SANDIA NATIONAL LABORATORIES
FCTP SYSTEMS ANALYSIS PROGRAM

QUARTERLY PROGRESS REPORT FOR JANUARY 2011–MARCH 2011

SUBMITTED BY: JAY KELLER (925-294-3316, JOKELLE @SANDIA.GOV)

RECIPIENT: SANDIA NATIONAL LABORATORIES

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MACRO SYSTEM MODEL: FY10Q4

COVERING PERIOD: JULY 1, 2010 THROUGH SEPTEMBER 30, 2010

DATE OF REPORT: OCTOBER 8, 2010

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PROJECT TEAM: MARK RUTH (NREL), VICTOR DIAKOV (NREL), ANDY LUTZ (SNL), TIMOTHY SA (SNL), MIKE GOLDSBY (SNL)

FY 2010 Q4 MILESTONES/DELIVERABLES

Task/Milestone Description	Planned	Actual	Comments
Task 1: Macro System Model			
1.1, Linking Component Models into MSM			
Updating links of GREET to MSM for H2A Power	11/09	Deferred	
Link of HYDRA to MSM (bidirectional)	5/10	7/10	Installed and tested on beta, installed on production.
Add extended emissions model (GREET2)	6/10	7/10	
Linking of H2A Power Model	7/10	Deferred	
1.2, General Improvements to MSM			
Added list-based model interface scripts		7/10	
Prototyped enhanced results output in GUI		8/10	
Added pathway dependent default input values		7/10	Installed on beta server
1.3, Infrastructure Systems Analysis			
Supported various systems analyses performed by NREL		Ongoing	

PROJECT OBJECTIVE

The goal of this project is to support the DOE Fuel Cell 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 fourth quarter of FY2010, the SNL Hydrogen Systems Analysis team, working together with Mark Ruth and Victor Diakov from NREL, completed a number of enhancements to the MSM.

1. Enhanced and stabilized production version of HyDRA web service. (HyDRA to H2 MSM direction). In addition to submitting jobs and receiving results, users can now monitor and cancel in-process jobs.
2. Installed production version of HyDRA client connection within GUI (H2 MSM to HyDRA direction).
3. Installed beta version of GUI using pathway dependent default input values (derived from data collected by Global Data Set monitoring).
4. Prototyped list-based format of model interface code that is more easily reconfigured to accommodate model changes. Placed in beta and production for HDSAM model.
5. Modified beta versions of run database and back end architecture to support prototype of enhanced GUI for viewing comprehensive job results in tree format using data based on GDS monitoring.

PLANS FOR NEXT QUARTER

In the first quarter of FY 2011, the team plans to install beta versions of:

- An enhanced GUI for viewing comprehensive results
- More robust error checking of user input values

The team also plans to install production versions of:

- GUI using pathway dependent default input values
- An extended emissions model (GREET2)

The team will also develop a strategy for user training sessions with a goal of improving the user experience by modifying the GUI according to user feedback. An annual planning session with NREL partners is scheduled for 12/10 and will be held at SNL, CA.

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.

MACRO SYSTEM MODEL: FY11Q1

COVERING PERIOD:	OCTOBER 1, 2010 THROUGH DECEMBER 31, 2010
DATE OF REPORT:	MARCH 15, 2011
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PROJECT TEAM:	MARK RUTH (NREL), VICTOR DIAKOV (NREL), ANDY LUTZ (SNL), TIMOTHY SA (SNL), MIKE GOLDSBY (SNL)

FY 2010 MILESTONES/DELIVERABLES

Task/Milestone Description	Planned	Actual	Comments
Task 1: Macro System Model			
1.1, Linking Component Models into MSM			
Added extended emissions model (GREET2)	6/10	10/10	Installed on beta
Updated emissions model (GREET)		10/10	Installed on beta and production
Updated delivery model (HDSAM)		11/10	Installed on beta server
Updating links of GREET to MSM for H2A Power	11/09	Deferred	
Linking of H2A Power Model	7/10	Deferred	
1.2, General Improvements to MSM			
Added pathway dependent default input values		10/10	Installed on beta and production server
Added vehicle fuel cycle chart		11/10	Installed on beta server
Added enhanced results output in GUI		12/10	Installed on beta server
1.3, Infrastructure Systems Analysis			
Supported various systems analyses performed by NREL		Ongoing	

FY 2011 MILESTONES/DELIVERABLES

Task/Milestone Description	Planned	Actual	Comments
Task 1: Macro System Model			
1.1, Linking Component Models into MSM			
Updating links of GREET2 to MSM	11/10		
Link the Consumer Vehicle Cost model	11/10		
Link H2A Power model for CHHP analysis	2/11		
1.2, General Improvements to MSM			
Incorporate GUI suggestions from a user workshop	9/11		

PROJECT OBJECTIVE

The goal of this project is to support the DOE Fuel Cell 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.

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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 FY2011, the SNL Hydrogen Systems Analysis team, working together with Mark Ruth and Victor Diakov from NREL, completed a number of enhancements to the MSM.

1. Installed beta version of enhanced GUI for viewing comprehensive results including a new vehicle fuel cycle chart.
2. Installed beta version of range checking for selected user inputs.
3. Installed production version of GUI using pathway dependent default input values (derived from data collected by Global Data Set monitoring).
4. Installed updated version of emissions model (GREET) on beta and production servers and installed extended emissions model (GREET2) on beta server.
5. Increased general robustness of back end processing on Windows OS.
6. Hosted annual planning session.

PLANS FOR NEXT QUARTER

In the second quarter of FY 2011, the team plans to:

- Conduct a user training session at a major energy conference
- Install beta version of enhanced scheduler that will prevent long jobs (i.e. multi-parameter runs) from delaying execution of short jobs (i.e. normal runs).

The team also plans to install production versions of:

- Enhanced GUI for viewing comprehensive results

- Range checking in GUI for selected user inputs
- An extended emissions model (GREET2)

PATENTS

No patents were applied for during this quarter.

PUBLICATIONS/PRESENTATIONS

The H2 MSM was presented at the 4th Transatlantic Infraday Conference Washington, D.C. November 5, 2010 (http://www.nrel.gov/docs/fy11osti/49544.pdf).

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.

MACRO SYSTEM MODEL: FY11Q2

COVERING PERIOD: JANUARY 1, 2011 THROUGH MARCH 31, 2011

DATE OF REPORT: APRIL 30, 2011

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FY 2011 MILESTONES/DELIVERABLES

Task/Milestone Description	Planned	Actual	Comments
Task 1: Macro System Model			
1.1, Linking Component Models into MSM			
Updating links of GREET2 to MSM	11/10	1/11	
Link the Consumer Vehicle Cost model	9/11		
Link H2A Power model for CHHP analysis	2/11	2/11	Backend work complete – GUI update in progress
1.2, General Improvements to MSM			
Incorporate GUI suggestions from a user workshop	9/11	3/11	Some suggestions incorporated

PROJECT OBJECTIVE

The goal of this project is to support the DOE Fuel Cell 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.

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PROJECT STATUS

Comparison of Progress against Project Goals

In the second quarter of FY2011, the SNL Hydrogen Systems Analysis team, working together with Mark Ruth and Victor Diakov from NREL, completed a number of enhancements to the MSM.

1. Installed production version of enhanced GUI for viewing comprehensive results including a new vehicle fuel cycle chart.
2. Installed production version of range checking for selected user inputs.
3. Installed extended emissions model (GREET2) on production server.

4. Conducted user training session at the Fuel Cell and Hydrogen Energy 2011 Conference and Expo (2/14/2011).
5. Enhanced the H2 MSM web site.

PLANS FOR NEXT QUARTER

In the third quarter of FY 2011, the team plans to:

- Install beta version of enhanced scheduler that will prevent long jobs (i.e. multi-parameter runs) from delaying execution of short jobs (i.e. normal runs).
- Update the GUI to include output from H2A Power model.

PATENTS

No patents were applied for during this quarter.

PUBLICATIONS/PRESENTATIONS

The H2 MSM was presented at the Fuel Cell and Hydrogen Energy 2011 Conference and Expo Washington, D.C., February 14, 2011.

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.

ANALYSIS OF THE EFFECT OF DEVELOPING A NEW ENERGY INFRASTRUCTURE ON THE EXISTING DOMESTIC INFRASTRUCTURE: FY10Q2

COVERING PERIOD: JANUARY 1, 2010 THROUGH MARCH 31, 2010

DATE OF REPORT: APRIL 27, 2010

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FY 2010 Q2 MILESTONES/DELIVERABLES

Task/Milestone Description	Planned	Actual	Comments
2. Analysis of Effect of Developing a New Energy Infrastructure on the Existing Infrastructure			
2.1 Stationary Power and Distributed Hydrogen Production			
Develop modules to simulate distributed CHP systems	2/10	Completed	SFC modules used in analysis of California.
2.2 Extend Analysis to Coal-Burning Region			
Modify model input and conduct infrastructure assessment analysis	8/10	Ongoing	

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 is accomplished through complex networks of interdependent systems comprised of energy resources, 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 transition to a hydrogen infrastructure. 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 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 FY09, Sandia developed a System Dynamics (SD) model for the penetration of electric and hydrogen vehicles and the response of markets for natural gas (NG), refined gasoline, and electricity generation within the state of California. The model includes plug-in hybrid electric vehicles (PHEVs) with an electric range of 40 miles to compete with the conventional and HFCVs. Vehicle adoption 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. The hydrogen for HFCVs is assumed to come solely from reforming NG.

The electricity model 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).

Following the change of the program to emphasize fuel cell technology, the future direction of the analysis in this project focused on using stationary fuel cell systems in distributed applications to begin the transition to hydrogen. The program managers emphasized concepts such as distributed energy systems which combine the local power production with use of the waste heat for either heating or cooling by heat-driven absorption chillers. In addition, the fact that fuel cell stacks usually operate with utilization factors less than one—incomplete consumption of the hydrogen inflow—can be used to advantage. Instead of recycling or venting the unused hydrogen, there is interest in making it available for vehicle transportation.

This quarter, we incorporated submodels for distributed fuel cell systems that use the waste heat for local building heating, absorption chilling for local air conditioning, and providing the unused hydrogen for distribution to vehicles. The combination of reduced electricity demand on the grid and reduced natural gas demand for reforming hydrogen for vehicles will is computed in the model. Using building penetrations for a selection of large buildings (offices, hotels, hospitals) and high-use single-family residences, the simulation implements enough stationary fuel cells to provide about 16% of the yearly electric generation for the state of California. The net effect on the state's CO_2 emissions is a 2% decrease. The reduction is due to the slight improvement in electrical efficiency of the fuel cells, as well as the displacement of some of the heating and cooling loads for the buildings. In addition, the hydrogen production potential from these distributed fuel cell systems can potentially supply nearly 2 million hydrogen-fueled vehicles in the state.

PLANS FOR NEXT QUARTER

In the third quarter of FY2010, we plan to modify the model and input parameters to consider a coal-burning region of the country. It is anticipated that the influence of stationary fuel cell systems will be much different when the natural-gas fired systems replace other types of generation, including a significant amount of coal-fired generation.

ANALYSIS OF EFFECT OF DEVELOPING A NEW ENERGY INFRASTRUCTURE ON THE EXISTING INFRASTRUCTURE: FY11Q1 AND Q2

COVERING PERIOD: OCTOBER 1, 2010 THROUGH MARCH 31, 2010

DATE OF REPORT: APRIL 27, 2010

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MILESTONES/DELIVERABLES

Task	Planned	Status
Task 2—Analysis of Effect of Developing a New Energy Infrastructure on the Existing Infrastructure		
Subtask 2.1— Analysis of dynamics of infrastructure transition to hydrogen		
Role of SFC in transition to hydrogen-based transportation	2/11	Completed
Subtask 2.2— Analysis of competition of refueling/vehicle technology alternatives		
Economics of low-carbon hydrogen pathways	7/11	Model changes in progress
Constraints of plug-in vehicle charging infrastructure	9/11	

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 is accomplished through complex networks of interdependent systems comprised of energy resources, 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 transition to a hydrogen infrastructure. The goal of this task is to use dynamic models of interdependent, regionally-differentiated infrastructure systems (natural gas, coal, electricity, petroleum, water, etc.) to analyze the impacts of widespread deployment of a hydrogen 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 FY09, Sandia developed a System Dynamics (SD) model for the penetration of electric and hydrogen vehicles and the response of markets for natural gas (NG), refined gasoline, and electricity generation within the state of California. The model included plug-in hybrid electric vehicles (PHEVs) with an electric range of 40 miles to compete with the conventional and HFCVs.

Following the change of the program to emphasize fuel cell technology, FY10 research included the use of stationary fuel cell systems in distributed applications to begin the transition to hydrogen. The fact that fuel cell stacks usually operate with utilization factors less than one—incomplete consumption of the hydrogen inflow—can be used to advantage. Instead of recycling or venting the unused hydrogen, there is interest in making it available for vehicle transportation. Our research showed that at a very aggressive penetration rate, stationary fuel cells could provide about 16% of the yearly electric generation for the state of California. The net effect on the state's CO_2 emissions is a 2% decrease. The reduction is due to the slight improvement in electrical efficiency of the fuel cells, as well as the displacement of some of the heating and cooling loads for the buildings. In addition, the hydrogen production potential from these distributed fuel cell systems can potentially supply nearly 2 million hydrogen-fueled vehicles in the state.

Feedback from our FY10 work included guidance to expand our analysis to regions outside of California. In FY11, we have completed changes to our model that allow simultaneous analysis of multiple regions. We choose to use NERC (North American Electric Reliability Corporation) electricity grid areas for the regions, dividing the country into 8 regions. We have also expanded the model to include 3 sizes of vehicles (small cars, large cars, and trucks) and more powertrains (gasoline ICE, PHEV10, PHEV40, battery EV, and hydrogen fuel cell), providing the ability to model 15 possible vehicle types.

Our results show that the effect of electric vehicles on emissions and petroleum consumption is limited because battery-dependent large vehicles are inefficient. In contrast, hydrogen vehicles have the largest impact in the large car and truck categories. The rate of hydrogen vehicle sales differs between regions due to natural gas price differences and also due to differences in vehicle sizes between regions. Overall, we find that alternative vehicles (PHEV, BEV, and HFCV) and make up 50% of the vehicle fleet by 2050 if gasoline prices increase over time. This vehicle fleet results in a 50% reduction in gasoline consumption in 2050 from 2015 levels.

Our FY11 work includes an examination of hydrogen co-produced at stationary fuel cells. While SFC-produced hydrogen can only supply a small fraction of the nation's vehicles, the availability of low cost hydrogen can have significant impact on the number of early adopters of hydrogen vehicles.

PLANS FOR NEXT QUARTER

In the third quarter of FY2011, we plan to modify the model to increase the number of hydrogen production pathways considered. Currently, we include stationary fuel cell H_2 production from natural gas, distributed SMR, and centralized electrolysis using wind power. We will add pathways for coal, coal with carbon sequestration, solar, and centralized NG SMR.

NOVEL DESIGNS FOR ADVANCED STATIONARY POLYGENERATIVE FUEL CELL SYSTEMS (PFCS): FY10Q4

COVERING PERIOD: JUNE 1, 2010 THROUGH SEPTEMBER 30, 2010

DATE OF REPORT: SEPTEMBER 30, 2010

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PROJECT OBJECTIVE

To evaluate the design of novel advanced stationary polygenerative fuel cell systems (PFCS) with chemical engineering models and techno-economic-environmental optimization models.

PROJECT STATUS

Between June 1st and September 30th, 2010, we advanced the development of chemical engineering fuel cell system (FCS) models and economic and environmental network models describing polygenerative fuel cell systems (PFCSs).

Chemical engineering models were advanced to include more details of the physics of both 1) combined cooling, heating, and electric power (CCHP) FCSs and 2) combined hydrogen and electric power FCSs (H_2-FCS). Chemical engineering models of CCHP FCSs were refined to analyze the thermodynamics of FCSs that produce heat and cooling power, instead of hydrogen, along with electricity. Chemical engineering models of H_2-FCSs were refined to analyze the amount of excess hydrogen that can be produced from a high temperature FCS, and how the FCS operating conditions affect the amount of hydrogen and electricity produced, and the H_2-FCS overall efficiency.

Techno-economic models were advanced

1. to include cutting-edge cost and performance data from all three leading FCS manufacturers (United Technologies Inc, FuelCell Energy Inc., and Bloom Energy Inc.);
2. to evaluate each manufacturer's system;
3. to expand optimization capabilities to include
    a. minimizing the human health impacts of air pollution emissions,
    b. minimizing greenhouse gases (GHG) emission impacts including the effects of carbon dioxide (CO_2) and methane, in terms of their carbon dioxide-equivalence (CO_{2equ}), and

   c. minimizing hydrogen fuel costs;
4. to simultaneously optimize the installed capacity of four different types of polygenerative FCSs either on their own or in combinations with each other. These four types include combined heating and electric power (CHP) FCS; CCHP FCSs; combined heating, hydrogen, and electric power (CHHP) FCSs; and combined cooling, heating, hydrogen, and electric power (CCHHP) FCSs.

3.1: Enhance and Integrate Chemical Engineering Models for Polygenerative Fuel Cell Systems

We developed and enhanced thermodynamic and chemical engineering models of novel stationary FCSs that produce CHP, CCHP and CHHP. In CCHP and CHHP systems, unrecovered heat from the FCS is used for producing either cooling power or hydrogen fuel, respectively. Reuse of unrecovered heat reduces the amount of fuel that needs to be burned for combustion heating. With this internal heat reuse, the amount of fuel used per unit of cooling power or hydrogen produced can be expected to be lower than other production methods.

3.1.1: Thermodynamic and Chemical Engineering Models of Hydrogen and Electricity Co-Production Fuel Cell Systems (H_2-FCSs)

The main goals of this work are to assess the thermodynamic feasibility of co-producing hydrogen from high temperature fuel cell systems, and to quantify the amount of hydrogen yield that can be expected, along with trends. A unique feature of our design approach is to evaluate hydrogen yield using only unused electrochemical heat alone. No heating is provided by combustion. This approach reduces the carbon footprint per unit of hydrogen produced. Models include

- a purely analytical thermodynamic model based solely on the heat of reactions of the exothermic fuel cell oxidation reaction and the endothermic steam reforming reaction,
- an AspenPlus™ model designed to mimic the analytical model (for model validation) but also account for ancillary compressor load,
- a detailed AspenPlus™ model designed to more realistically model incomplete reformation and heat transfer,
- and a similarly detailed AspenPlus™ model adapted to simulate a fuel cell system (FCS) which is running off biogas from a wastewater treatment plant (WWTP).

Two models are also included to simulate single-purpose generators of each product:

- an SOFC system that produces electricity only and no hydrogen, and
- a steam methane reformer (SMR) that produces only hydrogen and does not reuse unrecovered SOFC heat.

Model results indicate that, for the scenarios and operating conditions evaluated, the most significant design feature impacting hydrogen co-production yield is the extent of heat transfer between the hot exhaust streams and the cool inlet streams. With very low heat transfer between inlet and outlet streams, model results show that, the fuel cell stack may not generate sufficient heat to allow for appreciable quantities of hydrogen to be produced. This finding is under the constraint of only electrochemical heating and no combustion heating, However, with higher, more realistic heat transfer rates between exhaust and inlet streams, hydrogen co-production potential ranges from between 0.18 to 0.77 kiloJoules (kJ) of hydrogen (H_2) per kJ of total methane (CH_4) input (on a lower heating value (LHV) basis). This range depends significantly on the operating temperature and current density of the fuel cell, which affect the heat generation as well as the extent of preheating.

It is also shown that the addition of a hydrogen co-production subsystem amounts to either a small ancillary load increase, or a large ancillary load decrease, depending on whether the H_2 subsystem reduces the cooling requirement of the FCS. If the cooling requirement is not reduced, adding an H_2 subsystem amounts to a small gain in ancillary load. When compressing the fuel at ambient temperatures, the hydrogen-producing FCS (H_2-FCS) can typically provide greater than 98% of the electricity a non-co-producing FCS can provide. However, if the non-co-producing FCS is air-cooled, the addition of the H2 subsystem amounts to a sizeable decrease in ancillary load (up to a factor of eight).

Even when a portion of the H_2-FCSs heat and electricity must be devoted to running an upstream biogas plant, the system can still reach a combined efficiency (the sum of hydrogen and electrical energy produced, divided by sum of biogas and electrical energy input) of up to 76%. The steam-to-carbon ratio of the reformers (S/C) is shown to affect this efficiency, as well as the plant's water neutrality. If water neutrality is a constraint, the plant must either be run at lower current density and high temperature (producing more electricity and less hydrogen), or at a lower S/C (reducing combined efficiency).

3.1.2: Thermodynamic and Chemical Engineering Models Combined Cooling, Heating, and Electric Power (CCHP) FCSs

The goals of this research are to analyze the advances in overall system efficiency (the sum of electrical, cooling, and heating outputs divided by the power input determined from the higher heating value of the fuel plus any parasitic loads) through the incorporation of absorption or electric chillers and the recovery of waste heat. Specifically, FCSs will be modeled within AspenPlus™ software to create a simulation model that is used to compare and analyze the advantages and disadvantages in absorption and electric chillers. Models are created for absorption and electric chillers that replicate performance of industry-made chillers. Both chillers provide cooling power through the removal of heat from a water stream, and therefore, providing a cold water stream.

Absorption chillers operate at a coefficient of performance (COP) near one while being powered directly from the exhaust of the fuel cell. The main benefit of absorption chillers is the ability to create cooling power directly from the high temperature exhaust of the fuel cell. This means that additional power is not required for absorption chiller CCHP FCSs.

Electric chillers provide much promise for CCHP FCSs because they operate at a COP of 1.5 to over four. However, electric chillers require the consumption of electricity produced by fuel cell, and therefore reducing the available electricity for external uses. The electric chiller CCHP system will also produce a greater amount of available heat when compared to the absorption chiller system. Although, an electric chiller CCHP FCS will operate at a higher overall system efficiency, the performance is limited due to the reduction in available electricity.

3.2: Enhanced Techno-Economic and Environmental Network Models for Polygenerative Fuel Cell Systems

Energy network optimization (ENO) models were used to optimize FCS installations for cost savings, greenhouse gas emission reductions, and air quality improvement. The models analyze three different sized Direct FuelCell systems from FuelCell Energy, Inc. and take into account different economic incentives, extent of electricity sellback, heat-to-cooling COPs, and fuel cell models, all of which can significantly affect results. Air quality is typically most improved by implementing CCHHP FCSs based on smaller fuel cell models, since they can meet all demand while supplying the least excess electricity. Cost reduction is typically most improved by larger fuel cell models, since they produce more output per capital cost. CO_2 emission reductions are typically most improved by smaller fuel cell models. By using CCHHP FCSs, CO_2 emissions can be reduced by up to 42%, and 99.7% of the health cost of emissions can be eliminated. Using only CCHHP FCSs does not produce hydrogen at a price below that of competing generators, for the strategies tested. However, installing CHHP FCSs, can produce hydrogen at prices of $4.30/kg.

Three different paths for installing CCHHP, CCHP, CHHP, and CHP FCSs were analyzed for increased cost savings and reduced hydrogen prices. Installing different systems can affect costs because reformers and chillers are only installed on the number of FCSs required to meet hydrogen and cooling demand, instead of on all FCSs. For strategies that are load following heat before hydrogen, fulfilling the majority of heating demand before installing CHHP systems results in the largest cost savings, and the lowest hydrogen price (between $2.33 and $3.00/kg).

This research partly or fully sponsored these publications from June 1st to September 30th, 2010.

PUBLICATIONS

Peer-Reviewed Journal Articles

- Colella, W.G., "Optimal Design and Control Strategies for Novel Combined Heat and Power (CHP) Fuel Cell Systems: Part I of II – Datum Design Conditions and Approach," *Proceedings of the 8th International Fuel Cell Science, Engineering & Technology Conference*, (New York, NY: American Society of Mechanical Engineers (ASME), 2010), ISBN 9780791838754).
- Colella, W.G., "Optimal Design and Control Strategies for Novel Combined Heat and Power (CHP) Fuel Cell Systems: Part II of II – Case Study Results," *Proceedings of the 8th International Fuel Cell Science, Engineering & Technology Conference*,

(New York, NY: American Society of Mechanical Engineers (ASME), 2010), ISBN 9780791838754).

- Colella, W.G., "Designing Combined Cooling, Heating, And Electric Power (CCHP) Fuel Cell Systems (FCS)," *Proceedings of the 8th International Fuel Cell Science, Engineering & Technology Conference*, (New York, NY: American Society of Mechanical Engineers (ASME), 2010), ISBN 9780791838754).

Peer-Reviewed Journal Articles in Preparation

- Colella, W.G., Timme, R., "Chemical Engineering Models of Combined Cooling, Heating, and Electric Power (CCHP) Fuel Cell Systems (FCSs) using Electric Chillers," *ASME Journal of Fuel Cell Science and Technology*, (New York, NY: American Society of Mechanical Engineers (ASME), expected 2011.)
- Colella, W.G., Timme, R., "Thermodynamic and Chemical Engineering Models of Combined Cooling, Heating, and Electric Power (CCHP) Fuel Cell Systems (FCSs) using Absorption Chillers," *ASME Journal of Fuel Cell Science and Technology*, (New York, NY: American Society of Mechanical Engineers (ASME), expected 2011.)
- Colella, W.G., Tilghman, M. "Hydrogen Co-Production Potential for Solid Oxide Fuel Cells (SOFCs): Part I: Analytical Thermodynamic Modeling," *ASME Journal of Fuel Cell Science and Technology*, (New York, NY: American Society of Mechanical Engineers (ASME), expected 2011).
- Colella, W.G., Tilghman, M. "Hydrogen Co-Production Potential for Solid Oxide Fuel Cells (SOFCs): Part II: AspenPlus^{TM} Flowsheet Modeling," *ASME Journal of Fuel Cell Science and Technology*, (New York, NY: American Society of Mechanical Engineers (ASME), expected 2011).
- Colella, W.G., Margalef, P., Brouwer, J., "Enhancing Hydrogen Yield and Net Electric Power from Stationary Fuel Cell Systems (FCS) Co-Producing Hydrogen through Thermal Integration of the Hydrogen Separation Unit (HSU) based on Pressure Swing Absorption (PSA) Technology: Applying AspenPlus^{TM} Chemical Engineering Process Plant Models and Results," *ASME Journal of Fuel Cell Science and Technology*, (New York, NY: American Society of Mechanical Engineers (ASME), expected 2011).
- Colella, W.G., "Optimizing the Deployment of Advanced Combined Cooling, Heating, and Electric Power (CCHP) Fuel Cell Systems (FCS) for Low Costs and Minimal Environmental Impact using Techno-Economic-Environmental Optimization Models," *ASME Journal of Fuel Cell Science and Technology*, (New York, NY: American Society of Mechanical Engineers (ASME), expected 2011.)
- Colella, W.G., "Innovative Approaches for Co-Producing Hydrogen at Low Cost and with Low Emissions using High-Temperature Stationary Fuel Cell Systems (FCS): Techno-Economic-Environmental Models and Results," *ASME Journal of Fuel Cell*

Science and Technology, (New York, NY: American Society of Mechanical Engineers (ASME), expected 2011).

- Colella, W.G., "Reducing Building Energy Costs and Carbon Dioxide (CO_2) Emissions by Operating Stationary Co-generative Fuel Cell Systems (FCS) with Novel Strategies: Part I of II – Model Development," *ASME Journal of Fuel Cell Science and Technology*, (New York, NY: American Society of Mechanical Engineers (ASME), expected 2011).
- Colella, W.G., "Reducing Building Energy Costs and Carbon Dioxide (CO_2) Emissions by Operating Stationary Co-generative Fuel Cell Systems (FCS) with Novel Strategies: Part II of II – Example Results for a California Town," *ASME Journal of Fuel Cell Science and Technology*, (New York, NY: American Society of Mechanical Engineers (ASME), expected 2011).
- Colella, W.G., Tilghman, M. "Optimal Operating Strategies for Polygenerative Fuel Cell Systems (FCS) Simultaneously Generating Electricity, Heat, Cooling Power, and Hydrogen," *ASME Journal of Fuel Cell Science and Technology*, (New York, NY: American Society of Mechanical Engineers (ASME), expected 2011.)
- Colella, W.G., Sammes, N.S. "Unsupported Claims that the Electrical Efficiency of a Fuel Cell can Never be Greater than 50%," *Journal of Power Sources*, expected 2011.
- Colella, W.G., Schneider, S.H., Kammen, D.M., "Quantifying Regional Changes in Greenhouse Gas Emissions in California from Installing Stationary Fuel Cell Systems (FCS)," *ASME Journal of Fuel Cell Science and Technology*, (New York, NY: American Society of Mechanical Engineers (ASME), expected 2011).
- Colella, W.G., Schneider, S. H., Kammen, D.M. "Getting the Baseline Right: Reconciling Greenhouse Gas Accounting Data and Methodologies," expected 2011).

PEER-REVIEWED REPORTS

- Colella, W.G., Tilghman, M., Timme, R. Novel Designs for Advanced Stationary Polygenerative Fuel Cell Systems (PFCS), Sandia Report, Sandia National Laboratories, Albuquerque, New Mexico 87185, SAND2010-6187 P, September 2010.

KEYNOTE ORAL CONFERENCE PRESENTATION

- Colella, W.G., "Pioneering Devices for Mitigating Climate Change and Air Pollution," American Society of Mechanical Engineers (ASME) 8th International Fuel Cell Science, Engineering, and Technology Conference, Brooklyn, New York, USA, June 14-16th, 2010.

PEER-REVIEWED CONFERENCE PRESENTATIONS

- Colella, W.G., "Designing Combined Cooling, Heating, and Electric Power (CCHP) Fuel Cell Systems," American Society of Mechanical Engineers (ASME) 2010 8th

International Fuel Cell Science, Engineering & Technology Conference, Brooklyn, New York, June 14-16th, 2010.

- Colella, W.G., "Optimal Design And Control Strategies For Novel Combined Heat And Power (CHP) Fuel Cell Systems: Part I of II – Datum Design Conditions And Approach," American Society of Mechanical Engineers (ASME) 2010 8th International Fuel Cell Science, Engineering & Technology Conference, Brooklyn, New York, June 14-16th, 2010.
- Colella, W.G., "Optimal Design And Control Strategies For Novel Combined Heat And Power (CHP) Fuel Cell Systems: Part II of II – Case Study Results," American Society of Mechanical Engineers (ASME) 2010 8th International Fuel Cell Science, Engineering & Technology Conference, Brooklyn, New York, June 14-16th, 2010.
- Colella, W.G., "Generating Hydrogen (H_2) as a Byproduct of Operating Stationary Combined Heat and Power (CHP) Fuel Cell Systems (FCSs),"American Society of Mechanical Engineers (ASME) 2010 8th International Fuel Cell Science, Engineering & Technology Conference, Brooklyn, New York, June 14-16th, 2010.

BOOK CHAPTERS

- Sammes, Nigel M.; Suzuki, Toshio; Yamaguchi, Toshiaki; Awano, Masanobu and Colella, W. G., (authors) chapter in book, "Introduction to Solid Oxide Fuel Cells (SOFC)," *Handbook of Climate Change Mitigation*, (New York, NY: Springer, expected 2011), in print.

INVITED TALKS

- Colella, W.G., Novel Designs for Advanced Stationary Polygenerative Fuel Cell Systems (PFCS), U.S. Department of Energy, Energy Efficiency and Renewable Energy (EERE) Division, Hydrogen Program, Sandia National Laboratories L'Enfant Plaza Office, Washington, D.C., USA, Sept. 15th, 2010.
- Colella, W.G., Designing Innovative Microgrids to Reduce Energy Costs, Fuel Consumption, Air Pollution, and Greenhouse Gas Emissions, Interagency Working Group on Hydrogen and Fuel Cells (IWG), webinar-linked presentation between Sandia National Laboratories, Albuquerque, NM and Energetics Incorporated, 901 D. Street, SW, Suite 100, Washington, DC 20024, July 20th, 2010.
- Colella, W.G., Low Carbon Microgrids, Department of Chemical Engineering, Princeton University, Princeton, NJ, June 17th, 2010.

NOVEL DESIGNS FOR ADVANCED STATIONARY POLYGENERATIVE FUEL CELL SYSTEMS (PFCS): FY11Q1

COVERING PERIOD:	OCTOBER 1, 2010 THROUGH JANUARY 31, 2011
DATE OF REPORT:	JANUARY 31, 2011
PRINCIPLE INVESTIGATOR:	JUAN TORRES, (505)844-0809, JJTORRE@SANDIA.GOV
OTHER PARTNERS:	NONE
CONTACTS:	JUAN TORRES, (505)844-0809, JJTORRE@SANDIA.GOV JAY KELLER, (925) 294-3316, JOKELLE@SANDIA.GOV

PROJECT OBJECTIVE

To evaluate the design of novel advanced stationary polygenerative fuel cell systems (PFCS) with chemical engineering models and techno-economic-environmental optimization models.

PROJECT STATUS

Between October 1, 2010 and January 31, 2011, work was completed on the publications listed in the following section. The first two articles from this list below are being prepared for publication in the ASME Journal of Fuel Cell Science and Technology. The modeling work that was funded under this research grant provided the data and analysis that is used for the drafting of these articles. These articles are concerned with the potential efficiency improvements available through the application of combined cooling, heating, and electric power (CCHP) fuel cell systems (FCSs). Modeling results show that CCHP FCSs with absorption chillers produce electricity, heating power, and cooling power at an overall efficiency of 99%, while CCHP FCSs with electric chillers produce power at an overall efficiency between 125% and 145%. The third article also stems from this research knowledge base and is a collaborative effort with the Colorado School of Mines and the University of California. This article demonstrates that, in contrast to the claims of others, a fuel cell's electrical efficiency can exceed 50% even when operating at peak power.

PUBLICATIONS

Peer-Reviewed Journal Articles in Preparation

- Colella, W.G., Timme, R.J., "Chemical Engineering Models of Combined Cooling, Heating, and Electric Power (CCHP) Fuel Cell Systems (FCSs): Part A – Absorption Chillers," ASME Journal of Fuel Cell Science and Technology, (New York, NY: American Society of Mechanical Engineers (ASME), expected 2011.)
- Colella, W.G., Timme, R.J., "Chemical Engineering Models of Combined Cooling, Heating, and Electric Power (CCHP) Fuel Cell Systems (FCSs): Part B – Electric

Chillers," ASME Journal of Fuel Cell Science and Technology, (New York, NY: American Society of Mechanical Engineers (ASME), expected 2011.)

- Colella, W.G., Timme, R.J., Brouwer, J., Sammes, N.M., "Fuel Cell Efficiency Can Exceed 50% at Peak Power," Journal of Power Sources, (expected 2011).

INTERNATIONAL ENERGY AGENCY: FY11Q2

COVERING PERIOD: JANUARY 1, 2011 THROUGH MARCH 31, 2011

DATE OF REPORT: APRIL 30, 2011

PRINCIPLE INVESTIGATOR: SUSAN SCHOENUNG, 650-329-0845, SUSAN.SCHOENUNG@SBCGLOBAL.NET

DOE MANAGER: DAN SANCHEZ

PROJECT OBJECTIVE

To manage and participate in hydrogen systems analysis for the International Energy Agency Hydrogen Implementing Agreement Task 30 on Global Hydrogen Systems Analysis.

APPROACH

This contract has three subtasks:

1. Perform the activities of co-Operating Agent for Task 30, along with co-Operating Agent Jochen Linssen of Germany.
2. Perform the activities of Subtask A leader – Global Hydrogen Resource Study, together with partners at Sandia Laboratories and experts from Task 30.
3. Participate in the detailed modeling and analysis, along with the U.S. expert group at Sandia Livermore.

PROGRESS

As (co) Operating Agent for IEA Hydrogen Annex 30—Global Hydrogen Systems Analysis, Dr. Schoenung begun the work of (co) managing a new group of experts from 11 countries.

Dr. Schoenung is also the Subtask A leader for detailed resource analyses. She has met with Sandia partners to plan the Global Resource study for Subtask A. Dr. Schoenung has been collecting international data contributions to the resources template. A status report conference call took place in early January. All countries were represented except Japan.

A status report conference call with Carole Read took plakce at DOE HQ in February.

A second all-Task conference call took place in March.

Dr. Schoenung has worked with Sandia personnel to establish a Task 30 website, which was opened to experts in early January. Due to some glitches, the website needed to be reestablished and content resubmitted. The remaining Task 18 website materials were archived.

Dr. Schoenung has been working to establish a consistent basis for estimating resources and the time sequence for resource and demand development. This work was discussed on several conference calls, and during the Experts meeting in Paris in March.

Dr. Schoenung has also drafted a request for IPHE to consider how to help Task 30 get data from non-HIA member countries. A set of talking points was also delivered to DOE (Carole Read). Paul Lucchese of CEA will request an agenda item for the May IPHE meeting in Vancouver. Dr. Schoenung will present an overview of Task 30, while Mr. Lucchese will present the HIA request for a new annex to the HIA—IPHE MOU.

Dr. Schoenung co-led the Spring Experts meeting of Task 30, hosted by CEA in Paris. The 2 1/2 day meeting covered all aspects of Task 30 and included a half-day meeting with representatives from IEA Analysis activities: World Energy Outlook, Energy Technology Perspectives, and the Mobility Model.

Dr. Schoenung prepared the Task 30 input to the HIA 2010 Annual Report.

PLANS FOR NEXT QUARTER AND KEY ISSUES

Work will continue on the Subtask A modeling, and include new inputs from the Task 30 experts. A web conference is scheduled for May 18. Dr. Schoenung will present an overview of Task 30 at a meeting of the IPHE Steering Committee in Vancouver in May.

Dr. Schoenung will participate as co-Operating Agent in the HIA Spring Executive Committee meeting in Copenhagen, Denmark in June.

GLOBAL HYDROGEN RESOURCE ANALYSIS: FY11Q1 AND Q2

COVERING PERIOD: OCTOBER 1, 2010 THROUGH MARCH 31, 2011

DATE OF REPORT: APRIL 27, 2011

PRINCIPLE INVESTIGATOR: DAVE REICHMUTH, (925) 294-3393, DREICHM@SANDIA.GOV

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FY 2011 MILESTONES/DELIVERABLES

Task/Milestone Description	Planned	Actual	Comments
Global Hydrogen Resource Analysis			
Expert Task Definition mtg (Germany): Establish foundation and modeling approach.	9/16-17/10	9/2010	Complete
Development of dynamic models to describe resource availability and distribution networks at the country level. Initial analysis using models.	3/11	4/2011	Model development completed; data gathering ongoing
Participate in 2011 AMR.	5/11	5/2011	Pending
Analysis of international energy and fuel flows.	7/11		
Write draft implications to the U.S. energy markets in relation to world resources.	9/11		

PROJECT OBJECTIVE

The goal of the Global Hydrogen Resources Analysis Task is to perform comprehensive technical and market analysis of hydrogen technologies and resources, supply and demand related to the projected use of hydrogen in a low-carbon world with sustainable and including intermittent energy sources. This task is part of the IEA/HIA Annex 30 analysis activities. The specific objectives of this task are to prepare authoritative analyses which can be used to answer questions about hydrogen sources and utilization posed by the IEA HIA, the task members, the IEA, and government institutions.

PROJECT STATUS

This task begun in September 2010 with a kick-off meeting with IEA Task 30 participants. Since that meeting, the U.S./Sandia expert team has modified existing hydrogen delivery and use models to address the needs of the Task 30 analysis. Modifications include the ability to model multiple, interacting regions. The model is constructed to allow additional regions to be added with minimal effort. The data sources are held in Excel spreadsheet files. Because we use a widely-available file format, we can take data from new sources and quickly add them to the model. We currently can model 8 regions, 3 fuels, and 5 hydrogen production pathways (2 low-carbon pathways).

PLANS FOR NEXT QUARTER

Next quarter, we will complete our data collection for U.S. hydrogen production pathways with emphasis on collecting data on solar potential and costs. The model will then be used to report regional supply cost curves for the U.S. We will use sensitivity analysis to show key input variables that have a large impact on the supply cost curves.