is due to the expertise of the principal investigator.
- Some data would be helpful, in particular the vibration data and air filtering, to name a couple.
- No data or information is provided on the air filter development.
- How did IdaTech conclude that compressed hydrogen is unacceptable for maintenance vehicles?
- Insufficient information is provided to assess the progress in modifying the fuel cell systems.
- The project team has completed packaging of the fuel cell for the golf course vehicle.
- Dynamometer and shock and vibration testing should commence shortly to provide data.
- Much of the progress in developing the fuel cell and installing it in a golf cart has been accomplished through leveraging with project partners rather than with DOE funding.
- No final hardware yet.
- Concept is good, but implementation remains to be seen.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- The team seems to be collaborating well.
- Current source and properties of air filter should be described.
- Current and future role of Toro, if any, should be described.
- The project partners have enabled progress in securing a vehicle, designing an air filter, and providing shock and vibration profiles.
- Project partners with more robust off-road applications for the fuel cell should be considered.
- Good coordination with vehicle manufacturer.
- Project appears to be based on sound principles of user preferences, but other stakeholders, such as property owners, could be a valuable addition to the team.
- While the concept appears to be marketable, user, and property owner feedback will be vital to confirm this.
- Adding users and property owners to the project would be an enhancement.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.3** for proposed future work.

- The future proposed testing and development looks appropriate based on the objectives of the program.
- This reviewer would like to see more of the performance characteristics and the process layout/controls.
- Plan to complete the project is plausible
- A description of the planned shock and vibration testing would have been helpful.
- Testing on dynamometer and in real-world application will provide valuable data on the operation and additional research needs for fuel cells in off-road applications.
- Deployment of hardware is vital to accomplishment of the goals.
- Acceptance by the team and users and property owners remains to be seen.



### **Strengths and weaknesses**

#### Strengths

- Lawrance is a very credible engineer, especially for applications like this one.
- Demonstration for near-term application of transportation fuel cells.
- This project has leveraged the project partners to extend the value of the DOE funding.
- A fuel cell has been installed in a golf cart vehicle and is ready for real-world testing.
- Manufacturer input and feedback.
- Solid design.
- Good niche market.
- High value application.

#### Weaknesses

- Limited funding.
- Weak presentation.
- The golf cart application may not provide sufficient data to produce a fuel cell that can be used in more robust off-road applications. Golf courses are usually paved; thus, dust and shock and vibration issues may not be adequately assessed on golf courses.
- No working hardware yet.
- No users or property owners on the project team.

### **Specific recommendations and additions or deletions to the work scope**

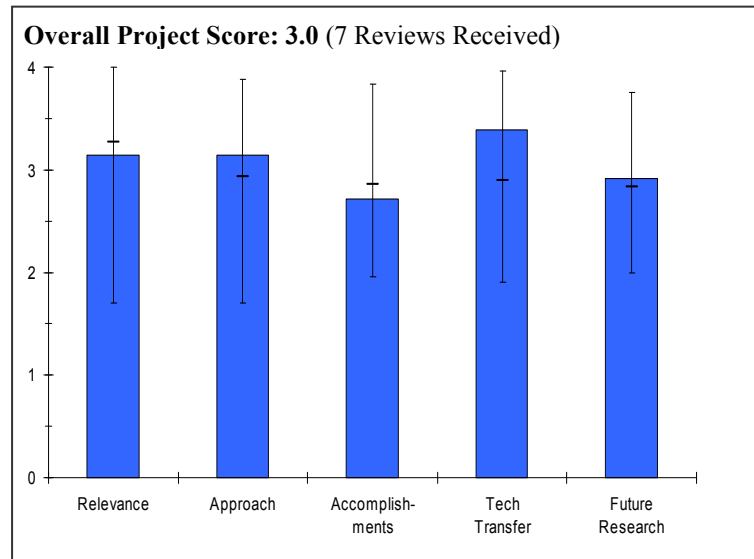
- Show more of the system layout and controls and lessons learned going forward.
- Perform efficiency comparison and cost/benefit analysis of the fuel cell powered vehicle versus the standard Toro Workman e2065 vehicle.
- Quantify barriers and results.
- Include partners with more robust off-road applications for the fuel cell vehicle.
- Include testing of the air filtration system.
- Reviewer suggests to moving this project to the Technology Validation subprogram.
- Add landscape managers, workers and decision makers to the team.
- Add property owners and decision makers to the team.

## Project # FCP-09: Market Opportunity Assessment for Direct Hydrogen PEM Fuel Cells in Pre-automotive Markets

*Kathya Mahadevan; Battelle*

### **Brief Summary of Project**

The overall objective for this project is to assist the Department of Energy in developing fuel cell systems by analyzing the technical, economic, and market drivers of polymer electrolyte membrane fuel cell adoption. The objectives of 2007 include 1) economic analysis of near-term markets in the federal and portable market sector; and 2) state and local agencies of emergency response market engagement. This includes 1) development of a candidate user database; 2) market engagement through targeted e-mailing of educational material and by facilitating teleconferences on polymer electrolyte membrane fuel cell applications and installations; and 3) conference presentation at venues frequented by the user community.



### **Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.1** for its relevance to DOE objectives.

- This project presents a survey of potential first-user applications among Federal government users.
- While the topic itself is relevant, the presentation did not fully assess market opportunities or production potential. As presented, the project only partially supports DOE goals and the President's Hydrogen Fuel Initiative.
- Relevant to the DOE program objectives.
- The general methodology and results to date are highly valuable in helping DOE provide relevant market signals to industry.
- Well-rounded approach to early market assessment that supports fuel cell market development.
- This project strongly supports the Hydrogen Fuel Initiative and the objectives of the Multi-Year RD&D Plan.
- It is evident that the first market opportunities for polymer electrolyte membrane fuel cells will be niche scenarios with less demanding cost and durability requirements than automotive applications. It is important to seek out and crack these opportunities while technology progresses on the challenges facing broader applications for fuel cells, due to the need to keep the supplier base engaged and in the game.
- Market analysis is essential in defining technical goals and 2012 targets.

### **Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- The comparison of first-use fuel cell applications with conventional, traditional power sources is interesting, but the approach does not present a compelling argument for a transition to fuel cell technology. Perhaps the problem is that the argument for the Federal government to lead a transition to fuel cells is more qualitative than quantitative.

- The presentation did not include any real breakthrough findings. During the course of its work, Battelle sought information from federal agencies but does not appear to have built on the data they were provided by otherwise preoccupied program managers, project members, and others.
- Market analysis techniques appear to be robust and thorough.
- The principal investigator used a multifaceted approach in identifying markets in two of the main early areas for polymer electrolyte membrane fuel cells. There are other early, small format markets as well, and using this approach will be very valuable.
- Primary research, particularly contact with potential users, is critical to understanding market needs.
- Stack life as a proxy for reliability may not be sufficient in early years of market development. System reliability, particularly for early systems, is a function of more than just stack life.
- Use of levelized hydrogen cost could downplay the impact of fueling infrastructure capital costs on decision processes for forklift applications.
- Approach is logical and well implemented following classical market analysis and early adopter conventions.
- In discussions with the principal investigator, it became evident that not a lot of follow up with respect to the earlier phases of this project (which focused on commercial niches as opposed to Federal and portable power) had been conducted. In other words, the project would benefit by fully understanding the results from the past with regards to fuel cell adoption in the commercial sector. Reconnecting with the decision makers in the commercial market that were previously identified as attractive opportunities by Battelle could help guide future project activities.
- To encourage adoption, there would be value in further support in the areas that have been identified as attractive near- and mid-term opportunities for polymer electrolyte membrane fuel cells. Even if the economics and technical attributes are there for specific applications, adoption of a new technology often requires considerable extra support and follow up.
- Another promising strategy for the future may be to facilitate the establishment of demonstrations for the applications that have been identified as most economically attractive.
- Approach is sound and logical. Methodology includes: market segmentation and identification of near-term applications; characterization of markets; identification of market and user requirements; selection of likely near-term markets using rating criteria; identification of lifecycle cost data for incumbent and polymer electrolyte membrane fuel cell technologies; and market penetration modeling and opportunity analysis.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- The progress this year in this project appears to be fairly limited – a lot of effort has been expended in this project but the results thus far could be considered obvious to an informed audience. Perhaps the value of this project is the addition of statistical confirmation.
- There was no apparent breakthrough to provide possible paths forward for hydrogen and fuel cells. While using extensive efforts to locate and survey activities, the project can leave a reviewer wondering just how in depth the collaboration really was.
- Analysis of the market opportunities that were identified in the project objectives have been completed.
- The results of the study can influence or at least validate some of the decisions on market positioning taken by the fuel cell developers.
- The methodology (slide 5) provides a good algorithm for industry to relate their capabilities and motivations into a plan for product development. Of particular note is the use of a Bass model in the market penetration step and judgment in the market opportunity analysis.
- The life cycle assessment for the Federal and portable power applications represent important groundwork for further work in aiding fuel cells to intelligently grow in the marketplace.
- Of particular note is the important message (slide 17) to DOE and the industry of the critical need for reliability data for the Federal Aviation Administration market segment. There are other market segments that need that as well.

- The project is addressing the barrier of early market identification, though it is difficult to ascertain overall progress against plan for this five-year project.
- The project has identified several areas in the Federal sector and portable power where polymer electrolyte membrane fuel cells can make a strong business case. Areas for further improvement including reliability have been identified.
- The business case for these areas has been elucidated laying the groundwork for further market adoption activities.
- Solid, consistent technical results and presentation therein.
- Good progress. Completed analysis of federal markets – October 2007; submitted draft reports. Completed analysis of portable markets. Conducted two state and local emergency response stakeholder teleconferences.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.4** for technology transfer and collaboration.

- Many participants have contributed input and information to the survey activity.
- While using extensive efforts to locate and survey activities, the project can leave a reviewer wondering just how in depth the collaboration really was.
- Collaboration took the form of extensive interviews with fuel cell developers and potential customers of the technology.
- The principal investigator collaborated well with US Fuel Cell Council in polling the industry for information.
- Excellent use of outside resources.
- There has obviously been extensive contact with potential adopters of the technology in the Federal and portable power markets, however there has been little collaboration with other firms specializing in market analyses and transformation. Other firms experience might have provided additional insight with regards to market opportunities and next steps to further facilitate adoption.
- Besides the National Renewable Energy Laboratory, there has been no other overt collaboration with national labs nor universities
- Collaboration is strong and effective. Demonstrated ability to gather and analyze information.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- Future plans appear to be reasonable to complete the project.
- As presented, the project could have focused more on the real challenges to market potential rather than an almost-cursory survey.
- Project is wrapping up and the objectives have been met.
- Fuel cells applications in wastewater treatment does represent a future market, but there are other similar niches that may be better to apply this effort towards.
- The project is winding down; therefore the proposed future work seems in line with the time remaining.
- Proposed future research for polymer electrolyte membrane fuel cells in wastewater treatment and data center markets makes sense. Combined heat and power in some applications may make sense and data center markets are highly attractive but do require extreme reliability.
- Would recommend that if this project or a similar one continues in the future that increased effort be placed not only on identifying other new market opportunities, but maximizing success in the ones already identified. Working closely hand and hand with potential adopters to tip the scales and achieve successful adoptions.
- Principal investigator needs to complete market opportunity assessments for fuel cells in wastewater treatment and data center markets. Suggest inclusion of biofuel opportunities. Also similar study should be done for small solid oxide fuel cell.

### **Strengths and weaknesses**

#### Strengths

- Despite a limited presence within and with Federal and other hydrogen and fuel cell programs, Battelle provided a well-organized and well-prepared document even though the discussion of market opportunities could have been improved.
- The study was very thorough.
- The principal investigator has a solid foundation for market analysis, and a detailed understanding of fuel cell market issues.
- Over all, this reviewer (with 14 years of fuel cell market entry analysis) thinks that this was an impressive effort.
- The project is well conceived and executed with good use of potential customers and industry participants.
- Very relevant to the Hydrogen Fuel Initiative and needs to breach the market for polymer electrolyte membrane fuel cells.
- Solid, methodical analysis that has done a good job identifying attractive opportunities and laying out business cases.

#### Weaknesses

- For a reviewer somewhat familiar with ongoing federal H<sub>2</sub> / fuel cell programs, the project offered little new knowledge, at best.
- It would be valuable to make this model generalized and available to users; the sooner the better.
- Hydrogen cost treatment could underestimate the impact of fueling infrastructure capital costs on decision process for forklift applications.
- Should incorporate other firms with market analysis and transformation expertise to enhance effectiveness.
- Develop deeper relationships with key decision makers in the areas of identified opportunities.

### **Specific recommendations and additions or deletions to the work scope**

- Project results would have been improved if the project had assessed or included unique strategies to advance implementation including the use of tax incentives or other early adapter strategy potential.
- It would be useful to extend this work to activities that can enable very small fuel cells in applications that translate to retail market space.
- Should go deeper in the future as opposed to broader and try to achieve some real market adoption successes with entities already showing interest in polymer electrolyte membrane fuel cells.
- Similar study should be done for small solid oxide fuel cells.

**2008**  
**Technology Validation**  
**Summary of Annual Merit Review Technology Validation Subprogram**

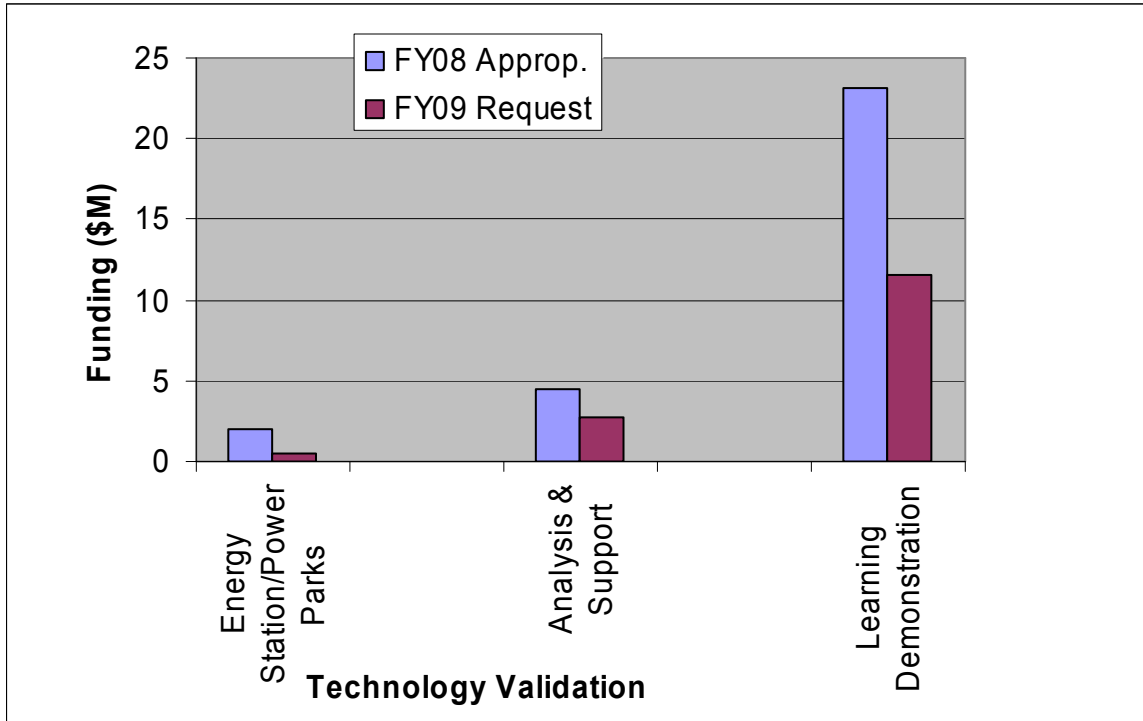
**Summary of Reviewer Comments on Technology Validation Subprogram:**

Reviewers consider the learning demonstration project to be a key element in determining whether the program's hydrogen and fuel cell activities are on course to achieve established research and development targets. In addition, acquiring "real world" operational data and experience is vital to making appropriate adjustments to the hydrogen program's research and development projects. Infrastructure demonstration elements provide hydrogen and validate fueling technology performance. There has been good progress in opening stations and putting vehicles on the road. Significant vehicle miles and hours are being accumulated on the vehicles in the learning demonstration. Codes and standards work is a very important aspect of technology validation and educational outreach to the public is an enhancement to the learning demonstration.

Reviewers thought that generation 2 vehicles have taken longer to deploy than the schedule might support and that the schedule should be analyzed. Insufficient effort is being made to maximize loading of hydrogen stations. However, an integrated electricity and hydrogen production facility is an innovative concept and promises to encourage the use of hydrogen fueling stations even when the vehicle usage might be low, at the start of deployment.

**Technology Validation Funding by Technology:**

The funding portfolio for Technology Validation stresses the continuation of the 6 year Learning Demonstration project as it enters its fifth year. Second generation vehicles will continue to be operated and data collection next year will provide information on meeting 2009 fuel cell durability and vehicle range targets. A high temperature fuel cell energy station will be funded and constructed in 2009 followed by a 6 month demonstration of the system. The FY2009 funding profile is subject to Congressional Appropriations. In FY 2009 the Technology Validation Activity is being transferred to the Vehicle Technology Program from the Hydrogen Program.



**Majority of Reviewer Comments and Recommendations:**

The Reviewer scores for the Technology Validation Subprogram were a maximum of 3.7, minimum of 2.5 with an average score of 3.2. The major recommendations by reviewers are presented below for each of the task areas. DOE will act on reviewer recommendations as appropriate for the overall Hydrogen Technology Validation effort.

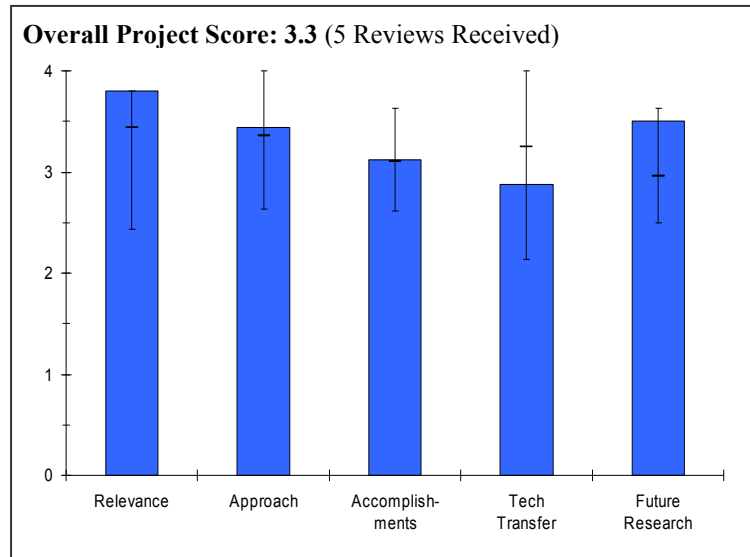
- **Learning Demonstrations** – The project is an important effort to demonstrate the feasibility of fuel cell vehicles and hydrogen infrastructure. Technology Validation project teams should work together on ways to take advantage of the technology validation infrastructure investments after the projects are completed.
- **Energy Stations** – The integrated electricity and hydrogen production facility is an innovative concept and allows the use of hydrogen fueling stations even when the vehicle usage might be low, at the start of deployment.
- **Storage** – The project focuses on one of the Department of Energy's key objectives which is to improve on-board hydrogen storage options available to the OEMs. Storage system should be better packaged in the vehicle so they do not intrude into passenger and cargo area.
- **Analyses** – These projects are vital to determining whether the Program's hydrogen and fuel cell activities are on course to achieve established research and development targets.

**Project # TV-01: Hydrogen to the Highways***Ron Grasman; DaimlerChrysler***Brief Summary of Project**

The main focus of the on-going Department of Energy (DOE) Fleet Validation and Demonstration Project is to collect data and evaluate the technology status of: fuel cell-powered vehicles (original equipment manufacturers) and hydrogen infrastructure (energy companies and suppliers); and validate DOE 2009 performance targets including 250-mile vehicle range, 2,000-hour fuel cell durability, \$3.00/gasoline gallon equivalent production cost.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.8** for its relevance to DOE objectives.



- This project is a key element in determining whether the program's hydrogen and fuel cell activities are on course to achieve established research and development targets.
- Acquiring "real world" operational data and experience is vital to making appropriate adjustments to the hydrogen program's research and development project mix and specific projects.
- This project is generating significant operational data.
- Project addresses Department of Energy needs and barriers in a general manner.
- Hard to evaluate the technical side of this from the presentation.
- This kind of information is critical to guide the more technical Research part of the program.
- Validation of hydrogen fuel cell vehicles in real world condition is clearly relevant to DOE objectives.
- This project is to drive and document progress in the next generation of fuel cell vehicles.
- Demonstration vehicles are critical for advancement of the technology.
- Deployment to varying climate areas is a good enhancement.

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- The primary element of a multi-dimensional approach is operation of Generation I and II hydrogen-fueled vehicles, with collection of detailed data sufficient to enable monitoring of performance relative to program targets.
- Infrastructure demonstration elements provide hydrogen and validate fueling technology performance.
- Safety initiatives have a high priority.
- Public education and awareness are also built into the project's activities.
- The point was made that detailed data are being generated for corporate use, in addition to that being provided to the National Renewable Energy Laboratory.
- This is not research, rather it is technical and product evaluation/marketing.
- The approach to the work appears adequate although there does not seem to be any major focuses on stressing systems to failure. This would be very useful from a safety point of view.
- Real world data acquisition is clearly the right way to validate hydrogen fuel cell vehicles, although it is unclear from the report what data is being collected.
- Codes and standards work is a very important aspect of technology validation.
- Good coordination with first-responders, including a fire vehicle.



## TECHNOLOGY VALIDATION

- Public and educational outreach is an enhancement.
- Standards efforts are good.
- Government fleets might be an improvement.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- An impressive listing of accomplishments was presented.
- Accomplishments include upgrading of the Gen-I fuel tank system to 70 MPa, and optimization of the vehicle software algorithm.
- Extensive support has been provided for safety codes and standards activities involving standards development and other organizations.
- The project's safety initiatives include "table top" crisis management exercises.
- Outreach and media events were detailed in the presentation.
- Since this project is not really research, this is an unfair assessment. The technical barriers are indistinct. However, the barriers to be overcome are the accumulation of product information to guide future research investment. The approach could be harsher, that is running the systems closer to performance limits could accelerate gathering of failure information that would be useful.
- Optimized software to improve fuel efficiency. This is why this project is important.
- 70 MPa storage on the vehicle.
- Codes and standards documentation, such as the best practices manual, is an important output of this program.
- Project was conducted in a safe manner, without incident.
- Vehicle numbers have met goals.
- Vehicle fueling stations are being open to support planned deployments.
- HAZOP approach is exemplary.
- It seems like the Generation II vehicles should have been deployed already. The schedule should be analyzed.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.9** for technology transfer and collaboration.

- The project team is fully engaged with many organizations addressing safety, and codes and standards, issues.
- Significant partnering and collaboration with government agencies, the media, and other organizations have enhanced the quality and results of outreach and education activities.
- There was no elaboration on how the project's primary partners are coordinating their activities.
- Co-ordination comes from Daimler plus Chrysler— this is weak.
- Performance data submitted to NREL.
- Detroit Edison Energy, NextEnergy, BP provide fueling stations for project.
- The program has good coordination relationships with various agencies and companies. This is a strength.
- Additional use by government fleets might be an improvement.
- The program seems to take full credit for standards released by CSA, SAE, ASTM, ICC and the DOE program in general. Although support by Daimler and Chrysler is certainly a factor in the release of these standards, dozens, if not hundreds, of additional experts from other corporations and other agencies were involved in the release of these standards. Taking full credit seems to be overstating the contribution of the contract.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.5** for proposed future work.

- Plans for future work were well summarized and clearly presented.
- Not sure what Generation II vehicles and improvements are.
- Lifetime test of Generation II fuel cell on test bench.
- Generation I vehicles continued to be tested by customers.

- Internal testing of Generation II vehicles for durability under different climate conditions.
- Daimler will continue their vehicle testing program and their cooperation with NREL and the technical evaluation assigned to NREL.
- The build-up to the release of Generation II vehicles is perhaps slower than the schedule might have supported. The schedule should be analyzed.
- The future planning seems consistent with the tasks remaining to be accomplished.

### **Strengths and weaknesses**

#### Strengths

- Significant vehicle miles and hours are being accumulated.
- Generation II vehicles are showing promise of significant improvement. There seems to be good utilization of the experience and knowledge gained from operations earlier in the project.
- Safety and outreach activities are important elements of the project.
- Experience is being gained in dealing with a variety of infrastructure issues.
- Reasonable number of vehicles involved. More would be better.
- Demonstrating technology status, developing codes and standards documentation, public outreach.
- Generation I vehicles were out early and have led the deployments of others, showing commitment and optimistic deployment of the technology.
- Good coordination with user agencies and hydrogen suppliers.
- HAZOP analysis is exemplary.
- Coordinating refueling stations is exemplary.

#### Weaknesses

- Generation II improvements are vague.
- Failure scenarios not pushed.
- It seems that hydrogen storage and fuel cells are being fit into a traditional car. Any plans to design the car form specifically for the fuel cell and hydrogen storage?
- It is unclear whether cost is a consideration when implementing the fuel cell and storage system into the vehicle.
- Quantified performance results not shown.
- The project might have benefitted from additional government fleet use.
- The project tends to take credit for standards that required an entire industry to develop. This might be better clarified.
- Generation II vehicles have taken longer to deploy than the schedule might support. The schedule should be analyzed.

### **Specific recommendations and additions or deletions to the work scope**

- It was stated that a project extension through September 2010 is being considered. While no addition to the project scope is recommended at this time, it is appropriate for DOE, this project team, and the other technology validation project teams to work on ways to take advantage of the technology validation infrastructure investments after the projects are completed.
- Add more "push to failure" scenarios. Lifetime durability acceleration schemes.
- Show system weight and volume specifications compared with DOE targets.
- Adding vehicles to government fleets might be able to better demonstrate the technology to early adopter markets.
- Accelerating the deployment of Generation II vehicles would be encouraged to keep up the momentum demonstrated by DaimlerChrysler during the Generation I deployments.

**Project # TV-02: Hydrogen Fuel Cell Vehicle and Infrastructure Demonstration Program Review**

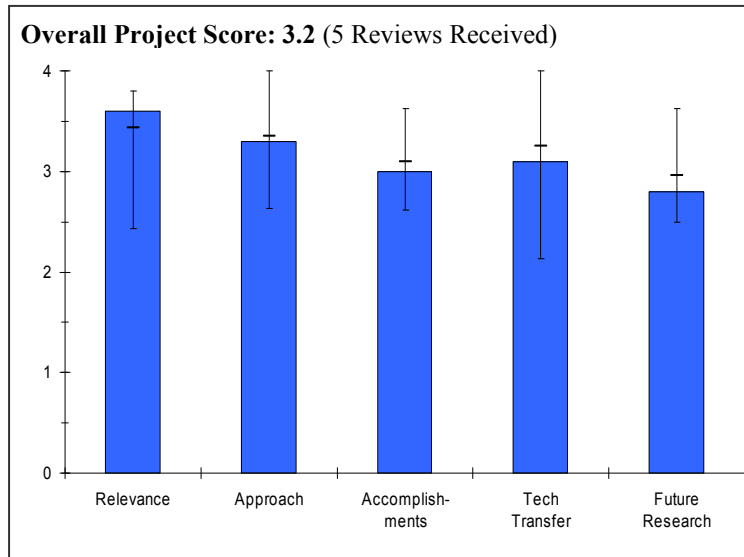
*Greg Frenette; Ford*

**Brief Summary of Project**

The objective of this project is to gain fuel cell vehicle operational data in differing climate conditions to direct and augment future design efforts. Objectives since the last review have been to 1) continue phase I vehicle operation; 2) report operational data; 3) maintain fleet; 4) survey customers; and 5) investigate updated concept vehicles and demonstration.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.6** for its relevance to DOE objectives.



- This project has direct relevance to the Department of Energy’s Multi-Year Program Plan and will help DOE achieve its goals.
- Based on National Strategic goals, the project supports National energy goals.
- The program appears to meet comprehensive hydrogen and fuel cell program goals including scope of deployment.
- It is extremely relevant to have major OEMs such as Ford involved in vehicle/infrastructure validation activities.
- Both the vehicle and infrastructure portions of the project predominantly support the Hydrogen Fuel Initiative and goals of the Multi-Year Program Plan.
- This project is relevant to the Hydrogen Fuel Initiative; however, its cost to DOE is very significant.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- Approach has not changed for both the vehicles and the infrastructure.
- The addition of a new location and a new hybrid vehicle are good additions and will enhance the approach.
- Applicant is clearly focused on overcoming technical barriers especially with respect to cold weather operations and onboard storage.
- There was very little discussion of teaming partners or expansion plans!
- Ford is providing vehicles and working with appropriate partners to provide potentially very valuable validation information. Unfortunately, very little detail was presented.
- Approach is conventional and targets principal barriers at the vehicle and infrastructure level.
- BP seems fully committed to safety of H<sub>2</sub> infrastructure.
- Number of vehicles involved (18) seems low for project of this magnitude. Unclear as to whether statistically valid sample sizes will be achieved.
- It is not overtly clear that strong efforts are being made to maximize the loading of the H<sub>2</sub> stations. No discussion of coordination with other entities to use these facilities for transportation (i.e. Hydrogen fueled internal combustion engine vehicles) or stationary H<sub>2</sub> applications.
- Approach used is as in similar tech validation projects; it has not changed since last year.
- Variation of geographic regions, in particular the latest addition of Iceland, is a plus.
- Impact of this project on advancing fuel cell technology for automotive applications is not obvious.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Added a 4th geographic region, Reykjavik, Iceland with a cooler climate. This will help analyze the fuel cells operation in a colder climate.
- Automated data collection takes into account the new HyWay 2/3 technology or next generation vehicle design.
- This project has many successes on the operation of the vehicle and supporting infrastructure.
- Flexible Series Hybrid data collection using the auxiliary power unit.
- Significant success on the infrastructure, i.e., Sacramento Municipal Utility District station.
- The applicant clearly presented that barriers existed but little was actually presented about scope of barriers or how they will be resolved.
- There was virtually no quantitative information presented so there is no way to determine the value of the efforts.
- It appears that relatively little effort went into developing the presentation.
- Information is high level making it difficult to fully assess technical progress. Side-by-side comparison of key project milestones and associated technical progress is not provided.
- Little data is provided on technical and cost targets achieved leading to questions with regards to transparency.
- Progress appears to have been made with respect to 700 bar refueling and storage systems and fuel cell stack beginning of life power requirements, sub freezing start-up, and lifetime.
- Project appears to be a continuation of previous effort, with relatively few modifications.
- Very little technical information makes accomplishments and progress difficult to judge independently, forcing reviewer to fully rely on rather general statements included in the presentation.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- This project has excellent collaboration with others.
- The project team was creative in its support for placing a vehicle in Iceland and mentioned that they had partners, but offered little discussion on the roles of those partners or whom their collaboration efforts were with.
- There appears to be excellent potential for collaborations, but there was little mention of actual interactions or information transfer except with energy partner, BP.
- Little mention of technology collaboration or transfer. Nature of project may preclude this at this point however it seems conceivable that collaboration with national laboratories/universities may facilitate solutions to stickier technical problems with regards to H<sub>2</sub> storage etc.
- Would be beneficial if information from this project could be shared with manufacturers of medium/heavy duty commercial vehicles such as buses. These applications are more likely in the near term and could benefit from lessons learned with H<sub>2</sub> light duty vehicles.
- Good collaboration with BP; role of other partners unclear.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- This project will redefine Phase II vehicle configurations and complete the 700 bar station.
- The presentation appeared thorough in its presentation of where Ford was and is, but appeared weak on future development and/or expansion plans.
- Even though little detail was given, the continuation of, and expansion of (with a new generation vehicle and 700 bar hydrogen), present efforts is very important.
- Plans exist for working toward near term commercialization opportunities for H<sub>2</sub> vehicles (curbside, people mover, etc.).

## TECHNOLOGY VALIDATION

- Further discussion indicated it is expected some of the refueling stations would remain operational after sunset of project, but no details were provided. Every effort should be made to keep all the refueling facilities open in some capacity even if their scope would require alteration.
- No major modifications to the project are anticipated.
- Little innovation.

### **Strengths and weaknesses**

#### Strengths

- Excellent management.
- Bringing a test vehicle to Iceland and obtaining DOE permission to locate a vehicle in Iceland goes a long way to further international deployment.
- Applicant's location of test sites across the nation, and in a variety of climates, is noteworthy.
- Ford and partners are major players with enormous combined capabilities.
- Addresses strong need for demonstration and evaluation information on H<sub>2</sub> vehicles and infrastructure.
- Convincing and thorough summary of "limiting issues."

#### Weaknesses

- None.
- The presentation did not adequately discuss their partners and the roles of those partners.
- There was no presentation on "What's next," specifically, how the program is to be developed from current state.
- The lack of detail in the presentation suggests the possibility that the project could have relatively low priority.
- Project seems somewhat stove piped and insular (Ford - vehicles, BP- H<sub>2</sub> fuel) with little outside collaboration or technology transfer.
- Given scope of project, number of vehicles and refueling stations seems limited.
- Insufficient effort is being made to innovatively maximize loading of H<sub>2</sub> stations.
- Below-target mileage accumulation is a drawback.
- There is little indication that this project will have an impact on overcoming challenges facing to fuel cell technology.
- Little technical content.
- Number of vehicles could be more in this project.

### **Specific recommendations and additions or deletions to the work scope**

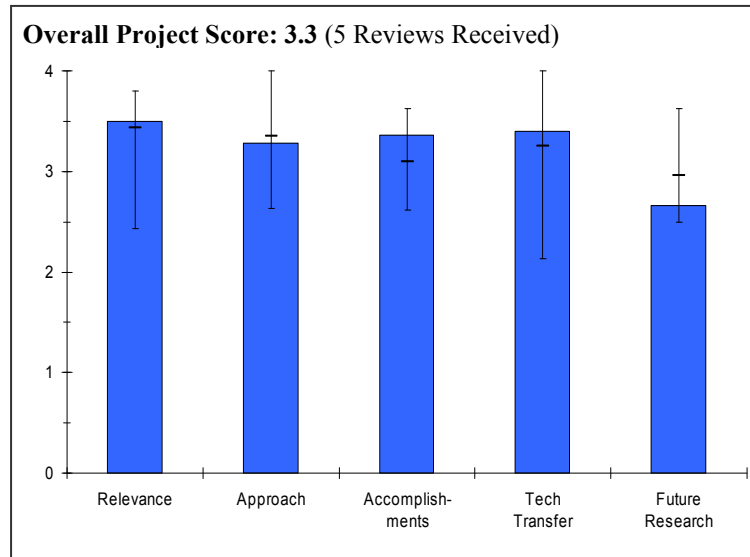
- Economic viability should be determined if possible for both vehicles and infrastructure.
- Develop the roles of your team members.
- Advise on the growth of the next step in deployment.
- Expand and enhance the technical discussion in the presentation.
- Include at least minimal quantitative information in future presentations.
- Propose specific approaches to identify some of the real-world adverse effects of normal operation.
- Fewer photos and more technical information would make this and similar technology validation presentations more useful to the community.

**Project # TV-03: Controlled Hydrogen Fleet and Infrastructure Demonstration and Validation Project***Dan Casey; Chevron***Brief Summary of Project**

Objectives for this project are to 1) demonstrate complete systems of integrated hydrogen fuel cell technologies for transportation and hydrogen infrastructure under real-world operating conditions; and 2) validate DOE 2009 performance targets including 250-mile vehicle range, 2,000-hour fuel cell durability, \$3.00/gasoline gallon equivalent production cost, and safe and convenient refueling by drivers.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.



- This project is a key element in determining whether the program's hydrogen and fuel cell activities are on course to achievement of established research and development targets.
- Acquiring "real world" operational data and experience is vital to making appropriate adjustments to the hydrogen program's research and development project mix and specific projects.
- This project is generating significant operational data.
- Addresses Department of Energy goals and objectives.
- The Department, in partnership with industry, is demonstrating contemporary fuel cell vehicle technology, and the hydrogen fuel infrastructure that supports those vehicles. This project is part of that activity.
- Refueling stations are essential to the program.
- Vehicle deployments are essential to the program.
- Hydrogen and electricity co-production is an innovative approach to meeting load factor needs of fueling stations.
- Like other similarly scoped technology validation projects in this group, this project is relevant to the hydrogen fuel initiative but does relatively little to identify major technical challenges still facing fuel cell technology.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- The slide addressing project approach was general and not particularly informative.
- Discussion of the approach by Mr. Casey was also brief and limited.
- Like to see some "push to failure" experiments - cold temperature examples given are good. Like to see more.
- Lessons learned from vehicle accident are examples of "push to failure" benefits. Try to design "accidents" into the project.
- Hydrogen and electricity co-production is an innovative approach to meeting load factor needs of early fueling stations.
- Including data from the Orlando station without cost to the DOE program is an enhancement.
- Diverse driving patterns are strengths.
- Relatively high number of tested vehicles is a plus; little technical information is a minus.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.4** based on accomplishments.

## TECHNOLOGY VALIDATION

- Year-to-year progress was shown for deployment of vehicles. 29 vehicles are now deployed.
- The data transfer and collection system has been upgraded, conveying impressive performance on this aspect of the project.
- Progress has been made on varied infrastructure development and utilization. Experience is being gained in dealing with multiple fueling station options and issues.
- Vehicles are being driven by a variety of operators, and used for a variety of purposes.
- Second generation vehicles have 700 bar tanks and supercapacitors for improved range and performance.
- Opened stations and vehicles are on the road. Significant progress.
- This is not research but product evaluation - good work in this respect.
- Good explanation of how the data is collected and analyzed by the Project and the National Renewable Energy Laboratory.
- Responded to reviewer comments from before re driver diversity.
- Explained Generation I to Generation II improvements.
- High pressure (700 bar) fueling hardware is being commissioned for the latest vehicles in the US fleet.
- Retraining of first-responders is a good improvement.
- Good analysis of "full fill" issue.
- Full deployment of vehicles and stations appears to be lagging behind what the schedule might have supported. The schedule should be analyzed.
- Interesting analysis of temperature effects during fueling.
- Technical progress difficult to assess due to very limited technical content of the presentation (not unusual for tech validation projects in general).

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.4** for technology transfer and collaboration.

- Work has been undertaken in collaboration with Gas Technology Institute on technology for co-production of hydrogen and electricity.
- Discussions are being undertaken with host sites about keeping fueling stations in operation after completion of the project.
- There was no discussion during the presentation about technology transfer initiatives, other than to point out that a case study had been done following a vehicle accident and that lessons learned from the project (e.g., station permitting and first responder re-training experience) was being communicated during the merit review.
- Seems to be adequate coordination between the partners and NREL.
- Chevron works with a group of excellent companies, a group of individuals who are operating, fueling, and evaluating the fuel cell vehicles. Chevron is also working with NREL, and with NREL's fuel cell vehicle testing program.
- Good coordination with other associations.
- Co-production of electricity and hydrogen is an innovation and inclusion is a strength.
- Strong partners with mutually complementary expertise.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.7** for proposed future work.

- There was minimal discussion of future work plans, focus and priorities.
- Future plans are not very exciting.
- The plan is to continue this activity until the next generation of fuel cell vehicles are thoroughly evaluated.
- Planning for future work appears to be limited. This is an area where additional effort might yield significant results.
- Continuation of the present effort; creativity & novelty are both missing.

**Strengths and weaknesses****Strengths**

- Significant vehicle miles and hours are being accumulated.
- The second generation of vehicles promises substantial improvement. There seems to be good utilization of the experience and knowledge gained from operations earlier in the project.
- Advancements in data gathering and transfer.
- Ability to work with host sites to install fueling stations with varied technologies, to provide a broad base of experience and information for comparison purposes.
- Good progress in opening stations and putting vehicles on the road.
- Lessons learned are good. Should be built upon.
- Good coordination.
- Electricity and hydrogen co-production.
- Almost all vehicles and stations have been deployed.
- Higher number of vehicles than in some other technology validation projects.

**Weaknesses**

- There is little evidence that education and outreach are important elements of this project.
- Other than brief discussion of a vehicle accident outcome, there was little or no mention of safety initiatives, activities, and contributions related to this project.
- Future plans are weak.
- Not all vehicles and stations have been deployed yet.
- Planning for future work seems to be lacking.
- Expensive. No obvious value to overcoming major technical challenges facing fuel cell power systems.

**Specific recommendations and additions or deletions to the work scope**

- While no addition to the project scope is recommended at this time, it is appropriate for DOE, this project team, and the other technology validation project teams to work together on ways to take advantage of the technology validation infrastructure investments after the projects are completed.
- Add future plans with more detail.
- It would be interesting to assign a test vehicle to a "car" magazine (such as Road and Track), and let a "wrench" (an automobile enthusiast) drive and write about one of the test vehicles.
- Additional planning for future work might yield significant results.



**Project # TV-04: Hydrogen Vehicle and Infrastructure Demonstration and Validation**

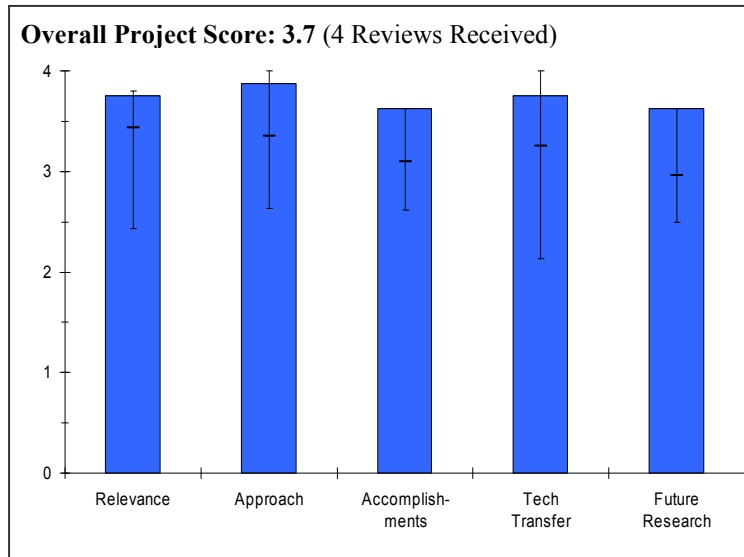
*Roz Sell; General Motors*

**Brief Summary of Project**

General Motors and energy partner Shell Hydrogen are deploying a system of hydrogen fuel cell electric vehicles integrated with a hydrogen refueling infrastructure to operate under real world conditions. The objectives of this project are to 1) demonstrate progressive generations of fuel cell system technology; 2) demonstrate multiple approaches to hydrogen generation and delivery for vehicle refueling; and 3) collect and report operating data.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.8** for its relevance to DOE objectives.



- The project expects to meet all of the Department of Energy goals in a timely manner.
- The DOE technical targets will remain the same in spite of the extension for this project.
- The project fully supports the President's Hydrogen Initiative and it is critical to the Hydrogen Initiative
- The General Motors project meets both technical and education goals.
- Very relevant to have major OEMs such as GM and appropriate partners involved in validation programs.
- This project strongly supports the Hydrogen Fuel Initiative and the technology validation aspects of the Multi-Year Program Plan for vehicle and infrastructure demonstration and evaluation.

**Question 2: Approach to performing the research and development**

This project was rated **3.9** on its approach.

- GM has extended this project in order to match DOE funding and to add second generation vehicles and increase the number of refueling stations.
- Phase 2 has started now with plans for 40 vehicles (Chevrolet Equinox).
- The General Motors program is working to address current and technical challenges, as well as the challenges to increasing fuel cell vehicle production.
- Both intent and execution of approach are excellent.
- The approach is well-developed, outlined, and targeted to barriers. Especially appealing is the fairly large number of vehicles (40) and refueling sites (5) being evaluated for DOE and attitude of open access where possible to the refueling sites.
- The project is also taking an aggressive posture with respect to vehicle demonstration and evaluation involving various government and private entities and citizens (Project Driveway), as well as public relations. The "driver relationship managers" is a proactive step to facilitate customers H<sub>2</sub> vehicle experience.
- The approach for H<sub>2</sub> station permitting is also strong emphasizing data collection and open access to a database of codes and standards, lessons learned, and processes to facilitate site permitting.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.6** based on accomplishments.

- This project successfully completed phase 1.
- Virgin Atlantic has partnered with GM to test vehicles at the Los Angeles airport.
- Commercial station with 700 bar refueling will be available this year at Benning road.
- Maintenance and training facilities are excellent additions to this project.
- They have purchased six 700 bar mobile refuelers to assist the customer on quick fills.
- The General Motor's presentation well-discussed fuel cell technical barriers, data collection, and ancillary technological requirements.
- General Motors has often raised concerns about hydrogen station quantity, location, and other concerns but they made clear that they are working to resolve.
- Overall the accomplishments are excellent and impressive. However, apparently relatively little was accomplished in the past year.
- Technical progress is somewhat more difficult to assess with respect to the vehicles due to the lack of a side-by-side comparison of targeted milestones and progress achieved.
- Progress is more clearly ascertained with respect to the fueling stations and appears to be on schedule.
- Overall, the task is making significant progress and is on schedule (or ahead) for completion.
- There is little mention of specific technical performance data (efficiency, life, cost, etc.).

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.8** for technology transfer and collaboration.

- Feedback from customers is essential.
- Infrastructure is essential and they need to collaborate with DOE to support this work.
- The presentation made it clear that General Motors greatly values all of its team members, partners, and customers.
- The General Motors team is demonstrating great creativity in bringing the technology to the public.
- From the presentation, it appears that collaborations and information transfers are excellent.
- Project has extensive list of partners especially with respect to the user demonstration component.
- There is no mention of outside collaboration with other projects or non-participating industrial or academic institutions.
- Project should in future consider technology transfer agreements with non competitive entities in the commercial heavy duty vehicle sector (i.e. buses).

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.6** for proposed future work.

- Deploy Phase 2 vehicles and inaugurate more stations.
- 700 bar fast-fill refueling is needed.
- GM is providing access for all automotive companies and their customers to this project's refueling stations.
- The presenter made it clear that General Motors current effort is built upon a large body of early work and that this current effort is the foundation for newer consumer products.
- Generally very good but no apparent plans to pursue any specific problem areas.
- Future work implies commitment to reaching the next level of hydrogen vehicle and refueling station deployment and utilization. No specific mention is made, however, of plans for hydrogen refueling facilities at the conclusion of project.
- Project is laying groundwork to significantly facilitate hydrogen refueling station permitting in the future.

#### **Strengths and weaknesses**

##### Strengths

- This project has excellent collaboration with other companies.
- Ms. Sell's presentation was very comprehensive and balanced.
- GM and partners represent a very formidable combined capability.

## TECHNOLOGY VALIDATION

- GM projects genuine enthusiasm for the project.
- Overall, relatively strong project clearly focused on technology validation barriers for H2 vehicles and refueling.
- Especially refreshing is the wide demonstration partner aspects of the project, public relations, and open mentality toward knowledge transfer on lessons learned and processes for hydrogen refueling codes and standards and permitting.

### Weaknesses

- None.
- The General Motors presentation was perfect until the slide that brought up ethanol.
- None of significance.
- No mention is made of near term commercial applications of hydrogen vehicle technology such as people movers, trams, etc.

### Specific recommendations and additions or deletions to the work scope

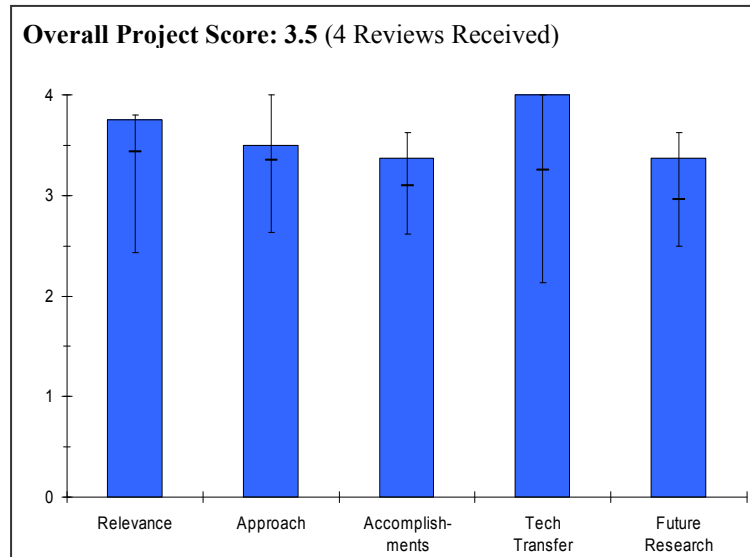
- Use the experience of the other 60 vehicles that do not collect data as part of this project.
- The General Motors presentation should delete references to ethanol unless they are addressing farmers.
- Put some effort into planning follow-up for the more severe problem areas encountered associated with vehicle/infrastructure.
- Add vehicle component targeting potential near term niche applications.

**Project # TV-05: Controlled Hydrogen Fleet and Infrastructure Analysis***Keith Wipke; NREL***Brief Summary of Project**

The objectives of this project are to 1) validate H<sub>2</sub> fuel cell vehicles and infrastructure in parallel; and 2) identify the current status and evolution of the technology including assessing progress toward technology readiness and providing feedback to H<sub>2</sub> research and development. Key targets are for a fuel stack durability of 2,000 hours, vehicle range of at least 250 miles, and hydrogen cost at station of \$3/gasoline gallon equivalent (gge) by 2009.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.8** for its relevance to DOE objectives.



- This project provides important and necessary end-user data and operating experience. Results should be used to provide future Department of Energy direction and emphasis and identification of technical areas that require additional and/or expanded emphasis.
- This project is considered to be the most important and critical element of the Technology Validation Sub-program, which receives a significant portion of DOE's Hydrogen Program funds.
- Acquiring "real world" operational data and experience is vital to making appropriate adjustments to the Hydrogen Program's research and development project mix and specific projects.
- This project is vital to determining whether the Program's hydrogen and fuel cell activities are on course to achieve established research and development targets. Without it, there would not be a way to evaluate the progress and public benefits deriving from the major automotive/energy company technology validation partnerships.
- Very relevant project performing a critical function.
- This project is relevant to the Hydrogen Fuel Initiative as a tool for summarizing where the technology is now.

**Question 2: Approach to performing the research and development**

This project was rated **3.5** on its approach.

- Excellent approach to maximize useful information from a massive amount of data.
- Intensive negotiations by National Renewable Energy Laboratory with industry performers and DOE have resulted in a superb system for collection, storage, securing, analyzing, and reporting on sensitive performance and other data submitted by industry.
- The approach includes providing analytical results for public use, as well as proprietary results for use by the companies providing raw data.
- The approach is dynamic, in that there are constant additions and improvements to the data collected, the systems for handling data, and the analyses provided.
- Presentation of 350 vs. 700 psi data in terms of percentages is somewhat misleading; absolute weight/volume data would be more revealing.
- Degradation analysis is an important part of the presented package; identification of clear cause(s) degradation would be welcome.
- High voltage = low current (redundancy in Slide 26).

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.4** based on accomplishments.

- Significant progress in assessing data from initial fuel cell vehicle operating experience.
- Impressive success in obtaining OEM data, both vehicle and fuel cell manufacturers, and treating it in a confidential way while still identifying important operating experience and trends.
- Major accomplishments and milestones since the project's inception in FY 2003 were communicated succinctly in an outstanding single slide.
- Mr. Wipke's presentation, backed up by additional well-constructed and informative slides, provided detailed accomplishments, such as data analyzed to date and NREL's Fleet Analysis Toolkit.
- Public results have been widely and proactively disseminated through numerous conferences, reports and publications. NREL's web site allows access to 47 Composite Data Products, plus reports and presentations.
- Many examples of information communicated, and associated initiatives, were included in the presentation.
- Accomplishments are good and in line with expectations.
- This project represents a comprehensive and needed summary of hydrogen fuel cell vehicle testing.
- Useful information on safety

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **4.0** for technology transfer and collaboration.

- Outstanding collaborative interactions.
- Mr. Wipke and the NREL team have earned the complete confidence of industry during the course of this project.
- Close collaboration with industry partners providing data is a primary contributor to project success. Site visits with industry on methodology and sharing of perspectives is commonplace.
- Working relationships and routine interactions have also been established with many other organizations having a stake in hydrogen and fuel cell progress. These include state agencies, analytical groups, and technical teams.
- Outstanding. Providing the necessary capability for companies.
- Project is collaborative in its nature as it relies on collaboration with OEMs.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.4** for proposed future work.

- Good future plans for keeping the analysis up-to-date and current.
- Plans for future work and initiatives were well summarized and clearly presented.
- Future plans are appropriate and adequately laid out.
- Future work should focus on identifying technical barriers limiting performance and efficiency of fuel cell technology for automotive transportation.

### **Strengths and weaknesses**

#### Strengths

- Strong analysis methodology and comprehensive input data.
- Mr. Wipke leads a strong, experienced, flexible team, which is committed to achievement of challenging project and hydrogen program objectives.
- The NREL team has gained the highest credibility with both industry and DOE.
- Collation of data from multiple teams.
- Project provides a good summary of factors of significant potential impact on fuel cell commercialization.
- Project offers a worthwhile compilation of "real-life" data.

Weaknesses

- Technical details are not immediately available. Can the participants provide more detail after a certain time interval?
- By its nature, this project does not offer solutions to existing challenges to fuel cell technology.
- Insufficient modeling/forecasting component in the project.

**Specific recommendations and additions or deletions to the work scope**

- Overall, this project represents a good summary of the state of hydrogen technology when applied to automotive transportation and should be continued.
- Forecasting should be added as an integral part of the project in the future.

**Project # TV-06: Validation of an Integrated Hydrogen Energy Station**

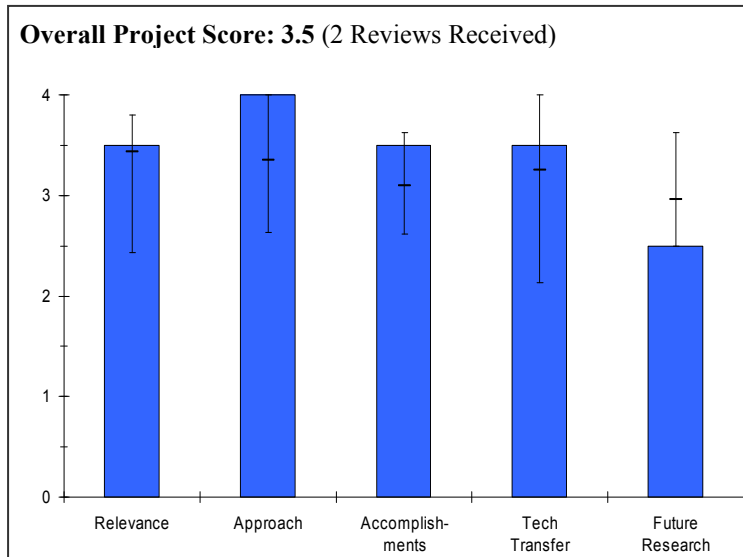
*Ed Heydorn; Air Products*

**Brief Summary of Project**

The overall objective of this project is to determine the economic and technical viability of a hydrogen energy station designed to co-produce power and hydrogen. Objectives are to 1) evaluate the feasibility of proton exchange membrane and high temperature fuel cell; 2) complete the preliminary system design; 3) complete detailed design and construction; and 4) operate station, perform testing and collect data.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.



- Based on the presentation and the expertise of the company, Air Products appears capable of performing this work so that the act of producing hydrogen and power can be improved.
- This project is critical to supporting the President's Hydrogen Fuel Initiative.
- The concept of an integrated electricity and hydrogen production facility is an innovative concept and promises to encourage the use of hydrogen fueling stations even when the vehicle usage might be low, at the start of deployment.
- Although an integrated co-production electricity/hydrogen system is not necessary for the deployment of hydrogen vehicles, it does support both high efficiency electricity generation and hydrogen vehicles.

**Question 2: Approach to performing the research and development**

This project was rated **4.0** on its approach.

- The project presentation was well-focused on addressing technical barriers, both the problems overcome and the work remaining.
- The Air Products presentation provided an ample amount of data that clearly demonstrated and justified the scope of the company's work.
- Seems to be an excellent approach to achieving the Program goals, including high efficiency and low cost of hydrogen.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.5** based on accomplishments.

- Air Products demonstrated and presented a great deal of technical progress to meet hydrogen development goals.
- Construction is in progress.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.5** for technology transfer and collaboration.

- Air Products made it clear that they coordinate closely with their Fuel Cell Energy colleagues and that the project depends on their teamwork.
- Good effort to proceed with permitting leveraged upon previous good experience with similar fuel cell units.
- Partnership is strong, but limited.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.5** for proposed future work.

- The project appears to be winding down and that there appears to be some lack of clarity for end of project completion.
- Plans for future work are somewhat limited.
- What is next, beyond validation?

#### **Strengths and weaknesses**

##### Strengths

- The research enjoys a great deal of metrics that clearly marks the team's progress.
- The project appears to benefit greatly from Air Products teamwork with fuel cell energy.
- Excellent concept.
- Strong partnership, experts in their fields.

##### Weaknesses

- If there was/is a well-defined plan for continuation or termination, further research and development or commercialization, it was not as clear as it could have been.
- Hardware and technology usage beyond the validation are not well addressed.
- What is next?

#### **Specific recommendations and additions or deletions to the work scope**

- A weakness of the project could be that they discussion did not discuss "What's next?" The presentation would have been closer to perfect if future options had been discussed.
- A power purchase agreement, with some sort of follow-on for the hydrogen generation technology would strengthen the project.

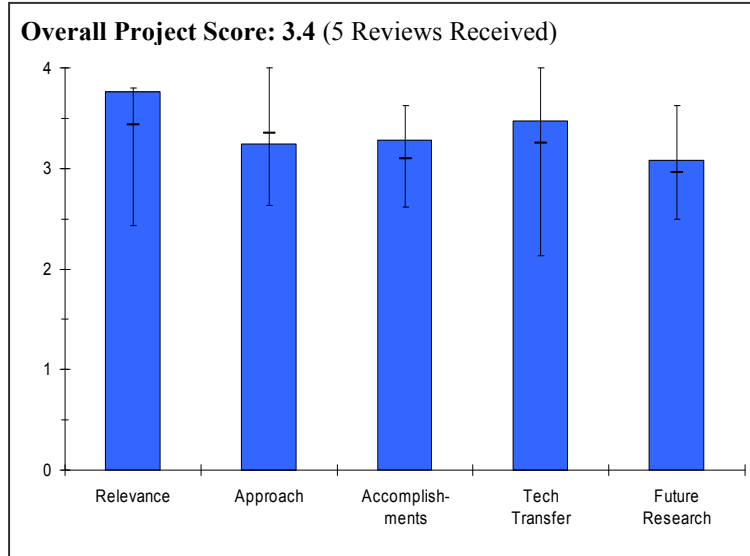


**Project # TV-07: California Hydrogen Infrastructure Project**

*Ed Heydorn; Air Products*

**Brief Summary of Project**

The objectives of this project are to 1) demonstrate a cost effective infrastructure model in California for possible nationwide implementation by designing, constructing and operating seven hydrogen fueling stations; collecting and reporting infrastructure data; documenting permitting requirements and experiences; and validating expected performance, cost, reliability, maintenance, and environmental impacts; and 2) implement a variety of new technologies with the objective of lowering costs of delivered hydrogen including the new delivery concept and the hydrogen-based unit.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.8** for its relevance to DOE objectives.

- The ozone analysis seems less relevant than the analysis of potential customers along the hydrogen pipeline and other hydrogen fueling options.
- Very relevant to have a major hydrogen producer involved in designs and fabrication of hydrogen infrastructure projects.
- Without hydrogen fueling stations, the hydrogen fuel cell vehicles are useless.
- This is a comprehensive project focusing on complete hydrogen infrastructure in a state, which is highly relevant to Hydrogen Initiative.
- Project is highly relevant to the Hydrogen Fuel Institute and the goals of the Multi-Year Program Plan focusing on expanding the number and variety of hydrogen refueling stations and reducing the cost of delivered hydrogen.
- This project has an interesting and relevant twist in its efforts to integrate hydrogen infrastructure with air quality modeling to understand and best maximize the urban benefits of hydrogen vehicles.

**Question 2: Approach to performing the research and development**

This project was rated **3.2** on its approach.

- Determine cost opportunities of delivered hydrogen at seven refueling stations operated in California.
- Identify interested parties to operate the stations.
- University of California, Irvine 350/700 Bar Station commercial station.
- Long Beach Mobile Fueler.
- Torrance Pipeline Hydrogen Fueling Station
- South Lake Tahoe Mobile Fueler.
- Novel Compressor system will be demonstrated in the next couple of weeks.
- Generally very good but perhaps too much emphasis placed on the use of liquid hydrogen. It is known to be energy intensive which would seem to make cost goals more elusive.
- Having both 350 Bar and 700 Bar hydrogen is a good approach.
- Mobile fueling is a good interim step for short duration or temporary demonstrations, but spending Program dollars on such short term options may not be the best use of Program funds.

- Innovative compression might provide cost or reliability improvements.
- Modeling work does not reveal any new areas of interest, but does validate existing modeling results.
- Well thought-through approach based on existing hydrogen resources.
- The project is very sharply focused on reducing the cost of the delivered hydrogen by exploring a variety of delivery mechanisms including pipeline, innovative liquid/gaseous bulk transport and storage, mobile stations, 350 and 700 bar dispensing, and technical advances with key technologies such as compressor systems.
- Hydrogen stations are appropriately focused in the highest need area—California.
- This project is coordinated with 4 vehicle OEMs supplying fuel cell and hydrogen internal combustion engine vehicles and California institutions.
- This project will document permitting requirements and experiences for hydrogen stations.
- No discussion however is provided on how to get the word out on hydrogen and to better educate the general public.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- Developed a new liquid hydrogen trailer.
- University of California, Irvine station is well used and is in a good location. There is continued interest from a broad base of customers. This is a commercial station.
- University of California, Irvine has done some excellent analysis on emissions, green house gas emissions, energy consumption and water consumption are outputs.
- Dispensing of hydrogen at University of California, Irvine station at 700 Bar is 4-5 dollars now, but it would drop if there were more than 25 kg per day.
- Very good accomplishments with mix of technologies being developed including transporter and single stage hydrogen compressor.
- Little was presented relative to permitting, installation, liability, etc. issues which seem to be major areas of concern.
- The University of California, Irvine portion of the presentation involved little useful information.
- Modeling results for fifty year scenarios may include so much climate and technology uncertainty that their results are of questionable use.
- Only one permanent fueling station has been put into service.
- Progress on the second permanent station has lagged behind the original schedule.
- Interesting and useful air quality analysis contributed by University of California, Irvine.
- Delays in hydrogen fuel cell stations represent some setback for this project.
- Excellent technical progress with the development of the New Delivery Concept (NDC), Hydrogen Based Unit (HBU), and novel compressor system.
- This project is aggressively exploring a variety of hydrogen station and delivery options.
- No actual data has been provided with regards to costs for any of the options so not able to ascertain economic feasibility. It would be expected that by this point in the project (which ends Sept 2008), operational and cost data would be available for the earliest options explored (University of California, Irvine 350/700 bar station and HF-150 mobile refuelers at least).

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.5** for technology transfer and collaboration.

- University of California, Irvine has helped analyze the infrastructure deployment in S. California.
- They developed a model from a lifecycle perspective. This model was used to analyze the distributed and centralized hydrogen generation.
- They also developed a model to analyze air quality impacts of Fuel Cell vehicle penetrations through the year 2060.
- There appears too is excellent collaboration with University of California, Irvine and various governmental groups.

## TECHNOLOGY VALIDATION

- A partnership with a university, as has been done with University of California, Irvine, is an excellent approach.
- A partnership with a vehicle manufacturer, or additional partnerships with automotive manufacturers, might help to provide better station utilization for the long term.
- Role of collaborators not clearly defined, except for that of the University of California, Irvine.
- Project appears to have a diverse set of partners including California institutions and vehicle OEMs.
- Little discussion, however, is provided as to formal technology transfer and collaboration amongst partners. It is not clear what each partner is doing, intellectual property arrangements, etc. On the surface, the "partnerships" appear not so much for the purpose of neither technology transfer nor collaboration but to gain access to certain sites or specific information.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Why develop the liquid hydrogen dispensing system?
- First pipeline station.
- Very good.
- Important that pipeline project is implemented.
- Proposed work should include studies to determine tradeoffs of costs between the uses of liquid hydrogen versus additional delivery trips of gaseous hydrogen.
- Continuing to provide demonstrations of mobile vehicle fueling does not support a permanent long-term hydrogen infrastructure and may not be the best use of program funds.
- Very sound list of proposed research task for the remainder of the project.
- The project is looking at a broad set of hydrogen refueling options and technologies, but has not adequately discussed the future for carrying on the stations once the project ends in September 08.
- Little discussion is provided on means to increase utilization of the hydrogen stations now and in the future either through additional hydrogen vehicles (such as buses) or other innovative means.
- No discussion is provided with regards to means for downselection of various hydrogen refueling options.

### **Strengths and weaknesses**

#### Strengths

- Using existing infrastructure such as the pipeline and trying to make sense of the cost and availability of customers.
- Technical capabilities, interactions with other groups.
- Partnership with University of California, Irvine.
- Air Products expertise in hydrogen.
- Combined liquid and gaseous hydrogen delivery.
- Overall, a strong and relevant project looking at a variety of hydrogen options with a strong emphasis on reducing cost.
- Solid technical progress in several areas.
- Seemingly broad and relevant team is assembled.

#### Weaknesses

- None.
- Possibly too much emphasis on liquid hydrogen.
- Little information relative to cost issues. Either not being done or done and not presented.
- Modeling studies of fifty-year scenarios may not be the best use of program funding.
- Schedule delays on the second permanent station.
- Only one permanent station has been installed and operated.
- Little if any discussion of actual mechanisms for technology transfer and collaboration amongst partners.
- Little discussion provided on means to continue existence of the stations at the end of the project and ways to increase hydrogen utilization.

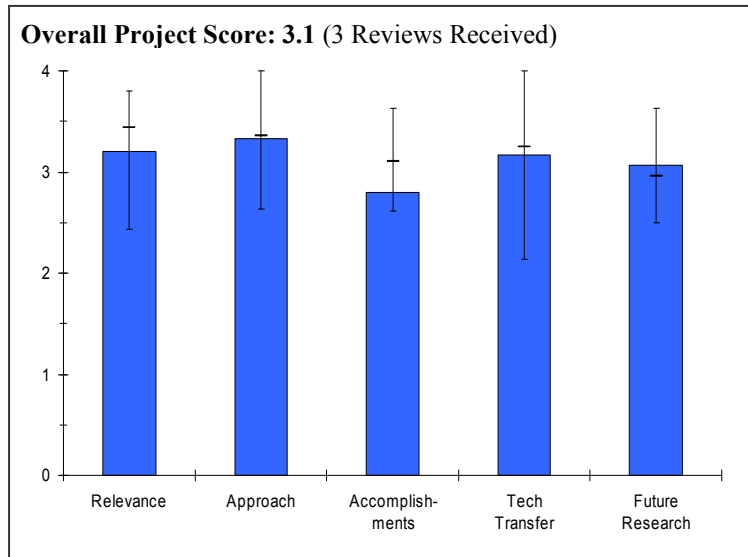
**Specific recommendations and additions or deletions to the work scope**

- None.
- Recommend more emphasis on cost issues.
- A better approach to the intent and results of the University of California, Irvine work would be useful.
- Additional permanent stations, in partnership with vehicle manufacturers, may strengthen the project.
- Funding for mobile hydrogen fueling stations might be redirected to permanent fueling stations to enhance the effect on the permanent hydrogen infrastructure.
- As this project is expected to end soon, there is no need for any modifications between now and the end-date.
- One-year extension could be of value to the DOE Program.
- Hydrogen cost analysis is needed.
- Put into place concrete plans for institutionalizing the hydrogen stations by assembling entities that would continue to use the facilities after the project ends.
- Establish means to increase awareness and acceptance of the hydrogen stations by the general public.

**Project # TV-08: Hawaii Hydrogen Center for Development and Deployment of Distributed Energy Systems**  
*Richard Rocheleau; Hawaii Natural Energy Inst.*

**Brief Summary of Project**

The objectives of this project are to 1) develop, validate and collect performance and cost data on the Hawaii Hydrogen Power Park, an integrated hydrogen system (electrolyzer, hydrogen storage, and fuel cell); 2) evaluate renewable hydrogen production from biomass including evaluating the H<sub>2</sub> yield potential of Pearson Technologies' gasification process and characterizing technologies for tar reforming and H<sub>2</sub> purification; and; 3) develop a strategic energy roadmap to identify economically viable technologies to transform the Big Island energy infrastructure including baseline models for electricity and transportation and identifying scenarios to facilitate acceptance of emerging new energy systems including hydrogen.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.

- The project presentation clearly demonstrates and greatly supports the President's Hydrogen Fuel Initiative.
- The project demonstrates on a micro level the complexities of using a variety of energy sources to provide grid/microgrid power.
- This project comprises four tasks. Each has some potential relevance in generating movement toward greater energy diversity and independence for Hawaii.
- Funding was provided in FY 04 and FY 05, and most work is completed. The results have provided some value in laying the foundation for activities that could have particular future energy benefits for Hawaii.
- The project is expected to have little or no benefit in terms of contributing to achievement of Department of Energy's Hydrogen goals, targets, and objectives.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- Approach is broad based. Appears to be larger than one person can over see when collaborations taken into account.
- Approach for use of biomass is weak and could easily be strengthened to be the center point of this project.
- The Hawaii Natural Energy Institute team addressed not only programmatic challenges but the technical challenges of developing and measuring a grid from multiple energy sources.
- The team demonstrated a great ability to integrate their work with other alternative energy research.
- The hydrogen power park task linked existing renewable infrastructure, a test bed for fuel cell technology, and analytical support by modelers at Sandia National Laboratory. The linkages and collaborations in this task resulted from a sound concept.
- Performing energy road mapping for the Big Island also seems like a good idea. It should have been implemented as part of an overall integrated plan for Hawaii's energy future, with the results of the integrated plan being used to determine project goals, priorities, and activities. It seems this was not how tasks were selected for funding.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- Amount of information generated by this project is minimal for the funding received. There is not long-term data collection or dissemination.
- Biomass clean up with ZnO is not new, this data is right out of literature. There are numerous better choices for sulfur remediation— consider rescoping this part of the project.
- The HNEI project team presented a great deal of data to demonstrate and measure the project's progress.
- To meet hydrogen and energy goals for the nation, many efforts such as this will be required to learn management requirements to integrate and wisely use alternative and renewable energy technologies.
- Completed and nearly completed tasks are resulting in incremental knowledge and experience for those who worked on them and relatively few others.
- It is doubtful that this project has contributed to meaningful progress toward a transition to hydrogen, or to achievement of DOE Hydrogen Program goals/objectives.
- Technical work on the hydrogen power park (task 1) and renewable hydrogen production from biomass (task 3) could assist in advancing technology. The results of this work should be communicated to those with appropriate expertise and an interest in related technologies.
- Outreach associated with task 1 is a good initiative.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.2** for technology transfer and collaboration.

- Collaborations are extensive, but how are they distinguished by task? Most appear to support power park work.
- The project clearly demonstrates a strong collaborative effort with a wide variety of public and private organizations.
- A number of cost share partners were identified in the slide presentation. Some collaboration was also identified in slides on project approach and accomplishments.
- There was little discussion or mention of collaboration and coordination with others during the oral presentation.
- There are working relationships established with officials, organizations, and communities in Hawaii.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- More elaboration on future R&D is warranted on tasks to be funded by DOE.
- The relevance of this project by HNEI is clearly applicable to meeting the nation's energy's requirements and managing a variety of energy sources to reliably meet community requirements.
- The presentation included recommendations for future hydrogen power park work, including Kahua Ranch education and outreach, and installation of a hydrogen fueling infrastructure at Hawaii Volcanoes National Park.
- Work on other tasks is evidently continuing under separate agreements.

**Strengths and weaknesses****Strengths**

- The presenter did a good job of conveying the difficulties of putting an alternative energy/hydrogen project together.
- Work on the tasks in this project should increase the visibility of hydrogen—and its potential—within Hawaii.

### Weaknesses

- Amount of information generated by this project is minimal for the funding received. There is not long-term data collection or dissemination.
- The work is not linked well with DOE's Hydrogen goals and objectives.
- It is not evident that a sufficiently developed, rigorous plan exists for guiding the project activities.

### Specific recommendations and additions or deletions to the work scope

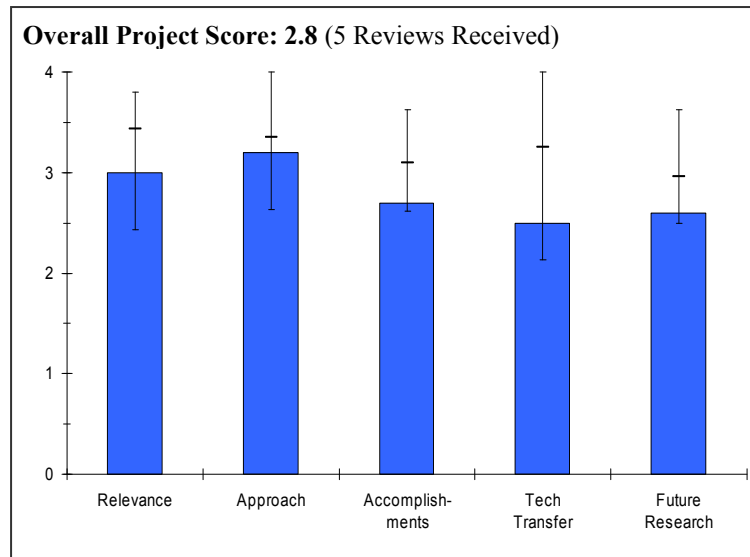
- Put into place concrete plans for institutionalizing the hydrogen stations by assembling entities that would continue to use the facilities after the project ends.

**Project # TV-09: Cryogenic Capable Pressure Vessels for Vehicular Hydrogen Storage***Salvador Aceves; LLNL***Brief Summary of Project**

The overall objective of the program is to demonstrate the practical advantages of cryogenic capable pressure vessels for hydrogen vehicles, including high energy density, no evaporative losses, flexible refueling and safety. The project has installed a pressure vessel in an experimental vehicle, and demonstrated long vehicle range (650 miles on a single tank), vacuum stability, and resolved technical risk of dormancy and high pressure.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.0** for its relevance to DOE objectives.



- This is a long-term project to develop cryo-tank development for hydrogen storage.
- Somewhat similar, liquid hydrogen storage is already in prototype vehicles (BMW).
- Interesting alternative storage system, since it opens up perspectives to reach specific volume and weight targets
- For automotive application it will not only be important to meet the specific technical targets (kg or liter per kWh), but the overall system needs to meet the packaging needs of the OEMs. As could be seen from the Prius pictures the 10 kg hydrogen storage is (although the specific values are not bad) not suitable for a compact to mid-sized vehicle. Cryo-compressed hydrogen storage shows an interesting perspective wherever larger amounts (>5 kg) need to be stored on-board. In terms of relevance for the program, the market perspective needs to be taken into account, since the fuel cell vehicles being developed by the OEMs usually range in the mid-size segment. This is also of relevance for the cost analysis, which is based on volumes of 500,000 units per year. This seems to be an unrealistically high volume assuming that most OEMs will start commercialization with high-pressure gaseous storage.
- The aspect of fuelling flexibility needs to be assessed further. In principle it is true, that these storage systems can be refueled either at a regular 5,000 psi gaseous station or at stations that offer liquid hydrogen. Whereas the regular 5,000 psi fueling does not offer advantages to the customer (why should he pay for the extra cryo-equipment?) the cryo-fill requires extra measures at the fueling station (which adds costs) and might require the combination with regular gaseous refueling to avoid wasting/blowing off hydrogen. This is relevant to the overall program since infrastructure build-up is one of the most critical issues which require cost effective concepts.
- Although boil-off does not occur since the hydrogen at low temperature and high pressure is in a supercritical phase, venting cannot be avoided once the maximum pressure is reached (dormancy time depending on customer driving habit). Hence the cryo-compressed hydrogen storage system is an open system which requires specific safety concepts on-board the vehicle. This has relevance to the overall Program in terms of safety concepts and RCS.
- In good alignment with 2010 goals but not 2015 as they stand.
- However, probably the best overall system available at present and potential to replace normal compressed gas.
- The project focuses on one of the Department of Energy's key objectives which is to improve on-board hydrogen storage options available to the OEMs.
- This project has achieved 10 kg of hydrogen storage on a vehicle in a reasonable sized tank. This goal of high density hydrogen storage on vehicles, in a safe manner, is extremely relevant to DOE's Hydrogen Program.



## TECHNOLOGY VALIDATION

- Excellent demonstration of potential affordability of this approach (slide 13) comparing this tank's costs to other hydrogen storage methods. Cryo-compressed could be more economical than other methods such as compressed hydrogen at moderate (5000psi) and high (10,000psi) pressures.
- Showing where cryo-compressed is now and where it needs to go, emphasizes the relevance of the research (slide 16). System capacity by volume and weight are important to continue to improve with this research.

### **Question 2: Approach to performing the research and development**

This project was rated **3.2** on its approach.

- Storage hybridization is a powerful way of resolving intermediate needs and this approach addresses that.
- However in the long run the approach has significant barriers which are beyond the scopes of this program to address.
- The main critical technical issues are dormancy time and vacuum stability which are addressed in the project.
- Cycling behavior as another critical factor is planned.
- Overall, it was unclear as to how specific automotive requirements are taken into account. This needs to be assessed further (mechanical and thermal stress).
- Generally good though not always clear what the integrated plan is.
- Not clear that liquid nitrogen fill makes sense in that the cooling of the tank will be expensive or slow.
- The technical approach to finding a unique hydrogen storage solution is excellent.
- The balance of both theoretical and experimental is perfect and a model for other projects to follow.
- This project is capitalizing on LLNL's extensive experience working with hydrogen over the past 40 years and related specialized equipment (such as high temperature/pressure ovens (slides 11 and 12), and high pressure containment rooms). This project is applying these valuable resources developed originally for other purpose for the hydrogen vehicle program.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- Progress in this project seems to have slowed significantly.
- Incomplete results in dormancy test and insulation outgassing tests.
- Dormancy time: Only one experiment was presented to assess the dormancy time. The predicted 3 weeks dormancy time is based on a weak experimental database as well as on the assumption that the lowest measured heat transfer can be maintained over a longer period of time. This needs to be assessed further. Mechanical and/or thermal stress arising from automotive use needs to be taken into account.
- The cost analysis compares 10.7 kg hydrogen in the case of cryo-storage with 5.6 kg in the case of high-pressure storage. The respective specific values are not directly comparable. Either both concepts address different vehicle types (in this case a direct cost comparison is misleading) or the two concepts compete in the range of 5-7 kg hydrogen storage. In the latter case a cost comparison needs to be based on the same amount of hydrogen stored.
- Important milestones in demonstrating vacuum stability and dormancy.
- Cost numbers look good.
- Only counting progress since 2007 Annual Merit Review, other progress earlier.
- Significant progress has been made in the last year, and experimental results are excellent.
- The Addition of both an OEM and a tank supplier will take this to the next level of maturity. Congratulations on securing these two partners.
- Demonstrated six days of dormancy (slides 4, 7, 8) and potential for three weeks of dormancy; plotted data (slides 7 and 8) is excellent; greater explanation needed for increase in temp and pressure at 135 hours — mentioned in talk not in slides (slides 7, 8).
- Demonstrated vacuum stability under warming (slides 4, 13).
- Outgasing and cycle tests.
- Plotted data on heat transfer into vessels is excellent.
- Demonstrated practicality of cyro-compressed hydrogen (slides 4 and 8) in a hybrid vehicle.
- Previously demonstrated long vehicle range (slide 4).

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.5** for technology transfer and collaboration.

- It appears to have limited interest from USCAR partners. USCAR partners have been engaged through several cyro-compressed workshops.
- No apparent partners or collaborations for this projects - although it was reported that some are in the negotiation stage. But it is not clear why there has been no interactions in the over three years that this project has been underway.
- Close collaboration with an OEM was mentioned, which is absolutely necessary to assure automotive feasibility
- Since the cryo-compressed storage concept has major impact on the infrastructure (especially on station design) it is highly recommended to start detailed discussions with energy companies.
- Questions regarding material behavior at low temperatures and high pressures should be addressed within the collaboration mentioned with a vessel manufacturer.
- A relationship with BMW would be appropriate as they are doing similar work.
- I look forward next year to hearing more about the benefits of the collaboration with your new industry partners.
- This project has spun-off its work to a major automotive company, which is trying to integrate this type of tank in their hydrogen cars.
- Finalizing CRADA with major auto manufacturer (slide 2).
- Negotiating CRADA with major pressure vessel manufacture (slide 2).
- The design and manufacture a new cryogenic pressure vessel for full cycle testing (slide 15) is very important to do with industrial partners.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.6** for proposed future work.

- Plan for future work is vague and not clearly stated.
- Building a next generation storage system and testing it under real-world conditions is the right approach. This requires a close collaboration with an OEM.
- More focus should be put on extensive testing under automotive conditions as well as the impact on infrastructure (including customer acceptance, i.e. will customers accept, that they get different filling-levels depending on the station they go to).
- Materials behavior at low temperatures and high pressures needs to be addressed.
- Direction is excellent.
- Details are hazy.
- More details could be provided about future work, such as how the next generation system build will improve upon your current generation
- What will change in the next generation system that will allow you to meet the 2010 goals?
- Demonstrating future cryo-compressed system capacity by weight and volume would be extremely helpful, especially if performance exceeds liquid hydrogen tank expectations.
- Design and manufacture a new cryogenic pressure vessel for full cycle testing (slide 15) is excellent to do with industrial partners, to better address the temperature and pressure profile of the tank during warm up and refueling. This kind of collaboration (between refueling station and tank developer) is necessary for success of the entire refueling system.

**Strengths and weaknesses****Strengths**

- The strength of this project is the combination of two well-established technologies for hydrogen storage.
- It builds on the positive aspects of each physical storage technique.
- Engineering developments.
- Interesting alternative storage concept for larger hydrogen quantities.
- Interaction with OEM and vessel manufacturer.
- Good concept, team has expertise in area and is responsive to input.

## TECHNOLOGY VALIDATION

- Higher density of hydrogen allows for smaller tank and thus cheaper than compressed hydrogen.
- Good balance of theory, experiment, and demonstration.
- Successful linkage for the future with industry partners.
- Valuable technical achievement toward DOE technical targets for storage.
- Demonstrated high range and vacuum stability.
- Excellent teaming with industry and spin-off of technology.
- The integrity of the research team is high, as well as their enthusiasm for this work and technical experience in this area. Very few research groups around the world could assemble this combination of excellent thinking and experience in hydrogen storage.
- This project is a hallmark example of "turning missile silos into plowshares." It is a superb example of converting the technical expertise developed for the weapons program into engineering science innovation for sustainable energy.

### Weaknesses

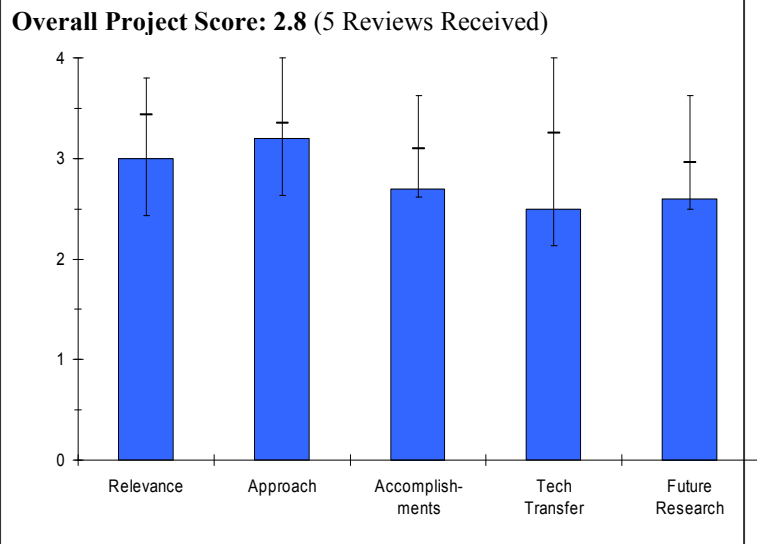
- Page 7 shows the fundamental technical limits of this concept (excluding the infrastructure and well-to-wheels efficiency shortcomings). Contrary to the presented interpretations, the data reflects why this technology is of limited use outside controlled fleet.
- It was reported that the shortened dormancy test was due to a valve failure, but this is very important since valves will surely be balance of plant components in any eventual system. This problem must be studied and solved.
- More experiments needed (automotive requirements).
- High cost structure limits progress, use of lower cost labor where possible would be wise.
- Probably can not meet 2015 goals, but since this is the leading new method of storage, do not emphasize that weakness.
- Tank more expensive than liquid hydrogen of same capacity.
- Lay out more detailed plans for future work.
- Describe improvements planned for next generation build.
- Speaker and presentation should clearly delineate previous years accomplishments compared with this year's accomplishments. For example, tank integration occurred in previous fiscal year (Jan 2007). Project could emphasize more strongly increasing system capacity by volume and weight. Project would benefit from some DFMA (Design for Manufacturing Analysis) taken into account in any tank re-designs. Please include a team member with DFMA experience during the tank re-design process that is being done in conjunction with industry.

### Specific recommendations and additions or deletions to the work scope

- Since this projects starts from a higher level of established development (prior art), it is reasonable to expect the team to address:
  - Storage module cost (as compared to either cryo or compressed system).
  - Infrastructure requirements.
  - Overall well-to-wheels energy efficiency.
  - Shortcomings in volumetric storage and finally a definite solution for over-pressurization/venting problem.
- It is recommended that this project be shortened and brought to timely conclusion.
- Objective: Demonstrate the practical advantages of cryogenic capable pressure vessels; 'practical' should be specified in more detail: automotive conditions and impact on infrastructure.
- Develop a clearer and more structured plan to reach 2010 goals and have DOE vet it.
- Work toward a more realistic packaging for your next vehicle demonstration (should not take up the whole trunk of a vehicle).
- Despite industry partner involvement for future and Cooperative Research and Development Agreement limitations, ensure that adequate technical results continue to flow out from this project.
- 1) DOE should fund further cryo-compressed tank prototypes, with updated designs and newer materials.
- 2) DOE would benefit by allowing the LLNL researchers who have developed this technology to take wider credit for this work. For example, peer-reviewed press releases from LLNL on their research should be encouraged. The DOE's image in the public eye can be enhanced by allowing its researchers to take credit for their work, so long as they emphasize the infancy of the technology and additional R&D contributions needed.

**Project # TVP-01: Florida Hydrogen Initiative***Pam Portwood; Florida Hydrogen Initiative***Brief Summary of Project**

The Florida Hydrogen Initiative is a non-profit organization incorporated under the laws of the State of Florida to move Florida to the forefront of the nation's hydrogen economy. The Florida Hydrogen Initiative has funded four projects to date 1) the HyTech Rest Area project to demonstrate the use of hydrogen derived from citrus waste in a fuel cell located at a Florida Turnpike rest area; 2) the development of location strategies for the initial hydrogen refueling infrastructure in Florida that would be required to support consumer demand and a hydrogen powered car rental fleet for Orlando, Florida; 3) designing and building a museum exhibit to tour 18 Florida science museums to inform and educate the public about hydrogen's potential and use as an energy carrying medium and the future role of hydrogen in energy distribution; and 4) the on-site reformation of diesel fuel for hydrogen fueling station application.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.4** for its relevance to DOE objectives.

- The four topics are excellent and will help the Department of Energy achieve its goals and objectives.
- This project is a set of relatively small sub-projects, which result from funding of proposals made to the Florida Hydrogen Initiative.
- At least two of the four projects discussed are expected to have little or no benefit in terms of contributing to achievement of DOE's Hydrogen goals, targets and objectives.
- Most of these projects seemed to address issues that are not core to the Program's mission
- This project consists of 4 discrete activities: 1)HyTech Rest Area, 2) Hydrogen Refueling Infrastructure and Rental Car Strategies, 3) Public understanding of hydrogen, and 4) On site reformation of diesel. Activities 2 and 3 are complete.
- 1) HyTech project shows solid relevance to Hydrogen Fuel Initiative goals including the use of local and renewable resources to generate power.
- 2) Rental car strategies project is relevant as a means to increase exposure to hydrogen vehicles and accelerate adoption. Given the cost of hydrogen stations it is imperative to maximize the use and location of each station. This project lends itself to credible strategies for doing this.
- 3) Public understanding of hydrogen project is a small but viable element to increasing public awareness and acceptance of hydrogen. Clearly dovetails into other education components.
- 4) It is highly unlikely that diesel fuel to hydrogen conversion will ever be viable economically or from an efficiency standpoint with other hydrogen distributed fuel pathways.
- Multiple projects, with multiple effects, all in Florida could improve the public perception climate for hydrogen, especially in Florida, while developing diesel reforming.
- Educational highway display.
- Citrus derived hydrogen.
- Hydrogen refueling location studies.
- Educational museum display.
- Diesel reforming.

## TECHNOLOGY VALIDATION

- This project has some relevance to overall DOE objectives.
- The project has 5 different, disconnected projects that do not appear to be at all integrated.

### **Question 2: Approach to performing the research and development**

This project was rated **2.6** on its approach.

- On-site reformer attempts to lower H<sub>2</sub>S to < 50ppm were not successful.
- The sub-projects selected for funding are each relatively small, independent activities. It would be preferable for each project to be funded in the context of an overall Florida Hydrogen Initiative plan that is linked to DOE's Hydrogen Program goals and objectives.
- Consideration should be given to using more project funds for hydrogen education initiatives in Florida.
- Most of the project approaches appear to be reasonable.
- HyTech approach is reasonable and methodical.
- Rental car strategies project approach is sound lending itself to optimal placement and utilization of each hydrogen station. However, it is questionable whether the general public will actually rent hydrogen vehicles ad hoc at this time due to perceptions with respect to safety etc. It is highly unlikely that a family coming to Disney World will rent a hydrogen vehicle. As mentioned later in the poster session, more likely early experimenters are techies, professors, etc. in university towns or at clusters of technical companies.
- Public understanding project approach is solid emphasizing hands on activities and touring expedition to increase exposure.
- The approach for the onsite diesel reformation project is not will detailed and is difficult to assess.
- Each separate task appears to be well managed and moving along well.
- Coordination between the project tasks is not addressed.
- The overall approach was not clearly presented.
- With 5 discrete projects, there was no recognizable cohesive.
- A few projects discussed approach, but not all.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.6** based on accomplishments.

- Were the HyTech Oct '07 and Jun '08 milestones accomplished?
- Completed sub-projects are resulting in incremental knowledge and experience for those working on them and a relatively few others.
- It is doubtful that meaningful progress toward a transition to hydrogen is enhanced by this work.
- The sub-project on reformation/de-sulfurization of diesel fuel could advance technology, but funding should be provided more logically from sources other than the Hydrogen Program.
- HyTech: Not clear if >32% efficiency will even be achieved, but it seems likely that other technology options would be more efficient and reliable.
- Hydrogen Refueling: Interesting model results and good use of existing information from the National Renewable Energy Laboratory model.
- On-site Reforming: Not clear how much funding was spent on this project.
- Technical accomplishments and progress are on schedule for HyTech although significant detail is not provided. Project appears to be schedule for completion in the Fall of 2008.
- Rental car strategies project is complete and appears to achieve its objectives.
- Public understanding project is complete and appears to have met objectives.
- Solid technical progress and accomplishments appear to have been achieved for the diesel reformation project.
- All project tasks are making good progress.
- With the exception of the on-site reformation of diesel fuel for hydrogen station fueling applications" project, technical accomplishments were weak. Seems like more should be accomplished by now (2 years into the project).

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.1** for technology transfer and collaboration.

- These projects make good use of academic organizations and demonstrate a high level of collaboration with industry.
- There has been some interaction with other modelers on the refueling infrastructure project that has been completed.
- In general, it seems that sub-project plans and results are not being sufficiently shared with those interested in the results.
- Work on the diesel reformation project should be discussed with DOE's Fossil Energy staff.
- Overall, these projects would benefit from working with more partners outside of the Florida hydrogen Initiative
- HyTech project has relatively broad connections with other entities (such as citrus ethanol producers), with the exception of drawing upon the experience of past stationary, biomass derived fuel cell power stations applications.
- Rental car strategies project collaborated well with other university researchers in Florida, but has no evident collaboration with others. This project would benefit from expanding its universe to other entities such as energy companies and Kennedy Space Center which has excess hydrogen capacity.
- Public understanding project has established and leveraged collaborations with important other entities including Disney, and US Department of Education.
- Only collaboration identified for diesel reformation project is Chevron. Project would benefit from other industrial entities experienced with stationary hydrogen fuel cell siting and application.
- Additional coordination between the project tasks might be helpful.
- Technology transfer and collaborations not directly addressed.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.5** for proposed future work.

- These projects (all 4) should be fully funded to complete the work
- Future sub-projects will be selected from proposals submitted to the Florida Hydrogen Initiative.
- Potential future work was not identified in response to questions, though more funding for the project will evidently be available.
- Proposed future projects for HyTech is reasonable if underdeveloped. As the project is nearing completion, extensive effort should be made to determine explicit economic targets necessary to commercialization viability and utilize knowledge learned to examine other possible biomass derived fuel cell power plant options.
- Proposed future research for rental cars strategies project is excellent especially as results could be equally applied to any alternative fuel. A good idea would be to work outside the university boundaries and look to coordinate a nexus using this tool with deployers of alternative fuels and other states.
- Public understanding project should consider being toured nationally as well.
- Proposed future research is reasonable for diesel reformation project.
- Projects continue toward realization of goals. The next year will be critical.
- Only the diesel reformer had much discussion of future work.

**Strengths and weaknesses****Strengths**

- Good use of funding for four distinct projects .
- Work on some sub-projects should increase the visibility of hydrogen—and its potential—within Florida.
- Some good work, but overall grouping of projects does not seem to fit with any one core objective.
- HyTech project is relevant for fuel diversification and utilization of local resources.
- Rental car strategies project provides good insight into hydrogen station deployment strategies to maximize utilization and cost effectiveness.

## TECHNOLOGY VALIDATION

- Public understanding project is a solid awareness and outreach effort for hydrogen.
- Good goals and approaches.
- Some of projects will have some good outreach value based on their high visibility (rest area project).

### Weaknesses

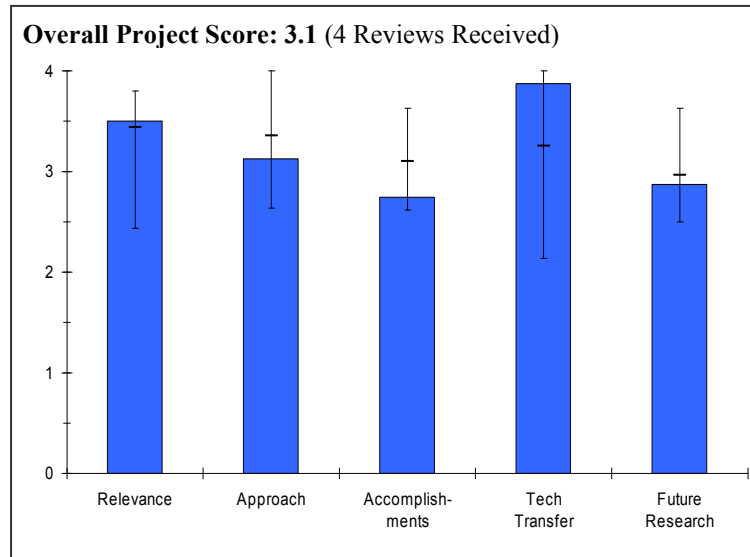
- The onsite reformer tested did not allow H<sub>2</sub>S scrubbing down to 50 ppm but the summary states the best metal to chelate system was capable of reducing H<sub>2</sub>S to <50 ppm. This is confusing. Only one statement can be true.
- The work is not linked well with DOE's goals and objectives.
- An overall plan for guiding the project activities is not sufficiently developed or rigorous.
- Too focused on one state.
- HyTech project would benefit from collaboration with other firms which have conducted similar biomass or renewable energy based fuel cell stationary applications.
- Rental car strategies project may benefit from reconsideration of strategy to utilize rental cars as initial "market" for hydrogen vehicles. Perception issues may make this a hard sell.
- Diesel reformation project ostensibly has no relevance to the other projects of the Florida Hydrogen Initiative and is surely not locally native to the state.
- Focus on Florida might be improved with additional coordination between the project tasks and additional coordination with other states and locales.
- There is no common thread among the projects, except that they are all in Florida. The projects really need to be reviewed individually as 5 separate projects
- Need to make more technical progress than has been demonstrated to date.
- At the poster, the presenter was a contracts administrator, not a technical person, so most of the information for this review had to be obtained from the PDF file.

### Specific recommendations and additions or deletions to the work scope

- Get NEPA permit for HyTech (as soon as possible).
- Terminate diesel reformation project as diesel to hydrogen reformation is highly unattractive from an efficiency and cost standpoint. Additionally, it does not fit within the context of the Florida Hydrogen Initiative.
- More integration between the project tasks
- More integration and coordination with other regions, states and the national programs.
- Given the overall weakness of the project as a cohesive package, the recommendation would be to separately review these projects (perhaps as posters) in the future so that reviews/feedback can be more direct and useful to the PIs.
- The station location analysis project probably has the most relevance to DOE's goals, so this project should be expanded.

**Project # TVP-02: Technology Validation: Fuel Cell Bus Evaluations***Leslie Eudy; NREL***Brief Summary of Project**

The overall objectives of the project are to 1) validate fuel cell and hydrogen technologies in transit applications; show progress of the technology toward commercialization; 2) provide “lessons learned” on implementing next generation fuel cell systems in transit operations; and 3) harmonize data collection efforts with other fuel cell bus demonstrations worldwide (in coordination with FTA and other U.S. and international partners). Objectives for 2008 are to 1) complete updated reports on AC Transit and SunLine; 2) begin data collection and analysis for first cold climate site, CTTRANSIT; and 3) provide a summary of the fuel cell bus experience and analysis of status.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- This project is essential if the Department of Energy objectives are to be met.
- This project appears to fully support the Presidents Hydrogen Initiative.
- Fleet program is an imperative step toward commercial variability.
- Accumulated data during real usage is valuable for fuel cell research and development.
- Although DOE is focused primarily on light duty transportation and the Department of Transportation is addressing heavy duty applications, it is extremely important that everyone understand the technology status and barriers that must be addressed prior to full commercialization of fuel cell vehicles.

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- The project collects data and compares to other international efforts.
- Barriers are addressed clearly.
- The approach to completing this project appears fully complete and well thought as documented in the team's presentation.
- As provided the data advises that a great deal of effort was accumulated and processed for use.
- Analysis seems to be superficial (simple data comparison). Deeper analysis, e.g. performance/failure analysis with usage profile should be more valuable.
- Excellent job of making real operational data available for all to view and use.
- Getting agreements with fuel cell manufacturers and being able to publish aggregated data is very important.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- Very clear, easy to read results. Related to DOE objectives.
- This project shows excellent progress. Results are clearly shown.



## TECHNOLOGY VALIDATION

- The project did a fine job of providing a snapshot of fuel cell bus costs, but the project could have been improved by comparing a history of costs and future trends. In other words, is a historical trend available and can one determine what future costs can be?
- Fleet data were just simply compared among three fleet programs. It would be more meaningful if the data is analyzed with usage profile and vehicle specifications.
- Unfortunately, a lot of time has been expended negotiating agreements on the collection and sharing of data.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.9** for technology transfer and collaboration.

- The transit companies participating embrace the whole community.
- From their presentation, National Renewable Energy Laboratory fully coordinated their collaboration efforts.
- Project organized and appropriate data publication.
- Progress on getting worldwide consistency in data collected and published is good.
- DOT is finally (planning on) participating with funding.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- This project should be fully funded for future work.
- The project appears to focus on completing their work in an "as is" data collection service. The project team might be able to improve their product if they could project from some of the observations.
- Data mining approach would be appropriate.
- Development of database for failure information and lessons learned would be valuable.
- Continuing the data collection and publication on the National Fuel Cell Bus Demonstration is excellent.

### **Strengths and weaknesses**

#### Strengths

- Good geographic diversity with various temperate real world conditions to evaluate performance and cost.
- Consistent data collection and evaluation of comparable; international efforts is highly desirable. This approach maximizes benefits and minimizes cost!
- The project is fulfilling a necessary requirement by measuring data.
- Access real world data.
- One location for all fuel cell vehicle data is extremely beneficial for everyone that has need for the data.

#### Weaknesses

- None.
- The project appears to focus more on accounting data, but could benefit from greater analysis.
- Data analysis methodology.
- More effort must be made to get the data publically available, especially aggregated proprietary data.

### **Specific recommendations and additions or deletions to the work scope**

- Fleet summary for HIISNA. Determine if there are any results for HI AIRFORCE Demo?
- The database and publications should include every fuel cell bus in operation.

## 2008

### Safety and Codes & Standards

#### Summary of Annual Merit Review Safety and Codes & Standards Subprogram

#### Summary of Reviewer Comments on Safety and Codes & Standards Subprogram:

In general, the Safety and Codes and Standards subprogram reviewers stated that projects were productive and successful. The Reviewers were impressed by the breadth of activities and the ongoing commitment to safety, codes, standards and information-sharing activities. They stressed that successes in this subprogram touch every other DOE hydrogen-related activity by fostering acceptance, collaboration and communication with critical stakeholders.

Reviewers stressed the importance of continuing efforts in critical areas such as hydrogen materials research, hydrogen codes, standards and permitting coordination efforts, hydrogen quality, and safety incident reporting and best practices. Suggestions for maximizing progress included leveraging the efforts of universities, standards organizations, national labs, complementary government agencies, and industry, as well as other subprograms.

Six safety projects were reviewed. The *Hydrogen Codes and Standards* work was praised for its varied engagement with industry, government, and researchers, particularly national laboratories. This work is seen as essential to fully address the Program barriers. However, reviewers felt that a better explanation of the relationship between computational fluid dynamics (CFD) activities and the codes and standards work was needed.

The *Hydrogen Materials Research and Development* project is focused on materials research to support the development of technically sound codes and standards to ensure the safe design of infrastructure for the storage and transport of high-pressure hydrogen gas. The project was praised for its highly relevant technical accomplishments, careful planning, and close collaboration with industry and Code Development Organizations (CDOs) and Standards Development Organizations (SDOs.) The availability of the pressure vessel for high-pressure testing was deemed a particular asset to this work. It was suggested that expanding the candidate materials for testing, perhaps by polling the Program at large, and adding test conditions reflective of particulate formation in a fueling system would enhance the project.

The *Hydrogen Safety Tools: Software and Hardware* project was considered to be valuable in terms of outreach to relevant groups. The open sharing of lessons learned exhibited in the incidents database was seen as the proper approach to take and a good complement to the rest of the Safety program. In addition, the construction of the hydrogen fuel cell vehicle simulator prop and the collaboration with first responders in the prop's development were seen as beneficial. It was suggested that focusing on incidents with commercial compressed gas storage might be more elucidating than focusing on industrial hydrogen practices. Reviewers also encouraged greater interaction with other transportation communities and NASA.

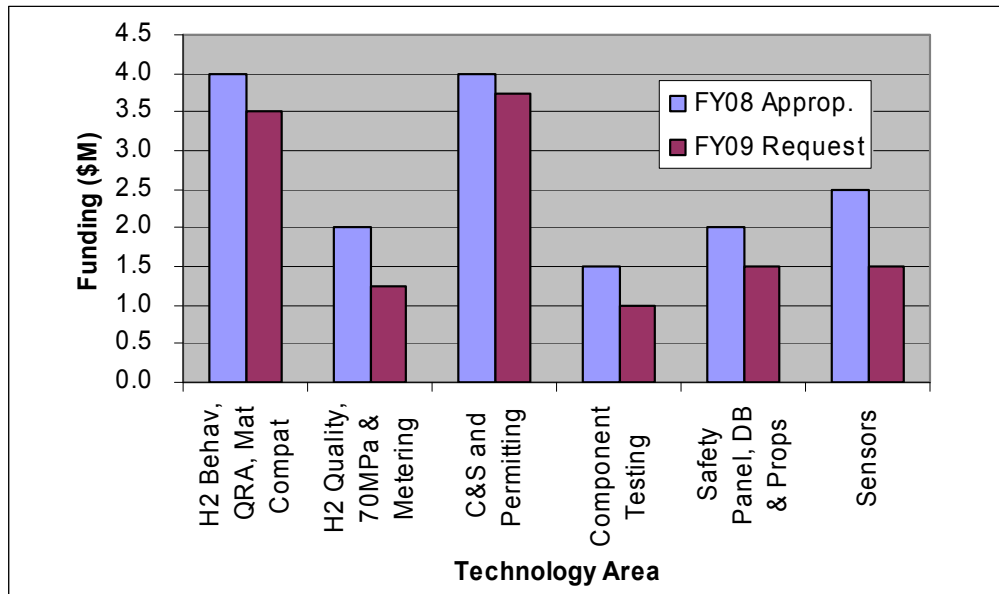
*Hydrogen Quality* work was praised for its strong underlying approach, emphasizing uniformity in data reporting, round-robin verification of methodology, and overall coordination of testing. Some reviewers noted that the project has not sufficiently taken advantage of the large amount of data in other subprograms. The Hydrogen Safety Panel was regarded as an important activity in which more work is needed. Industry representation was seen as a strength of the Panel, although some reviewers noted that more participation from automakers would be beneficial. The number of safety plans reviewed was

considered realistic given the time involved. However it was noted that there was room for improvement in terms of the number of safety reviews conducted.

Finally, the *Codes and Standards for the Hydrogen Economy* project, which is not a research and development activity, was seen as playing an important, although sometimes difficult, management and support role to codes and standards development organizations dealing with hydrogen technology. It was noted that the project strives to continually improve its business operations. However, it would be beneficial to emphasize the tracking of project deliverables.

**Safety and Codes & Standards Funding:**

Safety and Codes and Standards funding includes international activities as well as national development and coordination among several agencies. While funding had been a major concern in the past, the subprogram has received full funding for the past two fiscal years. This fiscal year, the subprogram received full funding.



**Majority of Reviewer Comments and Recommendations:**

Subprogram scores were average to high, with an overall average of 3.7. The planning and analysis for the Materials Compatibility effort was praised. The close collaboration exhibited in the Hydrogen Codes and Standards activity was seen as impressive. The database, best practices manual, and hydrogen fuel cell vehicle simulator prop were viewed as good ways to disseminate hydrogen safety information. The Hydrogen Fuel Quality work, which is seen as key to a successful transition to widespread adoption of hydrogen technology was praised for its coordination. The Hydrogen Safety Panel was viewed as important part of the continuous safety process.

Recommendations included:

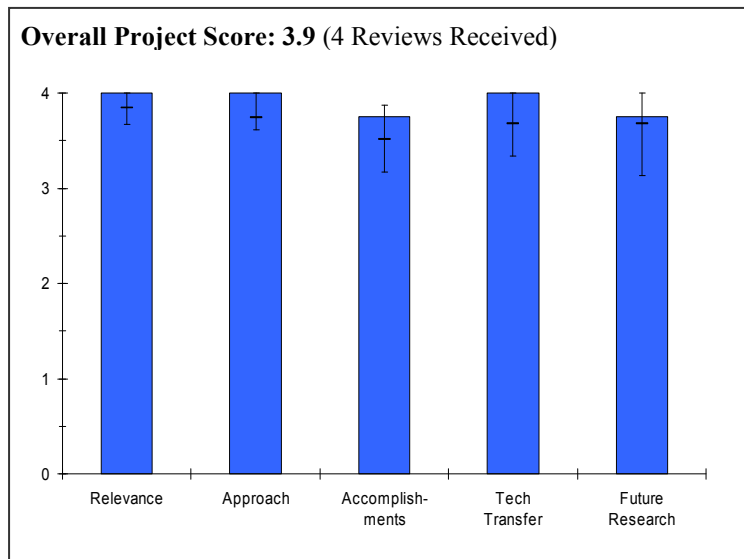
- Improve collaboration between international and domestic SDOs under the purview of the Codes and Standards activity.
- Expand materials set to include new materials and “legacy” materials. Effects such as brinelling and other materials degradation should be considered for the Materials Compatibility work.
- Garner content for the incidents database and best practices manual from commercial rather than industrial practices.
- Leverage data from existing projects and open sharing and cataloguing of data among researchers for benefit of the hydrogen fuel quality project.
- The Hydrogen Safety Panel should increase its output of safety reviews and white papers.

**Project # SA-01: Hydrogen Codes and Standards***Robert Burgess; NREL***Brief Summary of Project**

The objectives of this project are to 1) conduct research and development needed to establish sound technical requirements for hydrogen codes and standards; 2) support code development for the safe use of hydrogen in commercial, residential and transportation applications; 3) advance hydrogen safety, code development and market transformation issues by collaboration with appropriate stakeholders; and 4) facilitate the safe deployment of hydrogen technologies.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **4.0** for its relevance to DOE objectives.



- This project addresses a fundamental barrier to the introduction of hydrogen energy technologies.
- It addresses specifically and fully the listed program barriers.
- Developing technical requirements for hydrogen codes and standards is essential to the Department of Energy's Hydrogen Program to ensure that the codes and standards are developed in a manner that promotes the safe and successful commercial launch of hydrogen and fuel cell technologies without inhibiting technical progress. The National Renewable Energy Laboratory's contribution is vital in this way.
- Outstanding: domestic model code, design code, product standard, and material test method work are progressing apace with the evolution of the technology. The work is leveraging the synergy of the domestic standards development organizations (SDOs) to avoid redundancy, isolationism, and territorialism.
- The project addresses and leads to reduction of "barriers to trade" - roadblocks to technology deployment.
- This project is essential for market transformation.

**Question 2: Approach to performing the research and development**

This project was rated **4.0** on its approach.

- Strength: component and sensor testing; garage issues.
- Question on CFD activities: is there collaboration with the French group at INERIS/CEA concerning their garage experiments?
- Question: how do the CFD activities correlate with the codes and standards work?
- The research and development of the technical background ensures that the proper codes and standards will be developed.
- Additionally, the permitting workshops strongly support infrastructure development by educating AHJs and permit officials so the technical background behind the codes is understood.
- Outstanding. This activity is fully open to all parties and all parties are encouraged to contribute.
- This project has a focused objective to conduct the research and development needed to support sound technical requirements in consensus standards.
- Since codes and standards are by their nature collaborative activities, the approach emphasizing coordination, collaboration, workshops, and publications is exactly correct.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.8** based on accomplishments.

- Strength: excellent knowledge transfer strategy.
- Strength: excellent codes and standards coordination and development support work (e.g., ISO, SAE, NFPA C&D activities).
- Weakness: CFD/validation work concerning the garage/enclosed area problem is currently underway at CEA/INERIS as part of the DRIVE initiative (instrumented garage already available). Some collaboration would be nice for validation purposes.
- The National Renewable Energy Laboratory consistently proves itself to be a laboratory capable of conducting highly technical component testing. This project is no exception.
- Very good. Work is progressing as fast as industry is supporting it, as it should.
- The presentation documented eight diverse accomplishments, all valuable and well done.
- The presentation demonstrated good collaboration with the consensus standards community (e.g., SAE, CSA, ASTM, ISO, etc.)
- The principals demonstrated great leadership in the National Hydrogen and Fuel Cells Codes & Standards Coordinating Committee.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **4.0** for technology transfer and collaboration.

- Strength: there is tight integration and networking with international efforts.
- Strength: significant efforts have been made.
- There is much collaboration between the National Renewable Energy Laboratory and SDOs, key stakeholders, national labs, and industry. This collaboration ensures that the research benefits the industry as a whole.
- Outstanding. Being an open dialogue with all parties has established an open structure where input and information is flowing to where it is needed without presupposing who would need it.
- The principals demonstrated close cooperation with leading standards development organizations, as previously mentioned.
- The principals demonstrated great leadership in the committees on which they served.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.8** for proposed future work.

- Strength: strong and impressive program.
- The specific roles of the National Renewable Energy Laboratory and Sandia should be clarified in the future garage simulations/validations; they seem to have converging objectives
- The future work identified in the presentation is necessary. However, further research, particularly into hydrogen quality, is necessary.
- Outstanding. The future plans are to continue the course to completion.
- The proposed future work continues to be relevant and the approach continues to be good.
- The coordination between internally conducted research and development and external communities of interest continues to be well planned.
- The proposed work on back-up power for telecommunications is relevant to the program and well linked to past standards work (e.g., permitting workshop).

**Strengths and weaknesses****Strengths**

- This project is very strong in all of its objectives, particularly the codes and standards work.

## **SAFETY, CODES & STANDARDS**

- The National Renewable Energy Laboratory's research and collaboration with SDOs will help to ensure a safe roll out of the hydrogen industry.
- There is synergy and cooperation among all the contributing domestic parties.
- The codes and standards advanced by this work are essential in enabling technology deployment.
- There is excellent coordination and outreach.
- The external collaborations motivate and inform the internally conducted research.

### Weaknesses

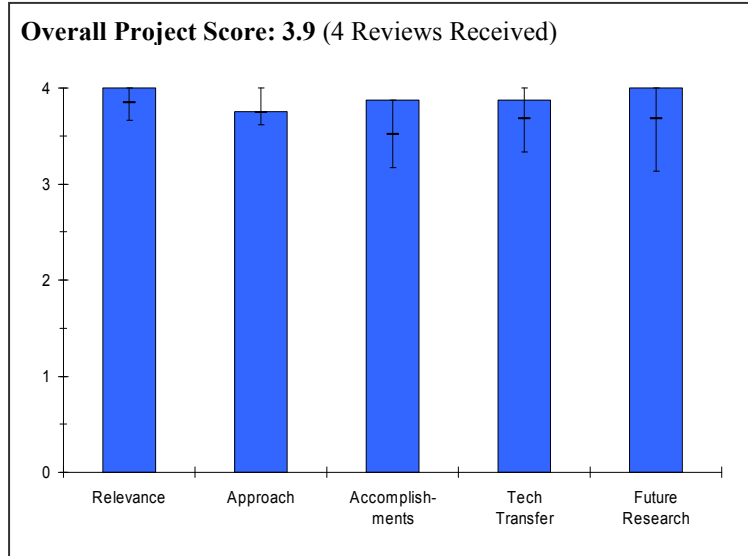
- An increase in the collaboration between international and domestic SDOs is necessary.
- There remains an attitude to focus activity and credit to ISO at the expense of the ANSI-recognized SDOs and code development organizations. It is important to note that state and local regulators use ANSI standards not ISO standards.
- Also, I believe that the fuel quality slide is inaccurate. See notes supplied to A. Ruiz for US Fuel Cell Council.

### Specific recommendations and additions or deletions to the work scope

- Underground garages and tunnels should certainly be a focus of the simulation group.
- Seek specific input on this project from HySafe.
- Leak rate measurements from components.
- Hydrogen quality research efforts should extend beyond ISO and SAE. Assistance is needed in ASTM D03.14 to develop proper test methodologies.
- A 70 MPa Particulate Sampling Adapter has not been developed. The 70 MPa Hydrogen Quality Sampling Adapter collects gaseous for constituent analysis, but particulate analysis is part of the J2719; thus the ISO and DMS report/guidelines/interim standards.

**Project # SA-02: Materials Compatibility***Brian Somerday; SNL***Brief Summary of Project**

The objectives of this project are to 1) enable development and implementation of codes and standards for hydrogen containment components; 2) evaluate data on mechanical properties of materials in hydrogen gas; 3) generate new benchmark data on high-priority materials; 4) establish procedures for reliable materials testing; and 5) participate directly in standards development. Sandia completed measurements cracking thresholds for SA 372 Gr. J, DOT 3T, and DOR 3AAX steels in high pressure hydrogen. Also, the effects of fabrication and service variables on hydrogen-assisted fracture in 316 stainless steel were evaluated.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **4.0** for its relevance to DOE objectives.

- Objectives are directly relevant to addressing the cited Department of Energy barriers.
- The research into materials compatibility and associated involvement with standards development organizations taking place at Sandia National Laboratories is vital to the DOE Hydrogen Program to ensure a safe and successful industry, specifically by providing a guideline for station or technology developers to follow for assurance of hydrogen compatibility.
- Material properties are essential to safe design of hydrogen systems.
- Safe design of hydrogen systems is essential to a safe hydrogen infrastructure.
- This work supports traditional design methods.
- Hydrogen embrittlement of structural materials is an important safety consideration in technology adoption; this project provides high-quality reference data and standards to enable appropriate engineering.

**Question 2: Approach to performing the research and development**

This project was rated **3.8** on its approach.

- Impressive experimental facilities.
- The applied research and standard development at Sandia has proven incredibly successful, from the materials reference guide to the direct input into KD-10. Enabling the development of standards has been and will continue to be exceeding expectations if Sandia continues using the current approach.
- Good selection of materials.
- Additional materials could enhance the usability of the project data.
- It is important to also check "legacy" materials where modern data is not available, such as existing pipeline materials and existing valve, pressure vessel, and appurtenance material where data is lacking.
- It is important to test materials that are candidate materials for advanced systems. This should be done by working with advanced tank and system designers in the Hydrogen Program.
- This project provides technical data and best practices to enable rational design of hydrogen storage containers (e.g., tanks and even pipelines).
- It is a solid approach to develop engineering data through research and then to allow the consensus standards community to interpret the data and to draw the conclusions from them.



**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.9** based on accomplishments.

- Strength: excellent progress on the hydrogen compatibility of materials information materials.
- The technical accomplishments at Sandia are phenomenal: thorough, directly applicable.
- Very impressed with the pressure vessel to evaluate fatigue crack growth.
- Good progress.
- Learning from the results as they go.
- The compilation "Technical Reference on Hydrogen Compatibility of Materials" is particularly noteworthy.
- The pressure vessel for high-pressure testing of hydrogen is an extremely valuable asset.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.9** for technology transfer and collaboration.

- International Energy Agency Task 22/Task 19 issues.
- Sandia's direct involvement, specifically with developing KD-10, is representative of Sandia's vast amount of collaboration with industry stakeholders to ensure proper information is shared.
- The project could be enhanced by polling the entire Hydrogen Program for candidate materials of interest.
- There is direct coordination with relevant standards development organizations, including ASME and CSA, and relevant industry (e.g., Swagelok and Fibatech).
- This work complements work being done under the Production and Delivery program element well.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **4.0** for proposed future work.

- Sandia's future research work extending beyond normal hydrogen (i.e., compatible materials fatigue testing) will add to the understanding of the mechanics behind hydrogen embrittlement and/or material fatigue associated with hydrogen. This extended understanding will assist in developing standards for safe design.
- Well-planned program.
- The proposed future research is a natural extension of on-going work.
- The work thus far emphasizes static loading. The proposed future work on fatigue crack growth rates and other deleterious effects of in-service vibration and pressure cycling would be very valuable.

**Strengths and weaknesses**

Strengths

- Technology, thoroughness, and a fantastic presenter.
- Excellent analytics.
- Learning from experience and data obtained.
- Supports traditional design methods, such as ASME.
- The development of fundamental engineering data by an impartial and competent laboratory is an essential part of the Hydrogen Program.

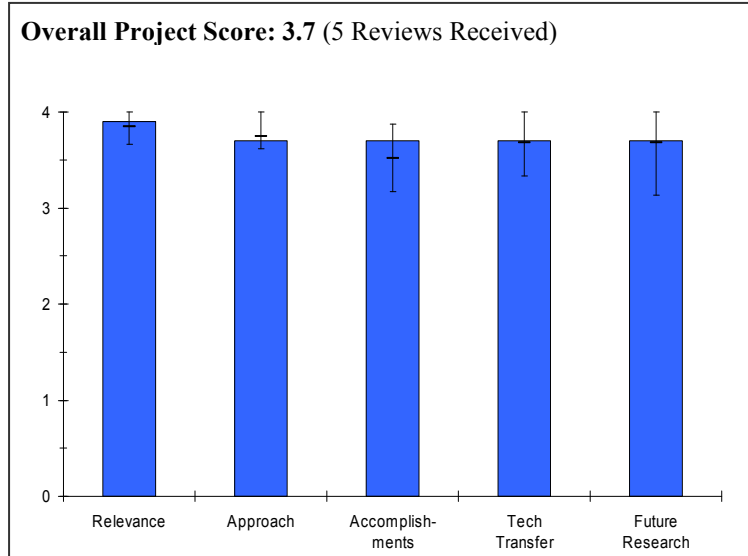
Weaknesses

**Specific recommendations and additions or deletions to the work scope**

- An understanding of particulate formation in a fueling system (such as nozzle brinelling or other material break-down) would assist in the development in hydrogen quality standards.
- Polling the Hydrogen Program, at large, for candidate materials might enhance the project.
- Higher-pressure testing might be an enhancement.

**Project # SA-03: Hydrogen Safety Tools: Software and Hardware***Linda Fassbender; PNNL***Brief Summary of Project**

The objectives of this project are to 1) capture the vast knowledge base of hydrogen experience and make it publicly available to those working with hydrogen and related systems, including those just starting to work with hydrogen; 2) collect information and share lessons learned from hydrogen incidents and near-misses with the goal of preventing similar incidents from occurring in the future; and 3) support the design, construction, commissioning and training use of a life-size mobile fuel cell vehicle burn prop that is hydrogen-specific.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.9** for its relevance to DOE objectives.

- The project fully addresses all three barriers that it targets and will contribute to increasing the acceptance of hydrogen energy technologies among authorities having jurisdiction.
- Capturing and reporting best practices and incidents is vital to avoiding future incidents.
- Very good. The work is generating useful guidance.
- The subprojects to capture data in a coherent form (Safety Best Practices and Incident Reporting) will lead to better consensus standards and better acceptance of hydrogen technology.
- The relevance as demonstrated by the NRC Phase 2 Report on FreedomCAR is documented on Slide 3.
- The simulator prop is very valuable for training first responders.

**Question 2: Approach to performing the research and development**

This project was rated **3.7** on its approach.

- The approach addresses all three barriers the project is supposed to address: best practices manual; fuel cell vehicle training (simulator prop); incident reporting (database).
- Web-based tools and hands-on props speak directly to the appropriate audience(s). However, an online submittal form may not provide industry members with sufficient confidence in submitting incident reports.
- Very good. The approach is rational and working.
- Need to reach out more to transportation communities, especially vehicle manufacturers (truck manufacturers associations) and maintenance organizations; for example, USDOT/PHMSA (pipeline safety and HAZMAT transportation); ASE; USDOT/PTA (hydrogen and fuel cell transit).
- The principals are to be commended for developing a well-organized and public website.
- The open sharing of lessons learned is exactly the approach best taken.
- The reporting tool is a good complement to the Safety subprogram.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.7** based on accomplishments.

- Strength: database, prop, and best practice manuals are all important contributions to hydrogen safety.

- Weakness: missing some important NASA input (the NASA Safety Standard and the NASA Glenn Safety Manual chapter 6).
- The websites and prop accomplish the goals of this project.
- Very good. The progress is where one would expect at this point in the project.
- The site is easy to navigate and use. A few "mouse-overs" need to be checked, they are hard to point to.
- Add "vehicle (car/truck/bus)" to choice of "settings" on hydrogen incidents page.
- Impressive accomplishments were made on all three subprojects (see, e.g., Slides 7, 9, 14, 17, and 18).

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.7** for technology transfer and collaboration.

- Strength: very good interaction.
- Weakness: is some NASA input to the database possible?
- It appears that the safety tools have most key stakeholders involved.
- Very good. This activity is being conducted with complete transparency.
- Overall, very strong. Should reach out more to vehicle operations and maintenance communities.
- Particularly impressive aspects of this project are its public face and the depth of data and design reviews conducted.
- The collaboration with firefighters (first responders) on the simulator prop is very good and beneficial to the Hydrogen Program.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.7** for proposed future work.

- The hydrogen fuel cell vehicle simulator prop should be integrated with current first responder training, already developed.
- Continuous updates to the websites will further help to avoid future incidents.
- Very good. This activity should continue the course.
- Need to consider needs of end-user communities with less engineering and technological expertise.
- The additional data proposed for the websites (Slides 10 and 15) are useful and appropriate.

### **Strengths and weaknesses**

#### Strengths

- Important contributions to facilitate the introduction of hydrogen energy technologies.
- Industry support.
- Highly accessible, comprehensive, "one-stop shop". Excellent progress, strong reporting, and posting of work in progress.
- The extent to which the public is clearly the "customer" of this project and the many steps taken to ensure customer satisfaction.
- The depth of data and design reviews conducted.

#### Weaknesses

- Focus on hydrogen, which is following industrial practice, and not compressed gas storage, which follows both industrial and commercial practices.

### **Specific recommendations and additions or deletions to the work scope**

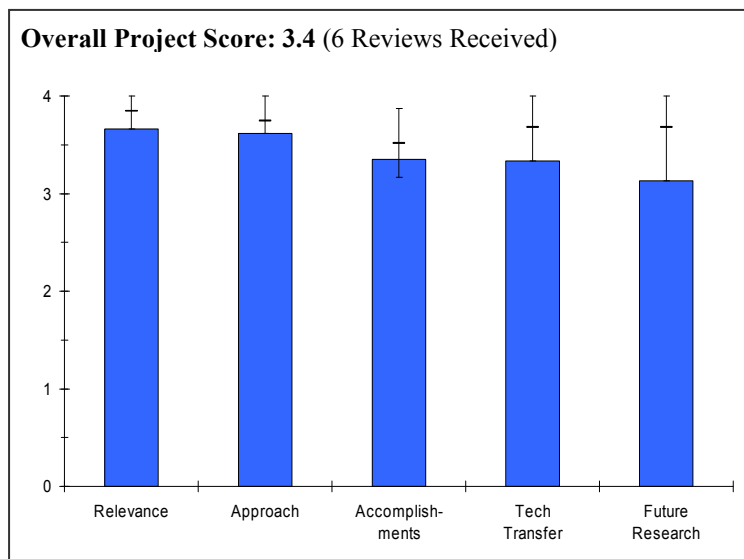
- Projects should actually be compelled to contribute incidents.
- A second database on commercial compressed gas vehicle incidents may be more instructive as far as lessons learned than monitoring industrial hydrogen practices.

**Project # SA-04: Hydrogen Fuel Quality***Tommy Rockward; LANL***Brief Summary of Project**

The objectives of this project are to 1) conduct gauge studies with testing labs and address experimental differences, thus increasing the confidence in the data; 2) create and standardize a Data reporting Format; 3) develop and test new analytical methods for detecting ppb levels of contaminants; and 4) test the critical constituents (NH<sub>3</sub>, CO, and H<sub>2</sub>S) and provide data sets to fuel cell modelers to establish predictive mechanistic models.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.7** for its relevance to DOE objectives.



- Excellent alignment with key barriers to achieving codes and standards for implementation of fuel cell technologies in the United States and for consistency with emerging international standards.
- The project is highly relevant and addresses important barriers.
- Hydrogen fuel quality has the ability to hinder the industry if inappropriate standards are set. Hydrogen quality research is vital to a successful industry launch.
- Very good. This activity has addressed a lack of coordination in the research in this area. The activity is now coordinated and the researchers are attempting to collaborate.
- The project is well in line with key Department of Energy objectives on hydrogen standardization.
- The smoothing of conflicts is particularly useful in U.S. situations with a variety of actors.
- Addresses an important barrier, the development of harmonized standards for hydrogen quality determination and requirements.

**Question 2: Approach to performing the research and development**

This project was rated **3.6** on its approach.

- Strong approach that leverages data from multiple sources for reliability and reproducibility.
- Good balance between understanding fundamentals of fuel impurity impacts, developing analytical methods for impurity detection, and developing codes and standards based on what is technically feasible.
- Very strong round-robin testing approach in which same cell tested by multiple participants with initial and final tests at Los Alamos National Laboratory.
- Strength: standardization efforts (reporting format, round robin verification of methodology) are a very worthwhile objective.
- Weakness: the study seems to address only specific contaminants. There is probably an effect from the storage technology used (chemical hydride storage, metal hydrides, adsorbents) on the level and the nature of impurities on the hydrogen released, and it would be important to perform such studies. This could actually help to qualify the usefulness of these storage strategies.
- Understanding the effects of constituents on the fuel cell stack and identifying proper analytical methods is the appropriate approach.
- The round-robin testing with the single cell utilizing the U.S. Fuel Cell Council procedure to calibrate all laboratories involved reduces potential future technical barriers.

- Outstanding. The round-robin activity forced the researchers to work together to generate and execute a detailed test method and resolve testing anomalies. This activity has resulted in data that is repeatable at a number of labs and reproducible among labs. This allows the merging of test data sets from multiple labs with a high degree of confidence.
- The approach is good with clear indication of activities to overcome the addressed barriers.
- The use of round robin requires better description in the way fuel cells systems, used as reference test sample, are chosen.
- The PI is not clear in distinguishing the role of round robin, which is addressed to verify data reproducibility on fuel quality in various test labs, from the research needs to analyze fuel impact, which mostly depend on fuel cell system design and operating conditions.
- Very good combination of determining what the sensitivity of testing is and then identifying the methods for testing for the critical impurities.
- The overall thinking is that technology development and codes and standards development should go in parallel. This project is carrying its own effort in parallel – learning about the impurities effect on fuel cells and identifying how the codes and standards should be developed. This is a good approach.
- There seems to be a great amount of effort in making sure that they "get it right." This is evident in the painstaking method of testing the cells before and after the round robin, and in running the round robin in an exhaustive manner. The amount of data gathering gives one confidence.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.4** based on accomplishments.

- Excellent progress in developing and demonstrating consistent testing protocols and results at a good number (4+LANL) test sites.
- Good progress developing data reporting format. Not sure if this format has been implemented yet or will be tried this coming year.
- Excellent progress assessing impact of H<sub>2</sub>S, NH<sub>3</sub>, and CO on fuel cell performance and understanding the mechanisms that lead to degraded performance.
- Longer duration contaminant studies will probably be necessary, and evaluation of recovery from higher impurity concentrations should be evaluated.
- Good breakthrough in developing method to assess sulfur ion concentration at very low concentrations.
- Strength: good progress so far on standardizing and validating measurements.
- Weakness: identifying contaminants and tolerance to contaminants (only sulfur was completed?) should probably have been an earlier priority, as this may affect the testing procedures.
- The collection of data thus far appears thorough and accurate.
- Very good. One barrier appears to still remain, the parochialism of the researchers to share unpublished data. This perceived barrier may delay completion of this effort beyond the DOE target dates.
- The results are valuable and interesting in harmonizing fuel quality analytical methods and specific equipment for contaminants determination.
- The round robin is instrumental to create a common basis for hydrogen fuel specifications and measurements.
- The PI does not clearly explain how contaminants analysis is related to fuel cell characteristics and operations, which makes this activity less relevant to harmonize fuel analysis methods to address DOE barriers.
- A large amount of progress appears to have been accomplished by the Los Alamos National Laboratory team.
- The team seems to have successfully moved from calibration and standardization, through Los Alamos National Laboratory and the round robin tests, to conveying with confidence that impurity data are not cell or test-method anomalies.
- The only minor issue here is that the presentation was a bit hard to follow in places. The presenter needed a pointer.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- Good collaboration among team members.
- Good effort to implement data reporting formation as part of standards community.
- Additional collaboration with ASTM and industry members should be included.
- Very good. The industry and academic cooperation is working well.
- The national testing network is well coordinated with good integration of testing laboratories and expertise.
- The PI describes the international activities well, along with the development of the data reporting format.
- The extensive collaboration with modelers and developers requires better description to identify actors and advantages for each.
- Seems like a good and successful use of the round robin participants.
- A bit unclear as to what the roles of the lab partners (SRNL, NIST, NREL, ANL) were.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Reasonable extension of prior activities.
- Need to address what the recommended impurity standards are going to be in terms of what can be measured and what is actually required for fuel cell performance. Focus seems to be too much on pushing the envelope on what is possible analytically in terms of detection without adequate tie-in to what level of analytical detection is required in terms of practical fuel cells.
- Strength: coherent future research that builds on past progress planned.
- Weakness: the effect of the production/storage/purification chain on contaminant levels should probably be addressed.
- Cannot wait to see the results of all of this hard work!
- Very good. The task is to follow through with the plan.
- The future activities are well-aligned with the DOE barriers and previous results.
- The planning must better focus on basic testing procedures definition with the extension to other laboratories and coordinate with international activities.
- The contaminant-effect analysis requires better specifications with clear identification of reference samples (fuel cell) and stakeholders.
- Their proposed future work appears to be just what is needed.
- The international portion may be difficult.

#### **Strengths and weaknesses**

##### Strengths

- Important project that could affect several aspects of hydrogen energy technologies – production, purification and storage technologies.
- Collaboration with industry and researchers.
- The project has created a large testing network with valuable collaborations to be used for further harmonizing common testing analytical methods.
- The international role is very important with adequate resources and expertise to fully support the action in ISO activities on fuel quality specifications and standards.
- Painstaking care in approach.
- Data look quite convincing.

##### Weaknesses

- Lack of a database of contaminants and their effect on fuel cell.
- Parochialism of researchers with data.
- The project must be sure to effectively represent in international setting bodies the complete needs and expertise in the United States.
- The planning does not clearly specify the existing collaborations and the technical background to make the contaminant analysis more effective.

## **SAFETY, CODES & STANDARDS**

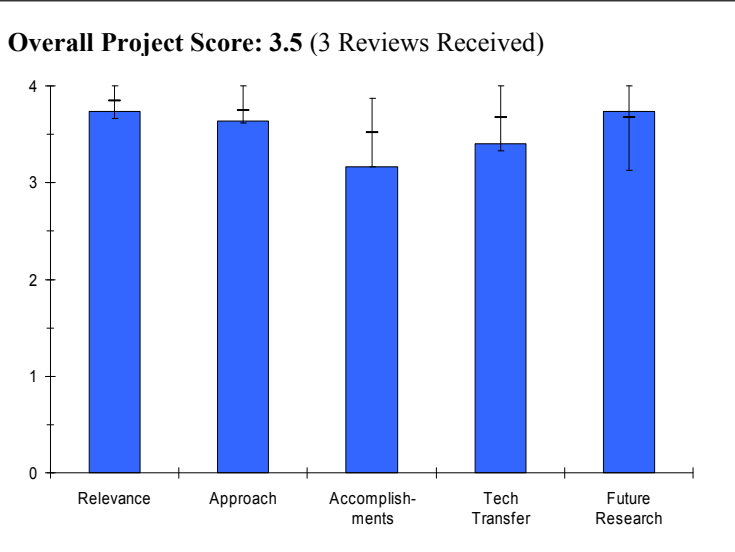
- The project is not sufficiently using the large amount of research work and results on testing methods and contaminants analysis coming from specific projects in other subprograms, such as Fuel Cells, Technology Validation, and/or Analysis.
- Some of the presentation was a little hard to follow. (Give the young man a pointer to use next time!)

### **Specific recommendations and additions or deletions to the work scope**

- Fuel impurities that would come from unconventional storage units. Coordinate with Storage activities, specifically, metal hydrides, physisorbents (also important in purification), and chemical hydrides.
- Evaluation of commercial and industrial cleansers. The hydrogen-containing components need to be cleaned to prevent contamination. The cleanser should not be a contaminant.
- The project must focus more on analytical methods and the creation of the large testing network for fuel quality analysis.
- The project must use more ongoing projects' results by screening and extending collaborations with other projects in different subprograms.

**Project # SA-06: Hydrogen Safety Panel***Steven Weiner; PNNL***Brief Summary of Project**

The objectives of this project are to 1) provide expertise and guidance to the Department of Energy (DOE) and assist with identifying safety-related technical data gaps, best practices and lessons learned; and 2) help the DOE integrate safety planning into funded projects to ensure that all projects address and incorporate hydrogen and related safety practices. Pacific Northwest National Laboratory will engage panel members, original equipment manufacturers, energy companies, international partners, first responders and other stakeholders in all aspects of the hydrogen safety program.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.7** for its relevance to DOE objectives.

- Safety should be the top priority of the Department of Energy's Hydrogen Program. The hydrogen safety panel ensures that all safety concerns are thoroughly investigated to reduce risks in the future, thereby ensuring the safety of all involved.
- Very good. The safety review of the DOE projects is an important activity.
- Very relevant. Need more work here.
- Make an effort to engage local agencies in some way – personally, meetings, briefs, etc.

**Question 2: Approach to performing the research and development**

This project was rated **3.6** on its approach.

- It is important to note that safety is a continuous process. As long as industry members are and will remain active, the approach is sufficient.
- Very good. The process is tried and true.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.2** based on accomplishments.

- It would be beneficial to see more whitepapers come from this group.
- Good. The number of safety plans reviewed (approximately two per month) is realistic. However, the conduction of only five safety reviews (about half a review per month) shows an area for potential improvement.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.4** for technology transfer and collaboration.

- More participation from automakers.
- Very good. This activity is being conducted with complete transparency.



**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.7** for proposed future work.

- Again, safety is a continuous process. The future work proposed is necessary.
- Very good. This activity should continue the course.

**Strengths and weaknesses**

Strengths

- The team has strong technical background, good industry input.
- Industry representation.

Weaknesses

- The number of safety reviews. It is not unreasonable to think that one project a month is attainable without overly taxing the volunteer membership. Focus should include the academic labs working with hydrogen and other compressed gases.

**Specific recommendations and additions or deletions to the work scope**

- The effects of these safety learnings on liability, insurance, etc. for station developers and/or owners was not shown as addressed in the presentation. There may become a more prominent need for the industry as stations are built if this is not already being investigated.
- Engage local fire and safety officials.
- Publicize panel activities on websites (e.g., EERE, PNNL, etc.).

**Project # SAP-01: Codes & Standards for the Hydrogen Economy***Gary Nakarado; Regulatory Logic***Brief Summary of Project**

The objectives of this project are to 1) accelerate the availability of appropriate codes and standards to ensure consistency and, if possible, uniformity of requirements and to facilitate deployment; 2) enable certification to applicable standards in order to facilitate approval by local code officials and safety inspectors; and 3) promote uniform standards because manufacturers cannot cost-effectively manufacture multiple products that would be required to meet different and inconsistent standards.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.8** for its relevance to DOE objectives.

- Very good in support of enabling the Department of Energy to support the development of model codes, design codes, and product standards and material test methods.
- Codes and standards are essential for technology deployment and risk management (insurance underwriting).
- Standards development organizations provide fora, but standards do not actually get written without determined and sustained leadership.
- Leaders are often volunteers and the individual financial burden (e.g., meeting travel) is more than they can personally sustain.
- This project provides support to leaders to ensure that codes and standards actually get written.

**Question 2: Approach to performing the research and development**

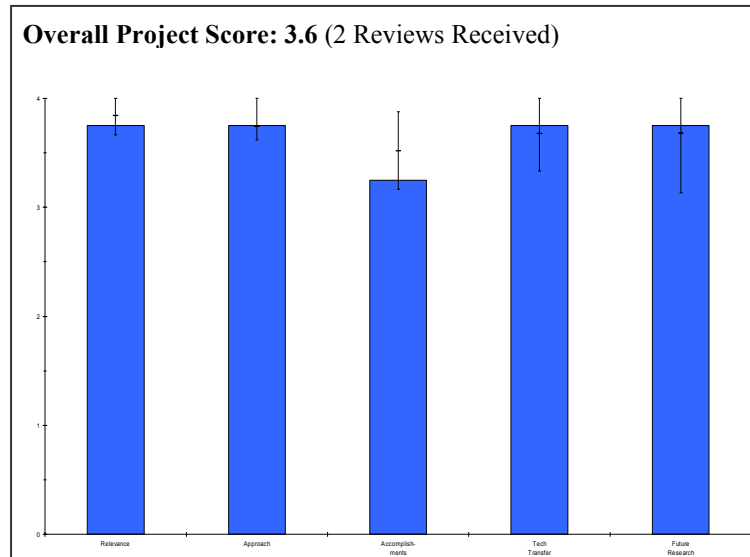
This project was rated **3.8** on its approach.

- Good in support of enabling DOE to generate the appropriate test data to support the development of the document types noted above.
- This project is outsourced, back office support for DOE at the National Renewable Energy Laboratory.
- The function of this project is to disperse support payments, using subcontracts, to standards development organizations (most often, non-profit organizations) or otherwise support standards development for the public good.
- This project performs low-overhead business services.
- This project, by its nature, performs no research and development and makes no technical decisions.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- Good in support of enabling DOE to meet its self-imposed scheduled deadline.
- The project is performing its business function well.
- In future reviews, presentation should clarify what the subcontract deliverables are and whether or not they are meeting expectations.



**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.8** for technology transfer and collaboration.

- Does not apply. The closest comment is that they appear to be properly supporting the DOE-selected standards development organizations.
- The essence of this project is collaboration within voluntary consensus standards organizations.
- The consensus standards process produces documents that describe best technology and practices, for general public benefit.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.8** for proposed future work.

- Does not apply. The closest comment is that they appear to be properly supporting DOE by directing additional research contracts as directed by DOE in direct support of the above discussed types of documents.
- The project strives for continuous improvement in its business operations.

**Strengths and weaknesses**

Strengths

- Supports DOE with financial administrative support.
- Unloads national laboratory assets.
- Appears to be more cost-effective and responsive than having the national laboratory administer.
- Codes and consensus standards take years of work and must be produced well in advance of technology deployment, which their absence can often frustrate.
- This project addresses the reality that standards are often written by volunteers (such as retired persons), who would otherwise have no source of support than their own personal funds.
- This project allows the sustained effort of volunteers, which they might otherwise be unable to provide.

Weaknesses

- Although this project does not make technical decisions, increased emphasis should be given to tracking the subcontract deliverables.

**Specific recommendations and additions or deletions to the work scope**

- None.

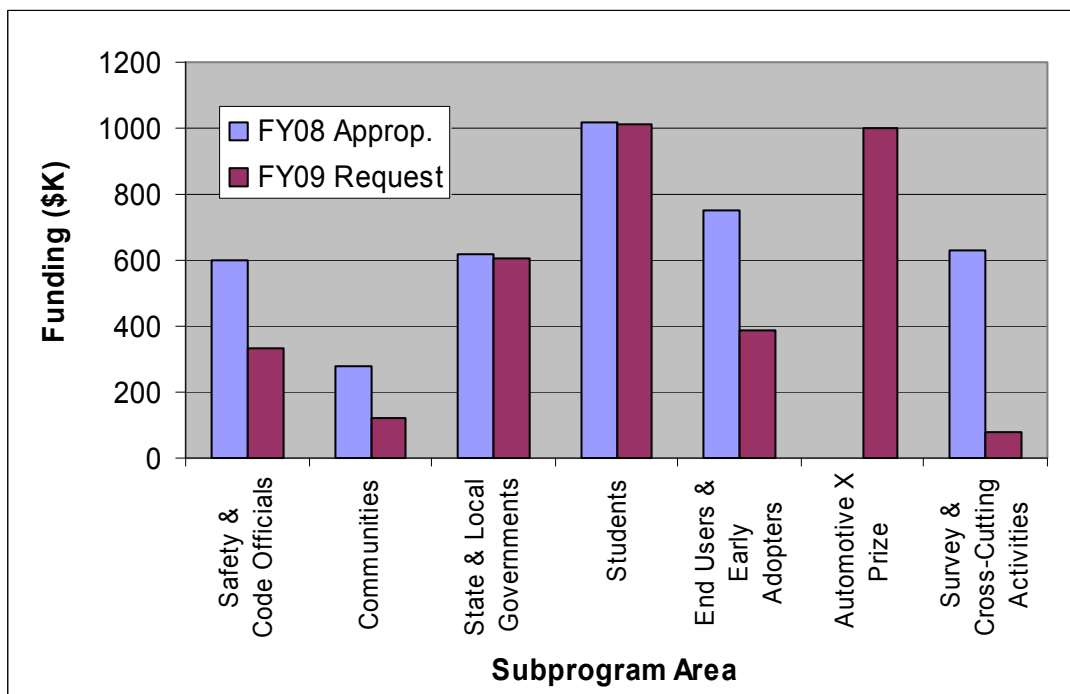
## 2008 Education Summary of Annual Merit Review Education Subprogram

**Summary of Reviewer Comments on Education Subprogram:**

Reviewers expressed the importance of education, raising awareness of hydrogen and fuel cell technology, and correcting false perceptions or misinformation. The education subprogram structure and focus were considered well-defined and appropriate, with projects well-aligned with DOE targets. Reviewer comments underscored the importance of metrics across all projects, collaboration with partners, and using new media to reach a “tech-savvy” audience that may be among the first to adopt hydrogen fuel cell technology. Reviewers also noted the daunting challenge of educating a largely uninformed public that is often confronted with mixed messages. Reviewers specifically commended the strong partnerships and efforts to collect input and feedback from industry partners and other experts to ensure technical accuracy and maximum usability of materials.

**Hydrogen Education Funding:**

The Education subprogram efforts are prioritized to focus on the target audiences involved in facilitating the near-term use of hydrogen and fuel cell technology. With funding at the request level, the FY 2008 budget allowed for support of projects across the education portfolio, including new competitively-awarded projects focused on outreach to state and local government officials and potential end users, as well as projects to develop and expand university hydrogen and fuel cell education programs. FY 2008 funds also support ongoing efforts to educate first responders and code officials, local communities, and teachers and students at the middle and high school levels. In FY 2009, the hydrogen education subprogram will move to the Vehicle Technologies Program to build on synergy with related education efforts in other alternative transportation fuels and energy-efficient vehicle technologies, including plug-in hybrids.



**Majority of Reviewer Comments and Recommendations:**

Reviewer scores for the education projects reviewed were average, with scores of 3.9, 3.4, and 2.8 for the highest, average, and lowest scores, respectively. Scores reflect progress made over the last year and reported plans for future activity. Key comments and recommendations are summarized below. DOE will act on reviewer recommendations as appropriate to the overall scope, direction, and coherency of the education effort.

**Knowledge and Opinions Assessment:** Reviewers noted the importance of the Knowledge and Opinions Assessment for helping to frame messaging and measuring progress. They felt the survey's statistical analysis is proficient and well thought-out, although for the public survey, many viewed the selected methodology of computer assisted telephone interviewing as being limited to a certain segment of the population. To remain statistically valid and adequately compare results over time, the follow-up survey methodology and survey instruments must remain the same as what was used for the baseline survey. Reviewers suggested coordinating the survey to align with other outreach projects.

**First responders:** This target audience is critical to successful market transformation. Reviewers credited efforts to pilot test, review, and validate the introductory course material prior to officially launching it, and noted successful usage. They also recognized the effective collaboration with first responder trainers at the Volpentest Hazardous Materials Management and Emergency Response (HAMMER) training facility and the importance of the steering committee, which includes representatives of both the hydrogen and first responder communities, to ensuring the appropriateness and usability of the new advanced-level, hands-on "prop course." For both the introductory course and the prop course, reviewers recommended a greater focus on near-term hydrogen applications such as forklifts.

**Code officials:** Reviewers felt that educating code and permitting officials is essential and highly relevant to the DOE Hydrogen Program. They felt that the project presented includes the right collaborations to ensure usability, and that as an interactive learning program, the e-learning modules should be effective. Reviewers suggested developing a more robust course deployment plan.

**Local communities:** Reviewers felt that public education activities are well-aligned with DOE objectives and reiterated the importance of ensuring that messages communicate realistic expectations for technology availability and the expected commercialization timeline. Both the "Increase Your H2IQ" and "H2 and You" public education efforts seek to engage the public through new media using simple and objective messaging, but cover different "space" using different tactics. Reviewers felt that both approaches are well-defined, yet recognized the need for partnerships as well as clear metrics to evaluate project success.

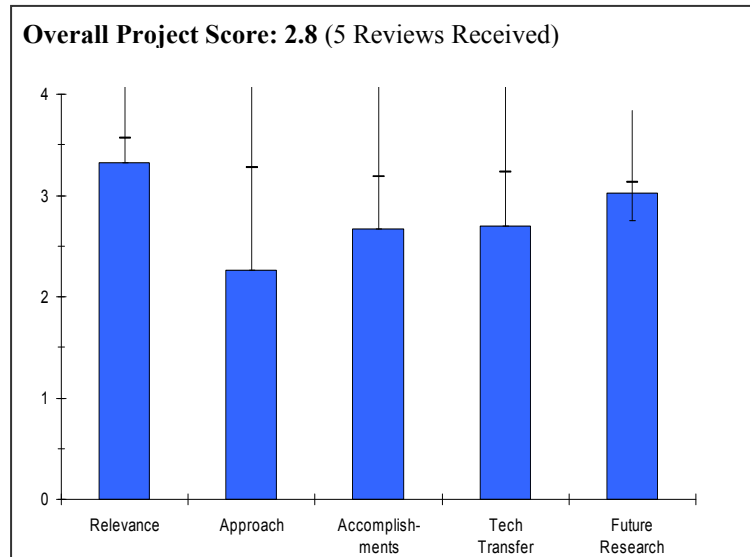
**Middle and high schools:** Reviewers felt that the middle school project is an aggressive, well thought-out effort to educate an important target audience. They also noted that the project team developed an excellent, collaborative approach that involves hands-on learning and addresses teaching standards. Reviewers noted the project makes great use of resources and partners; they suggested reviewing and possibly enhancing metrics. Note: The project focused on high schools was not reviewed because the principal investigator was unable to present due to illness.

## Project # ED-01: Hydrogen Knowledge and Opinions Assessment

Rick Schmoyer; ORNL

### Brief Summary of Project

The objectives of this project are to 1) measure the current level of awareness and understanding of hydrogen and fuel cell technologies in five target populations (general public, students, state and local government agencies, potential end users, safety and code officials); 2) compare the current level of awareness and understanding to results of the 2004 baseline; and 3) analyze and summarize results for use in developing strategies and tactics for the hydrogen education subprogram. A compendium of related surveys conducted since the 2003 literature review has been completed as well as the 2008 general public survey. The 2008 state and local government officials survey was underway during the week of the DOE Hydrogen Program Annual Merit Review.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Understanding the public's understanding and acceptance of hydrogen is important to future commercialization.
- Target populations for surveys are highly consistent with DOE H<sub>2</sub> Education Subprogram goals.
- Data gathered is very helpful for framing DOE's message and publications in education.
- The project is very relevant because it measures progress. Metrics are important to report success to Congress, the general public, and other stakeholders.
- Literature review to assess public hydrogen attitudes is important.
- Conducting controlled surveys of different public sectors is of interest.

### Question 2: Approach to performing the research and development

This project was rated **2.3** on its approach.

- Approach is sound but with some flaws based on "known" survey tools of cold-calling.
- Statistical analysis is very proficient and well thought out.
- Survey questions were well thought out and appropriate.
- The 4-year window between surveys may be longer than necessary to obtain statistically relevant results. A 2-3 year window may provide more timely input to the Principal Investigator.
- It is difficult to ascertain whether any increased target audience knowledge on hydrogen is attributable to efforts made by the DOE H<sub>2</sub> Program, or by general information penetration via other sources.
- Telephone interviews are hard because a lot of people only have cell phones (no land lines).
- [Many people] use Caller ID to screen calls.
- Hard to get large response or keep people on phone for entire survey.
- [The survey is possibly omitting] youth and tech-savvy people.
- Survey may not be the best approach, many (and, no doubt) specific demographics are not willing to spend time on surveys. Awareness, especially with the "general public" audience, is difficult to measure. It is not clear if the findings did more than validate expected outcomes.
- Literature review approach is good.

## EDUCATION

- Phone survey approach to assess hydrogen awareness in focus groups is good, but methodology based on land-line phones alone is somewhat flawed.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- Surveys were conducted and compared in 2004 and 2008.
- Statistical analysis was performed at a high level.
- Unsure of the validity of data based on people surveyed (cold-calling responders).
- When opinionated, the general public DOES appear to understand the connection between hydrogen technology and petroleum displacement.
- There is a need to work on increasing target audience response rates.
- Not quite finished but good data so far.
- The project is on-track to meet stated goals, such as numbers contacted, analysis, comparisons and reporting. It is not clear if the survey approach can help DOE overcome barriers. It is not clear if the survey findings have been used to help DOE develop strategies.
- Well defined tasks within the project and well-articulated progress in the given tasks.
- Results of survey possibly flawed due to limits of survey methodology.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.7** for technology transfer and collaboration.

- Use of outside company for surveys is well thought out and high collaboration is apparent.
- Collaborations are presented to exist with market research entities, however the Principal Investigator didn't provide much information on other collaborations.
- Review didn't speak much about collaborations.
- The project is not designed/intended to expand collaborations. Measuring awareness of state & local government officials does increase their awareness of hydrogen and fuel cells and DOE level of interest.
- No specific collaborations or technology-transfer activities were made clear.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- Future plans are good however they do not take into consideration the expansion of survey pool to more technically savvy people.
- Planned work does not differ from pattern/scope of past work, so there is no reason to believe volume or trends of survey results will improve.
- Survey still underway.
- The project addresses additional audiences and expands survey questions for other audiences. Additional analysis will be conducted that may assist in guiding future projects.
- Plan forward is clearly articulated with relation to the defined tasks.
- Should re-investigate limits of survey methodology to enhance quality of information.
- The survey tasks should be better coordinated to meet needs of providing metrics for the outreach projects.

### **Strengths and weaknesses**

#### Strengths

- Partner Opinion Research Corporation.
- Statistical analysis.
- Although survey results aren't strong, this project appears to have been successful at analyzing the data received by the Principal Investigator.

- The project also helps DOE measure progress and the data can be used to modify education and outreach approaches.
- Survey approach to assess hydrogen awareness in focus groups is good.
- Well-defined tasks and metrics.

#### Weaknesses

- Survey pool.
- The response rates are poor.
- Telephone surveys might be outdated. Think about other ways to interact – email, mail?
- Surveys are not the best way to measure awareness.
- Survey methodology based on land-line phones alone is somewhat flawed and should be re-investigated for better representation of focus group attitudes and awareness.

#### Specific recommendations and additions or deletions to the work scope

- Investigate and attempt to expand survey pool to people with technology savvy.
- The project should be better aligned with other H<sub>2</sub> "marketing"/outreach projects.
- Re-investigate survey methodology limited to land-line phone calls to improve results.
- The survey tasks should be better coordinated to meet needs of providing metrics for the outreach projects.

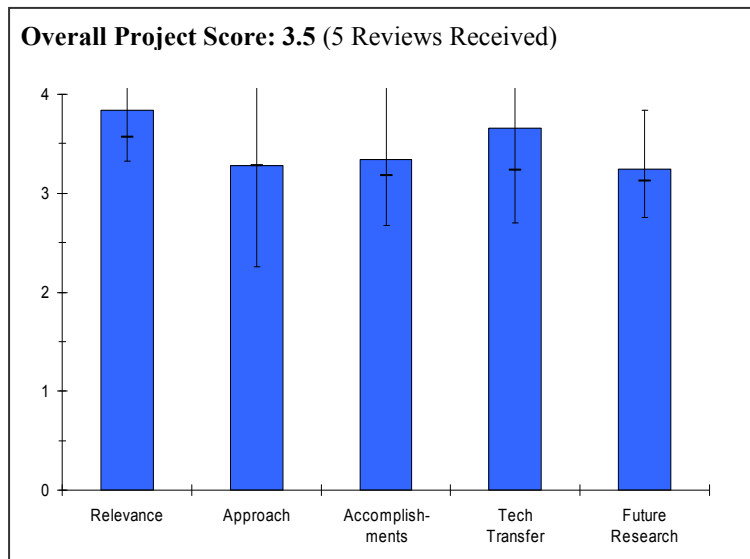


**Project # ED-02: Hydrogen Safety: First Responder Education**

*Marylynn Placet; PNNL*

**Brief Summary of Project**

The long-term objective of this project is to support the successful implementation of hydrogen and fuel cell demonstration projects and market transformation by providing technically accurate and objective information about hydrogen to first responders. The objective for fiscal year 2008 is to develop and disseminate first responder hydrogen safety educational materials, including an update of the awareness level course (first launched in fiscal year 2007) and a more in-depth, one day course. The more advanced course will include hands-on experience with a mobile hydrogen fuel cell vehicle prop developed in a companion project funded under the hydrogen safety, codes and standards subprogram.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.8** for its relevance to DOE objectives.

- Explaining and training first-responders on fuel cell technology is extremely important for the commercialization and safety of fuel cells.
- Awareness of first responders is the first step in making hydrogen accessible in communities – over 6000 unique visitors, 4000 in past year, 1700 in year one.
- Project objectives are highly consistent with Hydrogen Fuel Initiative and DOE Hydrogen Program objectives.
- Relevant to the Hydrogen Fuel Initiative in all aspects of project.
- Informs first responders on hydrogen.
- Development of first responders procedures for hydrogen-related emergencies is important to the hydrogen economy.
- Education of first responders in this area is critical.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- Approach is sound and has shown success thus far.
- Props are useful for training.
- Prop based course gives [first] responders a better framework for learning. Large numbers of reviewers of the course showed outstanding level of thoroughness. Online course helps get information dispersed to large numbers of responders – quiz is important for understanding accomplishment levels. Hearing voiceover added is helpful for some [first] responders.
- All tasks are well designed education dissemination strategies for the first responder audience.
- Great approach – especially the prop-based course for a "hands-on" learning experience.
- Well-defined approach for education and outreach using awareness-level course of clear benefit.
- Approach for prop-based course is also of clear benefit, but could be modified to include additional near-term fuel cell vehicles such as buses, tractors, forklifts, etc.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- Involvement/responsiveness has been very high.
- Have trained many first responders successfully.
- Have metrics: Good unique visitors, 4000 this year. Well-received by fire training/protection community. Steering [committee] is well rounded, lots of input from industry/responders.
- Task progress appears to be (mostly) timely and on schedule.
- Awareness-level course is highly developed, and includes a lot of interactive features to engage target audience.
- Tasks appear to be either strongly received or show strong interest from first responder community.
- Good progress. Tasks at various levels of completion with some key milestones/deliveries overrun.
- Good progress has been demonstrated.
- Awareness-level course use with feedback was a useful metric of progress.
- Formation of the Steering Committee is a critical positive step in this process.
- Prop-based course is good, but should also consider covering events associated with nearer-term vehicle applications, such as fuel-cell buses/ tractors/fork-lifts.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.7** for technology transfer and collaboration.

- Collaboration with HAMMER is successful.
- Clear, close work to achieve goals.
- Large number of reviewers from industry and emerging communities. Steering [committee for] prop based course showed strong effort to collaborate with stakeholders.
- The project has strong collaborations with highly relevant partners.
- Steering committee formation and input to prop-based course is a good coordination strategy.
- Excellent collaboration with relevant organizations (HAMMER, 100 representatives, etc.).
- Collaboration could be extended in the future.
- There is a limited list of collaborators cited.
- Participants involved in the Steering Committee should be included as active partners.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.2** for proposed future work.

- Future plans are good and are in-line with further expansion of training.
- Conducting courses and refining.
- The PI did not discuss a target number of future trainings, web-hits, CD's disseminated, etc.
- Could expand future work, but there are solid plans to use completed work to continue progress.
- Clear definition of plans to maintain and promote awareness-level course and to complete prop-based course.

**Strengths and weaknesses****Strengths**

- Partner.
- Website.
- On-site training.
- Appears to be a very well thought out initiative with phased approach.
- Very strong collaboration of industry.
- Modules for stationary and vehicles.
- Includes certificate of completion and train the trainer.
- Project deliverables are robust and close to on-time.

## EDUCATION

- Great educational tools – especially the prop. This makes material easy to understand and remember.
- Well-developed plan with well-defined tasks.
- Clear progress on each of the tasks.
- Steering committee formation including energy industry and firefighter representatives is a clear positive step.

### Weaknesses

- Not following up to understand first responder's opinion of hydrogen after training.
- Plans/costs associated with deploying training in future years were not discussed by Principal Investigator.
- Application of first responder education to hazards associated with stationary power and nearer-term larger-scale vehicles such as buses, tractors and forklifts should be more clearly addressed.

### Specific recommendations and additions or deletions to the work scope

- Follow up to understand first responder's opinion of hydrogen after training.
- Application of first responder education to hazards associated with stationary power and nearer-term larger-scale vehicles such as buses, tractors and forklifts should be more clearly addressed.

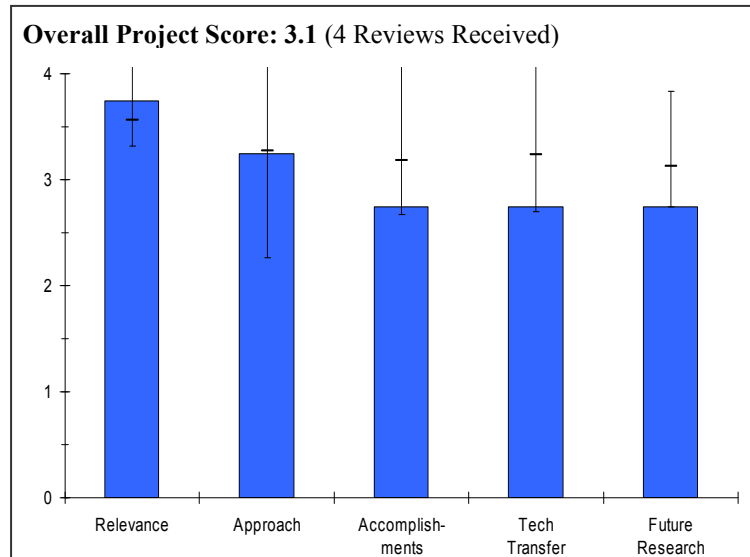
### Project # ED-03: Hydrogen Education for Code Officials

Melanie Caton; NREL

#### **Brief Summary of Project**

The objective of this project is to facilitate demonstration and deployment of hydrogen and fuel cell technologies by educating code officials on relevant safety, codes, and standards issues. Collaboration with codes and standards experts and consultation with code officials will help formulate appropriate content and ensure accuracy. Objectives for FY2008 include the development and deployment of this introductory information package for code officials.

#### **Question 1: Relevance to overall DOE objectives**



This project earned a score of **3.8** for its relevance to DOE objectives.

- Education of codes and standards officials is essential.
- Cannot get to implementation steps without educating code and permitting officials.
- The project aims to increase codes and standards knowledge of a critical target audience of the Hydrogen Fuel Initiative and DOE Hydrogen Program.
- The strategy and the goals of the project appear necessary and reasonable, but there may be a lack of understanding of what the code officials need.
- Highly relevant to the Program.

#### **Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- E-learning for code officials and testing provides good instant feedback for code officials. Makes it simple to get information.
- The e-learning modules each address key hydrogen codes and standards topics.
- Beyond designing the modules, the project does not include a strategy for delivering modules to the right audience or channeling the codes and standards community to the online modules.
- The project appears generally effective, but could be improved by a discussion on the extent that collected real world data can be provided through the education tool.
- Approach identifies effective methods to train; investigates current methods. The user may get engaged more than usual. Suggest adding audio/visual to grab the viewer.

#### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- Good progress on milestones also developing permitting links.
- Has a link with industry codes and standards database.
- Both vehicle stations, vehicles, and stationary.
- Can be used to educate other audiences.
- The Principal Investigator did not provide significant depth on the content and status of modules 2-5.

## EDUCATION

- The work on this project appears consistent with DOE goals, and while it doesn't appear to fall short, the project has room to [grow].
- Good progress and plan to complete work.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.8** for technology transfer and collaboration.

- Appears that the right people are being included.
- The project incorporates adequate collaboration to accomplish key milestones.
- The presentation appears to offer little in the way of collaboration beyond coordination with partners.
- Working with appropriate organizations.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- Planning to consolidate websites.
- Reviewing materials to make sure it is updated.
- Adding audio.
- All should boost usability and accuracy.
- Module dissemination needs to be emphasized in future work.
- As with earlier comments, project could be improved through a greater discussion of supporting goals. The fear is that the project outcome will not support code officials.
- Solid plans to use experience/lessons learned for future work.

### **Strengths and weaknesses**

#### Strengths

- Very focused toward regulator community that will be implementing laws is very important.
- Creates an interactive platform for codes and standards official education.
- The e-learning modules should be effective.

#### Weaknesses

- Does not include a deployment plan for the platform.

### **Specific recommendations and additions or deletions to the work scope**

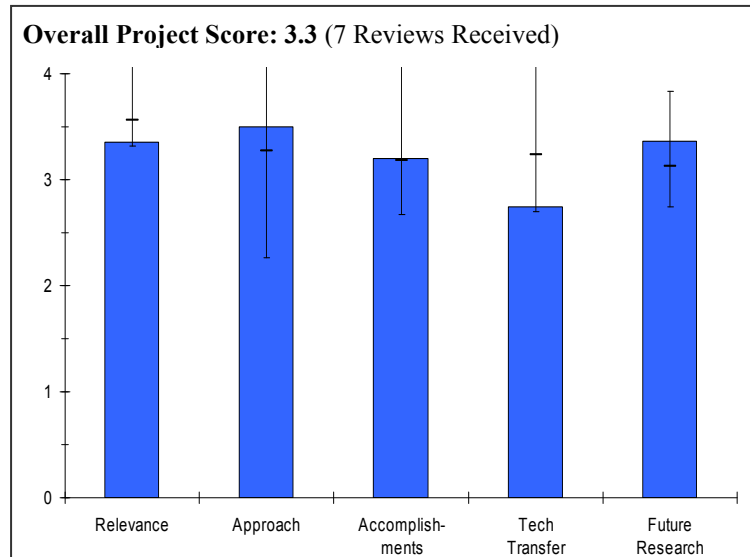
- The Principal Investigator should add a platform roll-out plan to ensure that the target audience actually uses to e-modules.

## Project # ED-04: Increasing “H2IQ”: A Public Information Program

Henry Gentenaar; The Media Network

### Brief Summary of Project

The objectives of this project are to 1) develop and disseminate resonant messaging that communicates to the general public basic facts about hydrogen as a fuel and fuel cells as an alternative to traditional power technologies; 2) transmit our message via communications channels audiences use; 3) generate interest, increase public requests for more information; 4) help raise knowledge levels to show progress toward education targets; 5) give the Hydrogen Program a communications mechanism with a flexible framework for reasons of timing and budget; and 6) make the most of Department of Energy resources and provide a gauge of success.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Educating/informing the public about fuel cells/hydrogen is aligned with the Hydrogen Initiative of the DOE.
- Not sure how important it is right now to engage general public because of spotty implementation with regard to achieving goals in the near term. Potential is much longer term but will be important in the future.
- The project engages a critical target audience (general public) of the Hydrogen Fuel Initiative/DOE Hydrogen Program.
- Supports overall education objectives to raise awareness.
- This well-prepared project expertly lays out a possible foundation for public education.
- Beyond advising the "how" of the project, the project also discusses the "why" of ideas presented.
- Project directly supports the Program on getting information to target audience on hydrogen – especially to the younger audience.
- The project is relevant and meets DOE's goal to reach 12-35 years olds. Unless fuel cell vehicles become available in a short period of time, it will be difficult to keep people interested.

### Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- Approach while using a lot of communication buzz words seems well thought out and viable.
- Website, podcasts, radio ads reach a wide technically savvy audience.
- Importantly promotes source of objective information.
- Consistent information.
- What's in it for me is a good message – simple message.
- Using new media: podcasts, MySpace, etc.
- Podcasts and radio broadcasts have good simple messages.
- Contemporary multi-media marketing strategies are central to the Principal Investigator's approach.
- MySpace is a great channel to youth market (and critical target audience).
- Very knowledgeable about changing/evolving way people receive information.
- Good message.
- As presented, the project makes sense while sharply focusing on requirements and tasks, as well as reasoning.

## EDUCATION

- Great look into what works and doesn't on getting information out to the public.
- It would be good to know the "attention grabber".
- MySpace page is a great tool and has significant potential to hit a wide audience.
- The project approach will be/is effective in planting hydrogen and fuel cell technology in the minds of the general [public] using the latest communications techniques for this target audiences is appropriate.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.2** based on accomplishments.

- Many different media tools have been used to reach public, websites, podcasts, radio, etc.
- Lack of measurable metrics makes it difficult to judge success.
- Finished ads and promos but have not followed up with metrics.
- Developed media campaigns (podcasts and radio spots) are high quality.
- It is difficult for the Principal Investigator to measure campaign progress/penetration.
- Great tie-in with NBA team.
- Frankly and clearly, this project advises marketing opportunities, how to penetrate, and why.
- Great progress – will have to visit the MySpace page.
- This project will inform the target audience about hydrogen and fuel cells.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.8** for technology transfer and collaboration.

- Looking for future collaborations with other agencies at both the state and federal level.
- Working with partners, who are potential partners?
- Collaboration efforts (outside of Orlando, FL) are still not developed.
- Great tie in with Orlando Magic – high visibility partners are important to entice and draw public in.
- There has been some collaboration (Florida) but presentation advises partnering is not yet complete. \*I really wanted to give a "4" here, but could not.
- Could use more collaboration. Find what else is effective.
- What makes a good radio spot? Good MySpace page (what grabs people).
- It is not clear if partners are a factor in this project.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.4** for proposed future work.

- Future plans are good and in-line with further expansion of education.
- Introduction and measuring of metrics will be useful to gauge success.
- Continue radio and MySpace.
- More markets.
- Measure response.
- Need to gauge results/response better – how many downloads, views, MySpace, friends, etc?
- This organization prepared a well-thought presentation and if they are involved in the implementation of these strategies, it is possible that DOE will be pleased with the results of its hydrogen education subprogram.
- Great plan moving ahead, progress on MySpace, more radio spots, building partnerships.
- Good to keep an eye on more social networks.

### **Strengths and weaknesses**

#### Strengths

- Principal Investigator is expert in the field of marketing; specifically to the key demographic.
- Using new media.

- Innovative marketing outreach methods are employed by the project.
- Think outside the box.
- The presentation was noteworthy for its clear, well-presented thought.
- Should hit wide audience with accurate information.

#### Weaknesses

- Lack of measurable metrics to gauge success.
- Should have some metrics by now – difficult to gauge without.
- Have not done a lot with fleets; should tap outreach to them in addition to this.
- Expanding program could be costly.
- No project weaknesses noted; there is a partnering requirement but the degree to which this project was completed and the quality of the work provided indicates that little partnering was required.
- Target audience could be expanded.

#### Specific recommendations and additions or deletions to the work scope

- Develop and use measurable metrics to gauge success.
- Expand media vehicles to include web banners and TV spots. For banners, if major sites are too expensive, even getting web banners placed on less-traveled sites and non-profit websites would help draw in people.
- This project should be coordinated with ED-01 (survey project).
- The Principal Investigator should weigh the cost/benefits between producing high-end podcasts that will be heard by a limited audience, with deploying strategically placed web banners that will draw in much greater numbers of people to DOE education web resources.
- Reviewing this project was enjoyable, no further recommendations provided.



**Project # ED-05: H2 and You: A Public Education Initiative by the Hydrogen Education Foundation**

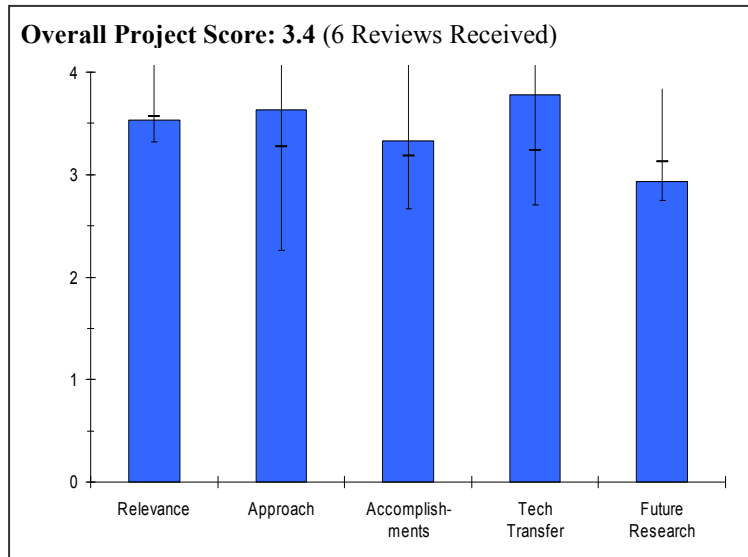
*Patrick Rooney; Hydrogen Education Foundation*

**Brief Summary of Project**

The overall goal is to increase understanding about hydrogen and hydrogen-fueled technologies. The objectives of this project are to 1) increase awareness and understanding of hydrogen and hydrogen-fueled technologies among the general public; 2) educate leading hydrogen influencers to validate hydrogen’s impact and potential; and 3) capitalize on related initiatives and resources from program steering committee partners. The program is guided and shaped by a steering committee of private and public sector organizations.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.



- Does not achieve much in short term, in terms of behavior.
- The project's objectives are highly consistent with Hydrogen Fuel Initiative and DOE Hydrogen Program objectives.
- Highlighting what is going on today is very important.
- Directly supports the Program in providing the public with information on hydrogen.
- The project works to dispel misinformation and promote the benefits of hydrogen.
- Use of up-to-date methods in internet and media and eminent interaction for promotion of hydrogen education is very important.
- The content of hydrogen education should be better coordinated with DOE Multi-Year Research, Development and Demonstration Plan goals.

**Question 2: Approach to performing the research and development**

This project was rated **3.6** on its approach.

- Industry eminent – key influences are brought in to collaborate.
- Have a general public influence.
- Easy to understand/strategy to communicate issues.
- Dividing approach across four issues platforms is a smart outreach strategy.
- The project targets very relevant websites and blogs where key target audiences convene.
- The project targets industry eminent that are critical to DOE Hydrogen Program communication goals.
- Blog monitoring – great idea, very practical.
- Approach lists a large audience and considers an effective means of getting information to the public.
- The project is designed well, includes metrics, and addresses DOE's target audiences.
- The partners are an excellent approach.
- Steering committee of public and private sector entities is a good approach for promoting hydrogen messages.
- The project's steering committee hydrogen messages need better coordination with the DOE's hydrogen messages.
- Use of internet and media resources is clearly a good and necessary approach.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- Metrics show positive responses to efforts.
- Measuring progress of effort through number of internet conversations is a shaky metric.

- Conversation "tones" have only been measured for 2 months, so the statistical relevance of these results is not strong.
- Obtain hard metrics that are very useful (online conversations/tour, etc).
- Can see improvement and growth in hydrogen conversation, making tune more positive.
- Great visibility. Accomplishing objectives.
- Number of conversations online is used as a metric, but it is not clear if the project has a direct influence on the changes. Media interviews and press are impressive.
- The approach of monitoring internet and blogs, and interacting with the media has great value, however project tasks, metrics, targets and progress against targets have not been clearly articulated.

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.8** for technology transfer and collaboration.

- Varied partners with different backgrounds in steering committee.
- Eminent are included.
- Working on more collaborations.
- The Principal Investigator has demonstrated outstanding collaboration on the project.
- Using NHA members to full advantage.
- Steering committee and other partners make sense. Includes government, OEMs and other relevant organizations.
- The project brings together an impressive array of private and private partners. The significant cost share shows the partners commitment to accomplishing the project.
- Impressive list of collaborators on the project steering committee.
- Better collaboration of steering committee with DOE is needed to coordinate the hydrogen message.
- Better technology transfer to the DOE of the developed internet and media resources would be useful.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- Media and consumer support loops.
- Future work should focus on building consensus messaging with steering committee members.
- Future work activities are good.
- Not detailed – "deepen and broaden" and "build a groundswell" doesn't really state what will be done.
- Plan forward is not clearly articulated with specific goals and metrics for success.
- Basic plan for future work is to continue work and hope to expand outreach.

#### **Strengths and weaknesses**

##### Strengths

- Has metrics on conversations.
- Lots of hang to the bucket.
- DOE budget is leveraged well.
- Getting good traffic on website and spending lots of time.
- Working well with media.
- Strong partnerships.
- Project is effective at reaching audience.
- Use of up-to-date methods in internet and media and eminent interaction for promotion of hydrogen education.
- Interesting progress in media and eminent outreach.

##### Weaknesses

- Affiliation with hydrogen industry could be viewed as biased.
- Poorly defined project milestones and metrics for tracking success.
- Good steering committee list, but their hydrogen outreach message not clearly linked to official DOE message.

#### **Specific recommendations and additions or deletions to the work scope**

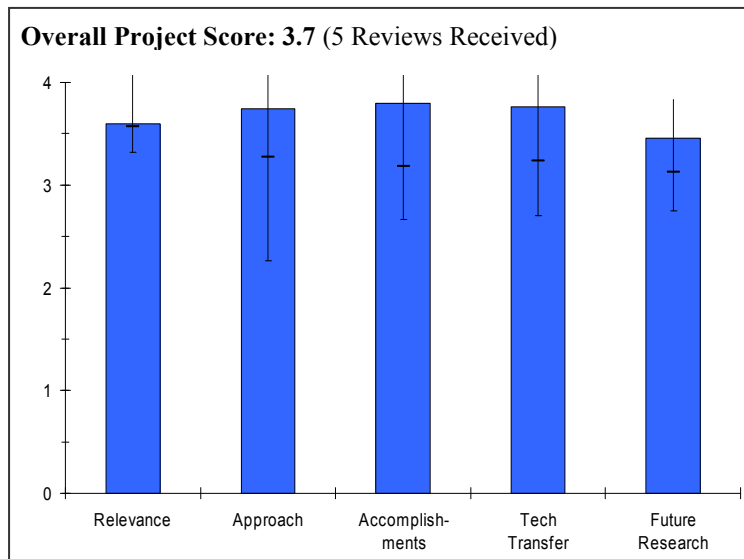
- Better coordination between DOE and project steering committee would be useful for promoting a more consistent outreach.

**Project # ED-07: H2 Educate! Hydrogen Education for Middle Schools**

*Mary Spruill; NEED*

**Brief Summary of Project**

The objectives of this project are to 1) develop, design and deliver a first class, comprehensive middle school hydrogen education program including: training, classroom materials, technical and best practices exchange, and evaluation; 2) design a program to link science and technology to the study of hydrogen and fuel cells; 3) deploy materials via teacher training and other professional development outreach opportunities; 4) provide technical support for schools that entered the program in year one and two; 5) collect data and evaluate for year two revisions; 6) work to expand the reach of the program with new partners able to support training workshops at the local level; 7) expand program for new localities and workshops; 8) continue to evaluate effectiveness and usability of materials; and 9) expand financial resources for workshops.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.6** for its relevance to DOE objectives.

- Project is critical to train teachers what they teach children who will be using fuel cells, studying in college, entering workforce, etc.
- Relevant to the DOE Hydrogen Program and will educate "future leaders" on what hydrogen is.
- Although the program is certainly worthwhile an effort of this scope will reach only a small fraction of teachers and students.
- An aggressive, well thought out program that reaches one of DOE’s primary target audiences.
- Education of middle school children is critical now to the future of the hydrogen economy.
- The exact message at the appropriate level for this age group is still in the process of evolving.

**Question 2: Approach to performing the research and development**

This project was rated **3.7** on its approach.

- Complying with standards – excellent.
- Community outreach – excellent.
- Upgrading labs and materials.
- Got information that could relate to audience (students).
- Good sequence with objectives.
- Generally good but probably there should be more emphasis on feedstocks, production, and energy, and less on molecular structure and periodic tables.
- Excellent approach that overcame finding and materials challenges. The approach is exceptional because it ensures that the program continues after the close of the grant.
- Working with the schools and teachers at this level is a great approach.
- The hands-on aspect is wonderful for the students.
- Alignment with national and state standards is very important and commendable.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.8** based on accomplishments.

- Reached a considerable amount of teachers per state even with zero funding for two years from DOE.
- Great progress with students and partners.
- Project complete – no major barriers preventing work to be accomplished.
- Project seemed ahead of schedule.
- Pre-/post-date indicates great success.
- On an absolute scale the accomplishments have been modest but relative to resources, they have been outstanding.
- Exceeded expectations in spite of funding challenges.
- NEED has deployed creative strategies and is one of the best projects.
- Good progress has been demonstrated.
- Somewhat less clear was the amount of progress since the last review.
- Survey metrics were a useful, though somewhat limited, indication of progress.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.8** for technology transfer and collaboration.

- Partnerships with utilities – excellent opportunity.
- Collaborations with state governments.
- More than a dozen partners including government, energy, national labs, industry, etc. This is great.
- The only way they could have accomplished what they have is through really good interactions with their partners.
- Brought many partners to the table to help reduce cost per unit and expand their reach.
- There is an impressive list of collaborators.
- The role of these collaborators and the extent of the collaborations was not made clear.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.5** for proposed future work.

- Need to expand but needs partners to do so.
- Expanding into technology education – YES!!
- Continued work to prove up-to-date information.
- Planned workshop (up to 10).
- Move beyond pilot project to training workshops.
- Continued alignment to national and state standards.
- Proposed work is appropriate for goals but apparently there are no plans for incorporation of lessons learned or for revisions to the student/teacher distribution materials.
- The grant closes in 2009, yet the program will continue because of the efforts of NEED to bring together additional partners and the high quality of the end product.
- Plans to continue with the regional workshops are good.
- Not clear if funding will be adequate to the future plans.
- Contingencies for reduced funding should be addressed.

**Strengths and weaknesses****Strengths**

- Making great use of resources and finding and integrating hydrogen into other curriculum (solar, wind).
- There are many willing participants for a technical area rapidly gaining national interest.
- Excellent project that exceeded expectations.

## EDUCATION

- Demand has exceeded the supply.
- Working in schools with teachers and students to develop hydrogen awareness is of clear benefit, and appears to be working well in the pilot schools.
- Hands-on projects for the students are a powerful tool for hydrogen education.

### Weaknesses

- Great success hinges on funding.
- Their main interfaces with the public are their distribution materials which are not particularly well done.
- Survey metrics for student and teacher development should be enhanced.
- Better integration into school programs to match the science education level of the students would be beneficial.
- The role of the collaborators should be more clearly defined and enhanced.

### Specific recommendations and additions or deletions to the work scope

- Put some time and effort into determining optimum messages to get to students and teachers and update the distribution materials accordingly. Also, put some effort into looking for additional innovative approaches for reaching target groups.

**2008**  
**Systems Analysis**  
**Summary of Annual Merit Review Systems Analysis Subprogram**

**Summary of Reviewer Comments on Systems Analysis Subprogram:**

The reviewers considered the Systems Analysis Subprogram an essential component to the Hydrogen Program mission and critical to the President's Hydrogen Fuel and Advanced Energy Initiatives. The projects are considered appropriately diverse and focused on addressing technical barriers and meeting targets.

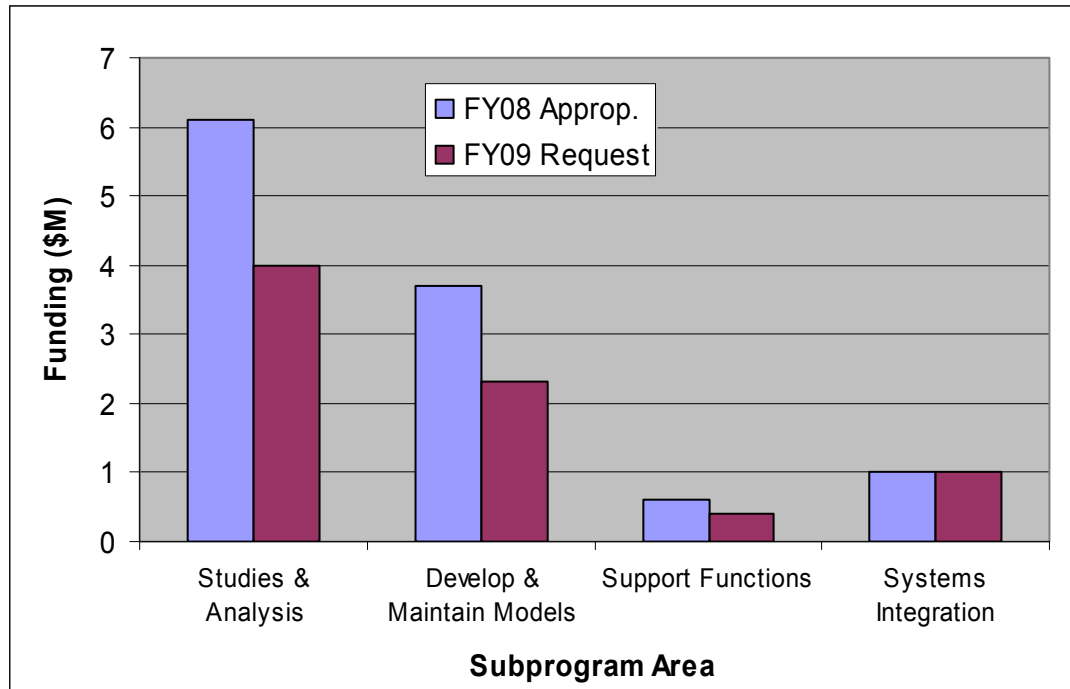
In general, the reviewers noted that Systems Analysis is a complex subprogram but is receiving the appropriate management attention. Some reviewers commented that the subprogram is well managed and has adopted an organized approach for analytical support of the Hydrogen Program, which is appropriate for addressing the comprehensive list barriers identified in the Multi-Year Research, Development and Demonstration Plan (MYPP).

Recommendations identified by the reviewers for Systems Analysis were: 1) a summary of assumptions should continue to be provided at the beginning of the Annual Merit Review for the Analysis Session; 2) a model discussion and demonstration should be provided prior to the Annual Merit Review for the Analysis Session; 3) fuel purity and the impact on performance and cost tradeoff analysis should continue; and 4) model validation and peer review is critical for sound and credible analysis. The Systems Analysis subprogram will continue to address these issues and reviewer feedback will be incorporated in the Systems Analysis Plan.

Finally, the reviewers commented that the analysis and model portfolio was complete and making good progress in addressing analysis topics. They indicated the analysis MYPP barriers were being addressed by the Systems Analysis subprogram and put into the proper perspective.

**Systems Analysis Funding:**

The funding for Systems Analysis primarily includes model development and analysis required for meeting the Hydrogen Program's technology readiness goal to enable commercialization of transportation fuel cell vehicles as well as model development and analysis for early market applications. The 2009 request-level funding profile, subject to Congressional appropriation, addresses the National Academies' Report recommendations and provides greater emphasis on transition, resource, and infrastructure analysis.



### **Majority of Reviewer Comments and Recommendations:**

In general, the maximum, minimum and average scores of the reviewers of the Systems Analysis projects were 3.9, 2.6 and 3.2, respectively. Reviewers commented that the diversity of the Systems Analysis project portfolio addresses the “analysis and modeling gaps” of the subprogram, and the resource, infrastructure, transition and early market analysis requirements. The major recommendations for the Systems Analysis projects are summarized below. The Systems Analysis subprogram will address these recommendations.

**Model Development:** Projects in model development received very favorable reviews. The majority of the projects were regarded as well-aligned with the current program goals and objectives. Reviewers consistently suggested the models be peer reviewed and validated with industry, academia and the National Laboratories. Reviewers recommended that models use a consistent set of inputs and assumptions; include plug in hybrid electric vehicles for well to wheel analysis of petroleum use and greenhouse gas emissions; and integrate the stationary power generation and transportation sectors.

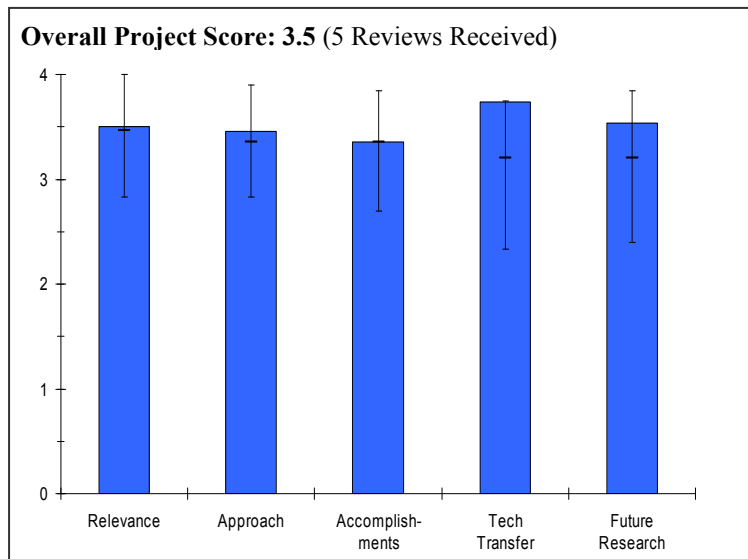
**Program Analysis:** The analysis projects were consistently ranked as good and the analysis projects supported the program goals. In general, the reviewers concurred that the analysis projects need to be peer reviewed prior to issue and publication, and that a consistent set of inputs and assumptions be used. The reviewers felt that the Lawrence Livermore National Laboratory (LLNL) Water Analysis project is important for hydrogen production but should be extended to include analysis of renewable hydrogen production pathways. The resource and infrastructure analysis with the new Hydrogen Demand and Resource Analysis Tool (HyDRA) was well received and encouraged by reviewers. The reviewers acknowledged that the environmental projects with University of Illinois and Tetra Tech, which are just getting started, are important to the Hydrogen Program in understanding how hydrogen production and use will affect the upper atmosphere and the environment. The TIAX platinum availability and leasing strategy project and the Argonne National Laboratory hydrogen quality project received good reviews and their importance was recognized in addressing fuel cell cost and performance.

**Lessons Learned Analysis:** In general, the reviewers agreed that understanding lessons from previous efforts to introduce new alternative fuels and power generation systems is important for developing a successful strategy to introduce hydrogen as a transportation fuel and fuel cells for stationary and transportation power. Use of a “lessons learned” analysis enables an understanding of past early market penetration issues which may be relevant to hydrogen production and fueling applications. Reviewers acknowledge the benefits of including industry in the analysis process.



**Project # AN-01: HyTrans Model: Analyzing the Transition to Hydrogen-Powered Transportation***David Greene; ORNL***Brief Summary of Project**

The objectives of this project are to 1) complete development of an integrated market model of the hydrogen transition; 2) construct and publish credible scenarios of the transition to hydrogen fuel cell vehicles; 3) collaborate with the International Partnership for the Hydrogen Economy/International Energy Agency to develop joint European Union and North America transition scenarios; 4) analysis the potential for a federal acquisition program to establish a sustainable North American non-automotive proton exchange membrane fuel cell industry; and 5) update and improve the HyTrans integrated market model. In fiscal year 2008, Oak Ridge National Laboratory is focusing on disseminating the results of the transition scenarios establishing international partnerships and building towards future assessments.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- Project objectives and intended results are consistent with DOE Hydrogen economy vision and related goals.
- Very good. Accurately summarizes the plight of the small non-transportation PEM manufacturer. Small companies, like Plug, ReliOn or Idatech, cannot continue to subsidize the price and remain solvent. These small units would probably use the same balance of plant hardware as the vehicles. Demand from either sector would be insufficient for a manufacturer to develop new, low cost components (valves, sensors, connectors, etc.). However, similar demand from the transportation sector and the stationary sector may generate enough demand to justify the manufacturer's investment and risk.
- This is a key component of the modeling and analytical work supporting hydrogen-related decisions by the Department of Energy and many other organizations.
- Dr. Greene and his associates continue to develop extensive, credible, and practical results through their sophisticated, "world-class" analytical activities.
- This project and model are extremely relevant.
- It is very important that the Program understand the transition from hydrocarbon to hydrogen.
- Resolving the chicken or egg issue is critical.
- Presented a good picture of what the vehicle roll-out transition looks like and the potential impacts during the transition period.
- Evaluate if the federal acquisition model is realistic for non-OEM PEM fuel cell manufacturers. Information appears to be preliminary and many assumptions have been made about fuel cell costs, durability, and the synergistic aspect of the private non-OEM companies working together.

**Question 2: Approach to performing the research and development**

This project was rated **3.5** on its approach.

- The technical strategy and approach to developing predictive analyses for phased transition from a hydrocarbon to a hydrogen economy is certainly challenging; the present work contributes to an understanding of issues and opportunities to some extent. The work is on-going. As of now the results are comprehensible and meaningful.
- The model results place the entire acquisition burden on the federal government; it does not identify government-private sector partnership. Issues on the program development, out-year funding requests, etc., for the massive acquisition process, etc., are not discussed. Although the study concludes that a transition to a H<sub>2</sub> economy is entirely a federal government responsibility, summary-level reports on why so and implementation approaches for policy and Deputy Assistant Secretary level readers are needed.
- The approach is very good. The polling of industry members was warranted. The polling does not appear to be as extensive as it might have been.
- The most advanced, state-of-the-art analytical and modeling methodologies are well understood and used by Dr. Greene.
- Prior work related to vehicle applications is now being extended to stationary hydrogen fuel cell applications in support of market transformation initiatives.
- The potential for hydrogen fueled internal combustion vehicle commercialization should be considered in the project approach. This is recognized by Dr. Greene.
- Market simulation to understand cause and effect will enable much better planning of research and development and the transition to commercialization.
- International collaboration is necessary because the hydrogen economy will be international.
- Developing and encouraging other PEM applications should help commercialization for transportation.
- The project approach appears a bit fragmented from the slides. Project covers HyTrans model as well as non-OEM fuel cell aspect.
- Dr. Greene needs to take a closer look at the uncertainties in the model.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.4** based on accomplishments.

- Significant progress toward accomplishing task goals has been completed or is in progress.
- The project's technical accomplishments and progress toward project goals is good. The modeling is interesting; assumptions are not noted.
- Information on many milestones and accomplishments was provided.
- These milestones and accomplishments include significant analytical and modeling results (e.g. HyTrans), reports, testimony based on analytical work, and responses to specific needs of the hydrogen program.
- Development of cost models plus greenhouse gas (GHG) impacts is impressive.
- The growth from 2000 units/yr federal acquisition to 35,000 units/yr federal plus private acquisition is encouraging.
- Need to further refine and/or update the HyTrans model based on updated versions of other models (H2A, GREET) to obtain more representative results.
- Need to look at what effect the success in automotive fuel cells (tougher cost & lifetime goals) might have on non-automotive fuel cell systems and the level of interdependency.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.7** for technology transfer and collaboration.

- National labs, two major auto manufacturers, fuel cell manufacturers, and universities are involved in this important, hydrocarbon-to-hydrogen energy technology transition study and analysis of issues, barriers, needs, and opportunities. The highly competent team with complementary expertise will make the study results meaningful and useful to decision makers.
- The project has good technology transfer/collaboration. The attempts to engage industry are laudable. The engagement of California Air Resources Board is important.
- Working with the Europeans shows a global focus.
- Dr. Greene's collaborations with others, both nationally and internationally, are extensive.

- The work on this project is done in the context of well-established partnerships and on-going communications/joint development work with colleagues in other national laboratories, industry, and many government organizations. Many were included in the presentation.
- Interactions with the international community, industry, and other research organizations are exceptional.
- Excellent work with other models and various public and private agencies.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.5** for proposed future work.

- The proposed future work is conducive to expanding the scope of the analyses.
- However, the analysis assumes that PEM will dominate the market; assumes that PEM material(s) has achieved commercial/market readiness. This assumption is not entirely correct.
- The analysis assumes that hydrogen is the safest fuel. Thus, the analysis does not address the safety and environmental issues for the hydrogen economy scenario from cradle to grave, that is the safety and environmental issues from the production of hydrogen to its end uses.
- The project's approach to and relevance to proposed future research is good.
- An excellent summary and discussion of future plans was provided.
- Planned work is appropriate for bringing this work to a worthwhile and useful conclusion.
- The PI is on the right track.

### **Strengths and weaknesses**

#### Strengths

- Technical, policy, and program management readers will get insights and understanding on the issues related to hydrogen energy technology deployment scenarios.
- The project's outreach to major OEMs and fuel cell manufacturers is a strength.
- A strong, experienced, committed analytical team led by Dr. Greene. It is highly respected for its body of analytical work, its expertise, and its responsiveness.
- The project has the strength of an excellent team with the right strategy.
- Incorporation of various models provides a good picture of hydrogen transition period.

#### Weaknesses

- The analysis depends on three private sector entities to determine that hydrogen energy technology R&D and related marketing efforts are all federal initiatives; opinions of federal and state policy makers should also have been included. Complementary technologies, such as hydrogen internal combustion engine, PEM material at its current state-of-the-art (i.e. its commercial readiness status), fuel dispensing, on-board and off-board storage, etc., have not been included in the study. Hydrogen sources, renewable, nuclear, fossil, comparative economics, etc., need to be included. Perhaps a comparison with battery powered vehicles, especially for local uses, along with its advantages and economics should also be included for a holistic approach to system studies.
- One purpose of system study is R&D guidance. Some prudent, mission-critical R&D needs and thrust should also be included.
- The project is missing the synergy on balance of plant hardware for both stationary and transportation applications.
- A huge gap between this federal acquisition and sustainable automotive production levels still remains, but Dr. Greene has plans to address this.

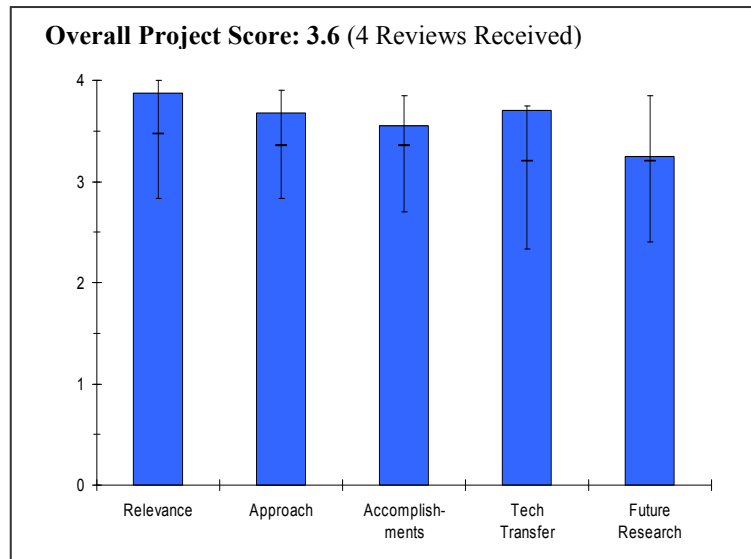
### **Specific recommendations and additions or deletions to the work scope**

- The weaknesses section discusses the limitations of the model and, in turn, recommends additional studies to make the overall study comprehensible to both technical analysts and policy makers.
- In his presentation, the Ford presenter's slide included "(1) hydrogen fuel storage is a significant challenge and (2) economic viability is uncertain."

- This work should address such challenges and make the analyses results and any predictive models more comprehensive.
- Poll the smaller companies active in this arena (for example ReliOn, Idatech, Alteryx, Bloom Energy, etc.) A more complete list can be obtained from A. Androsky of the USFCC.
- The approach to market transformation analysis could be extended to include an independent and more complete assessment of the nexus between fuel cell production capability and the timing of market demand.
- Expanding the outreach associated with the sustainable PEM fuel cells activity to companies beyond the three identified should be considered.
- A follow-up project or continuation of this project is needed to establish a viable path from federal acquisition of 1 kW to 5 kW fuel cells at 2000 units/yr to initial automotive production of 150,000 units/yr with power levels of 50 kW to 100 kW.
- Adding hydrogen fueled internal combustion engines as an additional element of market transition would be very helpful in establishing an understanding of the value/benefit of this for infrastructure transition.

**Project # AN-02: GREET WTW Analysis Results and Comparison of Advanced Vehicle Technologies***Michael Wang; ANL***Brief Summary of Project**

The objectives of this project are to 1) expand and update the GREET model for hydrogen production pathways and for applications of fuel cell vehicles (FCVs) and other fuel cell systems; 2) conduct well-to-wheels (WTW) analysis of hydrogen FCVs with various hydrogen production pathways; 3) conduct life-cycle analysis of hydrogen-powered fuel cell systems; 4) provide WTW results for Office of Hydrogen, Fuel Cells, and Infrastructure Technologies efforts on the Hydrogen Posture Plan and the Multi-Year Program Plan; and 5) engage in discussions and dissemination of energy and environmental benefits of hydrogen FCVs and other fuel cell systems. Data was obtained for hydrogen production pathways (open literature, H2A simulation results, process engineering simulations) as well as hydrogen FCVs and other systems (open literature, PSAT simulations, data from industry).

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.9** for its relevance to DOE objectives.

- This is a key component of the modeling and analytical work supporting hydrogen-related decisions by the Department of Energy and many other organizations.
- Dr. Wang and his team continue to build on their prior body of work to develop updated, credible, and highly regarded results.
- The objectives are essential to the provide projections and insights into the hydrogen pathway.
- GREET is used and respected throughout the community. It is imperative that it contain accurate models applicable to hydrogen fuel and fuel cells.

**Question 2: Approach to performing the research and development**

This project was rated **3.7** on its approach.

- The approach includes on-going activities to maintain and utilize current information on technologies of interest, simulation models, etc.
- Continuing to expand, update, and apply the GREET model is a major component of the project.
- Consideration should be given to confirming assumptions resulting from literature through discussions with knowledgeable individuals having "real-world" experience. This suggestion stems from the response to a question on assumptions about energy conversion efficiencies in stationary systems.
- Please clarify the data and the conditions for the calculations and the comparisons of calculated values versus measured ones.
- Approach is very good but it would be good to show how these models can be "validated" when possible.
- I am concerned that H2A and PSAT may not be validated for the simulations that are providing inputs to GREET. Unfortunately, they may still be the best available sources of information. Fortunately, where data is available, it is being used.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.6** based on accomplishments.

- Dr. Wang discussed GREET 1.8, which was released in March 2008.
- Fuel-cycle analysis of fuel cell forklifts and distributed power generation is being done in support of the hydrogen program's market transformation initiative. This should benefit government officials and others interested in acquisition of fuel cell technology. Dr. Wang presented the results of recent analysis.
- GREET is also being expanded to support analysis of hydrogen plug-in hybrid vehicles.
- Progress and additions to GREET are very impressive, but it is difficult to separate what has been accomplished with HFCIT funding and what has been accomplished through funding from other sources.

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.7** for technology transfer and collaboration.

- Dr. Wang's work with others, both nationally and internationally, is extensive. He continuously coordinates with other modelers and analysts, such as those working on H2A, PSAT and HyTrans.
- GREET is widely used and referenced worldwide.
- Indicate the data distributions.
- The model has a high number of simulation users which is a good sign of technology transfer.
- ANL should be commended for making GREET available to anyone and everyone and supporting the many researchers that use it.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.3** for proposed future work.

- An excellent summary and brief discussion of future work plans was presented.
- Future work will include analysis of biomass to hydrogen production options, as well as fuel cell plug-in electric vehicles.
- Use the metric system rather than the English system for the Greet international users.
- The proposed future research is good even if program is scheduled to end this year.
- Proposed future work is a good list; especially the FC PHEV Well to Wheel analysis should be given very high priority.

#### **Strengths and weaknesses**

##### Strengths

- A strong, experienced, committed, and highly regarded Principal Investigator and supporting team.
- Large amount of comparisons for the various selections for the future scenario.
- Very good distribution of software development to the world for use.
- This will be one of the most valuable models in the next administration when attention to greenhouse gases will escalate.

##### Weaknesses

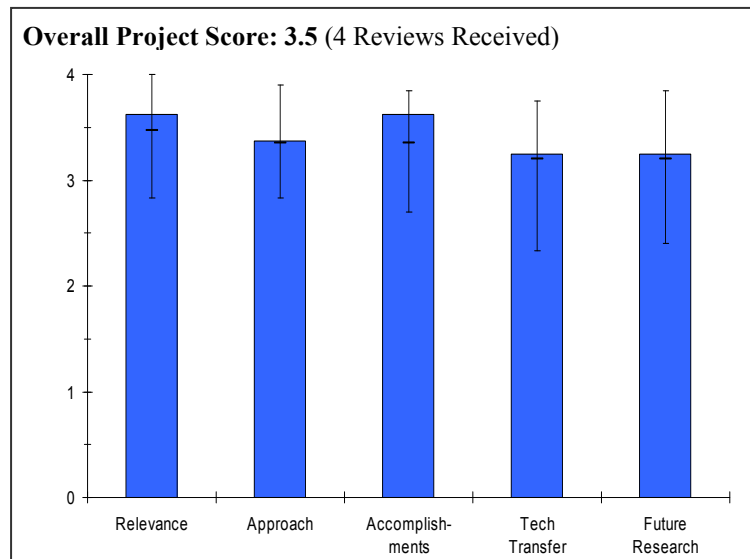
- No strategies on how to get feedback from all or any specific group of users about improving parameters and improving program accuracy calculations.
- There are so many pathways that need to be developed; maybe there should be a more visible prioritization process for selecting which ones to develop next.

#### **Specific recommendations and additions or deletions to the work scope**

- It would be good to understand the diversity of the end users of the program and how to get their feedback on the program's prediction.
- Minor issue, but might consider deemphasizing work directed at FC forklifts in favor of fuel cell vehicle (FCV) model development, such as the proposed fuel cell (FC) plugin hybrid electric vehicle (PHEV)'s Well to Wheel analysis.

**Project # AN-04: Macro-System Model***Mark Ruth; NREL***Brief Summary of Project**

The overall objectives of this project are to develop a macro-system model (MSM) aimed at 1) performing rapid cross-cutting analysis utilizing and linking other models and improving consistency of technology representation; 2) supporting decisions regarding programmatic investments and focus of funding through analyses and sensitivity runs; and 3) supporting estimates of program outputs and outcomes. The 2007/2008 objectives are to 1) improve the structure of the MSM and develop a graphical user interface; 2) update versions of component models; 3) add stochastic analysis capability; 4) validate MSM results; and 5) begin interaction between MSM and spatial and temporal models.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.6** for its relevance to DOE objectives.

- The project's objective is very good by having a simpler, faster, user friendly model. Common definitions and equations across platforms is a must.
- Ambitious project, but could be very useful for overall Hydrogen Program planning.
- The scope of this project is extremely relevant to the needs of the DOE Program.
- Looking at all aspects of hydrogen transition period is critical to the success of the infrastructure/vehicle roll-out in the future.

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- The project approach is very good. Designing a model that is compatible with other existing models is both cost-effective and wise.
- Need to be careful not to lose sight of the individual model assumptions. Some assumptions may not be reasonable, but setting up and running the Macro-System Model is a good way to identify (and hopefully change) those unreasonable assumptions.
- Technical approach is sound. The PI has focused on making the tool available to end users similar to what has been done for the H2A Model.
- Combining various models to look at technical, political, and environmental aspects to address key issues is a good approach.
- Need to consider making the model more user friendly since it is a different platform from other Excel-based models.
- Need to consider having more industry use/validation of the model.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.6** based on accomplishments.

- The technical accomplishments and progress are very good with the time and benchmarking in sync.
- Excellent progress has been made as shown by cost and performance results for various pathways.
- The PI is in the middle of the work plan and has demonstrated significant progress to date.
- More focus should be placed on making the model easier to use and making the list of assumptions used more explicit to the end user.

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- The technology transfer/collaboration of the project is good. The collaboration seems to be limited to other national labs and Direct Technologies, Inc. (DTI). No mention was made of academic or industry input.
- The PIs close collaboration with other participants and institutions were evident in the presentation, and this is essential to the project.
- The project/model has exhibited excellent collaboration with other models developed at other national laboratories. However, more industry and independent use/validation is needed.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.3** for proposed future work.

- The approach to and relevance of proposed future research is good. Electrical costs and quality requirements should probably have been addressed earlier.
- Additional model validation is necessary and will be challenging.
- The project is on track and future work is well organized for a successful completion.
- Need to consider independent validation of model upon successful linking with other models. Solicit feedback from end-users for model improvement.

#### **Strengths and weaknesses**

##### Strengths

- Commonality with existing platforms was incorporated in the model.
- Harmonizing existing platforms was incorporated in the model.
- The project has accomplished very good work on a very challenging assignment.
- The high level Macro-System Model (MSM) development will be very useful to others conducting analyses on technologies and applications for the hydrogen economy. Attention is being paid to the user interface, but it is very important to complete the work so that end users outside of the host lab are able to easily access the model and use it. The PI is very qualified in the field.

##### Weaknesses

- There are some questions based on the assumed efficiency of the distributed steam methane reformers. How does the efficiency of a smaller distributed unit become greater than the efficiency of larger central units? Economy of scale would suggest that the central units are more efficient.
- Consideration should be given to making reformation of ethanol (C<sub>2</sub>H<sub>5</sub>OH) a lower priority.
- There was no mention of collaboration or benchmarking the results with industry users.

#### **Specific recommendations and additions or deletions to the work scope**

- Clarify or amend items under weaknesses.
- Include academic input in the project/model. Possibly consult with T. Molter of University of Connecticut or Jean St. Pierre of University of South Carolina.
- Include electrical costs in the project/model.



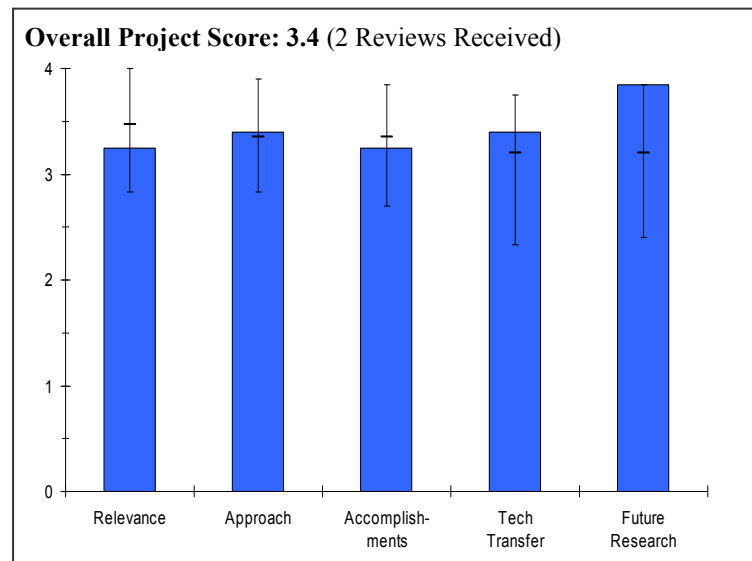
## Project # AN-05: Analysis of the Hydrogen Production and Delivery Infrastructure as a Complex Adaptive System

George Tolley; RCF, Inc.

### Brief Summary of Project

The purpose of this project is to deal with the chicken or egg problem between the supply of hydrogen fuel and the purchase of hydrogen vehicles, using agent-based modeling. The overall aim is to answer the questions: will the private sector invest in hydrogen infrastructure and what, if any, policy assistance is needed? The agent-based model explains the investment in a hydrogen infrastructure and purchase of hydrogen vehicles. Investors supply the infrastructure that makes hydrogen fuel available. The fuel demand is by drivers who purchase hydrogen vehicles.

### Question 1: Relevance to overall DOE objectives



This project earned a score of **3.3** for its relevance to DOE objectives.

- Very important that we do everything possible to understand barriers, risks, and tradeoffs to all aspects of commercialization.
- This project scope loses much of its value if stationary fuel cell systems can be used to co-produce hydrogen for refueling stations. This approach attenuates the chicken-in-egg problem.
- Model assumes interest rate of 5 to 15 %, which is too low for new technology and will underestimate costs.
- Economies of scale in mass-production of distributed hydrogen generators could out-pace centralized generation, particularly under the hydrogen co-production approach using stationary FCSs. Model omits this possible evolution.
- A constant price over time was exhibited for distributed hydrogen; model omits economies of scale in mass production for these units. This is an error.
- The exhibited policy conclusions by the model should be explained.

### Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- Approach is decent with the acknowledgement of barriers at hand.
- Agent based model approach is very informative.
- There are a few fundamental weaknesses of the "MBA" approach or NPV analysis. One is the inability to accurately predict future positive and negative cash flows. A more crucial weakness of the NPV approach relevant to this group of people is errors in accurately estimating the genuine risk of a new technology project. The methodology chooses a "similar" project of perceived similar risk. However, if a project is genuinely technically innovative, making analogies to previous new technology projects may not be appropriate. The discount rate for a new wind energy project may not be the appropriate discount rate as for a new tidal energy project.
- The model does not appear to necessary change the discount rate as the investor learns. This should be examined because as the investor starts out, the discount rate should be higher and as he/she learns more, it should decrease.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- The rate of progress for this project is low compared to the amount of money spent.
- Detailed business model is very impressive.
- FY08 accomplishments were not delineated clearly in the talk compared with FY07 accomplishments.
- The stated goal of this project is to "address the chicken-in-egg" problem for refueling stations. However, the speaker stated that he was considering the case of all the technical risks etc being worked out and therefore an interest rate of 5 to 15% was reasonable. This approach is financially incorrect. It fails to address the technology development-financial risk interface which is precisely the primary bottleneck in deploying these fleets and stations. One of the biggest bottlenecks to deploying stations and vehicles is their technical risk. This risk results in higher interest rate, which was ignored. In this way, the project fails to address the most important barrier to fleet deployment.
- Slide 16 shows valuable information about adopter traits vs. penetration, but was also shown at AMR 07. Has any new work been accomplished regarding this relationship?

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.4** for technology transfer and collaboration.

- For this kind of work, they need more partners.
- Industry cooperators provide a good connection to reality.
- Use of production and delivery models is good.
- Collaborations with these organizations will help make the project more relevant, used, and accepted: Argonne National Laboratory, BP, Ford Motor Co., Protium Energy Technologies and industry advisors.
- Collaborations should include data input from hydrogen electrolyzer manufacturers and a grid electricity-to-hydrogen via electrolysis scenario.
- Modeling work should include scenarios in which hydrogen is co-production in stationary fuel cell systems; this scenario is currently lacking as well as collaborations with industry to accurately describe this option.
- A common definition among collaborators for "chicken" and "egg" should be agreed upon.
- Is it realistic to have 76% penetration to passenger vehicles and zero for the rest of the broader vehicle fleet as exhibited?

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.9** for proposed future work.

- Carrying this through to include federal policy impacts is very important.
- Recommend that future work include coordination with David Greene.
- Fleet adoption should be considered in addition to household adoption.
- Analysis does not take into account financial benefits of "learning" how to design and deploy technology better as exhibited by the levelized cost of the stations being the same regardless of the year they are built.
- Analysis has not taken into account technology progress in the past few years. The model's assumptions about the performance and cost of the steam methane reformers (SMRs) are out-dated.
- Assumption that centralized production will be cheaper than distributed production may not be correct.

**Strengths and weaknesses****Strengths**

- This development could prove intuitive or something completely unexpected.
- Development and inclusion of upper management module is a strong point.
- Refueling stations have been built, but their utilizations (such as Praxair's station) are only 1%, due to a lack of vehicles. The project attempts to address this kind of impediment to fleet deployment, though not with great

accuracy given its assumptions of an overly low discount rate (5-15%) and no co-production of hydrogen from stationary fuel cell systems (a scenario that would tend to mitigate the concern of a lack of available refueling stations).

- The measurement units are not shown for Vehicle Adoption Rate.

### Weaknesses

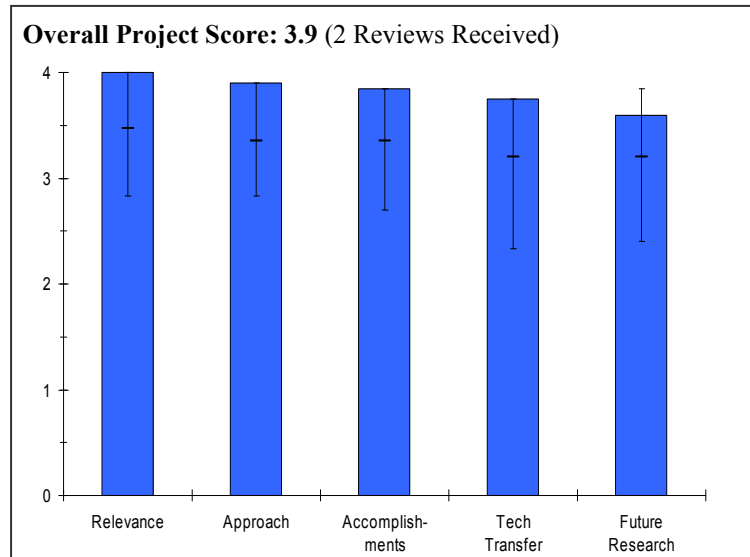
- Given the partners involved, the outcome is probably intuitive.
- The same usefulness of results could be achieved with a simpler model.
- Speaker recommends tax credit on the purchase of hydrogen vehicle but should indicate the amount of the tax credit. The presenter only plots the differential between the current vehicle price and the hydrogen fuel cell vehicle price.
- If the speaker is exploring the non-optimum, he should focus on the perceived risk / interest rate assumed and errors in estimating future revenues and costs.
- Results were not well-labeled or explained, such as showing the cost of station but not their size.

### Specific recommendations and additions or deletions to the work scope

- Program could use more diversity in partners, maybe international ones.
- Broader coordination with other models - others will benefit from this project.
- Consider expanding this approach to cover other aspects, such as vehicle commercialization.
- The amount of funding for this project, \$3 million, is much too high for the amount of work being contracted for and the quality of results presented. This project is a modeling project, and therefore is not as capital intensive as design and build projects. The project's budget should be cut to be more in-line with similar modeling projects.
- Please show more concrete results such as that shown in slide 10.
- Please reduce funding for this project significantly. The project's faulty input assumptions severely limit the utility of the results.

**Project # AN-06: Hydrogen Technology Analysis: H2A Production Model Update***Darlene Steward; NREL***Brief Summary of Project**

The H2A hydrogen production cash flow analysis tool was developed to 1) provide a consistent approach for tabulating the primary cost elements for hydrogen production over the lifetime of the facility; 2) provide a template for reporting analysis assumptions; and 3) calculate the annualized cost of hydrogen produced as a benchmark for comparison of technologies and measurement of progress. The objective for updating the H2A model is to focus the model updates to address the Hydrogen Program barriers.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **4.0** for its relevance to DOE objectives.

- It is absolutely necessary that there be one model that is used to calculate hydrogen cost.
- The H2A model, now with the new updates, is optimized and more accurately models cash flow for various pathways.
- The H2A model is important for standardizing the calculation of hydrogen production costs using a variety of feedstocks, technologies, and pathways.

**Question 2: Approach to performing the research and development**

This project was rated **3.9** on its approach.

- The presentation format of barrier strategy is excellent and shows thorough planning.
- The PI clearly addressed each key barrier and the corresponding strategy/update to the H2A model to address each barrier.
- The strategies/approaches to updating to version 2 are well defined.
- The new version appears to be much more user friendly.
- Making model more user-friendly is necessary for Macro-System Model (MSM) model integration and greater usage, but the speaker has not conveyed any intellectually stimulating results from this model update.
- It is not clear why the per unit costs are increasing between H2A version 1 and version 2. The benefits of this update are not conveyed.
- Model seems to be mixing current costs for some items with future expected costs for others. These two very different approaches to cost-estimates should be clearly separated in the model.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.9** based on accomplishments.

- Very impressive list of additions/enhancements made during the past year.
- All critical barriers have been addressed by the PI.
- This presentation did not show enough results, which makes the technical accomplishments to-date less impressive.
- Importance of model changes not demonstrated.

- Installing plant scaling is not a major accomplishment.
- "Use Excel variable naming to identify and locate critical input and output" is a limited achievement.
- "Provide detailed written documentation of methods and assumptions" should have done years ago.
- The information provided on "130% of daily production capacity" should be explained better.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.8** for technology transfer and collaboration.

- Very good, qualified team developing the model.
- Model availability and support is excellent.
- As evidenced by various studies/models that have referenced/used H2A model, the technology transfer & collaborations have been excellent.
- Acceptable partnering with other modelers, labs, and companies was incorporated in the model development.
- All acronyms should be defined in the presentation such as "CCS", "AEO", and "TOC".

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.6** for proposed future work.

- Plans for the coming year do not look as impressive as the accomplishments from the past year.
- There are more pathways to model and enhancements to be made.
- As more and more users are trying out the new version, feedback for improving the model needs to be monitored and factored in future maintenance and updating of the model.
- More validation of independent users based on real life data is needed for further refinement of the model.
- More detailed information should be provided about the planned "future work".

### **Strengths and weaknesses**

#### Strengths

- H2A is becoming the hydrogen cost standard.
- The new version 2 now builds in much needed updates to address critical barriers.
- Costs of carbon capture vs. plant size were plotted but more example results should be shown.
- Necessary model improvements appear to have been made, though not demonstrated to reviewers.

#### Weaknesses

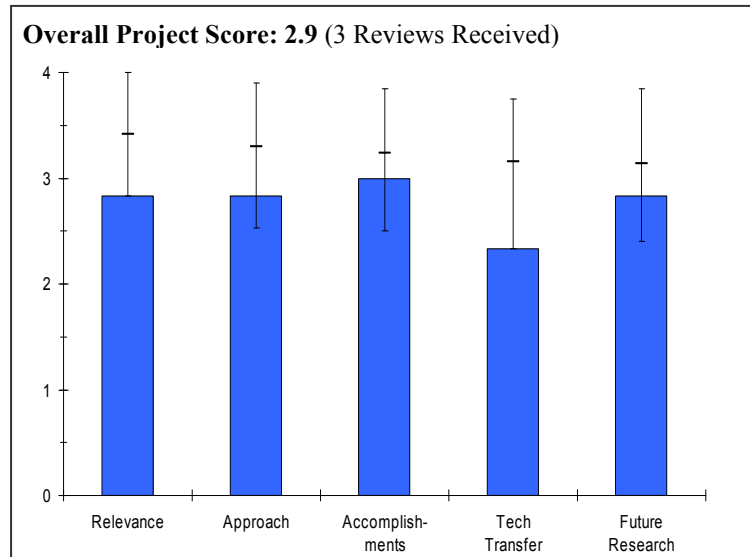
- Development effort seems to be tapering off.
- Perhaps more end-user education and feedback are needed.
- Importance of model changes not demonstrated.
- Plant scaling tool kit is not an impressive accomplishment.
- Lack of recent model validation is a weakness.

### **Specific recommendations and additions or deletions to the work scope**

- Become more aggressive in developing production pathways and enhancements to the existing pathways.
- A review session with modelers would be helpful to go over their models one-on-one.
- This presentation did not present any new research results. It showed that an inconsistent approach to modeling costs was being fused into the model (specifically, combining future costs for some items (carbon sequestration) with current costs for other items). It did not demonstrate enhanced model capabilities. As a result, funding for this research should be cut. This project is under-performing.

**Project # AN-07: Water Resource Analysis for Hydrogen Infrastructure***Rich White; LLNL***Brief Summary of Project**

The objectives of this project are to 1) characterize the water requirements for hydrogen production; 2) develop the framework for assessing the impact of water in hydrogen production; 3) conduct comparative analysis with water use for other fuel options; and 4) evaluate regional condition that may impact the adoption hydrogen production for a particular region. Water requirements will be assessed inside the hydrogen plant (water intensity, water quality, impact of water on hydrogen costs) and external requirements in support of hydrogen production (embedded water of input resources, source reliability, regional water influences).

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.8** for its relevance to DOE objectives.

- This analysis is not only important for hydrogen production, but needs to be extended (with funding from the Renewable Energy Biomass Program) to cover all potential renewable fuels.
- Though water is an important consideration in the production of hydrogen, it is not a critical factor in the Hydrogen Initiative R&D program.

**Question 2: Approach to performing the research and development**

This project was rated **2.8** on its approach.

- Sound approach beginning with literature search and ending in integration with the Macro-System Model (MSM) and benchmarking.
- Project is poorly designed. PI has chosen preliminary cases that may or may not be relevant, and it was not clear why or what were the underlying assumptions which justify the PIs choice of processes or process subsets. For example, biofuel from corn ethanol is not a relevant benchmark. There are numerous hydrogen production options that may indeed be most important in the future but these are not included in the project.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Project is less than a year old; however, excellent flow paths have been developed for several fuel pathways.
- The PIs early result that hydrogen water intensity can be kept low with new technology at small cost relative to the cost of hydrogen is a sufficient conclusion to the program and therefore further resolution in more detail is not that important. The comparison of hydrogen production to gasoline or corn ethanol production is like comparing apples and oranges and has no bearing on the assessment of water use between different hydrogen production options.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.3** for technology transfer and collaboration.

- Collaboration with other modelers is great.
- PI states collaboration with several labs, but there is no indication that there is any collaboration with industrial producers of hydrogen for establishing base case and benchmark realism.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- Please include comparison with other alternatives with the same assumptions.
- The project is working from a very good plan.
- The future plan was presented but it is difficult to see how the plan will extend or build upon the state of knowledge using the current results to generate knowledge that is meaningful beyond what has already been assessed.

### **Strengths and weaknesses**

#### Strengths

- Clearly shows the water requirement for the hydrogen production.
- Strength is in the team performing the research.

#### Weaknesses

- Need to be thinking about involving industry as an advisory group.
- No collaboration with industry, limited approach, uncertainty of assumptions, and unidentified project targets weaken this project considerably.

### **Specific recommendations and additions or deletions to the work scope**

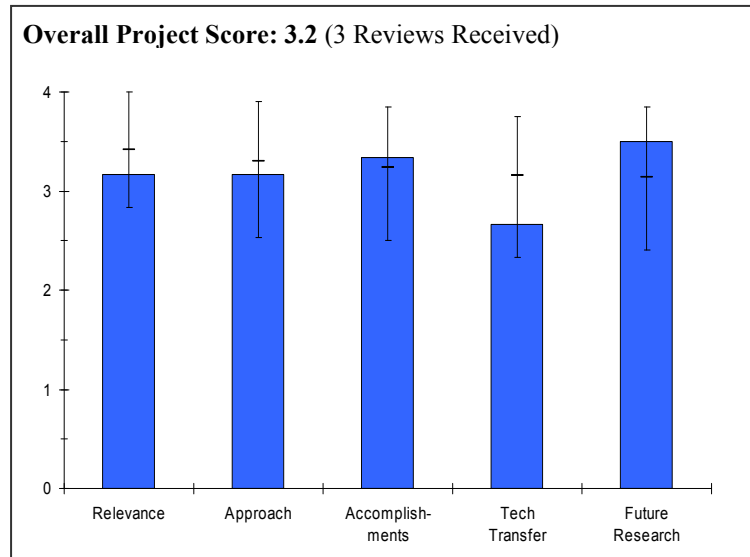
- Share the same assumptions with other energy alternatives such as biofuel.
- Indicate the absolute amount of water compared with other water consumption in the area
- This analysis needs to include other fuel pathways, such as coal-to-hydrogen.
- It is recommended that the current results be documented in a report and the project brought to a conclusion.

**Project # AN-08: HyDRA: Hydrogen Demand and Resource Analysis Tool***Witt Sparks; NREL***Brief Summary of Project**

The objective of this project is to develop a web-based GIS tool to allow analysts, decision makers, and general users to view, download, and analysis hydrogen demand, resource, and infrastructure data spatially and dynamically. For the fiscal year 2007/2008, 48 datasets viewable as graphical maps were created and integrated. Data manipulation and analysis tools, as well as application security, were implemented.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.



- The project aligns with Hydrogen Vision and the development of system analysis tools to analyze various hydrogen energy technology scenarios for providing technical inputs for R&D, deployment, market, and policy decisions supporting the overall Hydrogen Initiative.
- Understanding spatial resources, infrastructure, and potential demand data is important for correctly modeling the possible dynamics of transition to a hydrogen fueling infrastructure for particular regions; hence this project is important to the overall Systems Analysis effort.
- A graphical and simplistic view at the potential hydrogen demand and available feedstocks/resources to produce the hydrogen is in line of the overall objectives.
- Not entirely clear on the effectiveness/usefulness of the model.

**Question 2: Approach to performing the research and development**

This project was rated **3.2** on its approach.

- A useful feasibility analysis, user-friendly tool has been developed and further improvements in look, applicability, and effectiveness will be continued.
- This tool will help in identifying R&D needs for overcoming some known barriers--such as reducing hydrogen production costs—in addition to furthering understanding of issues and opportunities in large-scale deployment of hydrogen fuel.
- Project uses web server and GIS technology to make available resource, infrastructure, and potential hydrogen demand data in a visual manner, superimposed on maps of the United States. Approach seems reasonable and straightforward.
- Very good in pulling in data from various sources to predict demand and resource availability
- It is not clear that the factors/data considered will have a great influence on hydrogen demand in the future—the demand will be influenced by cost and reliability advantages of fuel cell vehicles over conventional technologies.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- Significant progress consistent with baseline objectives has been made within time and cost parameters.



## SYSTEMS ANALYSIS

- Project appears to have accomplished its objectives in a timely manner and has not run into any technical hurdles. Security issues prevent dissemination of some data on infrastructure to non-federal employees, which is outside the project's control.
- The PI showed great progress in compiling a great amount of data and the integration of the model with the other models.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.7** for technology transfer and collaboration.

- The project has some coordination with Mountain Top, LLC for its programming expertise.
- Outside consultant brought in to help w/ software development, which is a cost-effective approach. Collaboration w/ other projects as appropriate is planned (e.g. Macro System Model).
- Model needs to be validated by third party and industry.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.5** for proposed future work.

- Future work is well planned and will enhance the application of the tool.
- The list of planned work is impressive.
- Proposed future data sets to be added seem appropriate and helpful to overall goals of systems analysis program.
- Might need to consider adding a layer that contains information on hybrid vehicle purchases/uses around the countries. This will show public's willingness to embrace greener, more efficient technologies such as hybrids. These areas are likely to adopt fuel cell vehicles quicker, leading to the need for hydrogen demand/new infrastructure installation.

### **Strengths and weaknesses**

#### Strengths

- A useful, interactive tool to understand and analyze a variety of scenarios relevant to production, transport, and uses of hydrogen fuel is needed by technical, management, and policy people. This work supports that need.
- Project is well-structured and focused. Project has clear and rigorous methodology.

#### Weaknesses

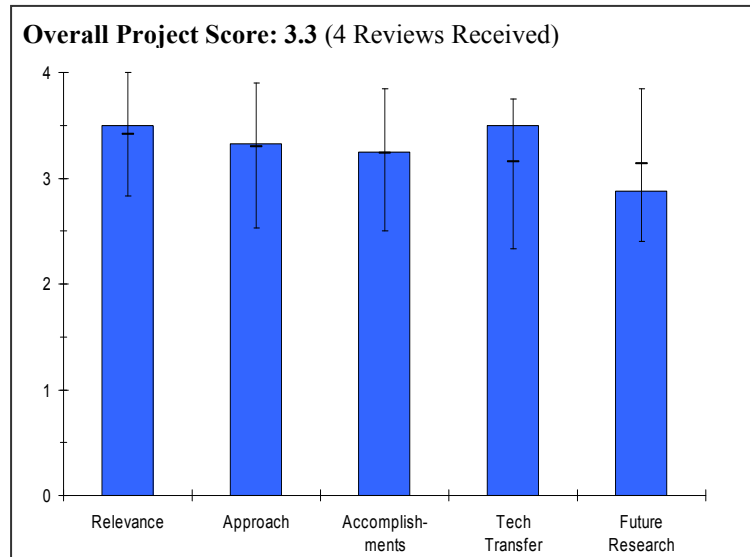
- No weaknesses were noted.

### **Specific recommendations and additions or deletions to the work scope**

- Build advanced capability by interfacing with other relevant models available in the hydrogen portfolio.
- Recommend considering adding data on local rates of taxation, labor, cost of construction, skills relevant to building & operating H2 stations, etc. as this could be helpful inputs to other models (e.g. H2A, or H2A through MSM) to be able to derive possible costs of construction for hydrogen fueling infrastructure.

**Project # AN-09: Lessons Learned for Fueling Infrastructure***Marc Melaina; NREL***Brief Summary of Project**

The objective of this project is to collect and articulate lessons learned from past experiences that can improve future decisions related to hydrogen fueling infrastructure development. Experiences to draw upon include 1) ethanol, natural gas and other alternative fuels for vehicles; 2) success with compressed natural gas vehicles in Argentina; 3) early development of the natural gas pipeline infrastructure; and 4) recent expansions of gasoline station networks in key urban areas. The approach consists of four tasks: 1) conduct a facilitate one day expert workshop; 2) collect empirical data on the success with natural gas vehicles in Argentina; 3) analogies to early natural gas infrastructure development; and 4) spatial evolution of urban gasoline stations.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- Very relevant to DOE goals—provides input on progress made and offers new options.
- Very good input on positive results and things that need correction.
- This program should provide insights into infrastructure deployment and expansion.
- Understanding lessons from previous successful and unsuccessful efforts to introduce new alternative fuels is important for developing a successful strategy to introduce hydrogen as a transportation fuel.
- Gaining understanding of other successful and accelerated introductions of fuel infrastructure can be very beneficial.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- Excellent approach in logically organized fashion.
- Includes alternative fueled vehicle H<sub>2</sub> station demo and innovation experience from expert organizations.
- Report summary is sent to participants for comments. This is very productive approach.
- Historical perspective of natural gas & gasoline vehicles is employed in a very useful way.
- It is unclear why natural gas vehicle data was collected from Argentina when the United States has years and years of natural gas vehicle deployments and end users. Consider approaching GM, Ford, and Chrysler along with the other fleet users for additional information about this database?
- Approach involved consulting relevant experts from industry, government, academia, and foreign experts. Approach seems reasonable and cost effective.
- Selecting compressed natural gas in Argentina as a study case is a very good place to start.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- Break-out session input is very well organized, analyzed and presented.
- Hydrogen value proposition (multi-purpose solution) is an important input from the analysis.
- Argentina's natural gas vehicle success story is a great example for United States.
- Study uncovered some previously unsuspected technical, economic, and administrative hurdles to be overcome, which is highly significant. For example, the study determined that expertise to design and build H2 fueling stations is a significant bottleneck. Also, siting and permitting processes are likely to take considerable time. Right now, perhaps insufficient effort is being put into addressing these problems by the DOE program.
- Starting in January and completing a workshop already is significant; although, scoring should not apply to this project.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.5** for technology transfer and collaboration.

- Workshop idea is a great tool and effectively utilized.
- Attaching with NHA conference was also a good way to get experience participants.
- Decent levels of participants but needs to have more participants from the United States.
- Experts from industry, government, and academia were consulted. Results will be widely disseminated via technical report.
- Focus on California is probably not representative of what could or will happen in the rest of the country.
- Recognize that it is early in the project; however, collaborations will need to expand for this project to thoroughly analyze lessons learned.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- Alternate vehicles should include hybrids, with hybrid FCVs being most important and especially as plug-in hybrids look very promising.
- Lots of possible future directions suggested, project needs to downselect. This reviewer suggests looking more in depth at factors contributing to successful introductions of compressed natural gas in Argentina, as well as ethanol in Brazil, compared with less successful efforts to introduce compressed natural gas in other countries.

### **Strengths and weaknesses**

#### Strengths

- The National Renewable Energy Laboratory has very good experience in collecting data and analyzing lessons learned.
- Collected good international data but a direct correlation to the behavior in the USA will be a big mistake. Different societies integrate technologies differently.
- Project is well-structured and focused. Project has clear and rigorous methodology.

#### Weaknesses

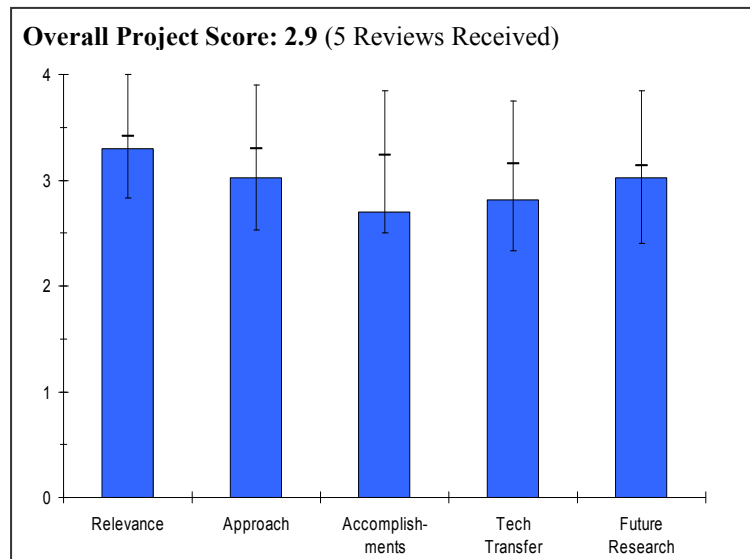
- Statistical data on success as well as issues are not presented. This may be very useful.
- The NGV graph regarding vehicles per station just does not look right. The USA has over 1000 Natural Gas Vehicle (NGV) fueling stations and quite a few NGV vehicles; however, this graph does not show it at all.
- Project has too many directions; it should develop a more focused scope. Suggest a downselect to concentrate on identifying factors behind successful and unsuccessful foreign introductions of CNG and ethanol.
- Project is so limited in time that it is going to be difficult to achieve the kind of results that will significantly impact future federal policy.

**Specific recommendations and additions or deletions to the work scope**

- Include H-CNG vehicles also for emission advantages.
- Include benefits of fleet vehicles to provide effective service at low cost.
- Lots of possible future directions suggested, project needs to downselect. This reviewer suggests looking more in depth at factors contributing to successful introductions of CNG in Argentina, as well as ethanol in Brazil, compared w/ less successful efforts to introduce CNG in other countries (e.g. Italy). Project should perhaps also pay special attention to possible cultural influences on success or failure of alt. fuel introduction efforts. Recommend less emphasis on studying infrastructure development in early 20th century, as this may have less relevance for today's situation (namely, the early automobile and gasoline were competing against less useful established modes of transportation, e.g. horse and buggy).
- This project will scratch the surface, but will not provide adequate information for DOE to recommend policy that will lead to sustainable hydrogen refueling.
- If DOE is really looking for information to guide hydrogen refueling introduction and growth, many additional successful and failed scenarios should be evaluated. Lessons learned must then be screened for applicability to the situation in the US.

**Project # AN-10: Hydrogen and Fuel Cell Analysis: Lessons Learned from Stationary Power Generation***Scott Grasman; U Missouri-Rolla***Brief Summary of Project**

The objective of this project is to collect and articulate lessons learned from past experiences that can improve future decisions related to hydrogen fueling infrastructure development. Experiences to draw upon include 1) ethanol, natural gas and other alternative fuels for vehicles; 2) success with compressed natural gas vehicles in Argentina; 3) early development of the natural gas pipeline infrastructure; and 4) recent expansions of gasoline station networks in key urban areas. The approach consists of four tasks: 1) conduct a facilitate one day expert workshop; 2) collect empirical data on the success with natural gas vehicles in Argentina; 3) analogies to early natural gas infrastructure development; and 4) spatial evolution of urban gasoline stations.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- Will provide useful information based on operating experience obtained from first time users of fuel cell technology.
- The project provides a good understanding about the synergy of stationary and transportation FC markets and linking them may keep both markets viable to support early entrant manufacturers solvent.
- Many different hydrogen and fuel cell systems have been demonstrated and deployed world-wide.
- It is appropriate at this time to take stock of how well they have worked out in meeting their test and demonstration goals, and to identify what significant issues have arisen.
- Understanding how stationary and other early market fuel cells are performing in the marketplace is relevant to the objectives of the DOE Hydrogen Program, specifically to efforts to advance fuel cell technology.
- It is very important that we learn from all relevant experiences relating to hydrogen as an energy carrier.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- A logical, structured approach with well-defined tasks including pathway analysis and ending with strategy recommendations.
- The project has a fair to good approach to performing the research and development. Information on market research or industry collaboration should be provided.
- The listed approach is systematic. It should lead to meeting the objectives of the project.
- No criteria were given or discussed as to how they would rate the success, or otherwise, of past or current fuel cell installations.
- It was not clear how the performance and other data would be obtained for the 2500 installations or demonstration projects.
- Project is collecting data on various fuel cell projects, and on what has worked to make them successful or not (Tasks 1-3). This seems like a reasonable approach. Examine the value of pathway analysis. The differentiation between Task 4 and Task 5 should be better defined.

- Well thought out plan that is thoroughly investigating stationary experiences.
- Changing from a workshop in St. Louis to a symposium at National Hydrogen Association in March is a great idea, as long as they retain the interactive breakout sessions and the sessions are well planned.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- Fairly new project. Good progress has been made to date.
- The technical accomplishments and progress toward project goals are fair. No evidence of progress was exhibited, just a check list stating level of completion.
- They have completed Task 1 and they are half-way through Tasks 2 and 4.
- No specific results were presented. It would have been useful if some detail of grouping of the 2500 projects was given, e.g., types of fuel cells, power ratings, combine heat and power (CHP) or not, co-generation of hydrogen or not, geographical and temporal distribution, current or past, or other deployment parameters.
- Progress to date has been unexceptional. Important project milestones are yet in the future.
- Very reasonable progress has been accomplished for less than a year of research.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.8** for technology transfer and collaboration.

- The project has some informed interactions but it wasn't clear what role these partners will play and what their specific contributions will be.
- The project's technology transfer/collaboration is fair but limited collaborations or sources were noted.
- The project should consider potential fuel cell demonstration sponsors other than DOE.
- An outside consultant is planned to assist with software development, which is a cost-effective approach. Collaboration with other projects as appropriate is planned (e.g. Macro System Model).
- Utilizing National Hydrogen Association as a forum to vet results is outstanding.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- The future project plan is adequate.
- Completing the data collection is good. Unsure of the need or reason to have a workshop.
- They propose to complete the tasks given in the approach section.
- No criteria are given for Task 3, Analysis and Lessons Learned, and Task 4, Pathway Analysis.
- Proposed future data sets to be added seem appropriate and helpful to overall goals of systems analysis program.
- Data collection followed by a workshop to consolidate and vet findings is great. Need to assure adequate planning for meeting at National Hydrogen Association to assure maximum benefit from a one day session with industry experts.

### **Strengths and weaknesses**

#### Strengths

- The project has a good approach.
- This project may help DOE support both stationary and transportation early adoption.
- The project has a systematic approach.
- The project is investigating 2500 applications.

### Weaknesses

- Presentation did not show any data collected to date. It would have helped to see where data collection is at. A few examples would have helped.
- There is a lack of apparent industry collaboration.
- The project needs to develop criteria for analyzing and rating success of past and current demonstrations.
- The project needs to identify how operating and other data will be obtained.
- The project needs to identify how they will sort through 2500 projects and 1000 fuel cell developers.
- The approach was not clearly explained, particularly Tasks 3 & 4.

### **Specific recommendations and additions or deletions to the work scope**

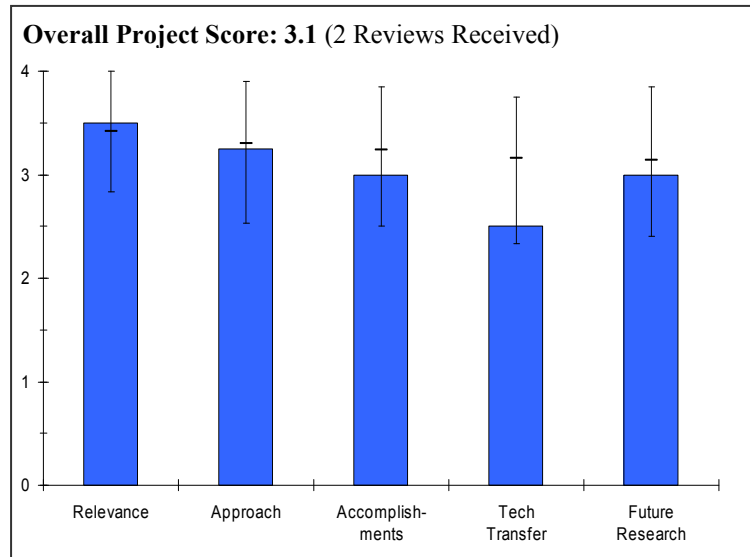
- Demonstration of industry collaboration to add fidelity to the analysis.
- The approach described in the summary at the end is not consistent with the 5-task approach discussed at the beginning of the presentation. Need to clarify what it is that they will do.
- Recommend looking at what alternatives to use of fuel cells would have been for each project evaluated, and factors that led to selection of fuel cells over the alternative. Recommend looking at whether fuel cell advantages/disadvantages for other markets are relevant to use of fuel cells for transportation.
- The project should include compression planning in meeting at National Hydrogen Association.

## Project # AN-11: Hydrogen Quality Issues for Fuel Cell Vehicles

Romesh Kumar; ANL

### Brief Summary of Project

The objectives of this project are to 1) assess how fuel quality influences the life-cycle costs and performance of the overall “hydrogen system” – production, purification, use in fuel cell vehicles, and analysis and quality verification; 2) identify information gaps and the research and development needed to fill those gaps; and 3) develop a roadmap that determines the significant cost elements, identifies challenges to reducing those costs and makes recommendations on how to address those challenges. Models will be developed to evaluate the quantitative effects of fuel quality on the costs of hydrogen system components.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Will provide useful input to FC developers regarding hydrogen quality and associated costs.
- This work is critical in recognizing the cost impact of purity levels and contributing input into set appropriate purity standard.
- Analysis of hydrogen quality/purity for fuel cell vehicles is extremely important
- Please explain the reasoning behind focusing on four contaminants primarily (slide 4) (N<sub>2</sub>, CO, CH<sub>4</sub>, CO<sub>2</sub>). These molecules found in hydrogen gas, air, and water, are impurities that can affect fuel cell performance.
- Understanding the trade-off between costs and contaminant levels is important (slide 4).
- Work is differentiated from other work by ASME and others, because of focus on life cycle costs, not just delivered cost of hydrogen.

### Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- Well-structured approach including cost analysis and trade-offs affecting life cycle cost. Approach based primarily on modeling rather than actual data collection.
- Looking at SMR + PSA product impurities and their effects on fuel cell performance & life cycle cost is a good approach. However, PI needs to consider other hydrogen production pathways and how fuel standard will have effects on these pathways' life cycle costs.
- The project might also need to look at tradeoffs of high temperature shift (HTS) + pressure swing absorption (PSA) vs. high temperature shift (HTS) + low temperature shift (LTS) + PSA vs. no water gas shift (WGS) + PSA vs. membrane vs. PSA, etc.
- Work should focus not just on pressure swing absorption (PSA) but also other technologies, such as EHS (electrochemical hydrogen separation), palladium membranes, preferential oxidation (PROX), methanation, etc.
- Integrating a portion of this work into the H2A model could be quite valuable.
- Were the models based on chemical engineering models or on experimental results? Are these ASPEN chemical engineering run results or a custom model? How does the custom model work?



- Sulfur is an odorant added to natural gas. However, the study considered a natural gas composition without any sulfur. This assumption is very favorable to fuel cells. A better explanation is needed to understand the reasoning for adding H<sub>2</sub>S to the water gas shift (WGS) outlet. Project needs to comply with conservation of mass principle.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Good progress has been made to date in modeling analysis and presentation of results.
- Good progress has been made to date. Would like to see some work/discussions/collaborations with groups/agencies working on hydrogen standards (International Organization for Standardization—ISO, California Fuel Cell Partnership—CaFCP, etc.).
- The project is producing excellent results. Work should receive a DOE award. Argonne National Laboratory's (ANL's) work adds great value to understanding impurity changes on the macro-system effects (hydrogen costs, mileage, etc.), and stack efficiency.
- Please show more results for additional impurities, not just CO.
- Database of critically assessed relevant published literature is very valuable.
- Integrating this information into existing models is extremely valuable.
- "Developed methodology to evaluate cost effects" using H<sub>2</sub>A is excellent accomplishment.
- The project demonstrates fascinating feedback loops between engineering system design and cost.
- More discussion of the drivers/reasons underlying results should be provided.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.5** for technology transfer and collaboration.

- Some work/discussions/collaborations with groups/agencies working on hydrogen standards (ISO, CaFCP, etc.) is needed as these type of work are valuable in helping these working groups setting realistic fuel standards.
- OEMs, Energy Companies, National Laboratories are good partners. Convened an excellent working group with different partners. Outreach meetings are excellent.
- Getting input from fuel cell developers, gas suppliers, etc. increases the relevance and utility of this study.
- Continued collaboration with industry is critical for project utility.
- Define the acronyms such as "TPSA" to increase audience understanding. Define recycle ratio, variables in table (delta\_V (change in voltage) and delta\_n (change in efficiency)) for the benefit of all audience members.
- This excellent work should be published.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- Good plan for future work based on extension of results to date.
- The project needs to look at other hydrogen production pathways.
- The project needs more collaboration with agencies in charge of setting hydrogen fuel standards.
- The project has nice ideas for future work. The project should consider "renewable sources" for hydrogen fuel generation such as anaerobic digester gas and landfill gas. These gases will have more impurities, be more difficult to clean-up, and will require more purification equipment. The project should perform a benchmark analysis on the "marginal cost" of going to a renewable fuel, in terms of the additional cost of the hydrogen purification equipment.

### **Strengths and weaknesses**

#### Strengths

- Interactive workshops with industry and international participants are quite valuable for the community.

- Integrating this work into the H2A model is valuable.
- The results for different inlet gas to the PSA cases, costs as a function of natural gas price, steam methane reforming (SMR) efficiency, and costs as a function of hydrogen purity level are extremely useful and demonstrate project progress.
- This presentation summarizes key results which is excellent. DOE should use this presentation's format emphasizing results as a model for other AMR presentations.

#### Weaknesses

- To improve this work, it should focus not just on pressure swing absorption (PSA) but also other technologies, including, but not limited to EHS (electrochemical hydrogen separation), preferential oxidation (PROX), methanation, etc.
- The reasons for focusing on only four contaminants (N<sub>2</sub>, CO, CH<sub>4</sub>, and CO<sub>2</sub>) should be more clearly justified. Other contaminants such as sulfur compounds can be equally or more of a problem for fuel cells.
- The focus on natural gas as a fuel should also be reconsidered. Expanding the feedstock fuels evaluated to biofuels (ethanol) and biogas, LPG could be even more helpful to some of the cutting-edge system designs taking place currently.
- A more detailed discussion of model inputs and function, and results for a wider array of cases should be provided.

#### Specific recommendations and additions or deletions to the work scope

- Some comparison with actual fuel cell operation conditions would be useful. Data would be available from Dr. Wipke of the National Renewable Energy Laboratory (NREL).
- This research should examine more contaminants in addition to N<sub>2</sub>, CO, CH<sub>4</sub>, and CO<sub>2</sub>.
- Convey more information about the assumptions, physics, and economics behind the model.
- Evaluate other hydrogen purification technologies (palladium membranes, electrochemical hydrogen separation) in addition to pressure swing absorption (PSA).
- Evaluate greater variations in natural gas composition than explored to date. Natural gas composition can vary significantly depending on the source, and regulations regarding purity levels and odorants.
- Consider "renewable sources" for hydrogen fuel generation such as anaerobic digester gas and landfill gas.

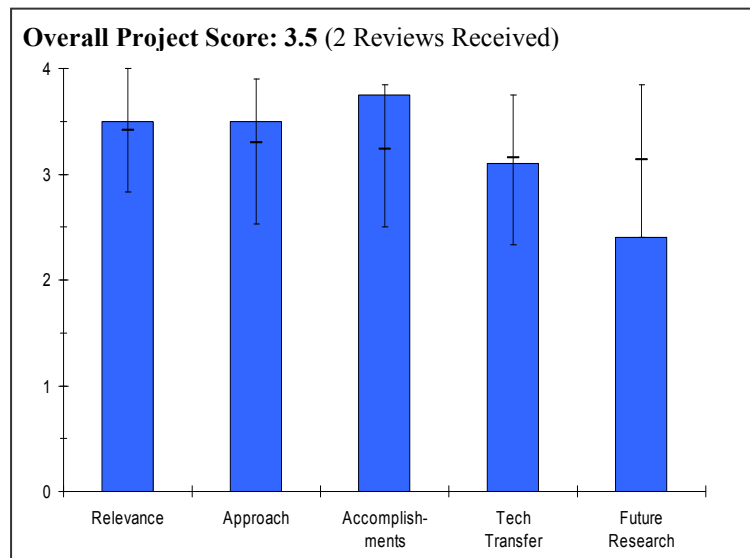
## Project # AN-12: Update on Platinum Availability and Assessment of Platinum Leasing Strategies for Fuel Cell Vehicles

Matt Kromer; TIAX

### Brief Summary of Project

This project updates a 2003 TIAX study on platinum availability and assesses the benefits of a platinum leasing program to support fuel cell vehicle (FCV) commercialization. The objectives of this project are to 1) assess constraints on platinum availability under high FCV penetration scenarios and 2) identify and quantify the benefits of alternative platinum ownership scenarios. The project hopes to answer the following questions:

- Are worldwide platinum resources sufficient to support high market penetration of FCVs?
- Can the platinum supply infrastructure meet the projected demand?
- Can upstream suppliers offer significant cost savings by internalizing the residual end-of-life value of platinum in an FCV's upfront cost?
- What are the risk factors and transaction costs associated with a leasing program?
- Given likely FCV supply chains, how could such a leasing program be structured and deployed?



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Adequate platinum availability for widespread fuel cell vehicle deployment is a recurring concern that has been voiced by many people.
- This concern has been heightened even more by the recent run-up in Pt prices to greater than \$2000 per troy ounce.
- Project is covering two extremely important issues.

### Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- The approach is systematic and logical.
- It is important to assess the level of confidence in the many different projections that are used in determining Pt demand over time (Slide 3).
- This project exhibited outstanding, straightforward research.

### Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.8** based on accomplishments.

- The project has presented a fairly comprehensive analysis and salient results of the analyses.
- The results show that platinum (Pt) accounts for roughly half of the fuel cell cost but that the supply should be able to meet the demand for the 50% market sales penetration scenario.
- The financial analysis shows that leasing of Pt (or the entire FCV) may not be a very attractive option for the consumer.
- The project was efficiently completed in less than a year.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- Platinum industry, the automotive OEMs, other interested parties were included in the project.
- Lots of resources used to complete the study.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.4** for proposed future work.

- The project is complete and no future work was presented.
- Completed project.

**Strengths and weaknesses**Strengths

- Logical approach, systematic analyses used in the project.
- The wide range of options was considered.
- Realistic inputs for the analyses were utilized from the Pt industry and OEM interests.

Weaknesses

- None.

**Specific recommendations and additions or deletions to the work scope**

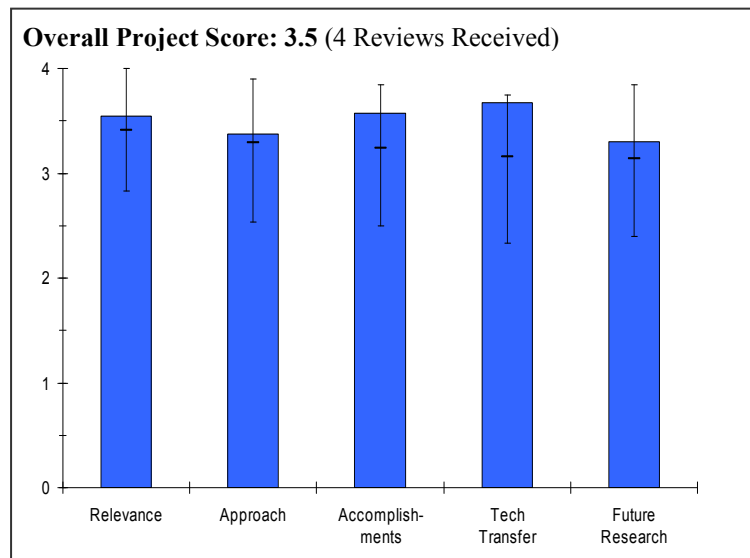
- No future activities are planned.
- The results presented should be useful to DOE and policy makers.
- Periodically, both of these topics should be reevaluated.

## Project # AN-13: Evaluation of the Potential Large-Scale Use and Production of Hydrogen in Energy and Transportation Applications

*Don Wuebbles; University of Illinois-Urbana-Champaign*

### Brief Summary of Project

The purpose of this project is to systematically identify and examine possible ecological and environmental effects from the production and use of hydrogen from various energy sources based on the Department of Energy production strategy and use of that hydrogen in transportation and power applications. This project uses state-of-art numerical models of the environment and energy system emissions in combination with relevant new and prior measurements and other analyses to assess the understanding of the potential ecological and environmental impacts from hydrogen market penetration. In the process, the Department of Energy will be provided with a capability for further assessing current understanding and remaining uncertainties for addressing the potential environmental impacts from hydrogen technologies.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- Project objectives and intended results are critical for both science and policy decisions to deploying hydrogen energy to stationary and mobile sectors and consistent with DOE hydrogen economy vision and related goals.
- Important work that is necessary to achieve DOE goals.
- This is an interesting project that is seeking to identify a range of potential effects of higher concentrations of hydrogen in the air as hydrogen production and use gets more widespread.
- Understanding how production and use of hydrogen would affect the environment is critically important to the overall DOE Hydrogen Program.

### Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- The study covers a wide range of relevant topics and answers or will answer many questions on the deployments of hydrogen energy technologies in both the stationary and mobile sectors.
- The study naturally cannot cover all related topics, but it will still contribute to the understanding and options to overcome some key barriers.
- The study covers safety and environmental topics from hydrogen production stage to its end uses; this is appropriate.
- The project approach appears to be sound.
- They are using atmospheric chemistry models to evaluate the potential effects of increased hydrogen concentrations on ground-level ozone and other pollutants on global and regional scales. They are also examining potential effects of hydrogen in the air on structural materials (e.g., embrittlement).
- Project is employing a variety of methods, including climate simulation, calculation of possible effects on materials, and measurements of hydrogen values near existing hydrogen sources. Methodology is extremely comprehensive and rigorous.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.6** based on accomplishments.

- Significant progress towards objectives have been accomplished and presented.
- Progress seems good except that there are a lot of things to finish by the end of FY08.
- They presented early results in many different areas of analysis.
- An interesting result is the much higher uptake of hydrogen by soils than what has been believed to be the case thus far. It should be noted, however, that these results still need to be validated by further testing and analyses.
- Project has already accomplished a number of calculations, showing likely consequences of elevated hydrogen on levels of atmospheric methane, likely composition of troposphere with widespread use of hydrogen, and likely rates of hydrogen uptake by soil and in buildings.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.7** for technology transfer and collaboration.

- National laboratories, University of Illinois, Queen's University, and Stanford University are involved in this important study.
- This team with complementary expertise will shed many insights on the health, safety, and environmental issues of deploying hydrogen to power production and transportation sectors.
- The technology transfer/collaborations seems to be good. The roles of the partners are clear.
- The project should include other universities and national laboratories.
- Projects involve significant collaborations between DOE labs and universities, and leverages relationships with companies involved in hydrogen production and use. Appropriately, cooperation is widespread and lots of data is being exchanged.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.3** for proposed future work.

- Each of the future work items is not only important and relevant, but legitimizes further, continued work to a complete understanding that large-scale production and wide-spread uses of hydrogen is truly safe. Another problem, as serious as ozone layer destruction, must not be created while solving greenhouse gas (GHG) issues.
- Future plans are not well developed particularly in FY09 and beyond.
- They have an ambitious future work plan outlined that includes modeling and experimental components.
- Proposed future research is aggressive and wide ranging, but seems largely doable since most of it involves calculations. Plans are very well focused on project goals.

**Strengths and weaknesses****Strengths**

- This study will create the awareness needed that there are issues with hydrogen fuel: its emissions during production, reactions with hydroxyl radicals in the atmosphere, its effect on the ozone layer, increased soil acidity, and, overall, the impact of the emissions on climate.
- The project will undertake extensive analyses.
- Project is well-structured and focused. Project has clear and rigorous methodology.

**Weaknesses**

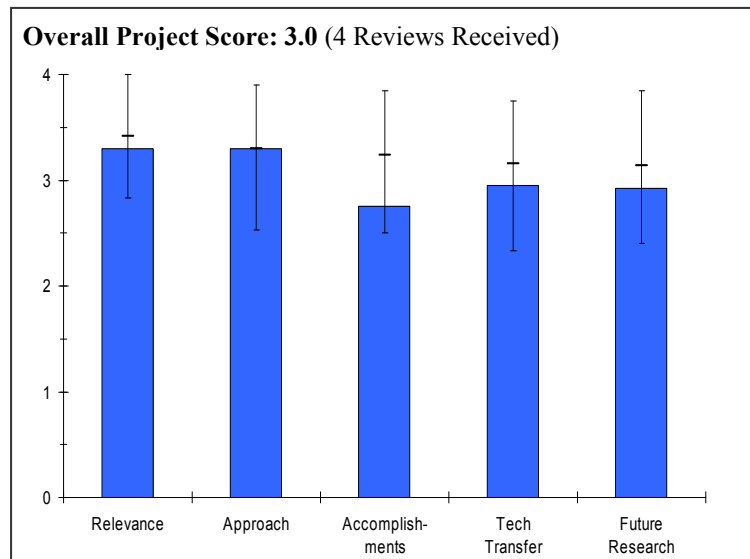
- The project needs to develop plans to validate modeling results.

**Specific recommendations and additions or deletions to the work scope**

- Conduct a long-term study on the effect of 5 ppm or more measured hydrogen concentration, such as in Mexico City and for the impact on steel and other metallic structures (simulated study is also appropriate).
- Consider different hydrogen production scenarios.

**Project # AN-14: Potential Environmental Impacts of Hydrogen-Based Transportation and Power Systems***Thomas Grieb; Tetra Tech***Brief Summary of Project**

The objectives of this project are to 1) compare emissions of hydrogen, the six criteria pollutants (CO, SO<sub>x</sub>, NO<sub>2</sub>, PM, ozone and lead) and greenhouse gases from near and long-term methods of generating hydrogen for vehicles and stationary power systems; and 2) evaluate the effects of emissions on climate, human health, ecosystem and structures. The following will be developed: 1) market penetration scenarios for vehicles; 2) market penetration scenarios for electricity generation; 3) emission-profile databases; and 4) soil uptake model. Changes in hydrogen and other atmospheric gases and aerosols in the troposphere and stratosphere will be predicted. Effects due to the implementation of two market penetration scenarios will be quantified.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- Study and understanding of potential environmental impacts of hydrogen-based transportation and power sectors is not only apposite but critical to the success of the engineering developments and ultimate deployment of hydrogen energy technologies.
- One purpose of systems analysis is research and development guidance; this and similar studies presented at the Annual Merit Review will allow technology research and development to overcome identified barriers to large-scale deployment of hydrogen fuel.
- This is critical work for policy goals and objectives.
- This is a useful study to assess the atmospheric effects of increasing hydrogen production and use over the near and long term time frames.
- Project seeks to evaluate impacts on criteria pollutants from widespread use of H<sub>2</sub> for light-duty vehicle infrastructure. This is relevant to understanding the possible benefits in addition to reducing CO<sub>2</sub> emissions that such an infrastructure might have.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- The technical approach and the task scopes are highly relevant and if successfully executed, the information will help in overcoming key barriers to deploying hydrogen fuel in the power and transportation sectors. Such system analyses studies are needed now, in parallel with the extensive technology research and development work on-going in production, delivery, and storage areas.
- Project addresses important sources of environmental impacts.
- The project seems to be a bit narrow but appropriate for the funding level.
- After developing emissions profiles as a function of hydrogen-based transportation and power production scenarios, they will conduct studies of the simplified global hydrogen cycle model to project changes in the concentrations of hydrogen and criteria pollutants in the air.

- Project will attempt to calculate production of criteria pollutants and green house gases from a variety of hydrogen production methods (including distributed steam methane reformation) and compare them to current (2005) emissions. Project will use two future scenarios for penetration levels of hydrogen fuel cell vehicles by 2050. The project combines environmental simulations and assessments.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- The project has summarized existing data and developed model scenarios to identify likely emissions and effects on climate, human health, ecosystem, and structures.
- The project, however, assumes that hydrogen is manufactured from renewable sources; this assumption is incorrect, fossil-based technologies will have to be used to produce hydrogen until renewable sources are fully technically developed; the hydrogen leakage intensity is different in the two production scenarios (fossil energy vs. renewable energy).
- Project has only been going 6 months, so modest progress seems satisfactory.
- The project is still at an early stage of execution. A major fraction of the background information has been collected but the analysis activity is just getting underway.
- So far, only scoping of problem has been accomplished.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.0** for technology transfer and collaboration.

- The project partner as of now is Prof. Mark Jacobson, known for modeling efforts, and the other partner is Potomac-Hudson Engineering.
- Stanford University's role is apparent, but the other partner's role is not.
- The collaboration is primarily in the form of using literature data and existing models.
- Project involves collaboration between industry and university. Results will be disseminated through reports and publications.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- Follow-up work building on results thus far.
- Both FY 08 and FY 09 task scopes are relevant and needed.
- The plans for the proposed project are limited.
- They have outlined an ambitious slate of analyses to be conducted in the remainder of the project term.
- Approach and relevance seem good, but could be improved - see comments below. Project should act as a useful check on previous studies/models, e.g. GREET.

### **Strengths and weaknesses**

#### Strengths

- This study will create the awareness needed that there are issues with hydrogen fuel. Its emissions during production and uses and the resulting impact on health, safety, and environment is a knowledge base that needs to be developed and comprehended.
- The project is utilizing the Stanford University modeling work.
- The project has a good strategy.
- The project has good scope and focus on studying hydrogen and atmospheric pollutants.

#### Weaknesses

- The project scope may be limited.
- None.



- Project's baseline scenario, assuming pollutant rates commensurate with 2005 technology for vehicles in 2050, is not a believable alternative to widespread use of H<sub>2</sub> vehicles. A more credible scenario is widespread use of plug-in hybrids or advanced electric battery vehicles which would be a future competitor for hydrogen and hydrogen fuel cell vehicles.

### **Specific recommendations and additions or deletions to the work scope**

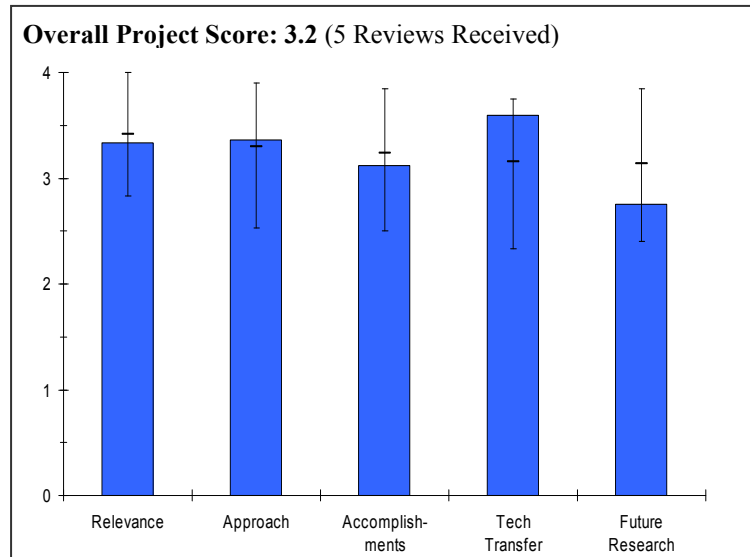
- Study of hydrogen dynamics in the troposphere and stratosphere is very important, but the project scope is limited. Suggest re-scoping for a more detailed study.
- Both fossil and renewable hydrogen production sources should be included in the study.
- Creating another problem as serious as the ozone layer destruction while solving the green house gas problem is not prudent.
- They should identify means to validate modeling results (i.e., how to determine confidence levels for the model outputs).
- Recommend considering changing baseline scenario to widespread use of electric battery vehicles instead of 2005 technology internal combustion engines. Alternative baselines to consider might be compressed natural gas vehicles, methanol internal combustion engine hybrids, or hydrogen internal combustion engine hybrids.

**Project # ANP-01: Hydrogen Technology Analysis: H2A Stationary Power Production Model***Michael Penev; NREL***Brief Summary of Project**

The objective of this project is to expand the capabilities of the H2A model to evaluate the stationary production of electrical power, heat co-generation and hydrogen co-generation. The H2A mission is to improve the transparency and consistency of cost analysis, improve the understanding of the differences among analyses and seek better validation from industry. The H2A model aims to make analysis consistent, transparent and comparable.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.



- Results of this work should be valuable for government personnel making decisions on market transformation.
- Expenditures related to stationary applications.
- Results should also be beneficial for private investors in stationary power, heat and hydrogen production.
- This work will reduce the time and cost for analysis of specific hydrogen applications.
- Stationary fuel cell systems are likely to have a significant presence in the marketplace well before the automotive fuel cells do. Therefore, this is a very worthwhile project to undertake.
- Model to calculate value proposition is very important.
- During the transition phase, stranded assets are a concern. The model allows evaluation of different approaches/solutions to this problem.
- Industry input is well-planned.
- Stationary fuel cell systems are not necessarily critical to the Hydrogen Fuel Initiative but this project at least rounds out the capabilities of H2A to include another option that may be of interest to some developers (perhaps help them decide to abandon certain development efforts).

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- The effort in this project seems to be linked well with prior H2A modeling work, and it also builds on it.
- The approach should provide a modeling tool which is broadly applicable to a variety of conditions.
- At present, their main activity is to develop the strategy for entering the hourly energy demand profiles into an H2A-compatible format. This energy demand will be met by a combination of reformat-based high temperature base load fuel cell system, a load-following direct hydrogen fuel cell system, and renewable electricity.
- The input energy sources are infrastructure fuels, grid power, and renewable electricity (the last one is yet to be added).
- The hydrogen demand is taken as a given at 100 kg/day.
- Extension of H2A model to multiple co-products is very useful.
- Ability to include time of day values of co-products allows the handling of high-peak and low demand scenarios.
- Cash flow analysis should include grid stand-by and demand charges.
- Overall, the approach is good. Detail is necessary in this case to make sure heat and power demands coincide.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- Not Applicable.
- The Principal Investigator stated the project is on track.
- There has been insufficient time to fully develop the model to the point at which specific tangible results could be cited.
- At this early stage of the project, only example input energy sources and demand profiles have been entered into the model.
- Preliminary distributions of the different sources and the demands for electricity (from the reformat fuel cell, the hydrogen fuel cell, and the grid) and heat (from the reformat fuel cell and a burner) have been obtained.
- The model is ready to be exercised for different applications scenarios.
- Program is relatively new.
- This project appears to be making very good progress for just \$70,000 of funding spent.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.6** for technology transfer and collaboration.

- The project plan includes collaboration with industry and the Risø National Lab doing modeling in Denmark.
- Feedback on the approach and project plan has evidently been received from only two companies.
- They are working with the H2A team at the National Renewable Energy Laboratory and Directed Technologies, Inc., and they are seeking input from various fuel cell developers as well as independent organizations that are active in installing demonstration units, such as Logan Energy.
- The project plans are excellent to share the model input-output with stakeholders.
- The project has good collaboration to date, but recommend talking to utility companies and perhaps US Fuel Cell Council

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- Not Applicable.
- After nine (9) months of work on this project, the result should be an important component of the H2A model.
- There are no specific plans or proposals for follow-on work at this time.
- They mention applying the model to a wide variety of stationary applications, but no specific examples are given, and neither is any rationale for the selection of applications to study given.
- There was no discussion of any effort to optimize the mix of input energy sources, or of alternative energy conversion subsystems, to meet the electricity, heat, and hydrogen demands at lowest life-cycle cost.
- Tri generation (co-production of heat, power and hydrogen) is a very important option.
- The project has the appropriate next steps.

**Strengths and weaknesses****Strengths**

- For a relatively small expenditure, this project will support individuals/organizations in making decisions on investments in stationary power facilities.
- All of the recognized benefits of the H2A model (consistency, transparency, accepted costing methodology, etc.) will accrue to this project as well, since it will be fully integrated into the H2A model.
- The model is flexible in that additional modules, such as for photovoltaics or wind power, can be added relatively easily.
- The National Renewable Energy Laboratory team is very well qualified.
- Input from equipment supplier ensures the results.
- Good modeling work.

Weaknesses

- None.
- This work is based on hourly or seasonal energy and hydrogen demand profiles, which are not readily available for the variety of applications that would be of interest.
- There is no strategy to optimize the mix of input energy sources and the energy conversion devices in the model to achieve lowest life-cycle costs.
- Inadequate plan to identify externalities and approach to internalize them (e.g. emission trading, industrial uses, etc.)

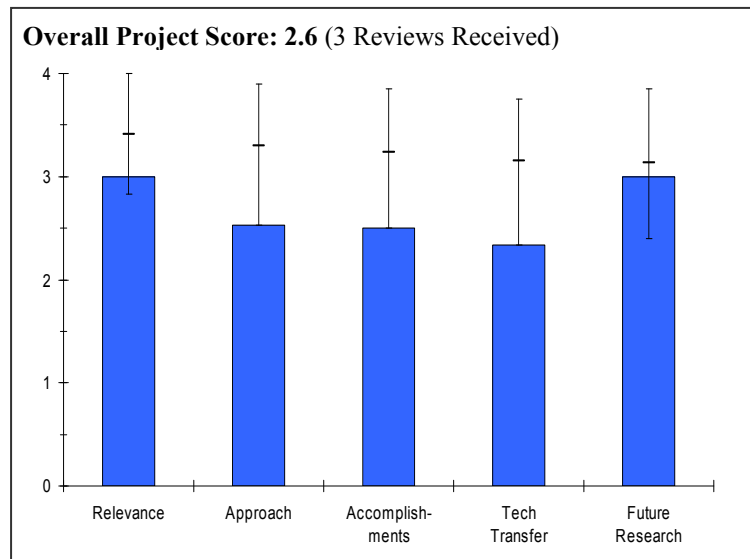
Specific recommendations and additions or deletions to the work scope

- Consideration should be given to a plan for disseminating the results to those who could productively employ this modeling tool.
- Consider optimization strategies for different scenarios. For example, consider these scenarios:
  - Different climatic regions.
  - Different mix and amounts of electricity, heat, and hydrogen.
  - Different costs (current, future) of the fuels, grid electricity, fuel cell systems (reformate and direct hydrogen) and renewable systems (photovoltaics, wind power).
  - Consider also the different sizes of the different fuel cells. For example, the high temperature fuel cells may be several hundred kW, the direct hydrogen fuel cells and electrolyzers may be only several to several tens of kW.
- The project should include all new opportunities to make positive impact on value proposition.
- The project should include renewable fuels.
- The project should include the impact of incentives (capital and O&M costs).

**Project # ANP-04: Hydrogen Infrastructure Analyses***Anthony McDaniel; SNL***Brief Summary of Project**

The objectives of this project are to 1) use dynamic models of interdependent infrastructure systems (natural gas, coal, electricity, petroleum, water, etc.) to analyze the impacts of widespread deployment of a hydrogen fueling infrastructure and 2) identify potential system-wide deficiencies that would otherwise hinder infrastructure evolution as well as mitigation strategies and unintended collateral effects on supporting systems. Sandia National Laboratories will provide analysis and insight into the dynamic behavior of complex systems and pose the following questions:

- Will the demand for steam methane reforming-derived hydrogen negatively impact natural gas distribution?
- Is there a potential for infrastructure interdependency issues to become problematic?
- Are there means to mitigate negative or amplify positive consequences?

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.0** for its relevance to DOE objectives.

- The project goals and approach require additional development before the relevance can be fully determined.
- The concept for the project of gaining insights into the impact of hydrogen use on other systems, such as natural gas infrastructure is sound.
- Useful project to answer detractors who ask how much will hydrogen drive up the price of natural gas and other feedstocks.
- The project looks at potential critical infrastructure and natural gas supply issues during initial fuel cell vehicle roll-out.

**Question 2: Approach to performing the research and development**

This project was rated **2.5** on its approach.

- It seems that the initial funding is being applied to developing the project's methodology and approach.
- The Principal Investigator and the Sandia staff have the capability to accomplish modeling and analysis that effectively complements hydrogen-related analysis already supported by other organizations, particularly other national labs.
- The Sandia team still has work to do on developing and vetting the approach.
- Hydrogen vehicle adoption rate needs to be a function of more than just "advertising effectiveness" and hydrogen price. Adoption rate should include assumptions/scenarios for hydrogen vehicle cost and vehicle benefits/consumer preference (e.g., green house gas emissions reduction), among other inputs.
- Model results would be more defensible if they just considered hydrogen vehicle adoption rate a model input rather than trying to predict the future performance/cost of hydrogen vehicles and then OEM and consumer's response to the future product (too many uncertainties).

- A localized (southern California) look might not be best representative of the US demand. It might be true that initial fuel cell vehicle penetration in southern California decreases gasoline demand and drives down gasoline price. However, gasoline price overall in the US and in the world might not really go down.
- Need to consider the real effect on the current distribution pipelines to see whether these pipelines can adequately handle the increase in consumption from numerous natural gas reformer systems (central and forecourt combined).
- Need to consider social factors (greener hydrogen from natural gas through CO<sub>2</sub> sequestration, hybrid fuel cells, etc.), green house gas emission factor, and public's willingness to embrace these technologies (willingness to pay more).

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.5** based on accomplishments.

- Not Applicable.
- This project is just starting, but they appear to be making good progress.
- Project has only started about 6 months ago. Model needs more refinement to achieve more accuracy and granularity.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.3** for technology transfer and collaboration.

- Initiative should be taken to work more actively with other entities such as national laboratories, states (e.g., California) and industry which have a stake in the results.
- This should be done during the project development stage of what could be a long-term, high-cost project.
- Seems like this project could be better integrated with other hydrogen analysis studies being conducted (or completed), especially on hydrogen vehicle adoption.
- Too early to tell since project only started in December 2007. Looking to collaborate with universities is a good plan.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- Not Applicable.
- Details of the initial project activity are still being developed.
- Good idea to incorporate water and electricity resources/capacities. Not sure how useful it is to roll this out to the rest of the country just yet.
- Factoring in electricity demand is a good plan since the majority of electricity produced in California is from natural gas.
- Might need to factor in potential spikes in natural gas price due to demand (locally, nationally and globally). This might to be disruptive (higher gas price = higher hydrogen price = fuel cell vehicle less attractive).
- Need to consider scenario of decreased gasoline demand in southern California might lead to decreased industrial gas demand (refineries no longer need as much natural gas to produce hydrogen for gasoline production). The increased natural gas demand by fuel cell vehicle roll-out might be offset (partially) by the decreased in industrial gas usage.

### **Strengths and weaknesses**

#### Strengths

- With the right team, approach and collaborations, this project could help fill a current gap in the hydrogen systems analysis program element.
- Provides a picture of what we need to be considered from the fuel and infrastructure standpoint (potential disruptive issues) during initial local fuel cell vehicle roll-out.

### Weaknesses

- Sandia staff needs to work intensively with others having a stake in the results during early project development to get feedback, recommendations and buy-in.
- The project needs further refinement because the project has too many assumptions and uncertainties at this point of the project.

### **Specific recommendations and additions or deletions to the work scope**

- Why is this project ending in 2015? Project budget and scope in future work should be complete by FY09.

## 2008 Manufacturing R & D Summary of Annual Merit Review Manufacturing R & D Subprogram

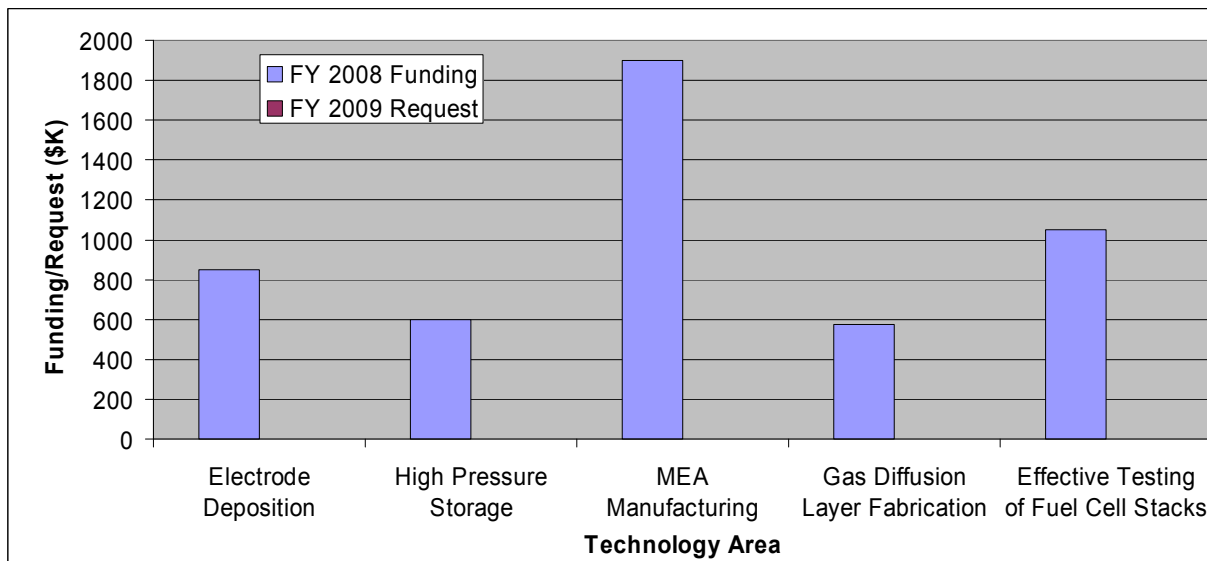
### Summary of Reviewer Comments on Manufacturing R & D Subprogram:

Reviewers consider manufacturing research a key element for fuel cell and hydrogen technology commercialization. Overall, the Manufacturing R&D subprogram was judged to be well-managed and focused on addressing program performance targets. Progress was considered good.

As a result of a competitive solicitation, six new R&D projects in the Manufacturing Research Subprogram are being awarded at the end of FY 2008. These new projects will be reviewed in FY 2009.

### Technology Focus:

The Manufacturing R & D subprogram continues to concentrate on reducing fabrication costs of the critical path technology, i.e. fuel cells and high pressure storage systems. Cost and quality of stack and storage components continue to be a key focus of the subprogram.



### Majority of Reviewer Comments and Recommendations:

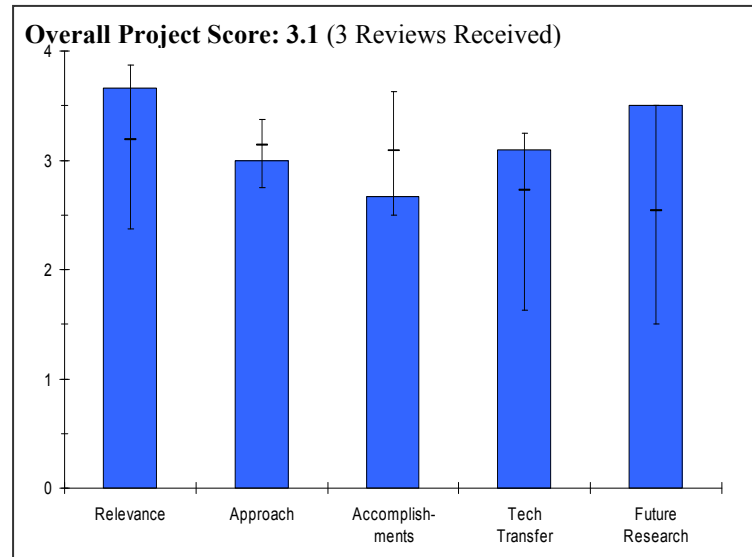
In general, the reviewer scores for the manufacturing projects were high to average, with scores ranging from 3.4 to 2.5 for the highest and lowest scores. The majority of the projects were reviewed by four reviewers. The scores reflect the technical progress that has been made over the past year, relevance to the DOE Hydrogen Program, technical approach of the project, extent of technical transfer, and proposed future plans for the project. Key recommendations and weaknesses are summarized below. DOE will respond to reviewer recommendations as appropriate for the scope and coherency of the manufacturing research effort.



The reviewers were most impressed with the Profile Composites project for rapid manufacturing of carbon composite high pressure storage, giving this project the highest scores for the sub-program in both project relevance and approach. In addition, reviewers were pleased with the progress Protonex has made in reducing cost with its novel fuel cell stack manufacturing process and with the progress by ASME Standards Technology in non-destructive quality assurance testing for carbon fiber hydrogen tanks. While reviewers were generally positive about the relevance of the projects to DOE goals, they demonstrated concern regarding the technology transfer and collaboration of more than half of the projects. Of the nine projects, the reviewers rated the National Renewable Energy Laboratory project highest for its future plans.

**Project # MF-02: Fuel Cell MEA Manufacturing R&D***Mike Ulsh; NREL***Brief Summary of Project**

The objectives for this project are to 1) evaluate and develop in-line diagnostics for membrane electrode assembly component quality control and validate in-line; 2) investigate the effects of manufacturing defects on membrane electrode assembly performance and durability; and 3) further develop and validate models to predict the effects of local variations in membrane electrode assembly component properties. Fuel cell system cost targets are based on a projection of 500,000 units/year. The supplier base needs high-speed manufacturing methods – and quality control methods to support them – to achieve these volumes.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.7** for its relevance to DOE objectives.

- In-line manufactured component quality measurement will be important to stack performance and durability.
- Project addresses the need to lower cost of manufacturing of fuel cells and membrane electrode assemblies, which directly supports Department of Energy objectives.
- In-line measurements of membrane electrode assembly components during the manufacturing processes will lead to better process control and lower costs.
- Manufacturing technology assures ability to make fuel cells in quantity and at minimum cost.
- This project stresses metrology of continuous-flow film processes for membrane electrode assembly construction, which is vital for in-process quality control.
- Manufacturing quality control is essential both for minimizing production costs and for ensuring long product life (for consumer satisfaction and acceptance of the technology).

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- One of the goals is to identify critical defect characteristics to help establish processing parameters and component quality specifications.
- The project is sharply focused on in-line measurements of membrane electrode assemblies and investigation of the influences of manufacturing defects on membrane electrode assembly performance.
- The approach includes both experimental techniques and modeling to understand these complex relationships, which is extremely important for solving manufacturing problems.
- Milestones are realistic.
- Approach in theory (Slide 5) is fine; approach in practice is lacking.
- It is not clear how, and if so in what way, current production lines at companies such as Ballard and Plug Power lack scalability to goal of 500,000 [industry-wide] units/year... It is not clear how this project is informed by current best-practices in existing production lines.
- Project lacks quantitative goals and objectives (e.g., measuring membrane thickness to specified resolution in nanometers with a specified measurement uncertainty).

- Project is spending significant effort in making qualitative (rather than quantitative) evaluations of measurement techniques on swatch samples, rather than in-process (simulated or real), flowing samples (e.g., Slides 7 and 8).
- Quantitative measurements—and advancing the art of quantitative measurements—are what would be essential for meeting quality-control goals.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- Decent progress for less than a year of effort.
- Some techniques evaluated and down-selected.
- Promising new technique described and proof of concept demonstrated.
- A comprehensive assessment was conducted comparing various techniques for measuring membrane electrode assembly characteristics.
- Unfortunately, results were not summarized quantitatively; therefore, it is hard to estimate the degree of effectiveness for any particular applications.
- Optical reflectometer approach seems to have great potential to measure multiple characteristics over large areas. Unfortunately, the technical details were not provided due to invention disclosure restrictions.
- There may still be significant barriers in achieving needed measurement resolutions.
- The results of initial model development are not obvious.
- Project could be much improved by stressing precision and accuracy of different measurement techniques.
- It is not clear what was modeled or what performance was demonstrated by the words, "Initial model development...complete", on slide 13.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- Several of the major membrane manufacturers are involved.
- The collaborations with other government laboratories and universities are right on target. These collaborations complement the expertise provided by each partner.
- Industry role seems to be limited to just providing guidance. Increased industry collaboration in developing and testing prototype measurement systems at early stages can help the technology transfer at the conclusion of the effort as well as providing some short cuts toward achieving the project goals.
- Partnerships with the Colorado School of Mines and University of Hawaii are positives.
- Project suffers for lack of partnerships with existing manufacturers with production-line experience.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.5** for proposed future work.

- Logical continuation to screen techniques and develop a new technique with interesting potential.
- Segmented fuel cell development is a great idea to achieve the objectives of this project.
- All future activities are well formulated based on the progress so far and overall objectives.
- "In-line validation of diagnostics with partners" is absolutely essential.
- Modeling is informed by good metrology, so should be only second priority.

**Strengths and weaknesses****Strengths**

- Good level of focus on the in-line measurements.
- Excellent potential for improving the fundamental understanding of the effects of manufacturing defects on membrane electrode assembly performance utilizing the combination of experimental and modeling approaches.
- This project addresses an important need.

Weaknesses

- It seems very difficult to generate well-controlled defects to carry out effective statistical analysis and/or validation of models.
- Early interaction with industry to validate techniques is very important for the success of the project.
- Lack of quantitative results presented (e.g., discussion of precision and accuracies of measurement techniques studied).
- Lack of partnerships with firms that have actual manufacturing experience.

Specific recommendations and additions or deletions to the work scope

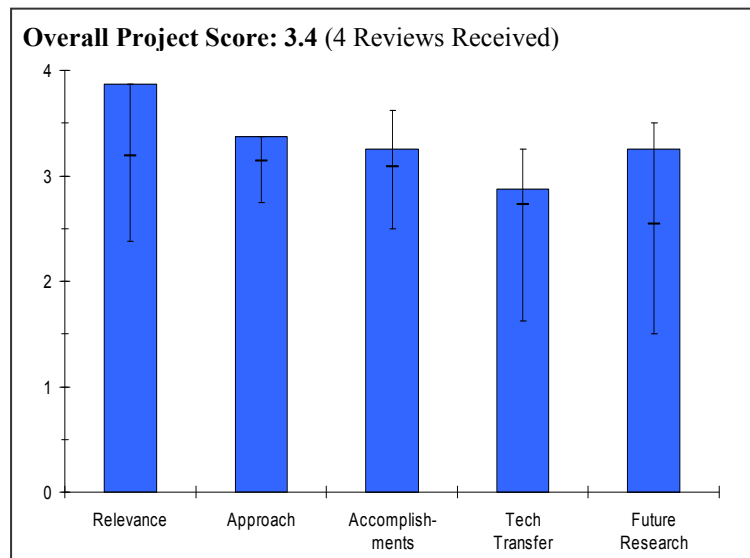
- None listed.

**Project # MF-04: Rapid Manufacturing of Carbon Composite High Pressure Storage Cylinders (an NCMS project)**

*Geoff Wood; Profile Composites*

**Brief Summary of Project**

The primary objective for this project is to demonstrate high-rate manufacturing of 35-MPa carbon composite hydrogen storage cylinders. An ability to achieve this objective requires 1) that no process stage take longer than 20 minutes; 2) all individual steps to be “production capable”; 3) all materials to be available in quantity and with potential for automotive volume production; 4) major process risk areas to be demonstrated physically; 5) cylinders to be validated by test program; and 6) showing a complete engineering analysis and process model to achieve under 10-minute production cycle time per cylinder for 70-MPa cylinders.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.9** for its relevance to DOE objectives.

- Rapid manufacturing focus is important to achieve Department of Energy goals.
- Vehicle cylinders address proton exchange membrane fuel cells for transportation sector.
- 350 Bar is one of the pressures OEMs will want to use.
- High-pressure hydrogen storage is an important aspect of the Hydrogen Fuel Initiative. This project addresses rapid manufacturing of carbon composite storage tanks.
- Although cost information was not provided, significant reduction in production time will eventually result in significant cost reductions.
- The project also claimed a decrease in capital investment for the manufacturing of the tanks.
- On-board storage is one of the major issues to overcome in achieving a competitive hydrogen pathway for fuel cell and other vehicles.
- Cost-effective storage capacity for achieving 300 miles is an overall DOE target—composite high-pressure tanks are an interim solution that would not achieve DOE overall goals, but are a feasible, nearer-term approach to storage.
- As stated in the manufacturing workshop background material, "The manufacturing processes for these (carbon fiber composite) containers are time consuming, very expensive and require multiple inspection steps. Scaling up production quantities while significantly bringing down unit costs will be particularly challenging." The purpose of this project is to address these issues, and particularly to identify and validate high-speed manufacturing operation.
- The primary objective is to demonstrate high-rate manufacturing of 35-MPa (5000 psig) as well as 70-MPa carbon composite hydrogen storage cylinders. Allow for production capacity off a single tooling line to approach that of specialty vehicle manufacturing over 20,000 tanks/line/year based on 3-shift operation (current technology defined by PI as 1000 tanks/line/year).
- This project is highly relevant because it would allow continued demonstration of fuel cell vehicles until other less-costly, greater-volumetric density storage alternatives are developed.
- Development of low-cost hydrogen storage tanks is an important function.

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- Focus on 20 minute rate of manufacturing is significant improvement.
- Approach also addresses both cost and performance of cylinders.
- Matching vehicle production rates allows for realistic scale-up.
- Good milestone schedule.
- The approach is very systematic and technically robust, covering a wide range of critical issues relevant to manufacturing of carbon composite tanks from design and materials, to manufacturing, testing, and commercialization.
- Very well thought out plan.
- Cost is not directly targeted, but natural outcome of the cycle time reduction and introduction of automation will be the cost reduction, which is correctly identified as an important barrier.
- The approach is to focus on design of updated composite fiber high-pressure tanks (design for new, unique process ability, manufacturability, and materials development); fiber/resin performance under accelerated cure rates and resin system designs; novel manufacturing processes and experimental development; design and development of an automated materials handling system; subscale cylinder burst pressure tests; subscale cylinder laminate tests; full-scale cylinder pressure and cycle tests; commercialization; and to demonstrate each process step in under 20 minutes.
- This is a logical approach formed by a knowledgeable and experienced team in an organized, systematic manner to achieve production capability for all operational steps, demonstration of novel manufacturing, and fabrication of full-scale cylinders for vehicle testing.
- The successful implementation of this approach would achieve the stated objective—considerably faster production of high-pressure tanks (7-9 hours present state-of-art to 20 minutes).
- The reduction to a 30-minute cycle time will benefit the industry.
- Quality control needs to be included in the program activity.
- Need to include reduction in fiber costs.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- Achieved 30-minute process time. On the way toward 20-minute time.
- Moving rapidly toward commercialization opportunities.
- Met similar process speed used by original equipment manufacturers for injection molding process.
- They have achieved excellent progress demonstrating the cycle time reduction from 7-9 hours to about 30 minutes, which is very impressive.
- There is a realistic chance to achieve the ultimate goal of a 10-minute production cycle time per cylinder with automation and fine tuning of the processes, which will meet the production target of 20,000 tanks/line/year.
- Although originally scheduled to end in June 2008, it was indicated that the project is 85 percent complete, which is some concern; however, I am optimistic that they will finish it by the new completion date of August 2008.
- Developed design of Type 3 tank (metal-lined) with separation of fiber placement and resin processing. Currently achieved 30-minute process cycle in FY 2008 with no automation. Designed automation systems to overcome major materials handling issues and implemented development of systems. Tests will be conducted next month.
- Developed a novel methodology to control fiber wrap, which allowed acceleration of fiber placement and improved processing materials.
- Demonstrated process for achieving 20 minutes, currently implementing more robust and repeatable systems. Tooling up for full-scale cylinder, re-designed tooling approach as required for control of overall process. Developed and designed and currently implementing third-generation materials handling system.
- Approach to achieve 10-minute overall cylinder production cycle time. It appears that 18-minute overall production cycle is best achieved at subsystem and suggests that 19 minutes at commercial scale is achievable.

- Progress appears to be reasonable but more needs to be done (additional tests to be conducted within the next six weeks) including demonstration of automation and handling system and process demonstration for complete manufacturing cycle.
- 70-MPa cylinder development would be done in FY 2009.-
- The 30-minute production rate is a benefit and should help this company in cylinder manufacturing for all applications. This is only at a small size.
- The benefits need to be demonstrated at a full size storage vessel.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.9** for technology transfer and collaboration.

- Coordinated well with rest of team.
- Not sure how other companies can benefit from this work as it doesn't appear this will transition beyond Profile, Inc.
- Still needs to be tested for hydrogen leakage. So far only hydraulic testing has been done.
- The project team includes all the key players: fiber producer, resin producer, machine tool builder, and the end-user.
- I was very glad to see a domestic machine tool builder is part of the team.
- There seems to be highly effective collaboration among the team members.
- The purpose of this task is to demonstrate commercial carbon composite tanks with the primary goal of achieving 35-MPa (5000 psig) tanks and also 70-MPa (~10,000 psig) tanks. Geoffrey Wood and his company produce carbon composite tanks. The cost sharing partners include Toyota, A&P Technology, Bayer, and MAG-Cincinnati with significant commercial interest and manufacturing capability.
- This project benefits this company and transfer of technology is not included.
- The project would not identify how they achieved the 30-minute cycle.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.3** for proposed future work.

- Identified appropriate follow-on target of research 700 Bar cylinders.
- Attempting to reduce manufacturing time even further, down to 10 minutes.
- The immediate future plan includes more testing, automation, and cost model refinement, which are on target for accomplishing the ultimate goal.
- Health monitoring is included in the longer term plans. It is correctly identified that health monitoring will be critical for the effective use of these tanks.
- The 70-MPa pressure cylinder development is also planned for FY 2009, which should be the next logical step in the development based on the knowledge and experience gained in the development of the lower pressure cylinder in the first phase of the project.
- In FY 2008 the principal investigators will complete a new tooling approach for full-scale cylinders; demonstrate the automation and handling systems; perform process demonstrations for the complete manufacturing cycle; refine the cost model and include automation factors; and complete the test cycle for cylinders and provide cylinders for partners.
- In FY 2009, the principal investigators will initiate systems for health monitoring of cylinders by beginning development for 70-MPa cylinders; and initiating production for 35-MPa cylinders.
- This future work must go on within a new contract.
- Limited details provided.
- It appears that the bulk of the future work would be done under a time extension or a new contract.
- The "proof of the pudding" will be the integrated production of the cylinders.
- The project addresses full size cylinders in the future. The research does not benefit the fuel cell community as a whole, but sponsors development at a single company.

**Strengths and weaknesses****Strengths**

- Very capable principal investigator/team with strong manufacturing focuses.
- The project team has used a systematic, technical approach.
- The project team has done a good job of utilizing the expertise of companies in the project team.
- A novel manufacturing approach led to significant reduction in cycle times (although not much information was provided about this novel method due to intellectual property protection issues).
- This is an important study because early to intermediate on-board storage will require high pressure tanks while other advanced storage technologies are developed and demonstrated.
- Cheaper tank storage will allow the validation of early fuel cell vehicles.
- This is a knowledgeable team with significant experience in high-pressure carbon composite tanks.
- The technology builds on high pressure tank experience from natural gas vehicles.
- Profile Composites appears to have good understanding of cylinder manufacturing processes.

**Weaknesses**

- The principal investigator cannot relate cycle time reduction to overall cost reduction.
- The project experienced a one-and-a-half-month slippage in schedule.
- Project will not benefit other manufacturers unless the principal investigator better shares information.
- Profile Composites did not provide much information was related to cost modeling and estimates.
- Profile Composites was not particularly aware of other research and development activities that are very relevant to this project (e.g. another National Center for Manufacturing Sciences project develops a health monitoring system using inexpensive acoustic emission sensing for defect detection).
- A high-pressure storage tank for hydrogen is just an interim solution.
- An integrated demonstration for complete manufacturing process remains to be done.
- The 70-MPa experimentation remains to be developed.
- Profile Composites needs to determine the final cost improvements.
- Profile Composites does not include quality control in the development activity.

**Specific recommendations and additions or deletions to the work scope**

- The principal investigator should upgrade the quality control activities.
- The principal investigator should increase the technology transfer activity.

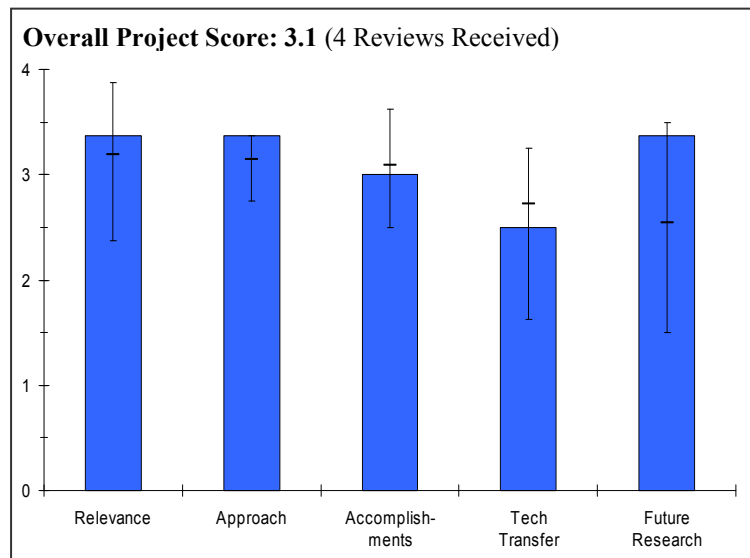


**Project # MF-05: Technologies for Mass-Manufacturable Manifolds and Durable Seals for PEM Fuel Cells in Transportation Applications (an NCMS project)**

*Patricia Cosentino; UTC Power*

**Brief Summary of Project**

The objectives for this project are to 1) evaluate/select material for manifolds and durable seals for polymer electrolyte membrane fuel cells; 2) develop a manufacturing process using those materials; 3) assemble a short stack using the new seals; and 4) assemble the seal into a full-size unit for in-house or field testing. Polymer electrolyte membrane fuel cells require inter-cell seals (interfacial seals) to separate reactants and coolant streams. Fuel cells utilizing external manifolds require a high-speed system for sealing the manifolds to the exterior of the stack. The current design for both these seals is expensive and has low yields.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.4** for its relevance to DOE objectives.

- Cost is one of the critical issues for the Hydrogen Fuel Initiative. These two projects approach cost reduction through materials selection and manufacturing technologies.
- Seals are expensive, currently have low yields, have too many components. Manifolds currently require 100 percent inspection. However, seals and manifolds are not critical cost or durability drivers.
- The project fully supports Department of Energy objectives by addressing the cost reduction needs of seals and balance-of-plant components.
- Rapid assembly of fuel cell components and the effects of seal additions is an important manufacturing issue.

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- The approach is logical and sound, progressing from materials selection to sub-scale proof and full-scale verification.
- The principal investigator had a go/no-go criteria built into milestone schedule and went through material selection with a 20,000-hour durability target in mind.
- UTC Power tried to find an existing product to qualify in the manifold.
- UTC Power tried to reduce the number of seal components.
- The principal investigator included full-size testing.
- This project is actually two projects – one for seals and the other for manifolds. I don't understand the logic of combining these projects into one project. This approach prevents the team from focusing sharply on the barriers.
- The technical approach seems to depend on mostly experimental comparison of materials; not much evidence was provided about any analytical study about material selection for compatibility.
- Well structured project with objectives identified. The speaker referenced use of Technology Readiness Levels as a means to judge progress.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Both projects have been successfully completed, resulting in significant changes in weight, cost, and inspection times.
- The project team realized a ten-times reduction in scrap by using a "cold sensor" tool.
- UTC Power reduced seal process time by 15 times.
- UTC Power reduced inspection from 100 percent to less than 5 percent.
- UTC Power improved the process capabilities and reduced seal components from 4 to 2.
- One part of the project was scheduled to finish in December 2007; it is only 80 percent complete. The other part is scheduled to finish in Aug 2008, and it is only 75 percent complete.
- It is not clear what is significantly new in the manufacturing process that resulted in the 10x reduction in material scrap.
- It is not clear how many different types of material were tested to down select to two.
- It is not clear what the results are of *in situ* testing on short stack, which was identified among the early steps in the technical approach chart.
- It is not clear what significantly new fabrication process was used that resulted in 90 percent cost savings.
- The information shared by this presentation did not allow a full evaluation of technical accomplishments. The presenter claimed good results but did not share details.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.5** for technology transfer and collaboration.

- The teams on the two projects are good.
- General Pattern was a good choice for a partner (injection molding).
- The project team includes a major seal producer, which should bring necessary expertise to deal with difficulties in seal production and testing.
- It was not clear what the roles of Lawrence Berkley National Laboratory and General Pattern are on the manifold manufacturing part of the project.
- There is no technical transfer of information. All technology belongs to UTC Power or to Freudenberg-NOK.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.4** for proposed future work.

- The manufacturing technologies project is complete.
- The low-cost/high-volume seals project has only a few months remaining. Future work will prove the concepts and techniques at full scale.
- Future plans include long-term short stack testing.
- The project will not require DOE funding for follow-up because UTC plans to do further testing and employ the technology.
- The experience gained in material selection and manifold manufacturing will help in design and assembly of full-size stack and durability tests.
- Automating the process for actual production is a natural next step in this development.
- Testing will be done on a subscale level. Full-size testing is anticipated.

**Strengths and weaknesses****Strengths**

- UTC Power will be able to employ the results immediately.
- Teaming with seal manufacturer was a strength of the project.
- UTC Power has identified a seal material that allowed process time reduction by a factor of 15.

## MANUFACTURING R & D

- UTC Power has identified the process and equipment for highly automatable application.
- UTC Power is well established fuel cell manufacturer.

### Weaknesses

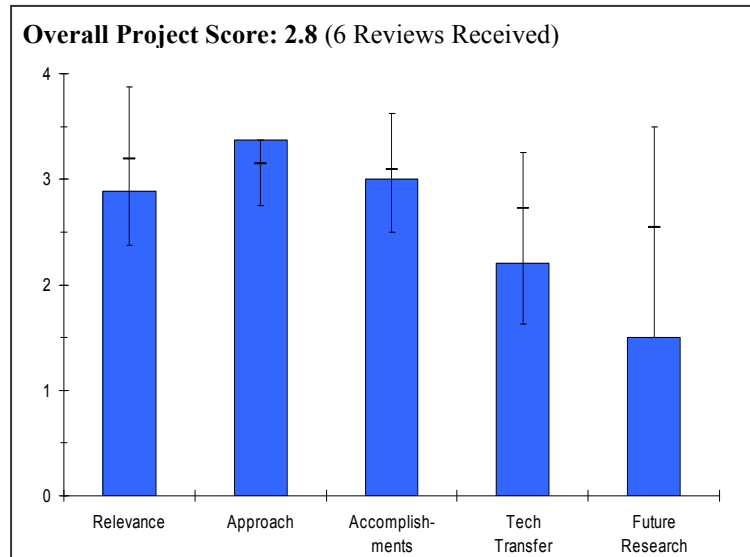
- The team has shown a lack of focus on the main technical barriers.
- The team has shown a lack of a clear technical plan for the manifold manufacturing part of the project.
- The project team developed injection molding, but does not have a market for this high-rate process. This focus appears to be a poor use of funding to develop unneeded manufacturing technology.
- The principal investigator did not provide sufficient information to evaluate the project's progress.

### Specific recommendations and additions or deletions to the work scope

- Increase information to evaluate success. Use marketing data to choose manufacturing projects.

**Project # MF-06: Develop Low-Cost MEA3 Process (an NCMS project)***Dennis Kountz; DuPont Fuel Cells***Brief Summary of Project**

The objectives for this project are to 1) develop a low-cost process for manufacturing DuPont's MEA3 and 2) develop product by process transfer functions. DuPont completed the study of low-cost MEA3 processes to understand the effect of manufacturing parameters on the performance of the MEA3. The feasibility of static screen versus a roll printing processes was studied for manufacturing direct methanol fuel cell MEA3s. A preliminary assessment of transfer function and MEA3 performance was also explored.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.9** for its relevance to DOE objectives.

- Evaluation of high-throughput screen printing addresses manufacturing cost.
- The project addresses the screen printing processes for low-cost membrane electrode assembly manufacturing, which fully supports the Department of Energy objectives.
- There are early market opportunities for adoption of direct methanol fuel cell technology for portable electronics.
- Adoption of direct methanol fuel cell technology requires lowering costs and providing more consistent product quality.
- Development of low-cost membrane electrode assemblies is an important and relevant activity.
- High-rate production of membrane electrode assemblies is an important aspect for fuel cell systems.
- The project addresses direct methanol fuel cell technology which is not in the mainstream of DOE projects.

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- DuPont's established rotary coater technology is being applied to direct methanol fuel cell membrane electrode assembly manufacture.
- The project is sharply focused on coating and laminating processes for membrane electrode assembly manufacturing. It considers all the important process variables such as yield, productivity, quality, capacity, and line balance issues associated with manufacturing.
- A systematic development path was identified.
- Project approach was well founded: A systematic variation of parameters (listed on Slide 9) in parameter space to maximize output performance.
- Approach appears good involving an adequate amount of ink formulation plus engineering development.
- The approach might be improved if the source of the voltage decay was identified.
- The rotary coating process provides high-rate production; however, it was not clearly explained how the rotary process for catalyst deposition worked with roll-to-roll processing.
- The approach identified important aspects of membrane electrode assembly fabrication; however, these aspects were not discussed in the handout or in the presentation.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Data were shown on graphs with no label values. Although improvement is shown, it is not possible to gauge the actual values of performance.
- A new screen printing method was developed with a new ink formulation, screen type, and relevant dimensions.
- Performance comparison tests were conducted demonstrating the improvement using this new process.
- The cost was reduced to a level acceptable by the customer.
- Results are shown on Slides 15 and 16: Variation in parameters resulted in incremental improvement over old technology at low current densities, and substantial improvement at higher current densities.
- DuPont has demonstrated impressive progress.
- DuPont reported success in developing roll-to-roll processing and a rotary printing method.
- DuPont reported improved performance with improvements in processing.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.2** for technology transfer and collaboration.

- A fuel cell company is involved.
- The main project partner is the customer of membrane electrode assemblies, but it is not clear what role this team member played in the development of this process.
- Project reporting suffered by lack of "lessons learned" that might benefit other industry participants.
- The role of Smart Fuel Cell, Inc was not clear.
- Some University collaborations might have given the project better fundamentals for such concepts as ink formulation, mechanical issues, adhesion, etc.
- There appears to be no technology transfer in this project.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **1.5** for proposed future work.

- The project is completed.

**Strengths and weaknesses****Strengths**

- DuPont demonstrated a very systematic development path.
- DuPont demonstrated improvement in fuel cell performance.
- The process is applicable to proton exchange membrane fuel cells as well.
- DuPont achieved demonstrable performance improvements in a direct methanol fuel cell system.
- DuPont brings extensive experience in roll-to-roll processing.

**Weaknesses**

- The methods of cost analysis and cost reduction were not made clear.
- The uncertainty and repeatability of performance measurements were not clear.
- The performance test details were not provided.
- Absent documentation of "lessons learned," the project benefits were unnecessarily limited for industry at large.
- The project did not provide sufficient detail to evaluate process.

**Specific recommendations and additions or deletions to the work scope**

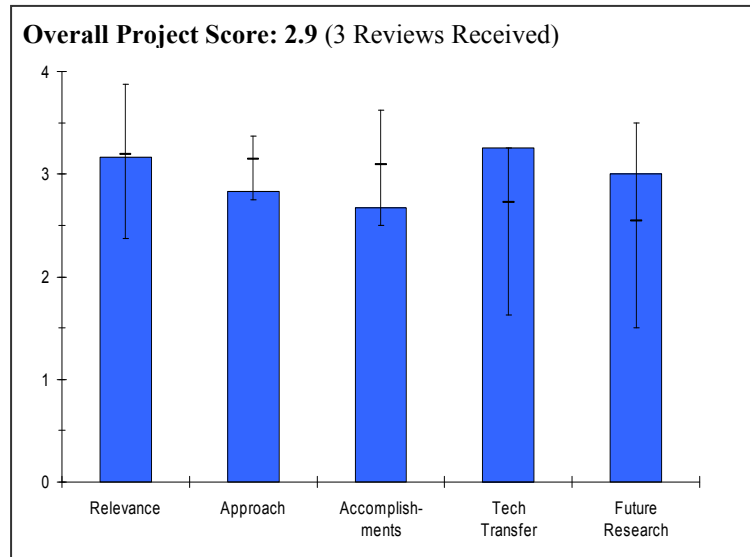
- This would have been more valuable with a fundamentals aspect that would provide information to the whole DOE program that could be used.

**Project # MF-07: NIST Fuel Cell Manufacturing Research Project Metrology for Fuel Cell Manufacturing**  
*Eric Stanfield; NIST*

**Brief Summary of Project**

The objectives for this project are to 1) develop a pre-competitive knowledge base of engineering data relating performance variation to manufacturing process parameters and variability; 2) identify and evaluate the capability and uncertainty of commercially available non-contact, high-speed scanning technologies for applicability to bipolar plate manufacturing process control; and 3) evaluate the suitability of Optical Scatterfield Metrology as a viable measurement tool for *in situ* process control of catalyst coatings.

**Question 1: Relevance to overall DOE objectives**



This project earned a score of **3.2** for its relevance to DOE objectives.

- Objectives are to establish the link between component, i.e., plate and catalyst coated membrane (CCM), characteristics and performance/durability of a cell/stack.
- It is not yet clear whether the high measurement accuracy is necessary.
- This very important activity will enable lower cost manufacturing.
- This project is likely to provide pre-competitive information that the entire industry can use to help achieve Department of Energy's ultimate objectives.

**Question 2: Approach to performing the research and development**

This project was rated **2.8** on its approach.

- The non-design-specific nature of the work is good.
- Evaluation of candidate non-contact measurement techniques may be applicable to plates, cloth gas diffusion electrodes, and membranes.
- The approach is good and the choice of the three areas is appropriate.
- Why do you think variation in manifold channels will affect performance?
- The approach is solid.
- Optical Scatterfield Metrology will elucidate ink and deposition problems but not Platinum content.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- Optical Scatterfield Metrology is interesting but it has not been conclusively demonstrated.
- The progress has been a bit slow due to slow funding arrival and needs to run faster now.
- The accomplishments are good considering the slow start.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.3** for technology transfer and collaboration.

- The interactions are broad and cover most of the relevant areas.
- There are lots of interactions with manufacturers.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.0** for proposed future work.

- The proposed future work is clearly laid out and includes Go/No-Go decisions.
- National Institute of Standards and Technology is following a logical path to identifying and evaluating non-contact measurement techniques.
- National Institute of Standards and Technology has good plans for the future.

**Strengths and weaknesses**

Strengths

- This work is appropriate for the Government Agencies to perform.
- There is a great need for online instrumentation.

Weaknesses

- The concept of "design for metrology" versus "design for manufacture" may not be unreasonable from a cost and performance standpoint.
- It is unclear whether the legal problems will hold up progress.
- The validity of targeted metrics should be questioned. Are these important and at what scale?

**Specific recommendations and additions or deletions to the work scope**

- None listed.

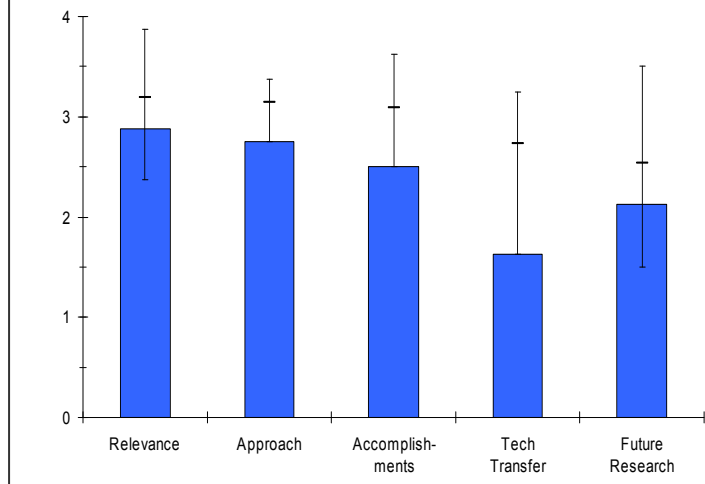
## Project # MFP-01: Innovative Inkjetting and Spray Deposition for Low-Cost, High-Performance Fuel Cell Catalyst Coated Membrane Manufacturing

Hanwei Lei; Cabot Corp.

### Brief Summary of Project

The overall goal of this project is to provide innovative solutions for low-cost, high-performance, durable next generation membrane electrode assembly manufacturing to accelerate direct methanol fuel cell commercialization. The objectives for this project are to 1) improve printing/deposition technology to manufacture membrane electrode assemblies with >95 percent production yield with improved performance; 2) demonstrate a manufacturing throughput of greater than 1,000 membrane electrode assemblies per month per shift; 3) identify two hydrocarbon membranes with lower methanol and water crossover and higher dimensional stability than Nafion; 4) demonstrate a hydrocarbon membrane electrode assembly with greater than 20 percent performance and cost advantages over Nafion; and 5) demonstrate hydrocarbon membrane electrode assembly durability greater than 1,000 hours.

### Overall Project Score: 2.5 (4 Reviews Received)



### Question 1: Relevance to overall DOE objectives

This project earned a score of **2.9** for its relevance to DOE objectives.

- The project addresses the needs for portable power applications.
- Although there are common threads for transportation applications, the gaps are not clearly identified. For example, the major focus is on direct methanol fuel cell commercialization. How can the technology developed in this project be extended to other fuel cell applications more common for transportation?
- The project addresses the need for development of low-cost catalyst coated membrane (CCM) for direct methanol fuel cells for portable applications.
- An earlier market entry of direct methanol fuel cell could assist in the development of a fuel cell manufacturing base; however, ink jetting of catalyst on CCM is not a likely technology to be used in the Hydrogen Fuel Initiative.
- This project develops technology for low-cost patterning of catalyst particles on membranes.
- The project goals are very relevant. Inkjet preparation is a feasible route for manufacture of membrane electrode assemblies.

### Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- The project is sharply focused on utilizing hydrocarbon membranes with significantly smaller catalyst particles than are commonly used and depositing them with inkjet printing and spray deposition technologies.
- Reducing the size of catalyst particles and spreading them more uniformly and in a better controlled manner will help reduce the cost of membrane electrode assemblies.
- Cabot has conducted a selection process for hydrocarbon membranes and applied the coating once the selection was completed.
- Cabot has addressed all the objectives they started out with.



- The presented info on project design is vague and without identification of specific barriers.
- The approach presented lacks enough detail to complete assessment.
- The approach ties to Department of Energy objectives and barriers not shown.
- This project supports manufacturing methods and the reduction of catalyst loading by depositing catalyst only where it might be useful.
- The idea of transferring an established technology—ink jet printing—to the new application of catalyst deposition is interesting.
- The approach appears good. However, the amount of detail provided in this presentation makes it hard to judge whether the presenter is accounting for likely problems.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.5** based on accomplishments.

- The principal investigator was able to reduce the size of catalyst particles to about 1 micrometer and develop necessary modifications to the inkjet printers to be able to deposit catalyst layer on the hydrocarbon membrane.
- Cabot carried out tests to compare the performance of hydrocarbon membranes with Nafion and demonstrated improvements.
- Cabot also claimed to have completed more than 1000 hours of operations in durability tests, but did not show any data from those tests.
- The timing of this project is not clear. According to the timeline, it was supposed to be completed in June 2006. In the Key Milestones, Phase II was mentioned, but it was not clear whether the accomplishments listed were part of Phase I or II. The presenter's response was also not clear.
- The principal investigator presented Limited quantitative metrics for parameters by which assessment of accomplishments can be made.
- The power density shown does not meet general objectives.
- The single set of comparative data shown is vague.
- For demonstration of attainment of manufacturing objective, statistical data as to yield, performance, cost, latitude, etc is needed.
- Technical results for Objectives 1, 2, 3 and 5 were not presented. Partial results for Objective 4 were shown qualitatively.
- The presentation stressed the slightly better performance of membranes produced using this method (and of different materials) than a Nafion reference.
- While cost reduction was the project objective, no data was presented on cost.
- While patterning was a project objective, no data was presented on patterning.
- While durability was a project objective, no data was presented on durability.
- The accomplishments seem good but the amount of detail provided is really inadequate.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **1.6** for technology transfer and collaboration.

- They mentioned one partner, but apparently that company is only their customer.
- The presenter claimed that their collaborations are proprietary and, therefore, did not reveal any useful information.
- No outreach shown to National Laboratories or Universities.
- Cabot is working with an US company (Mechanical Technology, Inc.), but no results were shown.
- The major effort is with a European Company (Smart Fuel Cells).
- Grantee worked with Mechanical Technology, Inc. to demonstrate membrane operation on a direct-methanol fuel cell platform.
- This project had no partners with a proton exchange membrane fuel cell platform.
- This project only utilized grantee's powered catalyst; transference to other catalyst formulations was not demonstrated.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.1** for proposed future work.

- The project seems to have achieved the major objectives. Even the durability demonstration listed as the future work has apparently completed. Improving manufacturing efficiency via better database management is not necessarily addressing any technical barrier.
- It is not clear what is planned for optimizing the depositing process.
- Only a generic description of future work presented. Not enough detail was provided to make an assessment of future work.
- The 1000-hour durability target is to be addressed in future, but no metric was given for "durability."
- Future plans include "further improve manufacturing efficiency," but it is not clear what the current manufacturing efficiency is (or what the future goal might be).
- Future goal of demonstrating durability was a goal of the project past.
- Not enough detail was provided even with discussions with the presenter.

**Strengths and weaknesses**Strengths

- The proposed technology provides much better control over the membrane electrode assembly geometry, enabling any shape of catalyst coated membrane, eliminating costly waste of catalyst layer.
- The process provides flexibility for the vendor to adapt to different end-user performance requirements.
- The use of a hydrocarbon membrane improves the catalyst adhesion, improving durability.
- The project is under budget.
- Some testing was performed and data shown.
- The principal investigator indicates the development is successful.
- The principal investigator presented a successful demonstration of a marginally better catalyst coated membrane than Nafion reference.
- The company has a strong position in carbon.

Weaknesses

- Not much hard data/information was made available due to the proprietary nature of the project.
- The comparison with Nafion was done solely by experimental means. There was no analytical study to assess a cost, performance, or durability comparison.
- The project timeline and budget information are inconsistent.
- The limited data presented makes assessment difficult.
- The stated objectives were not demonstrated.
- The current performance of the process is unclear.
- The applicability of the process to proton exchange membrane platforms and catalysts, in general, is unclear.
- It is not clear where the expertise in ink formulation is from. Not enough detail was provided to judge the project fairly.

**Specific recommendations and additions or deletions to the work scope**

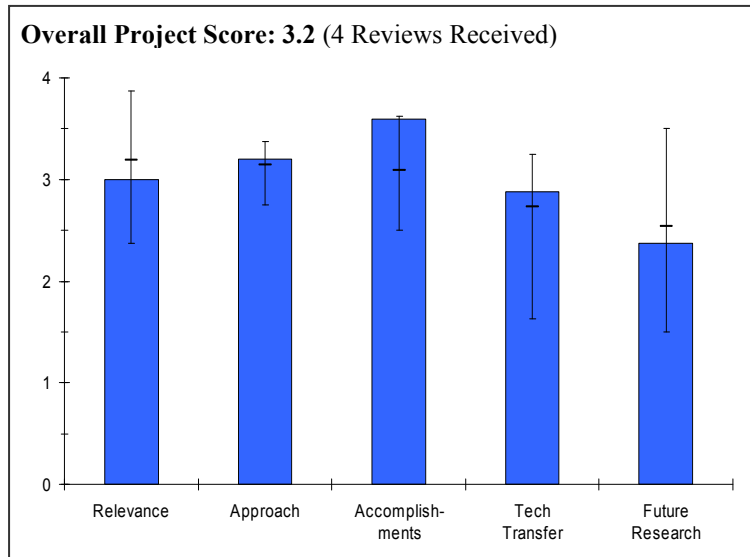
- Limited technical benefit was shown for support of the expected DOE manufacturing base.
- Specific objectives relevant to DOE Program barriers should be added. The accomplishments relative to those objectives need to be demonstrated and disseminated.

**Project # MFP-02: Novel Manufacturing Process for PEM Fuel Cell Stacks**

*Michael McCarthy; Protonex Corp.*

**Brief Summary of Project**

The Phase 1 objectives for this project are to 1) design and develop mass-producible stack architecture and components and optimize the stack assembly; 2) develop and optimize one-step integral casing/sealing of the stack assembly; and 3) establish technical and cost benefits of a one-step injection molding process. The Phase 2 objectives of this project are to 1) develop a concept modular assembly and balance-of-plant component integration; 2) design/develop and assemble sub-modules of the balance-of-plant components with appropriate interfacing of sub-modules with the fuel cell stack; 3) integrate a fuel cell system prototype using modularized balance-of-plant components; and 4) evaluate and demonstrate the system benefits of the modular balance-of-plant.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.0** for its relevance to DOE objectives.

- This manufacturing program's relevance to the Department of Energy's technical and cost targets is unclear.
- The project addresses manufacturing of proton exchange membrane fuel cell stacks for portable power applications (about 1-kW range). Scale-up issues for the automotive/transportation applications are not addressed (although it is listed as future work).
- The project addresses the manufacturability issues by reducing part counts and introducing novel sealing technology by injection molding. It also addresses the modular manufacturing and integration of balance-of-plant components into fuel cells to reduce the overall manufacturing costs of fuel cells, which is one of the main DOE objectives.
- The project focused on low-cost proton exchange membrane stack sealing and assembly/manufacture, as well as modular balance-of-plant design/build. The project addresses portable applications where earlier market entry would assist in the development of a fuel cell manufacturing base.
- Stack sealing and assembly/manufacture could be applicable to automotive stacks but the automotive industry would consider other approaches as well. The automotive supply chain would subcontract out bipolar plate and seals integrated as a component.
- The project fits well with the DOE's goals and objectives in its effort to design and develop fuel cell stack architecture, components, and an optimized stack assembly suitable for mass production.
- If successful, the project's outcome should enhance the manufacturing capabilities for fuel cells by providing techniques for handling high fuel cell production volumes and achieving better consistency and quality control.
- The project is aligned with DOE objectives with regards to its focus on the development of modular assembly and balance-of-plant integration. This aspect will provide simplicity and help achieve the cost reductions needed to move fuel cells from niche to mass markets.

**Question 2: Approach to performing the research and development**

This project was rated **3.2** on its approach.

- For small stacks (<1 kW), this sealed-stack concept may make sense. For much larger systems (>>1 kW), this concept will add size, weight, and cost.
- The project is focused on stack design to enable elimination of gaskets between individual membranes and bipolar plates.
- This project addresses the elimination of gaskets, which generate significant difficulties for stack assembly.
- The approach of using injection molding to achieve these objectives is impressive and proven feasible by this project.
- The technical approach addresses the development of a complete system integrated with balance-of-plant, which is a good indication of the developers' understanding of problems associated with early commercialization opportunities.
- The project continues development of Protonex's one-step sealing approach based on adhesive molded stack design.
- Additional detail on the project design and metrics for barriers is needed, i.e. how success is defined.
- The relationship to DOE barriers and specific targets is needed.
- The project is nearly 95 percent complete and the technical approach has enabled Protonex to reach this level within the stipulated period of performance (Sep-05 to Jun-08).
- All FY 2006, FY 2007, and most of FY 2008 milestones have been accomplished.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.6** based on accomplishments.

- The technical targets have been met.
- Although they have not provided direct cost figures, the four times reduction in build times is a good indication of manufacturing cost savings.
- They have designed, assembled, and sealed over 30 systems with integrated balance-of-plant demonstrating the feasibility of the technical approach.
- The project participants must have gained significant knowledge and insight with the impressive amount of tests (over 50,000 hours) they conducted; however, there is no publicly available paper describing the accomplishments for widespread understanding and criticism of those accomplishments.
- Significant progress exceeded the self-established target for stack power density.
- Stack manufacturing time reduced to 25 percent, but it is not clear whether this improvement meets the cost target, since the improvement is not identified quantitatively.
- The system endurance test results are promising, but no metric was identified for success of the test.
- All claimed accomplishments appear to have fulfilled all progress metrics and milestones.
- Unclear whether interim milestones were met within the stipulated cost and schedules, but overall the project's accomplishments are up to date.
- A finished modular fuel cell assembly was available for display at the poster session.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.9** for technology transfer and collaboration.

- An end-user (e.g., electronics or auxiliary power unit original equipment manufacturer) should be involved.
- There seems to be good collaboration between Protonex and Parker Hannifin. The presenter was from Protonex, but was knowledgeable about all aspects of the project.
- There may be a benefit to adding a membrane electrode assembly supplier to this project.
- Non-proprietary technology was not disseminated to benefit overall fuel cell community.
- The only other partner listed is Parker Hannifin, a manufacturer of motion and control technologies and systems. The company is well established and possesses the capabilities needed to cover product development, manufacturing, and sales/marketing needed to promote fuel cell products based on their past history.
- Given Parker Hannifin's competency in fuel cell balance-of-plant components and integrated subsystems, both companies will have the synergistic resources to focus on the commercialization of economic fuel cell systems for the portable power market.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.4** for proposed future work.

- The project has been completed.
- Future company plans are to scale up to higher power levels.
- Some key issues are identified such as expanding operational development and reducing balance-of-plant parasitic losses, but it is not clear if they are the main barriers left.
- Not much information was provided related to the approaches to be taken to address the outstanding issues.
- The goal to scale up to higher power levels is worthy to achieve DOE goals in transportation applications.
- Approach not sufficiently detailed to assess future efforts.
- Only generic, non-specific targets were identified.
- This manufacturing process may be relevant to other components.
- It was unclear whether the proposed future work is part of the an existing Statement of Work for the project or a future project with new funding. Given that the project is 95 percent complete and most goals and milestones have been accomplished, it is unlikely that the listed future work can be accomplished within the project's duration that ends June 2008.

**Strengths and weaknesses****Strengths**

- An impressive one-step injection molding process was developed to eliminate gaskets.
- Protonex has integrated balance-of-plant into the design and manufacturing of complete fuel cells.
- The project provides significant advances in design and assembly of fuel cell stacks and balance-of-plant.
- The project has developed, designed, and manufactured multiple stacks and systems demonstrating small volume manufacturing potential.
- The focus and targets for stack and balance-of-plant are appropriate for Protonex.
- Protonex demonstrated a single-step injection molding process for 250-W fuel cell stacks at a scaled-up manufacturing facility.
- Protonex demonstrated that their modular balance-of-plant components could be produced at reduced costs and improved reliability.
- Protonex created the opportunity to develop multiple systems for the Department of Defense and commercial markets.

**Weaknesses**

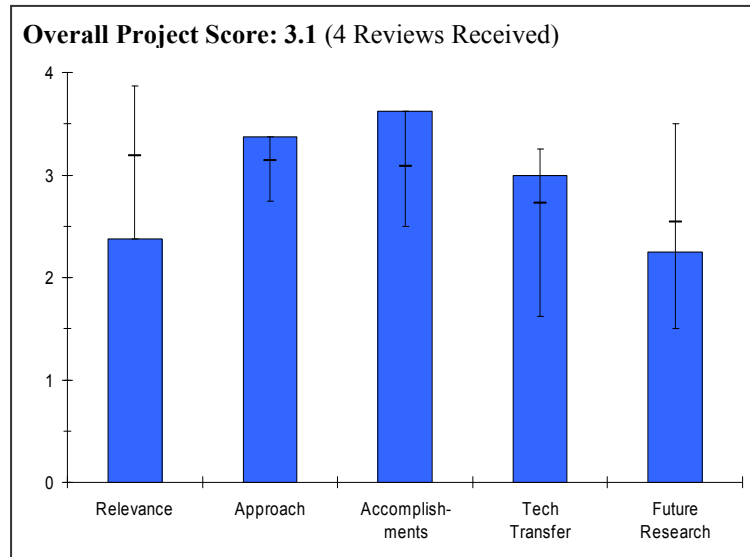
- The main focus is low-power applications.
- The focus in balance-of-plant integration is good in addressing near term opportunities for commercialization, but it is not highly relevant to DOE's goals and strategies for the transportation applications.
- Statistical data validating manufacturing accomplishments not were presented regarding the following: efficacy of manufacturing process (i.e. yield), component and system variability, unit cost and production rate, failure rates, performance, cycle times, etc.
- Non-proprietary results were not disseminated.
- There is limited applicability to automotive program.
- None - the project appears to have been completed on schedule while meeting all project goals.

**Specific recommendations and additions or deletions to the work scope**

- Complete the current program.
- None—the project is 95 percent complete.

**Project # MFP-03: Manufacturable Chemical Hydride Fuel System Storage for Fuel Cell Systems***Richard Mohring; Millenium Cell***Brief Summary of Project**

The objectives for this project are to 1) develop manufacturing concepts to reduce the process and product costs of chemical hydride hydrogen generation and storage technology; 2) develop a modified design to demonstrate high volume manufacturability of fuel cartridges based on Millennium Cell's patented Hydrogen on Demand<sup>®</sup> technology; 3) utilize strengths of the National Center for Manufacturing Sciences partners to achieve highly reliable fuel cartridge/tank performance (Dow – material selection, EWI – sealing techniques, NextEnergy – system testing); and 4) assess recyclability for all fuel system components consistent with performance and manufacturability.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.4** for its relevance to DOE objectives.

- The project addresses fuel storage systems for low power applications, which are not highly relevant to the Department of Energy's objectives related to transportation applications.
- There is no path to scale up to higher power applications.
- The project addresses the development of a manufacturable design for a low-cost chemical hydride generation and storage cartridge for portable applications where earlier market entry would assist in the development of a fuel cell manufacturing base.
- A direct application of this technology to the manufacturing base for transportation fuel cells is limited.
- This project supports early adoption of fuel cells in portable electronic devices.
- This project addresses the problem of fuel logistics by the development of a user-friendly fuel cartridge system.
- This project addresses manufacturing issues associated with hydrogen storage technology, which needs to overcome both technical and cost barriers.

**Question 2: Approach to performing the research and development**

This project was rated **3.4** on its approach.

- The approach presents a very comprehensive experimental evaluation of various materials, processes, and end products. However, analytical evaluation is not given any priority in selection of materials and understanding the processes.
- Barriers are identified and divided into subtasks which are addressed sequentially according to plan.
- Alternative paths identified and pursued where necessary.
- This project focuses on the development of suitable materials to make fuel cartridges affordable while maintaining their functionality.
- Significant technical and manufacturability issues were defined and addressed in this project in a well-designed work plan.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.6** based on accomplishments.

- A comprehensive experimental study was conducted resulting in significant cost reductions in manufacturing of a revolutionary fuel-on-demand system.
- Significant progress was made toward low-cost materials and manufacturing techniques overcoming indicted barriers.
- Final configuration indicated as a solution has not been fabricated and tested as of yet.
- The company achieved many, if not most, of its technical objectives.
- In this project the investigators made excellent progress toward meeting the objectives. The project is now complete.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.0** for technology transfer and collaboration.

- There is a good evidence of effective collaboration among the partners of the project. The nature of the experimental work requires such collaboration.
- Collaboration with other companies was beneficial to the project.
- Information was disseminated to the project partners. However, dissemination of information to the fuel cell industry is limited.
- The company has terminated the employment of all employees and has ceased operations; the intellectual property has not been transferred to a new owner.
- Little or nothing was published in the open literature, limiting technology transfer opportunities.
- Development was specific to grantee's fuel fluid; generalization to other means of chemical storage has not been demonstrated.
- The principal investigator worked with partners and collaborators effectively to understand the technical issues and to develop and test the component hardware.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.3** for proposed future work.

- Although some issues were identified as the future work, it appears that the Millenium Cell Company no longer exists and the presenter was not very optimistic that the research would continue unless another company would obtain the license. Therefore, I believe the future of this project is not very optimistic.
- Remaining barriers were identified and specific approaches to solutions were identified.
- The plans lack sufficient detail.
- The future of the company is highly doubtful and is dependent on fresh venture funding.
- Future plans would be dependent on the terms of financing arrangements or intellectual property licensing, if any.
- The future plan calls for scale up and optimization which is the next logical step in the process development. However, the current project has been completed successfully.

**Strengths and weaknesses****Strengths**

- The fuel-on-demand concept is revolutionary and this project demonstrated that it may be feasible for high-volume applications.
- The project is well organized and was managed according to plan.
- Critical barriers to project success were identified and addressed.
- The project team demonstrated systems engineering for portable, premium power.

Weaknesses

- This approach is not an alternative to hydrogen tanks for transportation applications.
- There is no clear path to scale up this approach for higher power applications.
- Applicability of project results to manufacture similar components for transportation application is limited.
- Statistical data validating manufacturing accomplishments was not presented regarding efficacy of manufacturing process, ie yield, production rate, component and system variability, unit cost and production rate, performance, etc.
- The future is uncertain, because the company ceased operations before the completion of development.

Specific recommendations and additions or deletions to the work scope

- The project is nearly complete at this time; continue to end of plan and end.



**Project # MFP-04: Non-Destructive Testing and Evaluation Methods**

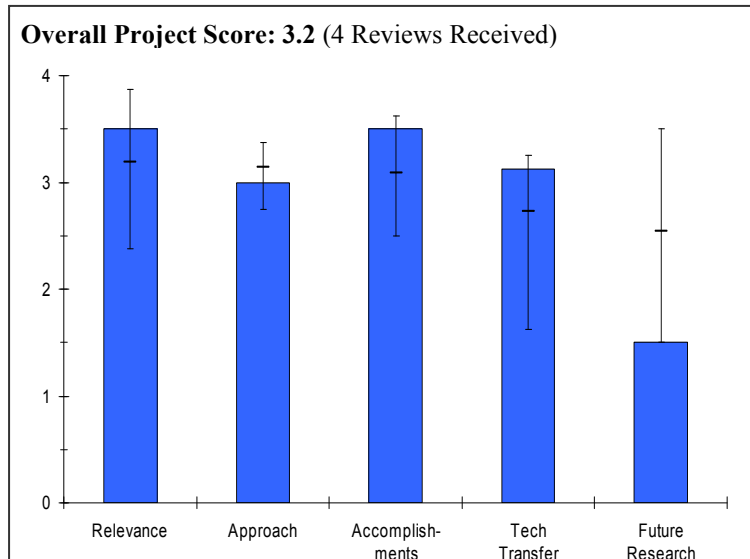
*Jim Ramirez; ASME Standards Technology*

**Brief Summary of Project**

The objectives for this project are to 1) investigate the feasibility of using nondestructive evaluation (NDE) methods in the evaluation of composite pressure vessels; 2) determine if nondestructive evaluation methods can be a suitable substitute to existing destructive testing currently used to determine pressure vessel integrity; and 3) investigate the use of stacked piezoelectric transducers in Modal Acoustic Emission (MAE) phased arrays for composite tank monitoring.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.



- The project addresses the non-destructive testing of carbon fiber hydrogen tanks. Thus, it fully supports the Department of Energy objectives related to hydrogen storage and manufacturing for hydrogen storage.
- As high pressure tanks are planned for the future transportation applications, it is critical to be able to test these tanks inexpensively and non-destructively for safety and security of commercialization.
- Project focused on investigation of feasibility of using Non Destructive Test Methods for composite pressure vessels, but concentrated on Modal Acoustic Emission technique.
- Other approaches addressed briefly in poster, but principal investigator not present at Annual Merit Review.
- This project supports both manufacturing (quality assurance) and safety.
- This project develops best methods to guard against the bursting of pressure vessels containing hydrogen.
- Non-destructive testing for quality assurance of pressure vessels is very relevant to DOE goals. However, this does seem to be something that industry should do on its own.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- The project is about developing a generic method and applying it to fuel cell storage and distribution applications. As such, it is not addressing all the technical barriers, such as cost reductions, to manufacturing of carbon fiber tanks.
- The project focuses on the application of non-destructive evaluation methods (phased array acoustic emission sensing) using inexpensive sensors with high signal/noise ratios.
- Barriers identified as fault sensitivity and nondestructive evaluation cost, but these were not quantified. Further information required, ie detectability vs. fault size, critical fault size, etc.
- Feasibility of techniques other than Modal Acoustic Emission were not evaluated technically.
- This project explored several methods of testing pressure vessels to ensure their integrity.
- The approach is sound.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.5** based on accomplishments.

- The project demonstrated excellent results using this technology and inexpensive Polyvinylidene film sensors.
- They were able to detect defects as small as 0.005 inches using phased array technology.
- By demonstrating feasibility of using Modal Acoustic Emission methods as an alternative to current destructive testing methods, they achieved the objective of reducing cost of hydrogen storage systems.
- Good progress was shown on Modal Acoustic Emission in reducing cost and increasing sensitivity with phased array, analog/digital result agreement, and use of Polyvinylidene film instead of piezoelectric sensors.
- Demonstrated that faults and location could be identified.
- Lower cost Modal Acoustic Emission materials could be permanently inserted in tank structure at manufacture to forewarn of failure.
- Modal Acoustic Emission representative (from Digital Wave) provided significant amplification of results.
- Since acoustic noise results from energy generated in initiation of failure process, the relationship between initial fault size and ultimate safe stress must be determined for each material.
- Although this was a multifaceted project, the speaker could only best represent the Modal Acoustic Emission method.
- Modal Acoustic Emission is strictly not a "non-destructive" evaluation method because it detects the formation of cracks under pressure.
- Modal Acoustic Emission is a useful tool for (a) engineering validation, (b) manufacturing inspection, and (c) real-time detection of imminent vessel failure.
- Good progress was made.

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- Although the main technical contributions are provided by Digital Wave, other participants seem to have good interactions providing realistic, commercial cases to develop meaningful solutions.
- No technology transfer or presentations indicated except among the team.
- Partnership with the American Society of Mechanical Engineers to document best practices promotes wide acceptance through the voluntary consensus standards process.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **1.5** for proposed future work.

- There are no future plans related to overcoming any barriers.
- The main plan is to package the system for end-user friendly applications.
- No future research plan shown.
- Project is finished and future work was not addressed.
- Voluntary consensus standards are subject to continual updates and periodic revalidation.
- Not applicable. Project completed.

#### **Strengths and weaknesses**

##### Strengths

- Very powerful approach for improving location sensitivity and signal to noise ratio.
- Modal Acoustic Emission definitely shows a potential for nondestructive evaluation of flaws in pressure vessels and should be explored further, but inadequate information was made available to make a definite decision regarding feasibility and efficacy.
- Utilization of the voluntary consensus standard process.
- Use of Modal Acoustic Emission as early warning signal of pressure vessel failure.

##### Weaknesses

- The method is ideal for detecting brittle fracture, which is observed in carbon fiber tanks. However, if different materials are used in the future, the method may not be as effective.

- No quantitative comparison was shown with other techniques re: sensitivity, cost, reliability, confidence level, etc. To be considered seriously much further work is required.
- No information was provided showing the use of Modal Acoustic Emission in other industries.
- I would have liked a fuller brief on the other technologies tested.

**Specific recommendations and additions or deletions to the work scope**

- If further Modal Acoustic Emission testing indicates feasibility of nondestructive evaluation process, statistical data showing fault detection efficacy should be developed.

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Appendix B

<i>Projects Not Reviewed</i>			
	<b>Title</b>	<b>Name</b>	<b>Organization</b>
MF-3	Advanced Manufacturing Technologies for Renewable Energy Applications - a DOE/NCMS Partnership	Ryan	NCMS
BES-1	Metal-to-Ligand Charge Transfer Excited States on Surfaces and in Rigid Media Application to Energy Conversion	Meyer	University of North Carolina
BES-2	Real-Time Atomistic Simulation of Light Harvesting and Charge Transport for Solar Hydrogen Production	Prezhdo	University of Washington
BES-3	Efficient H <sub>2</sub> Production via Novel Molecular Chromophores and Nanostructures	Nozik	NREL
BES-4	Regulation of H <sub>2</sub> and CO <sub>2</sub> Metabolism: Factors Involved in Partitioning of Photosynthetic Reductant in Green Algae	Ghirardi	NREL
BES-5	Fundamental Studies of Recombinant Hydrogenases	Adams	University of Georgia
BES-6	Catalyst Discovery Using Biomolecule Evolution	Feldheim	North Carolina State University
BES-7	Sunlight-Driven Hydrogen Formation by Membrane-Supported Photoelectrochemical Water Splitting	Lewis	California Institute of Technology
BES-8	Electrochemical Construction of High Performance, Low Cost Polycrystalline Photoelectrodes for Solar Hydrogen Production	Choi	Purdue University
BES-9	A Combinatorial Approach to Realization of Efficient Water Photoelectrolysis	Parkinson	Colorado State University
BES-10	Fundamental Investigations of Water Splitting on Model TiO <sub>2</sub> Photocatalysts Doped for Visible Light Absorption	Henderson	PNNL
BES-11	Catalyzed Water Oxidation by Solar Irradiation of Band-Gap-Narrowed Semiconductors	Fujita	BNL
BES-12	Photoactive Inorganic Membranes for Charge Transport	Dutta	Ohio State University
BES-13	Modular Designed Protein Constructions for Solar Generated H <sub>2</sub> From Water	Dutton	University of Pennsylvania
BES-14	A Hybrid Biological/Organic Half-Cell for Generating Dihydrogen	Golbeck-Bryant	Penn State
BESP-1	Hydrogenases of Methanococcus maripaludis	Leigh	University of Washington
BESP-2	Theoretical Research Program on Bio-Inspired Inorganic Hydrogen Generating Catalysts and Electrodes	Selloni	Princeton University
BESP-3	Identification of Enzymes involved in Syntrophic H <sub>2</sub> production	Krumholz	University of Oklahoma
BESP-4	Production and Engineering of Hydrogenase as a Biocatalyst for Hydrogen Fuel	Wang	University of Hawaii

**APPENDIX B: PROJECTS NOT REVIEWED**

BESP-5	Electronically Wired Semiconductor Nanoparticles: Toward Vectoral Electron Transport in Hybrid Materials	Armstrong	University of Arizona
BESP-6	Hydrogen Generation Using Integrated Photovoltaic and Photoelectrochemical Cells	Zhang	UC Santa Cruz
BESP-7	Tandem Hybrid Solar Energy System	Barber	Penn State
BESP-8	Photoelectrochemistry of Semiconductor Nanowire Arrays	Mallouk	Penn State
BESP-9	Strained TiO <sub>2</sub> Photoanodes	Guerra	Nanoptek Corporation
BESP-10	Highly Ordered Nanotube Arrays and their Use in Water Photoelectrolysis	Grimes	Penn State
BESP-11	Photoinitiated Electron Collection in Mixed-Metal Supramolecular Complexes: Development of Photocatalysts for Hydrogen Production	Brewer	Virginia Tech
STP-1	DOE Chemical Hydrogen Storage Center of Excellence Overview	Ott	LANL
STP-2	Chemical Hydrogen Storage R&D at Los Alamos National Laboratory	Baker	LANL
STP-3	PNNL Research as part of the Chemical Hydrogen CoE	Aardahl	PNNL
STP-6	Chemical Hydride Slurry for Hydrogen Production and Storage	McClaine	Safe Hydrogen, LLC
STP-7	Neutron Characterization and Calphad in support of the Metal Hydride Center of Excellence	Udovic	NIST
STP-9	Overview of the DOE Hydrogen Sorption Center of Excellence	Simpson	NREL
STP-10	NREL Research as Part of the Hydrogen Sorption Center of Excellence	Heben	NREL
STP-13	Metal Hydride Center of Excellence Overview, Repeat of talk on poster	Klebanoff	Sandia-Livermore
STP-14	Sandia work for MHCoE: expanded poster no review	Klebanoff	Sandia-Livermore
STP-22	Lightweight Intermetallics for Hydrogen Storage	Zhao	OSU
STP-23	Discovery of Novel Complex Metal Hydrides for Hydrogen Storage through Molecular Modeling and Combinatorial Methods	Lewis	UOP
STP-25	Hydrogen Storage by Reversible Hydrogenation of Liquid-phase Hydrogen Carriers	Cooper	Air Products
STP-30	H <sub>2</sub> Tank Manufacturing Optimization	Liu	Quantum
STP-31	Hydrogen Storage Research	Stefanakos	U of South Florida
STP-33	Advanced Concepts for Containment of Hydrogen and Hydrogen Storage Materials	Weisberg	LLNL
SAP-3	IEA Hydrogen Task 18: Evaluation of Integrated Demonstration Systems	Schoenung	Longitude 122 West
PD-6	Hydrogen Generation from Biomass-Derived Carbohydrates via Aqueous-Phase Reforming Process	Rozmiarek	Virent Energy Sys.
PD-9	High-Performance, Durable, Palladium-Alloy Membrane for Hydrogen Separation & Purification	Hopkins	Pall Corp.

**APPENDIX B: PROJECTS NOT REVIEWED**

PDP-1	Hydrogen Centrifugal Compression	Heshmat	MITI (SBIR)
PDP-5	PEM Electrolyzer Incorporating an Advanced Low-Cost Membrane	Hamdan	Giner Electrochemical Systems
PDP-6	High-Capacity, High Pressure Electrolysis System with Renewable Power Sources	Shimko	Avalence LLC
PDP-8	Inexpensive Delivery of Cold Hydrogen in High Performance Glass Fiber Composite Pressure Vessels	Aceves	LLNL
PDP-17	Integrated Short Contact Time Hydrogen Generator (SCPO)	Liu	GE Global Res.
PDP-20	Pipeline Working Group Support and Off-Board Hydrogen Storage Development	Klug	Concurrent Tech. Corp
PDP-24	Production of Hydrogen For Clean and Renewable Sources of Energy for Fuel Cell Vehicles	Deng	U. of Toledo
PDP-28	Hydrogen Compression	Hesmat	MiT
TVP-3	Hawaii Hydrogen Center for Development and Deployment of Distributed Energy Systems	Rocheleau	Hawaii Natural Energy Inst.
TVP-4	Detroit Commuter Hydrogen Project	Palombo	SEMCOG
FCP-6	Cost and Performance Enhancements for a PEM Fuel Cell Turbocompressor	Gee	Honeywell
FCP-7	Fuel Cell Testing at the Argonne Fuel Cell Test Facility	Bloom	ANL
FCP-10	Turbocompressor	Gee	Honeywell
FCP-11	Fuel Cell Testing at the Argonne Fuel Cell Test Facility	Bloom	ANL
FCP-14	Complex Coolant Fluid for PEM Fuel Cell Systems	Mohapatra	Advanced Fluids Tech.
FCP-15	Novel Non-Precious Metals for PEMFC: Catalysts Selection through Molecular Modeling and Durability Studies	Popov	University of South Carolina
FCP-16	MEA & Stack Durability for PEM Fuel Cells	Yandrasits	3M

## APPENDIX C: FY 2008 MERIT REVIEW AND PEER EVALUATION MEETING: FEEDBACK AND RECOMMENDATIONS

These notes summarize the comments received from various participants at the June 9-13, 2008 Review:

- Section 1:** Comments received from Peer Reviewers during feedback sessions held immediately after each subprogram track was completed. The comments received are organized with the particular subprogram session where they were received, although many comments are general.
- Section 2:** Scores and summarized answers to questions from the Review Questionnaire, filled out by approximately 78 of the participants.

### Section 1 – Peer Reviewer Comments

#### Analysis Reviewer Wrap-up Session

Tuesday, June 10, 2008, 10:30 a.m.  
Facilitator: Fred Joseck

#### Presentations

- Last year's subprogram presentation featured a slide at the beginning which introduced all the projects and showed their linkages to one another. Putting such a slide back into the presentation would be helpful.
- Assumptions should be discussed early on in the presentation.
- Reviewers would like to be able to see the models before the oral presentation is given on them.
- More information should be provided on why the particular approaches and methodologies chosen for each model were actually used.
- Projects with more funding should have longer presentations.
- The presentations did not always clearly state what improvements and changes have been made to the model since last year.

#### Projects

- Quality of the projects and presentations has increased since last year. Moving in the right direction. The quality of the work seems to be improving also – although this perception might be due to better presentation of the work.
- One reviewer suggested that the presenters should have approached more of the smaller companies in their research to obtain inputs, as opposed to just the larger ones. They wouldn't necessarily have to contact the firms individually to accomplish this action; they could have established contact with them through the U. S. Fuel Cell Council.
- Not always clear how the outputs from the models will be used.
- One reviewer requested justification as to why a simpler, more cost-effective model was not used. It often seems that overly complex models are used to produce basic results.

#### Reviewer Assignments

- Reviewers generally preferred to review several projects within one session, rather than have them broken up over time and across different program areas. This allows ability for Reviewer to get a general comparison of one presentation to others.

## **Education Reviewer Wrap-up Session**

Thursday, June 12, 2008, 6:15 p.m.

Facilitator: Christy Cooper

### **Review Comments**

- After solicitations are awarded, the Program should work with projects to determine goals and metrics.
  - Response: Metrics were proposed for the two student projects but because of funding cuts, they needed to revise their scope. Specifically, NEED partnerships have helped to sustain their work.
- It was unclear whether metrics were met. It was difficult to evaluate projects without metrics - they should have been presented with clear metrics. By establishing metrics, the Program can maximize "bang for buck." Projects should not have been presented without showing significant measurable progress.
  - Response: We included projects in the session based on funding for this year.
- Furthermore, metrics should be established for each market (target audience) to determine success scale.
- The budget for NEED was unclear. Did she say that the budget was zeroed?
  - Response: No, the Education budget was zeroed in FY05 and significantly reduced in FY06. As a result, we were unable to fund the MS-HS projects (NEED) and thus their total funding was reduced, not zeroed.
- Outreach and survey should be integrated in a more meaningful way – one should inform the other.
- H2IQ and H2 & You seem to be redundant projects.
  - Response: Through H2 & You, DOE works with partners in industry and academia to reach out through both traditional (newspapers, magazines, television, etc.) and new media (blogs, websites) to get the word out about hydrogen and fuel cell technologies. This NHA organized group can perform the rapid response work in the blogosphere that the government simply can't do. In contrast, H2IQ solely promotes the DOE hydrogen and fuel cell message by producing informational resources such fact sheets and podcasts to educate the public.

## **Fuel Cells Reviewer Wrap-up Session**

Thursday, June 12, 2008, 6:15 p.m.

Facilitator: Nancy Garland

### **General Review Comments**

- Colleague from Opel – first time – amazed at well-organized and stringent the meeting is. “Spectacular”.
- More adamant about the cell phones.

### **Projects**

- Why still psi?
- Hard time with recommendations and apply it to all three types of talk (industry, university, and labs). Unfair to expect that you'd rate a fundamental characterization project against addressing barriers. Complain more about people spreading thin. Assume project wouldn't be here, if not geared toward goals.
  - Should we review earmarks?
  - Presenters are given the review criteria. Sometimes that's hard to see. Maybe there should be better review of the presentations.
  - Agreement. Some projects will be five to ten years before commercially viable and some programs less than five, especially since moving beyond automotive. Makes it difficult to rate on the same criteria.
  - The numbers aren't as important as the comments? Try to give it a number, but I know they read the comments and try to put something that will help.
  - Scores are scrutinized very carefully, if they have a low score. Cut-off varies year-to-year.
  - Budget split can be affected by the scores.
  - The projects just about learning are a little bit more difficult.
  - Maybe green, yellow, red would be better?
  - Need a scale, though, in order to judge where you are.
  - Materials (fundamentals), characterization, applications, demonstration.

- Same categories, different guidance.
- Like the forms as they are, they provide continuity, and there's interpretation. Maybe DOE can provide guidance.
- Examples all go back to too high level.
- If they developed the tool, would you use it.

### Presentations

- Thirty percent of the slide is logo and all the graphics and text are un-readable.
  - Need a standard for what's allowed.
  - Max and min text size.
  - Only so many statements per slide.
- Too much detail w/o:
  - Maybe just a summary before the details.
  - Already required.
  - Maybe score on presentation.
  - But ... the presentation is sort of a formality – can't rely on presentation.
  - Sometimes, though, verbal more informative.
- Need a better method for identifying that time is running short.

### Evaluation Forms

- Need different forms for Technology Validation. The form as written is irrelevant to both.

### Reviewer Assignments

- Would have appreciated panels for review. Grouping reviews. Need to watch them all to review them.
  - Disagreement – review all would mean that you review all night long. A set of eight is tolerable.
  - Actually – not disagreement.
  - One vote for panel style.
  - Not concerned about back-to-back reviews, so long as in the same room.

### Reviewer Planning/Logistics

- We always have a conversation about grading after the review, might want discussion at the start.
- Reviewer logistics:
  - Many changes in the last week.
  - Understand that this happens due to things like COI forms, etc., but would appreciate some additional information.
  - A week ahead of time would be nice.
  - The first pass was too late.
  - A form ahead of time for COI.
  - Allow reviewers to pick which projects they can and cannot do.
  - Complaint about doing the work earlier.
  - “Educational class scheduling tools would help.”

## Production and Delivery Reviewer Wrap-up Session

Thursday, June 12, 2008, 6:15 p.m.

Facilitator: Rick Farmer

### Projects

- Seems like there is less and less to criticize (from a reviewer who has reviewed for the last 5 years).
- The cost per kg of hydrogen given by presenters should have supporting evidence. One reviewer does not believe the numbers. The hydrogen would be worth more if sold as natural gas at the higher price natural gas commands. Why sell hydrogen for less than \$3/kg when an equivalent amount of natural gas can command as much as \$11?

### Presentations

- Moderators did a good job keeping sessions on schedule.



## APPENDIX C: FEEDBACK AND RECOMMENDATIONS

- Production presentations on Wednesday afternoon were running 10 to 15 minutes ahead of schedule. This is a problem. Reviewers sometimes go from one session room to another and depend on adherence to the schedule in order to hear the presentations.

### Evaluation Forms

- The first question is always daunting – whether it meets the President’s Hydrogen Fuel Initiative. Some reviewers thought this was not a necessary question – the projects should be relevant, or are assumed to be relevant. However, a reviewer pointed out that programs do get off track, and that is why the question is asked.
- Perhaps the weighting should be changed around or the wording of the first and second question should be changed. It is difficult for reviewers to know what the shortfalls of the program are. Questions with more in-depth rating info for the 1-4 scores could help.
- The evaluation forms should include a place to evaluate evidence of creative activity. As an example, number of patent applications filed or number of articles published in peer-reviewed journals.

### Reviewer Assignments

- Reviewer felt it would be helpful if he reviewed the same presentation each year. However, another reviewer from six years ago feels that it is hard to know what the progress has been compared to six years ago. A third reviewer said it is helpful to look at the slides from last year before looking at this year’s slides, in order to see the progress.
- Reviewers would like to review a block of presentations within a specialty area.

### Reviewer Planning and Logistics

- The room was set up well, with outlets for laptop computers.
- A reviewer received last-minute assignment changes on Saturday night, and had to scrap all of the preliminary work he had already done for a bunch of evaluations.
- Reviewers should be asked which areas within production they are best equipped to review.
- Reviewers need to be told what milestones have been reached. The template for presentations needs to give the background history of this project. Presenters need to assume that their audience is made up of generalists, not experts on this specialty area. Presenters are getting too deep into the details. Reviewers are often not in the area being presented, so presenters need to make it clear and simple what is being accomplished and provide some basic understanding of the specialty area to understand this project.
- More laptop computers in the Reviewer Information Room on tables for use.

## Safety, Codes and Standards Reviewer Wrap-up Session

Thursday, June 12, 2008, 6:15 p.m.

Facilitator: Antonio Ruiz

### General Review Comments

- No major problems; indicative of documents arriving on time and when they are needed.
- Overall quality was very high.

### Projects

- Safety was more comprehensible than, for example, Storage.
- Overlap between NREL and SNL.
  - Response: CVD modeling is weak.
- Be clearer on defining the difference between NREL and SNL’s CFD work.
- FQ work gives reviewer “heartburn.” Companies that have big stakes in the outcome are not sufficiently at the table.

### Presentations

- Emphasize the relevance of what you are presenting, not elevator speech.
- Be fluid, don’t just read the slides.

- A presenter was giving a presentation that he did not write.
- People should time their presentations to fit in 15 minutes.
- All DOE TDMs should reinstitute that all presentations include a safety slide or reference (at the AMR).

#### Reviewer Planning and Logistics

- There was general disorganization of materials. Reviewers have to go to three different places. Should have one packet! Not several!
- Assignments and codes changed, SCS vs. SA.
- Need better communication with reviewers. Get back to reviewers before the meeting – one way or the other.
- Quicker comment/correspondence turn-around time.
- Orientation meeting was designed for veterans.
- Reviewers need to receive info and assignments at least a week and a half before the review – not the Friday or the night before!

#### Storage Reviewer Wrap-up Session

Thursday, June 12, 2008, 6:15 p.m.

Facilitator: Sunita Satyapal

#### General Review Comments

- Great meeting.
- Please turn down the air conditioner.
- 1<sup>st</sup> time reviewer (and international): It was interesting to see what happens when you throw a ton of money at a project; it was good to see that swinging back to good and interesting results.

#### Projects

- Very brave with research – they went with the down-selections.
- Regarding the basic research – different people but would be really nice to be able see what they are working on.
  - Response – the BES projects are rotated each year (not reviewed).

#### Centers of Excellence

- Understood the coordination in the Centers of Excellence – was explained better.
- Few cases where important to understand systems level requirement.
  - Response – we do try to emphasize this, will try to keep reiterating.
- Really think CoE concept is a success story for DOE, they foster collaboration beyond our wildest dreams. It will be interesting however what the future holds – there will be a decision point.
- Noticed going to downgrade tank. It will be very important to almost force communication between the different centers almost as much as within each individual center.
- When go forward with new CoE – have some reference on collaboration between existing.
- Should set up targets as systems targets. What really should happen – take system materials that really have most chance of making it and putting everything into them. (CoE).
- Regarding the engineering CoEs – recommend that regardless of the results generated (won't be much), try to highlight the CoEs that will show most promise. Support the OEMs, would like to hear the opinion.
  - Response – we can't show all projects, but need feedback on projects that are really good and also those that aren't so good (funding decisions are made). This is why there's a spread of both good and bad projects.
- Clarification – specifically talking about the engineering CoE – what are researchers discovering, specifically for next year?
- Project management of individual CoEs is excellent, but papers, etc. sound more like a conference, not an AMR. Would like to see more emphasis on connectivity rather than the technical goals and aspects.

## APPENDIX C: FEEDBACK AND RECOMMENDATIONS

- Natural consequence of the engineering CoE – as get more materials, would like to see some real studies not involving pure hydrogen. In the real world we won't be using pure hydrogen.

### Presentations

- Should definitely encourage presenters to present to a more general audience... not everyone is necessarily an expert – a generalist, not an idiot.
  - Response – should let know if you feel something is not appropriate.
- Presentations don't have to necessarily be last-minute, up-to-date – reviewers being more prepared should be more important.
- One presenter used titles in his presentation that matched the areas on the evaluation forms. This made his project extremely easy to review.
- Couldn't the evaluation forms and presentation templates just match? In the template that gets sent out, make the titles the same – particularly for the CoE presentations.

### Evaluation Forms

- One reviewer said the CoE form was better/improved.
- Another said the CoE form is redundant. He wondered whether these forms get sent to presenters and noted that some questions on the form weren't really answered by any of the presenters.

### Evaluating Projects

- PIs did distinguish more clearly what they did this year vs. what they did in past years, with the exception of section 3. How are reviewers to rate the performance – just past year or overall?
- Feedback in Storage compared with that in other sessions – FC reviewers appear to be a lot rougher on relevance.

### Reviewer Assignments

- One who didn't have too many projects said it wasn't too bad.
- One longtime researcher but new reviewer said 9 reviews is a lot to review for a new reviewer. He would like more time to be able to review. He recommended that new reviewers should be warned to prepare before hand

### Posters

- One reviewer felt a little uncomfortable with the number of posters he was given in a single poster session. He was not able to give posters as much time as the oral talks. With posters it's difficult to get more than 5-10 minutes without dominating the presenter. It was recommended to have a brief 30 minute poster session for reviewers only prior to the open session. It was noted that presenters would not be anonymous, but then again are they really anonymous?
- Another reviewer's comment on posters was that someone should give a 30 minute overview of all the projects presented as posters.
- 1<sup>st</sup> time attendee and reviewer – What is the difference between posters and orals – how do you select which is poster and which is oral?
  - Response – there are various criteria. Projects that are relatively large with a lot of results are preferred for an oral presentation, major project/significant results are oral; also try to vary so not oral every year
- Would it be possible to not have posters? Have 15-minute presentations in place of the posters?
  - Response – don't really have time unless 2 weeks, 15 min is too short to present so much
- DEER conference has done that is effective – allow 2 minutes for each poster presenter to say something about their projects (cut them off after 2 minutes) – as an introduction to the posters could have directly following the oral session on the night of the posters

### Reviewer Planning/Logistics

- hard to review presentations in such a short time – a day or so – would be better to know something about what presenter is doing before hand
- want the presentations and assignments earlier
  - Response – get presentations 2-3 weeks... want to have reviewers only in storage

## Technology Validation Reviewer Wrap-up Session

Monday, June 9, 2008, 6:15 p.m.

Facilitator: John Garbak

### Projects

- Seems like there is less and less to criticize (from a reviewer who has reviewed for the last five years).
- Seems like virtually every fuel cell development has batteries as a major component – the trade-off is between the size of the batteries and capacity of fuel cell.
- Some of the Fuel Cell projects are doing very similar work, as well as some projects in analysis.
- For future projects, should ask: Does it advance the state of the art? Or the state of the research?

### Presentations

- A brief history of the technology validation subprogram (review that and provide some substance) would be useful in the subprogram presentation. Also, give more specifics and more substance than the plenary presentation yesterday.

### Evaluation Forms

- Is there a way to enable spell check in Excel?
  - The evaluation form must be locked in order for the data to be correctly extracted. Locking the file disables spell check in Excel.
- We should look at what are we now starting to learn and what we should we do next? Recommendation to add to evaluation form: How do we take this ahead?
- Trouble talking about and rating relevance – at this point, in Technology Validation, shouldn't it be relevant if it is at the point of demonstration? Recommendation to change evaluation forms to better fit the Technology Validation activity area? (One reviewer mentioned that he had volunteered to help out with a new form previously.)
- There's the possibility that something is relevant but it is inappropriate for the government to fund. For example, if the BMW fleet was a project being funded (it's not), it would be a relevant but inappropriate project for the government to fund.
- Maybe combine the relevance question with "appropriateness for the government to fund." Or even just make that question a box to check rather than score. Is it sufficiently high-risk for the government to fund? If industry is going to do it by itself, the government should not fund.

### Reviewer Assignments

- One reviewer commented that he would rather review all of the projects on similar topics – instead of just doing every other one. He brought up the point that assigning a group of reviewers to a single group of projects with similar projects. That way, each project would have the same high and/or low scoring reviewers.
- One reviewer stated he would not like to review projects consecutively.

**Section 2 – Review Questionnaire**

**Evaluation Questionnaire Results - 2008 DOE Hydrogen Program Merit Review and Peer Evaluation Meeting**

<b>2007</b>	<b>2008</b>	
<b>61</b>	<b>78</b>	<b>Demographic Questions</b>
		1 a What is your role in the review?
<b>14</b>	<b>19</b>	Peer Reviewer
<b>11</b>	<b>23</b>	Presenter of a Project -- Oral or Poster
<b>1</b>	<b>1</b>	Presenter of Program Overview
<b>34</b>	<b>36</b>	Attendee, neither Reviewer nor Presenter
		b What is your affiliation?
<b>0</b>	<b>2</b>	Government agency directly sponsoring the program under review
<b>16</b>	<b>31</b>	National/government lab, private-sector or university researcher whose project is under review
<b>16</b>	<b>16</b>	In an industry directly involved in the program under review
<b>6</b>	<b>4</b>	In an industry with interest in the work under review
<b>3</b>	<b>3</b>	Government agency with interest in the work
<b>11</b>	<b>4</b>	National/government lab, private-sector or university researcher not being reviewed, but who has an interest
<b>5</b>	<b>13</b>	Other (descriptions below)
		<b>Questions for ALL Attendees</b>
<b>4.6</b>	<b>4.6</b>	2 Purpose and scope of the Hydrogen Program Review were well defined.
<b>4.3</b>	<b>4.4</b>	3 The plenary presentations were helpful to understanding the direction of the Hydrogen Program.
<b>4.3</b>	<b>4.3</b>	4 Sub-program overviews were helpful to understanding the research objectives.
		5 The quality, breadth, and depth of the following were sufficient to contribute to a comprehensive review:
<b>4.1</b>	<b>4.2</b>	a Presentations
<b>3.9</b>	<b>4.2</b>	b Question & Answer periods
<b>3.8</b>	<b>3.9</b>	c Answers provided concerning programmatic questions
<b>3.9</b>	<b>4.1</b>	d Answers provided concerning technical questions
<b>4.2</b>	<b>4.4</b>	6 Enough time was allocated for presentations.
<b>4.0</b>	<b>4.2</b>	7 Time allowed for the Question & Answer period following the presentations was adequate for a rigorous exchange
<b>3.8</b>	<b>3.7</b>	8 The questions asked by reviewers were sufficiently rigorous and detailed.
		9 There were no problems with:
<b>4.5</b>	<b>4.4</b>	1 Groupings of projects by technical area
<b>4.3</b>	<b>4.4</b>	2 Proprietary data (should not be any at this Review)
<b>3.9</b>	<b>3.9</b>	3 Quantity/level of the information presented
<b>4.5</b>	<b>4.7</b>	10 The review was conducted in an organized fashion.
		11 The frequency (once per year) of this formal review process for this Program is:
<b>59</b>	<b>73</b>	about right
<b>0.0</b>	<b>3</b>	too frequent
<b>1.0</b>	<b>0</b>	not frequent enough
<b>0.0</b>	<b>0</b>	don't know the frequency of reviews
<b>4.6</b>	<b>4.5</b>	12 Logistics and amenities were satisfactory
<b>4.0</b>	<b>4.3</b>	13 The visual quality of the presentations was adequate. I was able to see all of the presentations I attended.
<b>4.3</b>	<b>4.5</b>	14 The audio quality of the presentations was adequate. I was able to hear all the presentations I attended.
<b>4.3</b>	<b>4.7</b>	15 The hotel accommodations were satisfactory.
<b>4.5</b>	<b>4.4</b>	16 The information about the Review and the hotel accommodations sent to me prior to the Review was adequate
		17 What was the most useful part of the review process ? (Enter below)
<b>4.3</b>	<b>4.4</b>	19 Overall, how satisfied are you with the review process?
		20 Would you recommend this review process to others and should it be applied to other DOE programs?
<b>56</b>	<b>68</b>	Yes
<b>0</b>	<b>3</b>	No
		21 Please provide comments and recommendations on the overall review process (Enter below)

**Answers to the question: *What was the most useful part of the review process?***

- Presentations - all, especially those for other Centers of Excellence.
- The presentations. (3)
- Both presentations and breaks were good.
- CD & presentations
- Good quality presentations, fairly uniform format of presentations - having slides on CD.
- The CD
- CD of talks to allow review prior to presentation.
- Review process was well organized. As an attendee, it was a good experience.
- Networking
- Opportunity to network.
- Opportunity to network with other researchers.
- Networking with DOE and researchers.
- Interacting with other researchers.
- Talking/interacting with PIs
- Opportunities to discuss projects, often outside the review itself is often useful in the formation of alliances between projects and parties involved.
- Networking and benchmarking with colleagues and competitors, and gaining awareness of industry/government trends.
- Opportunities to chat with other participants between sessions.
- Meeting people, making contacts.
- Meeting everyone at the same place and time.
- Access to presenters.
- Opportunity to meet DOE program managers.
- Interacting face-to-face discussion with DOE managers.
- Face-to-face
- Meeting and talking to people.
- Talking with various people working on projects of interest.
- Hear what other people are doing in the same field.
- Increased opportunity for collaboration.
- To see the whole program in one place. The opportunity to discuss with others in the program.
- The ability to see a lot of areas within the program all in one short week.
- Getting a big picture of all aspects of fuel cells from H production to market transformation. Great networking opportunity.
- Knowledge of the current status of the research.
- Getting an overview of all the different DOE activities under the hydrogen initiative.
- Good overview for my postdocs. Good opportunity to hear all 3 storage centers.
- Program overviews and project presentations.
- Overview.
- Overviews.
- I got an overview of the DOE H2 program.
- Getting an overview of the projects.
- Good overview.
- Plenary session overview was very helpful.
- Plenary session. It's helpful to understand overall results in this year.
- Plenary talks.
- Plenary.
- Technical session, Plenary.
- Information exchange & quality of presentations.
- So many presenters & project reviews!!! Great!!!
- Presentations and posters.
- Poster session - like interaction with researchers 1 to 1.
- Nice breaks - good to get a chance to talk and mingle.

## APPENDIX C: FEEDBACK AND RECOMMENDATIONS

- Thank you for keeping on schedule.
- Feedback from reviewers.
- Q&A after each presentation revealed the most relevant information.
- The Q&As.
- Entire program was useful.
- A chance to see a large diverse program.
- Assessing the importance of current research in meeting program goals (i.e. which accomplishments are particularly important and why).
- Good to see a Manufacturing Session on the program.
- Target/Budget objectives are clear and constant.
- Learning about the progress.
- It gives me a breadth of H-program with an update on the progress.
- Excellent facilities!
- The presentations to start and end at the same time made it possible to move from room to room. The arrangement of the talks maximized my attendance to various talks.
- New info gathering.
- The presentations to start and end at the same time made it possible to move from room to room. The arrangement of the talks maximized my attendance to various talks.
- New info gathering.
- Chance to see and talk with others in the fuel cell community.
- Liked later starting time for oral sessions.
- I have been involved in the AMR since the beginning of the Grand Challenge effort. Each year, the organization is better and the presentations have improved - this not only speaks to the good work being done by the individual investigators, but it also is an indication of the great work being done by the DOE organizers and technical program leads.
- DOE is doing a great job of organizing and coordinating the AMR. I hope that the benefits of the review don't get diluted somehow by the proposed expansion to include an entirely new R&D community next year.
- Providing overview of collaborations between program partners.
- Excellent job. This is the best technical program I have attended.
- To see all projects together and in context is very useful.

### Answers to the question: *What could have been done better?*

- Plenary session in one morning would be preferred.
- In the name tag, organization font could be larger.
- Standardize font size in presentation.
- Screen presentations in advance to make sure they are legible from the back of the room. Too much information on some slides. It may be excellent work, but if it can't be understood by the audience, it isn't making the impact it could.
- It was hard to look the slides because sometimes I found many busy slides.
- Presenters put up data in small font, the viewgraphs are crowded yet there's a limited amount of information possible to extract.
- Quality of audio and screen (larger). Typically, there is too much material on any given slide which translates into fine print or legends that are not legible from the back of the room. Possible answers: discourage the use of crowded slides or use larger screens??
- I was disappointed that Steve Chalk was a no-show for the plenary session.
- Print out of CD as a book so reviewer can follow the presentation and take notes directly in the book correspondingly.
- EARLIER selection and notification of reviewers. I was not asked to review until three days before the conference!
- Actually, it was a good conference.
- Presentations and Q&A need much more time to be comprehensive.
- Quality of information presented was poor for companies, reasonable for academics.
- Some presenters had slides for much smaller rooms.

- Sub-program overviews were too general.
- More thorough overview presentations showing accomplishments including efficiencies, costs, goals, etc. and comparing various technologies.
- Better problem statement review before presentations - presenters sometimes assumed existing familiarity with work or issues.
- I think the program REVIEW is well run but some "tutorials" on methods should be held to take advantage of experts who are present. These could insure everyone is "on the same page." Major topics could be fuel cell I/V curve, conductivity, H<sub>2</sub> store density, etc.
- Make the session smaller, such as each session individually, instead of four together at one time. So it will be easier to interact with people who are doing similar work.
- Lunch talk (Wednesday)
- Temperature control in technical sessions, especially in Salon V-VI.
- Several presenters seemed to resent tough questions from the reviewers and did not give satisfactory responses. If this is really a review - some egos will have to be bruised and sloppy work must be discussed and corrected. Wednesday's fuel cell session particularly poor in this regard.
- Longer Q&A.
- There are still questions to the relevance of some of the work.
- Keep everyone on time.
- Presenters need to be held to a stricter time limit, especially in the fuel cell talks many presenters went 25 and 28 minutes leaving no time for adequate questions. This shows 1) they have no concept of timing their presentation, and they just take as many slides to cover every piece of data, and 2) there is less time to question their data, since we move on the next speaker to stay on time.
- Some presentations too long - 20 minute slot enough for some
- More rigorous control of speakers - many ran on for 28 minutes with no interruption from moderator - too few questions were then asked (nice trick when your data are less than adequate . . .) 7 minutes for questions is probably the right number.
- For presentations, the screen should be positioned higher. Often I could not see type near the bottom of the screen.
- Screens need to be a few feet higher
- Some presenter's fonts were too small.
- Presenters need to use larger fonts, especially on figures.
- Wider focused discussion with researchers, DOE managers and industry on direction and strategy adjustments.
- Technical planning.
- Release detailed program earlier.
- Education Projects: It would be helpful for reviewers if the presentations include metrics - #s to be reached and #s reached; or produce a certain number of radio spots. It was hard to determine how much progress was made on some of the projects.
- Very crowded, almost claustrophobic in common areas.
- Break hall gets congested.
- Presentations are good but format seems to limit some presenters. Could format be optional to get best and most interesting talks?
- Less expensive accommodations. Conference rate sold out too early.
- Facility too expensive, poor sound.
- The structure of the presentations. It was dictated as if every presentation was done by a company representative. University research is different from company activities. Milestones and go/no-go decisions are not well defined. Research results should be allowed to be presented in standard ways used in Academia.
- I would like to suggest the bigger ballroom for the poster sessions. This year was too crowded and it's hard to hear and walk around in the ballroom.
- The poster session was very crowded and noisy. Two rooms might have alleviated these issues.
- Many talks seemed very focused on discussions administrative/collaborative aspects of the projects at the expense of technical details.



## APPENDIX C: FEEDBACK AND RECOMMENDATIONS

- Focus presentation efforts more on technical data rather than foundation establishment/communication/collaboration.
- Just right

### *Comments and Recommendations on the overall review process:*

- This is my 4th year attending. It's well organized and I would not recommend making any significant changes - it runs well.
- I would like to see two levels of review - 1. independent experts 2. those in audience. I attended several excellent presentations and a few bad ones. I was not a reviewer but would like to have had the opportunity to note thumbs-up or thumbs-down. The two levels can, of course, be weighted differently.
- Outstanding in presentations and amount of work prepared for this review.
- Reviewers should be notified well in advance - this helps plan out schedule at the review meeting and also familiarize ourselves with the project.
- One of my presenters could not make it to the conference at the last minute - thus the opportunity to ask questions was lost. There should be a request for presenters to have a back-up presenter (who is knowledgeable) in the event they cannot make it.
- I thought there was a lot more honesty being applied to the difficulties in moving to a hydrogen economy rather than "pie in the sky" rosy predictions to meet potential expectations. Let's keep it real and not fool ourselves. If not us, then who?
- Very few probing questions generally. Talks were well presented with (usually) good slides.
- Why do you consistently find the more expensive venues to hold this meeting?
- Getting informal and objective peer reviewers is always a challenge so reviews of detailed, technical projects are meaningful. It is also important to rebut comments of reviewers (by project proponents).
- Outstanding planning and facilitation of the meeting by Rich Bechtold and associates. Facility is top-notch. Food excellent. Other DOE offices should follow this blueprint for successful program reviews.
- Vegetarian lunch options were not all that tasty.
- Need more healthy options at all feeding opportunities.
- Compared to a DOE NETL review I recently attended in Pittsburgh, PA, this review is more informative, educational and much better for networking.
- Great idea to do this type of review. Great info & idea sharing.
- Presentations should be a bit longer (25 min) and Q&A shorter (5 minutes is enough) - because the time allotted for presentations is too tight. In my opinion, the presenters often cram too much in their slides (and it becomes an eye test to read their material) or lots of good work is just not presented.
- It was very difficult for ME to understand presentations outside my area of expertise. I think one slide on background material would be helpful. Also I think the objective should be very specific and the presentation should revolve about the objective. I don't think the milestones slide adds much.
- If you are not familiar with the material, then it is hard to understand most of the presentations.
- Presenters should be very clear about what problem they are addressing. It would be helpful to have more background material at least one slide.
- Please change the guidelines (template) Current template of go/no-go decisions, etc. is very restrictive. It does not allow a research to present his/her research in the best possible way.
- While theory and idealized concepts provide the foundation for the H2 storage progress, applied technologies should be emphasized as the focus of the presentations. Funding should reflect the progress made in the fiscal year otherwise it should be redistributed.
- Have a drop-off box for these forms in the Reviewer's room so we don't have to make 2 stops.
- Very nice opportunities to grasp advance of development.
- Some reviewers did not seem impartial in there reviews/questions.
- Food/accommodation/organization were excellent.
- The plenary should be more dynamic, and you should get someone outside of DOE to give a talk. That would generate more interest, especially if you continue to have the plenary on a "non-review" day.
- I saw a trend in several program areas where researchers are doing things that either have been done by others previously and/or were doing non-relevant research (i.e. whatever they want to do -- they do). I suggest that DOE take a hard look at some of these and complete those activities. The DOE does not have enough funding to allow "white collar welfare."

**APPENDIX C: FEEDBACK AND RECOMMENDATIONS**

- Excellent.
- It does not make sense to fund university-led R&D (except in Basic Energy Sciences) for fuel cells of H2 storage when they have no production intent or knowledge.
- Manufacturing Session should be expanded - else the industry will remain in R&D only!
- Very well run meeting.
- Many presenters skipped the slides required by DOE and went straight to technical issues. Rather than have Ned and Carole get up on stage and stand awkwardly next to presenter to let them know time is up, provide a clock or time check of some kind.
- Provide 1-2 drink tickets for poster sessions . . . \$7 for a beer is ridiculous.
- Don't schedule talks during lunch, nobody listens and it's very rude to the speakers.
- Separate reviews for storage, fuel cells, etc. would make the meeting size more manageable and would significantly shorten the meeting and allow for a more detailed technical discussion.
- This meeting is very helpful for me. But, this year most of the results were disappointing. I hope they will be better next year.
- I feel that the review is fair and equitable. It provides everyone (including the presenters) with a focused opportunity to evaluate the overall program, identify areas where increased emphasis is needed, and note areas for diminished work or mid-course corrections. An important side benefit is the opportunity the "network" across all elements of the program.
- It's ok as it is.

**2007    2008**

		<b>Questions for Peer Reviewers ONLY</b>	
3.6	3.5	22	Information about the program/project(s) under review was provided sufficiently prior to the review session.
4.0	4.2	23	Review instructions were provided in a timely manner.
3.4	3.8	24	The information provided in the presentations was adequate for a meaningful review of the projects.
		25	The evaluation criteria upon which the review was organized were clearly defined and used appropriately.
4.2	4.2	1	Relevance
4.2	4.3	2	Approach
4.2	4.4	3	Technical Accomplishments and Progress
3.5	4.2	4	Technology Transfer/Collaboration
3.5	4.3	5	Proposed Future Research
		26	Explanation of the questions within the criteria was clear and sufficient.
4.0	4.5	1	Relevance
4.2	4.5	2	Approach
4.2	4.5	3	Technical Accomplishments and Progress
3.8	4.5	4	Technology Transfer/Collaboration
4.0	4.4	5	Proposed Future Research
		27	The right criteria and weightings were used to evaluate the project(s)/program.
3.9	4.2	1	Relevance
4.3	4.3	2	Approach
4.1	4.4	3	Technical Accomplishments and Progress
4.2	4.3	4	Technology Transfer/Collaboration
3.9	4.2	5	Proposed Future Research
3.9	4.4	28	During the review, reviewers had adequate access to the Principal Investigators.
4.4	4.7	29	Information on the location and timing of the projects was adequate and easy to find.
		30	The number of projects I was expected to review was
1.9	3	a	Too Many
2.3	3	b	Too Few
4.0	5	c	About right
3.8	4.3	31	The reviewers in your session had the proper mix and depth of credentials for the purpose of the review.
7.0	13		**Don't know their Credentials
3.7	4.0	32	Altogether, the preparatory materials, presentations, and the Question & Answer period provided sufficient dep Enter additional comments below.

## APPENDIX C: FEEDBACK AND RECOMMENDATIONS

### *Additional Peer Reviewer Comments:*

- Since a lot of projects will end in 2009 or 2010 it could be of interest to ask the reviewers which topics they would focus on in a next DOE-funding phase.
- Ten reviews was too many for me. Each review takes a lot of time. Doing 10 of them was a bit overwhelming.
- Review of posters was more difficult than review of oral presentations. I think that we need to find a way to streamline the poster review process (e.g. have special time for reviewers to meet one-on-one with presenters??).
- As a reviewer, I would find it useful if each presenter would include a one-page (bulletized) summary that is a concise statement of their response to the reviewer criteria: Relevance, Approach, Accompl., etc. Some presenters do that, and I find it very helpful.
- It is not clear how reviews are assigned.
- Getting the information about the projects under review a week earlier would have been better.
- There has been steady progress and improvements over the several years.
- The presenters could be clearer/be required to focus more on metrics.
- Information on the location and timing of the projects was not easy to read.
- Too many meaningless required slides and not enough time for technical details.
- Recommend sending reviewer assignments earlier (minimum 2 weeks in advance to adjust for conflicts within 1 week).
- Production and Delivery sessions need more (and expert) reviewers.
- The "relevance" should be automatic - if DOE funded, that is relevant (by definition).
- Relevance - should be a yes or no question with no weighting.
- Future work was always just plodding along. Maybe the "future" should be moved ahead to cover the next funding cycle - sort of a proposal of what PIs would like to do. Grading or collaborative was also arbitrary because there was no way to judge the value (to DOE) with these interactions.
- The presentations alone are not adequate for a peer reviewer. The peer reviewer should receive more detailed project reports in order to understand progress and prepare questions. Also: Presentations were old and some PIs had made significant progress. Try to close the time gap between collecting all the materials and the actual presentation.

2007	2008	Questions for Presenters ONLY
4.7	4.7	33 The request to provide a presentation for the review was provided sufficiently prior to the deadline for submission.
4.8	4.7	34 Instructions for preparing the presentation were sufficient.
4.8	4.3	35 The template for the presentation was helpful.
4.8	4.3	36 The PDF format provided adequate functionality for my presentation.
4.9	4.0	37 The time limit for my presentation was adequate to present the information needed by reviewers.
4.8	4.4	38 The audio and visual equipment worked properly and were adequate.
		39 The evaluation criteria upon which the review was organized were clearly defined and used appropriately
4.5	4.6	1 Relevance
4.5	4.7	2 Approach
4.6	4.6	3 Technical Accomplishments and Progress
4.5	4.4	4 Technology Transfer/Collaboration
4.6	4.8	5 Proposed Future Research
		40 Explanation of the questions within the criteria was clear and sufficient.
4.5	4.5	1 Relevance
4.5	4.5	2 Approach
4.7	4.5	3 Technical Accomplishments and Progress
4.5	4.5	4 Technology Transfer/Collaboration
4.6	4.5	5 Proposed Future Research
		41 The right criteria and weightings were used to evaluate the project(s)/program.
4.6	4.5	1 Relevance
4.6	4.5	2 Approach
4.6	4.6	3 Technical Accomplishments and Progress
4.7	4.6	4 Technology Transfer/Collaboration
4.5	4.5	5 Proposed Future Research
4.2	4.2	42 During the review, presenters had adequate interaction with the reviewers.
4.4	4.0	43 Altogether, the preparatory materials, presentations, and the Question & Answer period provided sufficient depth. Enter additional comments below.

*Additional Presenter Comments:*

- I had much more to present that had to be omitted. Time constraints needed because of the number of presentations did not provide me with an adequate time limit to present the information needed by reviewers.
- In terms of a/v equipment, we need a better pointer.
- Review materials, presentations, and Q&A were good where technical points presented. Some people were very vague.
- As a progress review I thought the program was very well run.
- I think tutorial on important topics could expedite the rate and reliability of progress in technology development and discovery.
- Poster sessions are too long. They should not be more than 2 hours. It's very tiring to keep on standing and talking for 3 - 3.5 hours at a stretch. Other option is to split it over 2 days: 60 - 90 minutes each day.
- Could you have a stool or chair next to each poster board during the poster session so that poster presenters have somewhere to sit?
- Some projects are just at the beginning stage, some of them are final. It may not be fair to use the same standard to judge these two together. Some professors have been doing similar work for 10 years, the lab is well established, but some labs are new, so it is not apple to apple to compare these two. Otherwise, the new groups will never get the chance to get funding.
- The poster session was crowded, noisy too; it was difficult to hear/carry on a detailed discussion.
- To find deadline, we had to go through 2 -3 pages to get to the poster deadline. Please highlight or provide DIRECT link in email.
- I had trouble with the laser pointer.
- Consider beginning the sessions at 8am so the reviews don't drag into Friday!
- This is a great forum to learn, provide feedback, interact and network.

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APPENDIX D: EVALUATION FORMS

**DOE Hydrogen Program 2008 Annual Merit Review & Peer Evaluation  
Project Evaluation Form**

**Project Number:**  **Reviewer:**

**Presenter Name:** \_\_\_\_\_ **Presenter Org:** \_\_\_\_\_

Provide specific, concise comments to support your evaluation -- and, write clearly please.

**1. Relevance** to overall DOE objectives – the degree to which the project supports the President’s Hydrogen Fuel Initiative and the goals and objectives of the applicable Multi-Year RD&D plan. **(Weight = 20%)**

**4 - Outstanding.** Project is critical to Hydrogen Initiative and fully supports DOE RD&D objectives. **score**

**3 - Good.** Most project aspects align with the Hydrogen Initiative and DOE RD&D objectives.

**2 - Fair.** Project partially supports the Hydrogen Initiative and DOE RD&D objectives.

**1 - Poor.** Project provides little support to the Hydrogen Initiative and the DOE RD&D objectives.

**comment**

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**2. Approach** to performing the R&D – the degree to which technical barriers are addressed, the project is well-designed, technically feasible, and integrated with other research. **(Weight = 20%)**

**4 - Outstanding.** Sharply focused on technical barriers; difficult to improve approach significantly. **score**

**3 - Good.** Generally effective but could be improved; contributes to overcoming some barriers.

**2 - Fair.** Has significant weaknesses; may have some impact on overcoming barriers.

**1 - Poor.** Not responsive to project objectives; unlikely to contribute to overcoming the barriers.

**comment**

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**3. Technical accomplishments and progress** toward overall project and DOE goals – the degree to which research progress is measured against performance indicators and to which the project elicits improved performance. **(Weight = 40%)**

**4 - Outstanding.** Excellent progress toward objectives; suggests that barrier(s) will be overcome. **score**

**3 - Good.** Significant progress toward objectives and overcoming one or more barriers.

**2 - Fair.** Modest progress in overcoming barriers; rate of progress has been slow.

**1 - Poor.** Little or no demonstrated progress towards objectives or any barriers.

**comment**

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**4. Collaborations** with other institutions – the degree to which the project interacts with industry partners, universities and laboratories. **(Weight = 10%)**

- 4 - Outstanding.** Close, appropriate coordination with other institutions; partners are full participants.
- 3 - Good.** Some coordination exists; Necessary coordination could be accomplished easily.
- 2 - Fair.** A little coordination exists; Necessary coordination would take significant effort.
- 1 - Poor.** Most work is done at the sponsoring organization with little outside interaction.

**score**

**comment**

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**5. Proposed future research** – the degree to which the project has effectively planned future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and when sensible, mitigating risk by providing alternate development pathways. **(Weight = 10%)**

- 4 - Outstanding.** Plans clearly build on past progress and are sharply focused on barriers.
- 3 - Good.** Plans build on past progress and generally address overcoming barriers.
- 2 - Fair.** Plans may lead to improvements, but need better focus on overcoming barriers.
- 1 - Poor.** Plans have little relevance toward eliminating barriers or advancing the program.

**score**

**comment**

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**Project strengths**

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**Project weaknesses**

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**Recommendations for changes to the project scope**

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**Project Number:**

**Reviewer:**

**DOE Hydrogen Program 2008 Annual Merit Review & Peer Evaluation  
Education Project Evaluation Form**

**Project Number:**  **Reviewer:**

**Presenter Name:** \_\_\_\_\_ **Presenter Org:** \_\_\_\_\_

Provide specific, concise comments to support your evaluation -- and, write clearly please.

**1. Relevance** to overall DOE objectives - the degree to which the project supports the President's Hydrogen Fuel Initiative and the goals and objectives of the Multi-Year RD&D plan. **(Weight = 20%)**

- 4 - Outstanding.** Project is critical to Hydrogen Initiative and fully supports DOE RD&D objectives. **score**
- 3 - Good.** Most project aspects align with the Hydrogen Initiative and DOE RD&D objectives.
- 2 - Fair.** Project partially supports the Hydrogen Initiative and DOE RD&D objectives.
- 1 - Poor.** Project provides little support to the Hydrogen Initiative and the DOE RD&D objectives.

**comment**

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**2. Approach** to performing the work - the degree to which technical barriers are addressed, the project is well-designed, feasible, and integrated with other efforts. **(Weight = 20%)**

- 4 - Outstanding.** Sharply focused on technical barriers; difficult to improve approach significantly. **score**
- 3 - Good.** Generally effective but could be improved; contributes to overcoming some barriers.
- 2 - Fair.** Has significant weaknesses; may have some impact on overcoming barriers.
- 1 - Poor.** Not responsive to project objectives; unlikely to contribute to overcoming the barriers.

**comment**

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**3. Accomplishments and Progress** toward overall project and DOE goals - the degree to which progress is measured against performance indicators. **(Weight = 40%)**

- 4 - Outstanding.** Excellent progress toward objectives; suggests that barrier(s) will be overcome. **score**
- 3 - Good.** Significant progress toward objectives and overcoming one or more barriers.
- 2 - Fair.** Modest progress in overcoming barriers; rate of progress has been slow.
- 1 - Poor.** Little or no demonstrated progress towards objectives or any barriers.

**comment**

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<p><b>4. Collaborations</b> – the degree to which the project interacts with other entities and projects. <b>(Weight = 10%)</b></p>	
<p><b>4 - Outstanding.</b> Close, appropriate coordination with other institutions; partners are full participants.</p> <p><b>3 - Good.</b> Some coordination exists; full/needed coordination could be accomplished easily.</p> <p><b>2 - Fair.</b> A little coordination exists; full/needed coordination would take significant effort.</p> <p><b>1 - Poor.</b> Most work is done at the sponsoring organization with little outside interaction.</p>	<p><b>score</b></p> <div style="border: 1px solid black; width: 40px; height: 40px; margin: 0 auto;"></div>
<p><b>comment</b></p> <p>•</p> <p>•</p> <p>•</p> <p>•</p> <p>•</p> <p>•</p>	
<p><b>5. Proposed Future Work</b> – the degree to which the project has effectively planned its future, considered contingencies, built in optional paths or off ramps, etc. <b>(Weight = 10%)</b></p>	
<p><b>4 - Outstanding.</b> Plans clearly build on past progress and are sharply focused on barriers.</p> <p><b>3 - Good.</b> Plans build on past progress and generally address overcoming barriers.</p> <p><b>2 - Fair.</b> Plans may lead to improvements, but need better focus on overcoming barriers.</p> <p><b>1 - Poor.</b> Plans have little relevance toward eliminating barriers or advancing the program.</p>	<p><b>score</b></p> <div style="border: 1px solid black; width: 40px; height: 40px; margin: 0 auto;"></div>
<p><b>comment</b></p> <p>•</p> <p>•</p> <p>•</p> <p>•</p> <p>•</p> <p>•</p>	
<p><b>Project Strengths</b></p> <p>•</p> <p>•</p> <p>•</p> <p>•</p> <p>•</p> <p>•</p>	
<p><b>Project Weaknesses</b></p> <p>•</p> <p>•</p> <p>•</p> <p>•</p> <p>•</p> <p>•</p>	
<p><b>Recommendations for Additions/Deletions to Project Scope</b></p> <p>•</p> <p>•</p> <p>•</p> <p>•</p> <p>•</p> <p>•</p>	
<p><b>Project Number:</b> <input style="width: 100px;" type="text"/></p>	<p><b>Reviewer:</b> <input style="width: 100px;" type="text"/></p>

**DOE Hydrogen Program  
2008 Annual Merit Review & Peer Evaluation  
Sub-Program Evaluation Form (plenary and opening sessions)**

**Reviewer:**

**Title of Sub-Program** \_\_\_\_\_

**Presenter Name** \_\_\_\_\_

Using the following criteria, rate the work presented in the context of the Program objectives and provide **specific, concise** comments to support your evaluation. <sup>\*\*\*</sup> Write/print **clearly** please. <sup>\*\*\*</sup>

**1. Was the Sub-program area was adequately covered?  
(include information presented in the Plenary presentation of the Sub-program if appropriate):**

**2. Were important issues and challenges identified?  
Are plans identified for addressing them? Are there gaps in the project portfolio?:**

**3. Does the Sub-program area appear to be focused, well-managed, and effective in  
addressing the DOE Hydrogen Program R&D needs?:**

**4. Other Comments:**

**DOE Hydrogen Program  
2008 Annual Merit Review and Peer Evaluation Meeting  
Hydrogen Storage Center of Excellence Evaluation Form**

**NOTE: This evaluation form is only for the evaluation of the Center of Excellence overall presentation (NOT for partner evaluations)**

Project Number:  Reviewer Name:   
 Title of Project:  Center of Excellence Overall Presentation  
*(Sorption, Metal Hydride, or Chemical)*

Using the following criteria, rate the work presented in the context of the program objectives and provide specific, concise comments to support your evaluation.

**1. Approach to performing the R&D** – the degree to which the DOE EERE Multi-year Program Plan (RD&D Plan) technical barriers are addressed; the overall CoE effort is well-designed and technically feasible. The technical approach clearly leverages partners’ unique skills to complement activities and avoid duplication. The CoE management approach includes, and has demonstrated, effective down-select/decision points and criteria. CoE progress and technical direction are periodically internally “audited” for effectiveness, efficiency, and benefits.

(Weight = 25%)

- 4 - Outstanding. The overall center is sharply focused on one or more key technical barriers to development of onboard hydrogen storage technology (focused on 2010 targets). Difficult for the approach to be improved significantly.
- 3 - Good. The approach is generally well thought out and effective but could be improved in a few areas. Most aspects of the center projects will contribute to progress in overcoming the barriers.
- 2 - Fair. Some aspects of the center projects may lead to progress in overcoming some barriers, but the approach has significant weaknesses.
- 1 - Poor. The approach is not responsive to project objectives and unlikely to make significant contributions to overcoming the barriers.

**score comments**

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**2. Technical accomplishments and progress toward DOE goals** – the degree to which the CoE research has achieved progress across the center. CoE’s actual progress and technical accomplishments are measured against performance indicators and quantitative milestones as related to DOE’s RD&D plan. (Weight = 25%)

- 4 - Outstanding. The overall CoE has made excellent progress toward objectives and overcoming one or more key technical barriers. Progress to date suggests that the barrier(s) may be overcome.
- 3 - Good. The overall CoE has shown significant progress toward its objectives and to overcoming one or more technical barriers.

2 - Fair. The overall CoE has shown modest progress in overcoming barriers, and the rate of progress has been slow.

1 - Poor. The overall CoE has demonstrated little or no progress towards its objectives or any barriers.

**score comments**

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**3. Proposed future research approach and relevance** – the degree to which the CoE has effectively planned its future, considered contingencies, built in optional paths or off ramps, etc. (Weight = 20%)

4 - Outstanding. The future work plan clearly builds on past progress and is sharply focused on one or more key technical barriers in a timely manner.

3 - Good. Future work plans build on past progress and generally address removing or diminishing barriers in a reasonable period.

2 - Fair. The future work plan may lead to improvements, but should be better focused on removing/diminishing key barriers in a reasonable timeframe.

1 - Poor. Future work plans have little relevance or benefit toward eliminating barriers or advancing the program.

**score comments**

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**4. Coordination, collaborations and effectiveness of communications within the CoE** – the degree to which the partners interact, interface, or coordinate with other partners within the CoE. The center coordinator provides a mechanism to foster partner interaction, interface, or coordination within the CoE. The center coordinator has helped to leverage resources to achieve progress and obtained maximum benefit from the center’s overall funding. Technical progress gained from the CoE has benefited from the group effort as opposed to a group of independent projects.

(Weight = 20%)

4 - Outstanding. Close coordination is evident among the majority of partners with continuing cross center communications and collaborations; partners are full participants.

3 - Good. Some coordination exists; full and needed coordination could be accomplished fairly easily.

2 - Fair. A little coordination exists; full and needed coordination would take significant time and effort to initiate. Some partners appear to be insufficiently aware of other work occurring in the CoE.

1 - Poor. Communications among and between partners appears to be insufficient. It appears as if unnecessary duplication of work may be occurring.

**score comments**

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**5. Collaborations/Technology Transfer Outside the CoE** – the degree to which the CoE interacts, interfaces, or coordinates with the other DOE CoEs and with other institutions and projects.

(Weight = 10%)

- 4 - Outstanding. Close coordination with other DOE CoEs and other institutions is in place and appropriate; the CoE is formally leveraging other work occurring in the subject areas.
- 3 - Good. Some coordination exists; full and needed coordination could be accomplished fairly easily.
- 2 - Fair. A little coordination exists; full and needed coordination would take significant time and effort to initiate. The CoE does not appear to be fully aware of other major R&D efforts occurring in a particular subject area.
- 1 - Poor. Most of the work done within the CoE; has little outside interactions or collaborations.

**score comments**

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**Overall Center Strengths**

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**Overall Center Weaknesses**

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**Recommendations for Additions/Deletions to Center Scope**

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**Project # AN: Systems Analysis***Fred Joseck; AN***Degree to which the Sub-Program area was adequately covered and/or summarized**

- Well. Goals of Sub-Program were clearly explained, as were projects that were funded to address each goal. History of the sub-program was also clearly explained.
- Sub-program was well addressed, but it would be good to include a chart showing the relationship of all analysis projects.
- Overall, Mr. Joseck provided an excellent summary of his sub-program, which encompasses a diverse set of projects that supports the entire hydrogen program.
- An easy-to-grasp overview was provided for the FY 2008/2009 budget.
- The "Analysis Portfolio" slide assisted significantly in understanding of the major program elements. The "Systems Analysis Progress" slide and discussion were most helpful in briefly conveying the history and evolution of the sub-program.

**Were important problem/issue areas and challenges identified/discussed, including plans for addressing these items in the future?**

- Yes, challenges identified included analyzing transition scenarios and modeling potential impacts on existing infrastructures (e.g. water, electricity, NG, petroleum).
- Issues have been identified and as funding is available, they are being addressed.
- The description/discussion of issues and challenges was too brief and general.
- There was insufficient attention devoted to how the work being done in the sub-program is addressing the complex challenges and resolving the issues associated with model integration, policy impacts, etc.

**Does the Sub-Program area appear to be focused, managed well, and effective in addressing the Hydrogen Program R&D needs?**

- Yes, there is a clear focus on the problems of analyzing benefits of hydrogen technology vs. costs, as well as analyzing transition issues, including impacts on existing infrastructures (fuel, water, electricity).
- Subprogram has well thought out progression from identifying issues to policies.
- Accomplishments cited and the discussion of future plans conveyed a sense that good progress is being made in achieving analysis that is better integrated, focused, and relevant for making program decisions.
- During the past year, there seems to be progress in getting more benefit from the Systems Analysis budget. Results of activities such as the transition scenario analyses are being communicated and disseminated so as to assist organizations and decision-makers outside DOE as well.

**Other comments:**

- Mr. Joseck's sub-program is funding a number of outstanding analysts and modeling initiatives. Significant attention must be devoted to assuring that communication among the various project performers is sufficient and productive. The challenge in accomplishing this is particularly acute in the management of analytical projects other than those being conducted by DOE's national laboratory teams.
- It is recommended that more attention be paid to analyzing viability of potential competing technologies, including plug-in hybrids, advanced ICE (e.g. HCCI running on CNG, DME, Methanol, etc.). Also, it is recommended potential ways in which hydrogen-based transportation fueling infrastructure might be preferable to alternatives like electric battery vehicles or plug-in hybrids, or widespread use of biofuels be evaluated. Hydrogen might have advantages in terms of efficiency of turning feedstock energy into useable transportation energy, for example.

**Project # FC: Fuel Cells**

*Nancy Garland; FC*

**Degree to which the Sub-Program area was adequately covered and/or summarized**

- Fuel Cell subprogram area was covered adequately.
- The program was very well-covered this year. There were about 60% more oral presentations than in the past. I was impressed.
- Comprehensive presentation of the goals, the work, the achievements and the plans was given as well as allocation of money to the various fields

**Were important problem/issue areas and challenges identified/discussed, including plans for addressing these items in the future?**

- Programmatic problems, challenges, and solutions were discussed in wrap-up sessions.
- Problem areas were discussed. Reviewers were not shy about asking questions.
- Issues and challenges were well-addressed.
- Plans for future listed areas of work in sufficient detail.

**Does the Sub-Program area appear to be focused, managed well, and effective in addressing the Hydrogen Program R&D needs?**

- With the exception of the earmark projects, the program focusses effectively to meet DOE H<sub>2</sub> program needs.
- Yes, it does. The sub-program does need to shift greater emphasis to catalysts (over membranes), but the recent solicitation indicates that this is understood.
- Simply and clearly: YES!

**Other comments:**

- Significant efforts on some projects are focussing on meeting interim targets, sometimes with the Pis employing approaches that are not likely to meet long term targets. I would recommend downplaying the interim targets if not part of primary path to meet final targets.
- The general goals are addressing consumer electronics as well.
- There was no presentation concerning that; if this is true and the program is focusing on automotive and stationary this would be good.
- Maybe DOE can think about Fuel Cells for aeronautic applications (reducing CO<sub>2</sub> and other emissions from air transport is a big issue in Europe).
- In general: another well-prepared and well-run Review Meeting - Congratulations!

**Project # MF: Manufacturing***Pete Devlin; MF***Degree to which the Sub-Program area was adequately covered and/or summarized**

- Manufacturing R&D sub-program addresses the manufacturing issues to achieve the cost targets of mobile and stationary fuel cells and storage systems. It was very well summarized. Critical focus areas were described clearly. Ties between manufacturing and market transformation were also covered adequately. It was also very clearly stated that one of the important objectives of the sub-program is to enable the growth of the domestic supplier network. This issue should always be in the forefront of the discussions related to priorities associated with the U.S. hydrogen programs.

**Were important problem/issue areas and challenges identified/discussed, including plans for addressing these items in the future?**

- Critical problems areas are clearly and well identified. The timelines for accomplishing critical milestones toward achieving cost targets were presented.

**Does the Sub-Program area appear to be focused, managed well, and effective in addressing the Hydrogen Program R&D needs?**

- The sub-program area is very focused and well-managed. It is the critical component of the DOE Hydrogen Program R&D needs. It was disappointing to hear that there was no allocation for this area in the FY 2009 budget request. Using Manufacturing Readiness Levels to assess current and future technologies is a very effective tool in managing this area.



**Project # PD: Production and Delivery**

*Monterey Gardiner; PD*

**Degree to which the Sub-Program area was adequately covered and/or summarized**

- Excellent overview! This briefing was at the right level for the AMR.
- The program was summarized satisfactorily via barriers and funding proportions but it could have highlighted the specific projects that were funded.

**Were important problem/issue areas and challenges identified/discussed, including plans for addressing these items in the future?**

- Issues, priorities and plans were well covered and put the subprogram into perspective.
- Issues were addressed but future plans were not addressed.

**Does the Sub-Program area appear to be focused, managed well, and effective in addressing the Hydrogen Program R&D needs?**

- Distribution of funds appears to be well aligned with barriers and priorities.
- The sub-program seems to be reasonably focused but there seems to be too much emphasis on hydrogen liquefaction.

**Other comments:**

- Great to have an enthusiastic manager presenting the subprogram.

**Project # SA: Safety, Codes, & Standards***Antonio Ruiz; SA***Degree to which the Sub-Program area was adequately covered and/or summarized**

- The description is well-balanced and clear with well-justified actions.
- A list of projects and their focus would be helpful in clarifying the effective Sub-program actions.

**Were important problem/issue areas and challenges identified/discussed, including plans for addressing these items in the future?**

- The key issues are identified well and presented with synthetic but clear actions to address them.
- Plans present acceptable actions for future Sub-program implementation.
- The Global Technical Regulation (GTR) effort is not clearly stressed.
- In the past, with limited or standing funding, the emphasis and efforts on the Global Technical Regulation were better motivated and described.

**Does the Sub-Program area appear to be focused, managed well, and effective in addressing the Hydrogen Program R&D needs?**

- The Sub-program is well managed with clear vision of the necessary actions to meet DOE needs and address DOE barriers.
- The collaborations with other sub-programs must be improved due to the cross-cutting nature of the Safety, Codes and Standards activities.
- The international activities require better specification.

**Other comments:**

- The use of prenormative research occurring in other sub-programs (FC, TV, ST) should be used more to levelize funding and synergistically integrate resources and expertise.

**Project # ST: Hydrogen Storage**

*Sunita Satyapal*

**Degree to which the Sub-Program area was adequately covered and/or summarized**

- The overall Storage Program effort was covered well given the short time allowed. The presenter assumed everyone in the audience was totally familiar with the program and that may not be true. More time could have been spent to explain and review the slide that shows the program organization relative to the CoEs, independent projects, etc. It was not clear if the program had any prioritization among the three areas of sorption, chemical hydrogen storage, and metal hydride materials. That left one to assume the program believes all three have an equal chance of success and should be funded at about the same level.
- Program was very well summarized. The shown graphs and plots will once again be used as a "master plot" for other world-wide research activities, as previous slides from earlier reviews have been already widely cited and copied.
- Excellent, concise summary by DOE. All the key sub-program elements and issues were adequately addressed.
- Good placement of emphasis on what the storage targets really mean and on the fact that the storage capacity targets are not the only ones that matter.
- The progress chart showing where systems are with respect to the temperature and gravimetric targets has great value. Perhaps we need one like that for volumetric storage versus temperature and another for kinetics versus temperature.
- Sub-Program was covered in the program plenary session and the storage technical session review. However, a copy of hydrogen storage session review was not available.
- Clear and complete, challenges noted but congratulations on progress both technical and administrative [are] offered.
- The Team leader delivered a comprehensive snapshot of the current state of the storage subprogram while also discussing its strategy, technical goals, and highlighting main achievements and future directions. Quite an achievement given the timeframe of the presentation. An excellent overview putting this subprogram in perspective.
- The coverage was appropriate in terms of annual progress and the future work.
- Great overview of project organization, challenges, key accomplishments, and targets. Charts were easy to understand from the back of the large room.
- DOE targets were highlighted, with the important challenge that all targets need to be met simultaneously.

**Were important problem/issue areas and challenges identified/discussed, including plans for addressing these items in the future?**

- The presentation did a good job of reviewing the storage program targets and key challenges. The emphasis was on the gravimetric and volumetric capacity targets and some of the other important targets only got a quick mention. In particular the cost target should also have been emphasized since it is perhaps the toughest target and should not be neglected.
- All important issue areas have been discussed and future plans to address them have been mentioned.
- It was once again important to remind the scientific community to the fact, that DOE targets are SYSTEM targets. As there are so many examples out there, where the target are misinterpreted or incorrectly cited. Additionally, it was important to mention that DOE targets not only consist of gravimetric and volumetric densities. Hydrogen capacity versus operating temperature is also one of the most important key graphs for the whole storage project.
- Another very comprehensive is the slide of the progress of the storage densities over the last years.
- This was done in sufficient detail to highlight the major issues.
- If the truth be told, none of the CoEs, independent projects, etc. that comprise the Hydrogen Storage Sub-Program is comfortably close to meeting all the "system" targets by December of 2010 which is only 30 months away.

- Yes. Problem of DOE targets referring to systems rather than materials has been addressed and emphasized.
- Yes, plus the downselect process.
- Important issues, persisting problem areas, and challenges facing the storage activities were clearly identified and discussed within the time constraints of the presentation. Main accomplishments were also highlighted and attention was drawn to research gaps and future R&D directions.
- There was adequate identification.
- Material Capacity versus temperature plot was very informative. It highlights the importance of systems integration, and not just material capacity.
- Progress towards DOE targets was shown. Progress towards meeting the volumetric requirement seems to be lagging, and was acknowledged.

**Does the Sub-Program area appear to be focused, managed well, and effective in addressing the Hydrogen Program R&D needs?**

- The Storage program is outstanding and very well managed. There are two aspects of the program that could be looked at: (1) It appears that the DOE is providing about equal funding to each of the three routes being researched, Sorption, Chemical Carriers, and Metal Hydrides. Based on the information that has been generated by this program and other researchers, it might be appropriate to de-emphasize metal hydrides and carbon based sorption options at this point in time. This would enable greater funding of the other sorption systems and the best chemical carrier systems and/or other parts of the DOE Hydrogen and Fuel Cell Program. (2) If a material solution is not found, it appears that high-pressure cold hydrogen gas or perhaps supercritical hydrogen is the best alternative. There is very little funding within the Storage Program that would lower the cost and improve the performance of these approaches. It may be appropriate to significantly increase the funding for these approaches. This may need to include research to reduce the cost of the carbon fiber needed for high-pressure tanks.
- The Sub-Program is focused very well. Especially, this has been impressively shown by the down-selection process of different storage technologies, which will not fit the DOE targets.
- The sub-program is very well managed. The team in that office always looks very tired. They really are working hard.
- The CoEs are equally well organized and managed. The CoE overviews were very well orchestrated and got positive messages across. The down selecting done by two of the CoEs was much needed and was done reasonably well. I would have set the bar a bit higher, e.g., >9 wt.% H instead of >6 wt.% H. The Hydrogen Sorption CoE didn't do much down selecting-- if they had, just about all of the systems they are studying would have fallen by the wayside.
- Yes. Making the hard choices needed to make good progress. Offering help to all researchers as well.
- The storage sub-program is efficiently managed and sharply focused on technical targets. It has a robust portfolio, responsive to R&D needs, getting more refined, and constantly evolving in the right direction.
- This is a very difficult technical field. In short there is room for improvement in this area. So the sub-program could use a strategic revision as well as tactical improvements. Of course considering the remaining length of the program, the options are limited.
- The project seems clearly focused on finding storage technologies that meet DOE targets both on-board and off-board vehicles. It was evident from the presentation that there is a well managed down selection process for storage technologies.

**Other comments:**

- What I call back-of-the-envelope calculations can show that many of the single materials and composite embodiments under study in the sub-program right now have no chance of meeting one of or in many cases either of the 2010 capacity targets. In a system context, it will almost always be the case that the system will add amounts of weight and volume roughly equal to the fully charged storage material by itself. The word "system" as used in the description of the targets has put the matter of agreeing on an acceptable material capacity in a broad gray area. Proposers recognize that the targets are system based up front in their proposals then claim success when they achieve material capacities equivalent

## APPENDIX E: SUBPROGRAM EVALUATIONS

to the system targets. More simply said, a material or composite structure better achieve 9 wt.% H to be put on the table for system development. Then of course there's all the other targets.

- Reviewed what was wanted of reviewers as well, and why it was important, plus allied work audience might care about.
- It appears that hydrogen storage will be part of a long-term national research portfolio. This program is/was a first step. As part of the lesson-learned efforts, technically and strategically, it is imperative to start a self-critical analysis of the effectiveness, progress, and the methodology for future research program portfolio design.
- (i) It is important to further encourage strong cross-CoE interactions and closer collaborations to address commonalities, avoid duplication of efforts, particularly in cross-cutting issues, and optimise use of resources. An example - the aerogel work: need to share experiences between the MH and the Sorbents CoEs. (ii) Ensure that there is a continuous interaction of the materials CoEs with the soon to be established Engineering CoE - this very point could also be considered as one of the performance indicators for the materials CoE.

**Project # TV: Technology Validation***John Garbak; TV***Degree to which the Sub-Program area was adequately covered and/or summarized**

- Good overview; however, there was not a good picture of all the projects funded and how they related to each other.
- Mr. Garbak provided an excellent overview of the Technology Validation sub-program during the opening plenary session on June 9.
- The overview was repeated in opening the Technology Validation session on June 10. It would have been preferable to use this opportunity to convey more details of sub-program history, evolution, highlights, accomplishments, results and plans.
- An easy-to-grasp overview was provided for the FY 2008/2009 budget and budget request.

**Were important problem/issue areas and challenges identified/discussed, including plans for addressing these items in the future?**

- The most important issue of fuel cell life was discussed.
- On June 10, the description/discussion of issues and challenges was too brief and general.
- There was insufficient discussion devoted to how the sub-program's activities, plans and initiatives are addressing the challenges and resolving the issues, both those within the sub-program and those related to the overall hydrogen program.

**Does the Sub-Program area appear to be focused, managed well, and effective in addressing the Hydrogen Program R&D needs?**

- Sub-program is certainly well focussed on validation of the technologies that have been developed.
- It would be beneficial to show/discuss what is being learned from the infrastructure and vehicle demonstrations and how this is being fed back into the HFCIT R&D Program.
- This important and well-funded sub-program is getting good results for the expenditures being made. However, this conclusion is not the result of the brief overview provided by Mr. Garbak at the opening of the session, but more by the project presentations delivered throughout the day.
- During the coming year, the projects other than the four major automotive/energy company projects should be objectively scrutinized to better understand their potential for contributing to achieving hydrogen program goals and targets.