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QUARTERLY PROGRESS REPORT

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Project Title: Hydrogen Systems Analysis

Covering Period: January 1, 2008 through March 31, 2008

Date of Report: April 29, 2009

Recipient: Sandia National Laboratories

Contact(s): Jay Keller, (925) 294-3316
jokelle@sandia.gov

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QUARTERLY PROGRESS REPORT

Project Title: Hydrogen Systems Analysis: Task 1 – Macro System Model

Covering Period: January 1, 2008 through March 31, 2008

Date of Report: April 20, 2009

Recipient: Sandia National Laboratories

Subcontractors: None

Other Partners: Mark Ruth, NREL
(303) 384-6874
Mark_Ruth@nrel.gov

Contact(s): Andy Lutz, (925) 294-2761
aelutz@sandia.gov
Jay Keller, (925) 294-3316
jokelle@sandia.gov

Project Team: Mark Ruth (NREL)
Andy Lutz (SNL)
Tim Sa (SNL)
Mike Goldsby (SNL)

Project Objective: The goal of this project is to support the DOE Hydrogen, Fuel Cells, and Infrastructure Technologies Program in the development of a Macro System Model (MSM) that will enable existing or new component models to be linked together to analyze crosscutting issues involved with the production, distribution, or use of hydrogen for light-duty vehicle transportation. Among the many types of models to be linked are models that determine feasible or desirable schedules for deployment of hydrogen infrastructure, models that compute the costs for producing hydrogen, models that determine the costs of building delivery and distribution infrastructure, and models that determine the emissions produced from various pathways for producing, distributing, and using hydrogen. Some of the crosscutting issues the MSM is being used to examine include identifying critical / risky links in potential hydrogen pathways, determining if the Program's current technical targets are appropriate or best, and looking for interdependencies between the technical targets.

BACKGROUND

In a 2004 report, the National Research Council recommended that a systems analysis function be formed within the DOE to analyze the systems and subsystems under development, the character of competitive approaches for providing energy services, potential future energy scenarios, and how proposed technologies might fit into a national system. When this systems analysis function was stood up, it recognized that the Hydrogen Initiative had already developed or had begun developing many models covering different aspects of a possible hydrogen infrastructure for light duty vehicle transportation.

The Systems Analysis function determined that a macro-system model (MSM) would be necessary for analyzing cross-cutting issues because no existing model encompasses the entire system sufficiently. For example, no single model adequately represented all of the phenomena involved in the early stages of deployment of a hydrogen fuel infrastructure and hydrogen fueled vehicles. In addition, developing the MSM was expected to expose inconsistencies in methodologies and assumptions between different component models that arose because the individual models were developed under different philosophies and without thought of eventually integrating them.

In 2005, the Systems Analysis function of the DOE Hydrogen Program designated an investigator from NREL, Mark Ruth, as the Macro System Model Engineer, responsible for developing and implementing a plan for building the MSM. Mark Ruth and the DOE Hydrogen Program also determined in late 2005 that SNL had expertise in integrating component models that would be useful for building the MSM. Consequently, beginning in FY 2006, SNL undertook to construct the MSM, with Mark Ruth providing guidance and requirements.

PROJECT STATUS

Comparison of Progress against Project Goals:
In the first quarter of FY2009, the SNL Hydrogen Systems Analysis team, working together with Mark Ruth and Victor Diakov from NREL, completed a number of enhancements to the MSM. Following last quarter's testing of the concept of running a virtual machine for each invocation of the model, this quarter the ability to execute multiple runs (~1000) of the MSM was demonstrated and tested. This is important in avoiding problems that occurred when running the Excel-based models repeatedly to perform parameter studies. An early prototype of a GUI for this capability has been developed.

The SNL team also developed a new directory structure that is appropriate for the different environments of the server, back-end, and development machines. This will streamline the work-flow in the future as versions of the software are transferred from one environment to another.

The third significant area of progress is the enhanced GUI with detailed model inputs. Following the local SNL testing in the past quarter, the enhanced GUI is now available on the beta server for testing by the NREL members of the team. In addition, a portable, stand-alone version of the GUI has been prepared for the purpose of giving demonstrations of the MSM.

.Implementation of new models HyPRO and HYDRA is beginning with HyPRO this fiscal year. We are working with the NREL team to identify the necessary input/output communications. In stand-alone mode, HyPRO reads and writes Excel files. The team decided to implement xml input files: one to provide data that are fixed, and another for parameters that will be changing through the MSM interface. In addition, data from the Excel output file will be extracted for processing in the MSM.

In preparation for the goal of including a distributed power model, the team began investigation of the capabilities of the H2A Distributed Power model and the H2Lib Power Park Simulation, which includes exergy calculations. The NREL team is testing the H2A Distributed Power model, while the SNL team is looking into the software issues of compiling the H2Lib Power Park model to stand-alone from the Simulink software that it was developed in. Discussions also considered the relative merits and appropriateness of these two models for incorporation into the MSM.

The Hydrogen Systems Analysis team demonstrated three important capabilities of the local version of the MSM: multiple runs with each run in its own virtual machine, a GUI with detailed model input capability, and a new, more robust directory structure.

PLANS FOR NEXT QUARTER

In the third quarter of FY2009, the team plans to implement the new GUI and multiple-run capabilities on the production server. Additional models to be incorporated into the MSM include HyPRO, HYDRA, and a distributed power model (H2A Distributed Power and/or H2Lib Power Park simulation).

PATENTS

- No patents were applied for during this quarter.

PUBLICATIONS/PRESENTATIONS

- No publications were made this quarter.

WEBSITES

- http://h2-msm.ca.sandia.gov

COLLABORATIONS:

- The SNL team continued fruitful collaborations with researchers from Argonne National Laboratories (ANL), NREL, and Oak Ridge National Laboratories (ORNL) in the process of conducting analyses and validating the MSM.

FY09 AOP Milestone Status Table:

Task/Milestone Description	**Planned Completion**	**Actual Completion**	**Comments**
1. Macro System Model			
1.1 Integration of Component Models into Macro System Model			
Linking of HyPRO to MSM	3/09	Ongoing	Investigating HyPRO

			input file;
Linking of H2A Stationary Model	5/09		
Link of HYDRA to MSM	7/09		
Linking of Power Parks/Cogeneration Simulations (H_2LIB)	10/09		Investigating compile of stand-alone Simulink code, required for MSM integration.
1.2 Enhancement of Graphical User Interface (GUI)			
Enhance GUI with additional MSM component configurations	9/08	Done	
Deploy enhanced GUI on Beta server	4/09	Ongoing	GUI in place on beta server; under initial testing.
Develop GUI for multi-parameter capability	6/09	Ongoing	
Add stand alone feature to GUI	3/09	Done	Facilitates local runs and improves testing
1.3 Infrastructure Systems Analysis			
Demonstrate multi-parameter runs		12/08	Multiple runs, each in a virtual machine demonstrated on local machine.
Provide assistance to enable utilization of the alpha version of MSM	As Needed		
1.4 Develop/Deploy Model Run Database			
Implement/test new directory structure	2/09	Done	Developed new structure locally (12/08); applicable to server, back-end, and development machines.
Deployment of first version of database (improvements throughout FY09)	4/09		Deferred

QUARTERLY PROGRESS REPORT

Project Title: Hydrogen Systems Analysis: Task 3 – Analysis of the Effect of a Developing Hydrogen Infrastructure on the Existing Domestic Infrastructure

Covering Period: January 1, 2009 through March 31, 2009

Date of Report: April 29, 2009

Recipient: Sandia National Laboratories

Subcontractors: None

Other Partners:

Contact(s): Andy Lutz, (925) 294-2761
aelutz@sandia.gov
Jay Keller (925) 294-3316
jokelle@sanida.gov

Project Team: Dave Reichmuth (SNL)

Project Objective: This project supports the DOE Hydrogen, Fuel Cells, and Infrastructure Technologies Program by analyzing the potential impact of an emergent hydrogen fuel infrastructure on existing infrastructures, and by providing technical guidance as systems evolve over time. Production and delivery of energy to the transportation sector is accomplished through complex networks of interdependent systems comprised of energy sources, coupled to conversion and distribution systems, which deliver fuel and electricity. In order to effectively navigate infrastructure evolution, decision makers need reliable information detailing the impact of public policy and capital investment on future markets and infrastructure reliability. This is especially critical in the future of hydrogen powered transportation where rapid introduction of new technology will be an important driver. The goal of this task is to 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, identify potential system-wide deficiencies that would otherwise hinder infrastructure evolution, and identify mitigation strategies that will support growth and acceptance.

PROJECT STATUS

In FY08, Sandia developed a System Dynamics (SD) model representing the dynamic behavior of natural gas (NG), refined petroleum (RP), and electricity generation (EG) infrastructure markets within the state of California, in an effort to assess the effects of large scale steam methane reforming (SMR) derived hydrogen needed to support a successful hydrogen-fuel cell vehicle (HFCV) adoption plan. The initial model development showed that a successful rollout of HFCVs will not dramatically increase demand for NG in the state of CA. However, the simulation suggests that a significantly larger NG price increase may occur if the high-penetration of HFCVs is combined with a high demand for gas from a specified increase in EG. Limitations of the existing model were that the electricity demand was a single value that could be adjusted to increase NG demand. In addition, the vehicle penetration model considered HFCVs as the only alternative to conventional gasoline vehicles, using a simple model for adoption of these alternative vehicles.

Progress this quarter involved developing the model to include plug-in hybrid electric vehicles (PHEVs) with an electric range of 40 miles to compete with the conventional and HFCVs. The vehicle model competes three vehicles: PHEVs, HFCVs and conventional gasoline vehicles. Vehicle adoption now depends on a willingness-to-adopt equation with parameters for the effects of marketing and word-of-mouth, as well as an affinity variable that factors in the relative cost per mile of the vehicles. Learning curves for the new vehicles bring their cost per mile down over time. As in the previous year's work, the hydrogen for HFCVs is assumed to come solely from reforming NG.

In addition, a detailed model for electricity demand now uses hourly demand data for the state and fills the demand with "must run" generation (nuclear, hydro, and renewable options) and then various amounts of generation from NG plants. The load-following is entirely met using NG, which then couples electricity demand and price to the natural gas demand and market price. As is the case presently, nearly one-third of the electricity demand is filled by imported power from neighboring states, which includes a significant amount of coal-power (~50% of the imported power).

The initial projections of the dynamic model are demonstrated in Figures 1 and 2 for a reference case designed to achieve vehicle penetration similar to the scenario proposed by David Greene (ORNL study) at last year's merit review. For the first couple decades, the HFCVs cannot compete due to high capital costs. However, PHEVs compete with conventional gasoline vehicles, because their high efficiency in both electric and gasoline modes (48 mpg) allow them to overcome a slight capital cost disadvantage to displace a large fraction of the conventional vehicles. By 2025, when the learning curve has reduced the cost of HFCVs, their high efficiency on hydrogen allows these vehicles to begin displacing the PHEVs. Overlaid on the vehicle competition is the assumption that oil prices rise linearly from about 60 $/bbl to about 140 $/bbl in 2030; this affects both the conventional and the PHEVs, which travel one-third of their miles in gasoline mode.

The market prices for the energy carriers are depicted in Figure 2. NG experiences the largest relative increase, due to the fact that both electricity and HFCVs (by reforming NG to H2) contribute to demand. The hydrogen price is simply proportional to NG price, since the model at this point only allows the one path to producing it. The refined gasoline price actually shows a flat period with no price increase, despite a linearly increasing oil price; this may occur in the model, because the refined price of the gasoline is modeled with a supply/demand elasticity that allows decreased demand to reduce the refining margin on the wholesale price of the fuel. However, after the period of soft gasoline price, the rising oil price causes the gasoline price to increase at a linear rate. Lastly, the electricity price increases with time, mainly because the NG price is providing a fraction of the electricity generation.

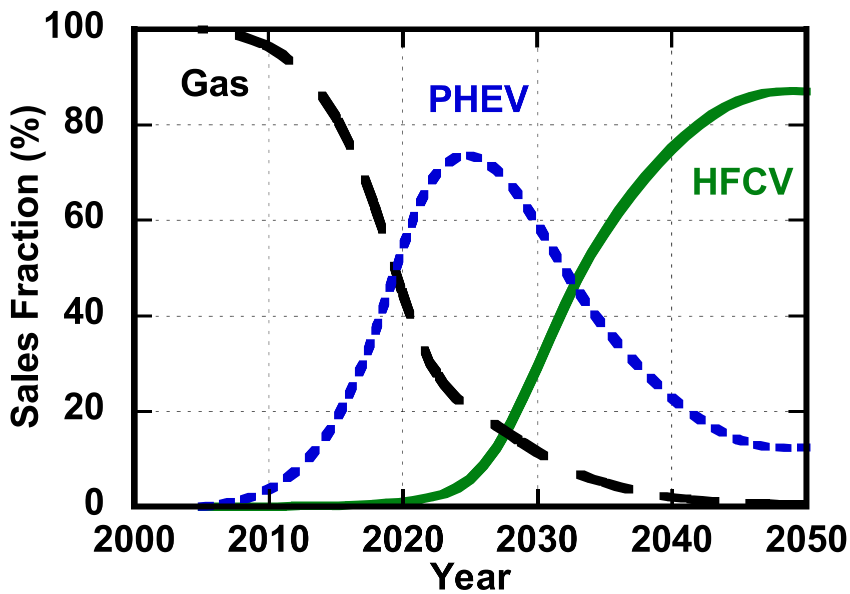

Figure 1. Fraction of total vehicle sales projected by the infrastructure model as a reference case for large-scale adoption of and PHEVs and HFCVs.

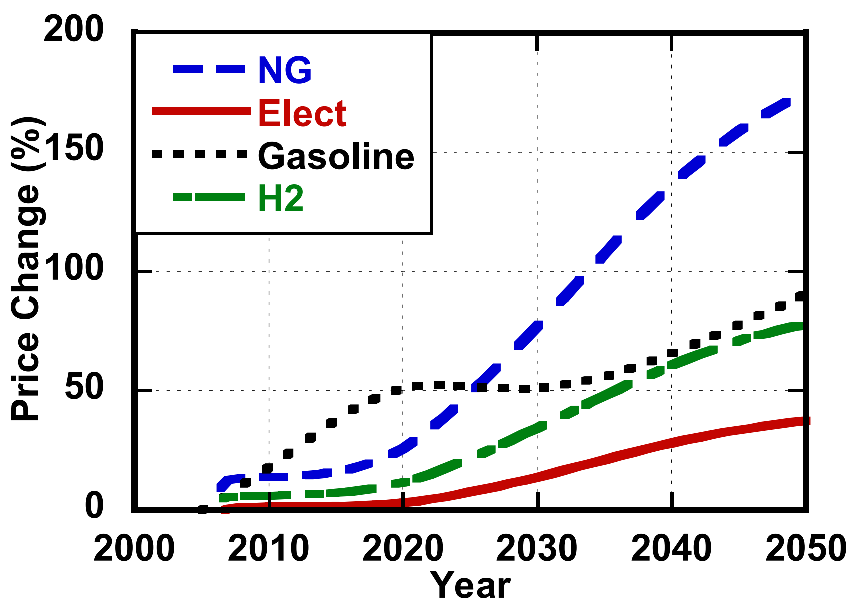

Figure 2. Price change (in percent) for the energy commodities: NG, electricity, gasoline, and hydrogen in the state of CA during the coming half-century.

PLANS FOR NEXT QUARTER

Plans for next quarter are to focus on developing a more detailed model for the NG infrastructure for the state of CA. The results of the model project that CA will likely reach the capacity of the pipelines that import gas into the state. Consequently, it should be interesting to model the pipeline dynamic capacity, along with in-state storage, to determine what happens as the demand approaches the capacity. Imports of NG to the state vary with season, and even week-day or week-end, due to the demands within source-regions (Canada and bordering states), such that CA imports more gas in spring/fall than in winter. Resolving these seasonal variations should be interesting in understanding the NG market.

Lastly, the EG market in the state of CA is faced with meeting the Renewable Portfolio Standard (RPS) of 20% renewable electricity by 2017 and growing to 33% by 2020. Meeting the RPS, may incentivize renewable production of H2 by electrolysis. The RPS will likely involve using solar, wind, or biomass to produce electricity. The model could consider the effects of meeting the RPS on the price of electricity in the state, which in turn influences the prices of NG and hydrogen in the market dynamics. The existing model only considers H2 reformed from NG, so addition of H2 electrolysis allows a path to renewable H2.

FY09 AOP Milestone Status Table:

Task/Milestone Description	**Planned Completion**	**Actual Completion**	**Comments**
3. Analysis of Effect of Existing Infrastructure on Development of Hydrogen Infrastructure			
3.1 Coupling of EG Market			
Define EG market economics	03/09	Done	
Include PHEV penetration model	04/09	Done	
Analyze the impact of PHEVs and HFVs on demands for H2 and electricity	06/09	In Progress	Initial results presented at Annual Merit Review in May

QUARTERLY PROGRESS REPORT

Project Title: Hydrogen Systems Analysis: Task 4 – Evaluating Novel Strategies for co-producing Hydrogen with Stationary Fuel Cell Systems

Covering Period: October 1, 2008 through December 31, 2008

Date of Report: January 12, 2009

Recipient: Sandia National Laboratories

Subcontractors: None

Contact(s): Whitney Colella, (505) 844-8534
wgcolel@sandia.gov
Ellen Stechel, (505) 845-1277
ebstech@sandia.gov
Jay Keller, (925) 294-3316
jokelle@sandia.gov

Project Objective: The goal of this project is to support the DOE Hydrogen, Fuel Cells, and Infrastructure Technologies Program in evaluating the viability of co-producing hydrogen within a stationary fuel cell system for refueling hydrogen vehicles.

PROJECT STATUS

***Subtask 4.1*— Develop Novel H_2-PFCS Designs with Low Marginal H_2 Production Cost**
We reviewed relevant literature, identified expert collaborators with key skills and experience, down-selected from available modeling tools, and solidified modeling approaches.

Subtask 4.2— Develop Novel H_2-PFCS Designs that Release Low Levels of Greenhouse Gas Emissions fueled by Biogas

We reviewed relevant literature, identified expert collaborators with key skills and experience, down-selected from available modeling tools, and solidified modeling approaches.

Subtask 4.3— Actively Collaborate with other DOE Labs to Contribute to Related Models and Research

We actively collaborated with the National Renewable Energy Laboratory (NREL) and other DOE labs to develop a workshop on hydrogen co-production and to contribute to related models and research.

Contributing to the Oct. 2008 Hydrogen Co-production Workshop:
We teamed with NREL and others to hold the October 27th, 2008 *Transportation and Stationary Power Integration Workshop* in Phoenix, AZ. The meeting materials are available online at http://www1.eere.energy.gov/hydrogenandfuelcells/power_integration_workshop.html. Prior to the workshop, we attended several phone meetings with other DOE lab members to develop ideas and modeling suggestions related to this research. For the Workshop, we suggested a series of technical discussion topics and appropriate invitees from industry and government agencies. At the Workshop, we provided technical and economic information to participants, answered questions from industry and other participants wherever possible, and explained modeling approaches and desired input data for these models. In the twenty-person breakout sessions and in the broader sixty-person gatherings, whenever possible, we provided valuable technical suggestions. We also informally met with other DOE modelers and industry participants to exchange feedback 1) on our modeling approaches (for example, with Dr. Paul Leiby of Oak Ridge National Laboratories (ORNL)), 2) on detailed technical descriptions of hydrogen co-production systems (for example, with Dr. John Hansen of Haldor Topsøe A/S and with Dr. Pinakin Patel of FuelCell Energy Inc.), and 3) on our related research findings (for example, with Dr. Amgad Elgowainy of Argonne National Laboratories (ANL)).

Contributing to Hydrogen Co-production Models and Research:
We provided very detailed feedback on next generation versions of NREL's H2A model updated for hydrogen co-production. We provided constructive comments to Darlene Steward, Michael Penev, and Marc Melaina of NREL on models they developed in three separate rounds of discussions over the quarter.

On November 7th, 2008, we communicated comments to Darlene, Mike, and Marc in reference to their presentation at the Workshop and to their models. Based on comments at the Workshop, we helped translate breakout groups' comments into suggestions for enhancing models. For example, three suggestions for enhancing their model include 1) to more clearly identify the more economical and more energy efficient designs, 2) to update data for hydrogen refueling demand over time to reflect the behavior of a nascent fleet with low numbers of vehicles and more sporadic refueling demand patterns, and 3) to show a clear comparison between the new approach (hydrogen co-production) and the benchmark conventional approaches (for example, distributed stand-alone steam methane reforming). These comments were summarized in a two page e-mail.

On December 4th, 2008, at Darlene Steward's request, we again met with Darlene by phone to provide constructive feedback in two main areas: 1) the model's usability/user interface and 2) the model's assumptions regarding the cost and performance of fuel cells and electrolyzers. These comments were discussed by phone and summarized in a four page memo. For example, three suggestions were for the model 1) to include the additional control costs of adding more components and complexity to the energy system, 2) to incorporate the expected increase in fuel cell system component lifetime over time through learning curves, and 3) to clarify the intended thermodynamic definition of "hydrogen purification efficiency".

On December 23rd, 2008, we met again with both Darlene Steward and Michael Penev by phone to discuss their modeling further. These comments centered on the models' assumptions about the electrochemical performance and dynamic response of fuel cell systems, on the overall thermodynamic efficiency of the entire modeled energy system, and on their modeling philosophy and objectives. We suggested key publications that describe fuel cell system performance using precise data and standardized methods.

PLANS FOR NEXT QUARTER

Subtask 4.1— Develop Novel H_2-PFCS Designs with Low Marginal H_2 Production Cost

We are developing first generation computer models describing novel H_2-PFCS designs intended to produce H_2 at a low marginal cost. Simulation studies will attempt to identify novel H2-PFCS designs that 1) address DOE longterm targets for production unit capital cost and total hydrogen cost and that 2) produce hydrogen at a lower marginal cost than the full cost from single-purpose generators. Compared with a single purpose generator, a H2-PFCS can be expected to achieve a higher capacity utilization of the equipment and be able to optimize for cost more effectively by having multiple product streams. In this way, it can be expected to produce hydrogen at lower cost. For example, a reformer can be designed for providing hydrogen for a vehicle. When vehicle demand for hydrogen is low at certain times during the day, it can also be used to provide hydrogen for a fuel cell to produce electricity. As the equipment is used a larger percentage of the time (a higher capacity utilization), the capital costs associated with any particular task, such as hydrogen generation, generally could be expected to decrease. A H2-PFCS can also capitalize on the financial resources normally allocated to separate conventional electricity, heating, and water delivery systems. For example, as a H2-PFCS produces a potable water stream that garners revenue, the marginal cost of hydrogen declines. Because hydrogen costs decrease with higher capacity utilization, simulations will focus on increasing the percentage of the time equipment is used by optimizing the system for generating multiple products.

Subtask 4.2— Develop Novel H_2-PFCS Designs that Release Low Levels of Greenhouse Gas Emissions fueled by Biogas

We are developing first generation computer models describing novel H_2-PFCS designs intended to release low levels of greenhouse gas emissions and to be fueled by biogas. Simulation studies will identify novel H_2-PFCS designs that produce hydrogen with lower greenhouse gas emissions (CO_2, CH_4, N_2O, etc) than single-purpose generators. To do this, simulation studies will focus on increasing efficiency through thermal integration strategies and the use of natural gas and renewable (low carbon) fuels. These renewable feedstock fuels may include some of the different types of biogas that can be consumed by fuel cell systems: 1) anaerobic digester gas (ADG) from a) human waste (both liquid and solid, as from waste water treatment (WWT) facilities), b) food waste, c) agricultural waste, and/or d) packaging waste, and 2) landfill gas (LFG). Simulations will evaluate different emission levels from various H_2-PFCS designs, installations, and control strategies.

Subtask 4.3— Actively Collaborate with other DOE Labs to Contribute to Related Models and Research

We are actively collaborating with NREL and other DOE Labs to contribute to models and research related to hydrogen co-production. We will provide constructive feedback on the next generation of NREL's H2A model for hydrogen co-production. It is planned that this more advanced model will invoke a different type of fuel cell system design. While initial models were based on Phosphoric Acid Fuel Cell (PAFC) systems, these next generation models will include Molten Carbonate Fuel Cell (MCFC) system designs as well.

FY09 AOP Milestone Status Table:

Task/Milestone Description	Planned Completion	Actual Completion	Comments
4. Evaluating Novel Strategies for Co-Producing H_2 with Stationary Fuel Cell Systems			
4.1 Develop Novel H_2-PFCS Designs with Low Marginal H_2 Production Cost			
Complete computer simulations	3/09		
Describe optimal designs	06/09		
4.2 Develop Novel H_2-PFCS Designs with Low Greenhouse Gas Emissions fueled by Biogas			
Complete computer simulations	06/09		
Describe optimal novel designs	09/09		
4.3 Actively Collaborate with other DOE Labs to Contribute to Related Models and Research			
Teaming with NREL hold co-production "workshop"	01/09	10/08	We teamed with NREL and others to hold the October 27, 2008 *Transportation and Stationary Power Integration Workshop* in Phoenix, AZ. The meeting materials are available online at http://www1.eere.energy.gov/hydrogenandfuelcells/power_integration_workshop.html.
Teaming with NREL hold co-production "workshop"	09/09		