SAND2009-3198P

QUARTERLY PROGRESS REPORT

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

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Recipient: Sandia National Laboratories

Subcontractors: None

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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

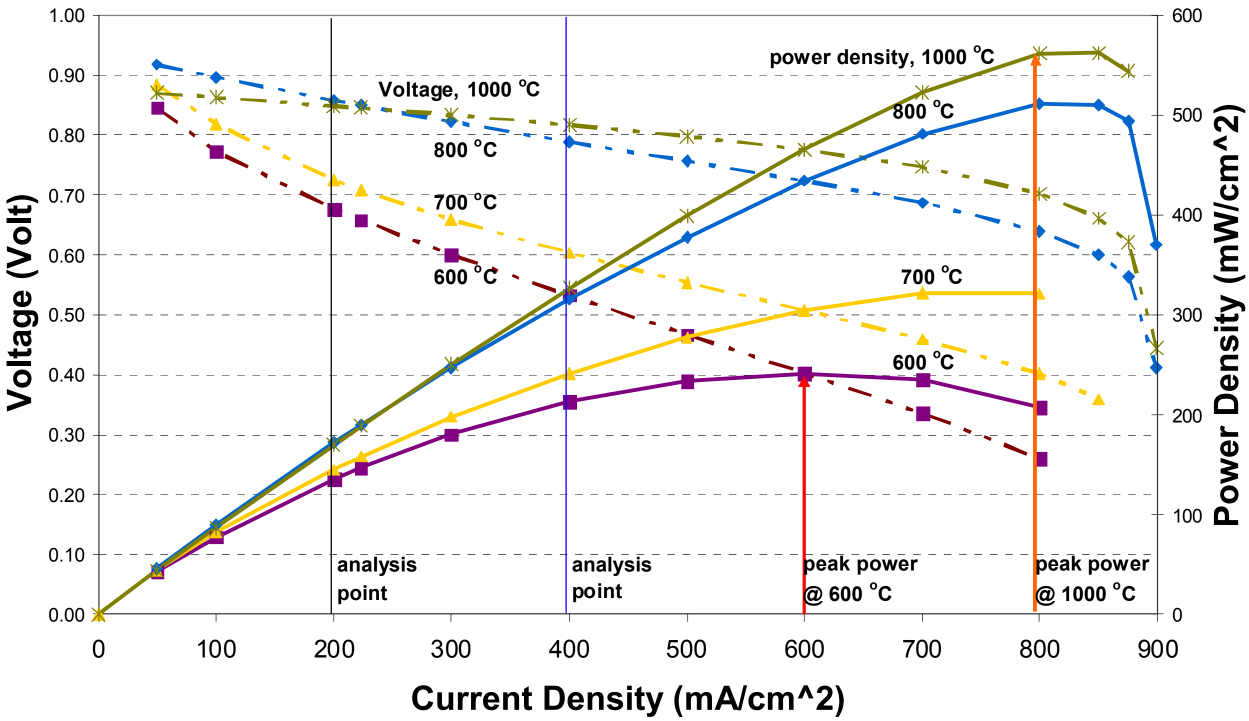
Subtask 4.1— Develop Novel H_2-PFCS Designs with Low Marginal H_2 Production Cost

4.1.1: Developing engineering, economic, and environmental models and analyses

In this first of three distinct modeling efforts, our engineering, economic, and environmental model shows that low marginal hydrogen (H_2) production prices could be achieved through the use of novel operating strategies such as networking, employing a variable heat-to-power ratio, and using various load following constraints. Our model minimizes total yearly electricity, heat, and hydrogen costs by changing the installed capacity of stationary polygenerative fuel cell systems co-producing hydrogen (H_2-PFCS) for different operating strategies. Our model considers a particular location's climatic region, building load curves, fuel cell system type, and competitive environment. A fuel cell system's load following controls will match the hourly demand if it is within the physical constraints of the system. All demand not supplied by the fuel cells is purchased from competing electricity, heat, and hydrogen generators. To meet the DOE Hydrogen Program's goals of hydrogen production with low fuel consumption and carbon dioxide emissions (CO_2), our model focuses on H2-PFCS designs that reuse internal waste heat from the FCS to provide heat for the endothermic steam methane reforming process for hydrogen production such that no additional fuel need be consumed. For the case studies evaluated here, the competing hydrogen generators are stand-alone steam methane reformers and the H2-PFCS are assumed to be connected to the grid, allowing them to sell back un-used electricity at market price. For these case studies, our model assumes that hydrogen production is for just-in-time use with no hydrogen storage, is limited at 5% of the total fuel energy entering the system, and the additional hydrogen production and separation equipment results in a 25% increase in fixed costs over the more standard fuel cell system without hydrogen co-production. For these cases, our model shows that electricity, heat, and hydrogen can be produced with the lowest costs for strategies that combine electrical and thermal networking, a variable heat-to-electric power ratio, a variable hydrogen-to-heat ratio, maximum electrical output, and then hydrogen and heat load following.

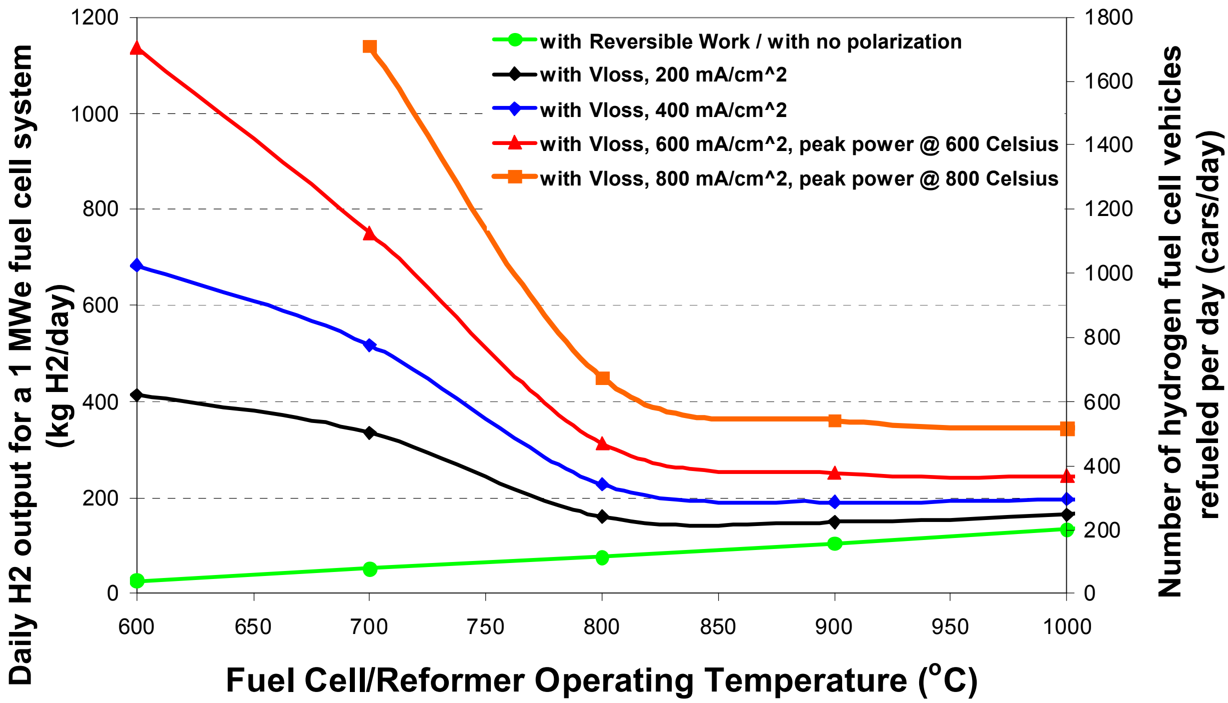
4.1.2: Developing thermodynamic models

In this second of three distinct modeling efforts, we have chosen a theoretical approach this quarter to understand the upper bounds for cost savings, fuel savings, and excess available hydrogen. During this quarter, we developed an analytical approach towards benchmarking the quantity of excess hydrogen available from high-temperature Solid Oxide Fuel Cell (SOFC) and Molten Carbonate Fuel Cell (MCFC) designs with no marginal increase in fuel consumption or greenhouse gas emissions. We derive the theoretical limit of excess hydrogen from electrochemical waste heat alone. The methodology involves hypothetically partitioning fuel cell stack waste heat into a quantity that meets the minimal energy requirement to provide heat to reform fuel solely to run the stack and a quantity that is potentially accessible to produce excess hydrogen. The steam reforming reactions can provide hydrogen (A) for the fuel cell's anode or (B) for excess hydrogen production. For benchmarking a hydrogen co-producing system against a standard system, we analytically separate the two processes – (A) and (B) -- in two "virtually" separate steam reformers – REFA and REFB. REFA produces enough hydrogen for the fuel cell to provide electric power. REFB produces excess hydrogen (for vehicles, etc.) We analyzed the excess hydrogen as a function of temperature between 600°C and 1000°C under different fuel cell stack polarizations and operating conditions. Our polarization expressions and constants are from the peer-reviewed literature, industry, and our collaborators at UCI. The resulting polarization and power density expressions are plotted in the figure for an SOFC. We studied the impact of ideal and non-ideal



1) cell operation and 2) system-wide heat transfer. For example, for non-ideal cell operation, the excess heat is greater at higher current density due to greater voltage loss. The benefit of

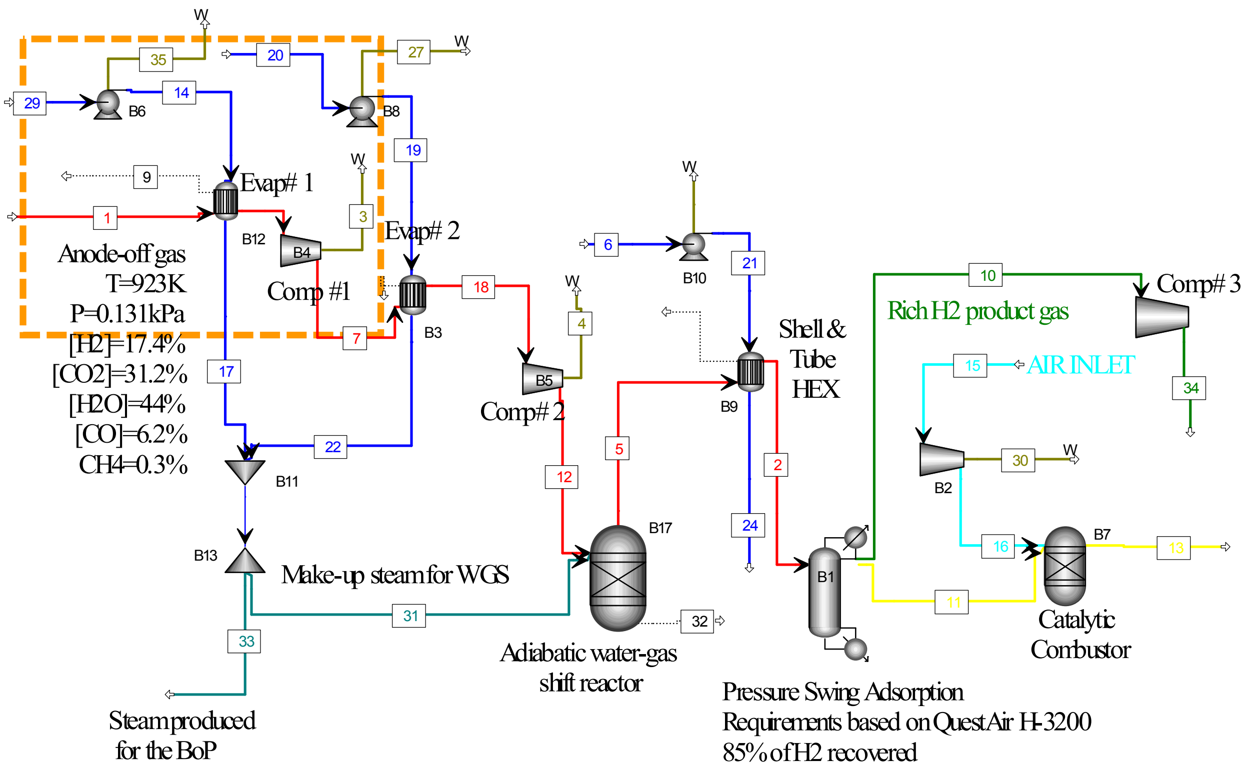
excess hydrogen diminishes significantly if anode off gas and cathode inlet gas are not thermally integrated. We have validated our analytical results using AspenPlus chemical engineering process plant simulations. Applying this hypothetical model to real-world operation, a 1 megawatt electric (MWe) fuel cell operating between 800 and 1000ºC could make ~150 to 450 kg of hydrogen /day without added fuel consumption or greenhouse gas emissions, as shown in the figure.



4.1.3: Developing chemical engineering process plant models and analyses
In this third of three distinct modeling efforts, we model the thermodynamics of the overall hydrogen tri-generation system using detailed chemical engineering process plant simulations in ASPENPlus. A one MWe MCFC system, based on a similar commercial product from FuelCell Energy (FCE), Inc., has been thermally integrated with a hydrogen separation unit (HSU). Pressure Swing Adsorption (PSA) has been selected as the hydrogen separation technology due to its commercial readiness.

PSA technology requires inlet gas at relatively low temperature (323 K) and high pressure (20 bar). Since the anode-off gas of a MCFC is at high temperature (923 K) and low pressure (1.06 bar), a significant energy penalty could be associated with the required compression (146 kWe) and heat extraction (600 kWt). In addition, if hydrogen is separated prior to the catalytic combustor that is part of the current FCE system design, less heat is available for preheating of fuel cell reactants. This leads to an overall thermal energy deficit of 123 kWt for steam generation and air and fuel preheating. The designed HSU system integrates the fuel cell balance of plant with the heat extraction steps required for the PSA (Figure 1). With this configuration, 435 kWt are recovered to produce high quality steam for the fuel cell operation. In addition, compression work requirements have been minimized by reducing compressor inlet gas temperature. Furthermore, since anode-off gas temperature is dropped below its saturation point, steam condensation takes place in both evaporators. As a result, liquid water can be separated from the gas stream lowering compression work and PSA separation requirements. A water-gas-shift reactor (WGSR) has been integrated into the system after the compression stage. As a result, hydrogen yield increases by shifting carbon monoxide and steam into hydrogen and carbon dioxide.

Through scenario analyses, the team has identified an optimal HSU cycle design that combines heat recovery and WGS reactions to increase H2 yield by 132%. Individual contributions to the increase in H2 yield are: 1) 102% due to displaced H2 combustion; 2) 15% due to WGS; and 3) 132% due to both. This design consumes 11% of gross electrical power and reuses 73% of available waste heat. In summary, we have shown that daily hydrogen production can be increased by over 132% when the FCS reuses internal waste heat for hydrogen production.



We continued to review relevant literature, collaborate with expert researchers with key skills and experience, and solidify modeling approaches.

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

4.2.1: Developing engineering, economic, and environmental models and analyses

In this first of three distinct modeling efforts, our engineering, economic, and environmental model evaluates scenarios in which hydrogen is co-produced with no additional, marginal increase in carbon dioxide (CO_2) emissions. Our model shows the potential carbon emission reductions when combining novel operating strategies with H2-PFCS designs. Our model analyzes greenhouse gas emission reductions when compared to a base case in which no H2-PFCS are installed and all energy is purchased from competing technologies. Total yearly greenhouse gas emissions are calculated based on the total fuel consumption from the fuel cell systems and competing generators. When optimizing for greenhouse gas emission reductions, the model changes the fuel cell system installed capacity to minimize the total greenhouse gas emissions produced by on-site power. Compared to a base case with no FCS, our novel strategies with H2-PFCS installed reduce CO_2 emissions by 40%. When accounting for the displaced CO_2 caused by selling electricity back to the grid, our novel H2-PFCS strategies reduce CO_2 emissions by an even larger quantity, 50%. Under optimal design and operating conditions, H2-PFCS potentially could not only provide a cheap method of fueling hundreds of H_2 fuel cell vehicles a day, but also do so with no marginal increase in CO_2 emissions. While most of our model results focus on natural gas fuel, we also are conducting scenario analyses for biogas fuel operation.

4.2.2: Developing thermodynamic models and analyses
In this second of three distinct modeling efforts, we explored different feed compositions for calculating the theoretical excess hydrogen co-produced in our SOFC and MCFC designs. Compared to pure methane, the biogas will require more throughput for the fuel cell stack due to CO_2 dilution of fuel input. The analytical approach from this quarter is being used to differentiate the impact of different feed compositions on excess hydrogen based on our heat of reaction balances at different temperatures. This work is being extended to real flowsheet designs in AspenPlus flowsheet to consider other process considerations, such as higher throughput, hydrogen separation unit, compressors, and heaters to evaluate different realistic thermally integrated designs.

4.2.3: Developing chemical engineering process plant models and analyses
In this third of three distinct modeling efforts, we develop models with significant design and operational flexibility that allows one to vary and define inlet fuel compositions. To-date, analyses have focused primarily on natural gas fuel, but models are also being built to be flexible enough for expansion to biogas. There is a growing interest and emerging technology developments that involve operation of fuel cells and also H_2-PFCS on biogas (typically anaerobic digester or landfill gas) to produce "green" or "renewable" hydrogen and power. Anaerobic digester gas (ADG) produced in waste water treatment plants (WWTP) represents a great opportunity for tri-generation of electricity, heat and hydrogen from a locally produced renewable fuel. Analyses show that the state of California has enough WWTP to produce 316,824 m^3 of ADG/day. Other regions of the U.S. contain similar significant renewable fuel resources that will be considered in the future H_2-PFCS systems analyses.

We continued to review relevant literature, collaborate with expert researchers with key skills and experience, and solidify modeling approaches.

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

We collaborate with academia, industry, and federal entities to greatly advance research and development, and technology transfer. Our primary collaborators are shown in the table.

#	Collaborator	Relation-ship	Entity Type	In DOE H_2 program?	Extent of Collaboration
1	University of California at Irvine, Mechanical & Aerospace Engineering Dept.	sub-contractor	academia	yes	Actively collaborating on a daily basis to develop chemical engineering models of hydrogen separation units thermally integrated with fuel cell systems. Conducting related energy system analyses.
2	Fuel Cell Energy, Inc.	partner with data disclosure sensitivity	industry	yes	Actively partnering on a bi-weekly or monthly basis to validate model inputs, assumptions, and operating data. Verifying molten carbonate fuel cell (MCFC) performance, system integration approaches with fuel cells, design cycle configurations, and curren
3	Technology Management Inc.	partner with data disclosure sensitivity	industry	no	Actively partnering on a monthly basis to validate model inputs, assumptions, and operating data. Verifying solid oxide fuel cell (SOFC) performance, system integration approaches, operation on low-carbon fuels.
4	Transportation and Stationary Power Integration (TSPI) team: SNL, NREL, LANL, ORNL, BNL, ANL	research team partners	federal	yes	Sandia National Laboratories (SNL), National Renewable Energy Laboratory (NREL), Los Alamos National Laboratories (LANL), Oak Ridge National Laboratories (ORNL), Brookhaven National Laboratories (BNL), and Argonne National Laboratories (ANL) are meeting o
5	National Renewable Energy Laboratory (NREL)	partner	federal	yes	SNL has provided three separate rounds of detailed technical feedback on nascent versions of NREL's H2A model. SNL and NREL collaborated to develop TSPI invited workshops.
6	Fuels Pathways Integration Technology Team (FPITT)	technology transfer	federal and industry	yes	Federal laboratories -- including SNL, NREL, ANL, and Lawrence Livermore National Laboratories (LLNL) -- develops models related to alternative transportation supply chains, and industry -- including Exxon Mobil, Shell, ConocoPhillips, and Chevron critica
7	International Energy Agency (IEA) Advanced Fuel Cells Annex: Stationary applications Annex XIX and Annex 25	knowledge transfer	federal, industry, and academia	no	Sandia presented model results to IEA stationary fuel cell systems working group experts and included their feedback in subsequent model development and proposed future work.

Sandia actively collaborates with other DOE labs through the Transportation and Stationary Power Integration (TSPI) team. As part of this team, Sandia National Laboratories (SNL), National Renewable Energy Laboratory (NREL), Los Alamos National Laboratories (LANL), Oak Ridge National Laboratories (ORNL), Brookhaven National Laboratories (BNL), and Argonne National Laboratories (ANL) meet on a monthly basis by phone to enhance their engineering, economic, and environmental models to include H2-PFCS scenarios. We attended several phone meetings with the other DOE lab members to develop ideas and modeling suggestions related to this research. Sandia has provided advice on relevant H2-PFCS literature, analyses, model results, and model feedback to team members either individually or as a group. Whenever possible, we provided valuable technical suggestions. For example, we have discussed modeling efforts 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)).

SNL has provided three separate rounds of detailed technical feedback on nascent versions of NREL's H2A model updated for hydrogen co-production scenarios, and are now engaged in a fourth round of feedback on more advanced model versions. We engaged with Darlene Steward, Michael Penev, and Marc Melaina of NREL to prepare this fourth round of feedback. SNL and NREL collaborated to develop a TSPI invited workshop in October and are now developing a second one for June.

On March 17^{th}, 2009, Sandia presented model results to the Fuels Pathways Integration Technology Team (FPITT) working group and included feedback in subsequent model development. As part of the FPITT, Federal laboratories -- including SNL, NREL, ANL, and Lawrence Livermore National Laboratories (LLNL) – are developing models related to alternative transportation supply chains, and industry members -- including Exxon Mobil, Shell, ConocoPhillips, and Chevron are critically evaluating these model results.

Sandia presented model results to International Energy Agency (IEA) stationary fuel cell systems working group experts and included their feedback in subsequent model development and proposed future work. Leading international research organizations have also advised us on our model development. These include the École Polytechnique Fédérale de Lausanne (EPFL), Laboratoire d'énergétique industrielle (Swiss academia); E4Tech (European industry); and the Fraunhofer Institute for Solar Energy (ISE) Systems (German federal & industry).

PLANS FOR NEXT QUARTER

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

We are developing more advanced 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. Having completed initial computer simulations that explore a narrow band of operating conditions, we are now continuing to expand this operating regime to include more realizable designs.

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. Having developed the framework for initial computer simulations, we are now expanding this operating regime to include more realizable designs.

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 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 initial computer simulations	3/09	3/09	We completed initial computer simulations that explore a narrow band of operating conditions. We continue to expand this operating regime to include more realizable designs.
Describe optimal designs	06/09		
4.2 Develop Novel H_2-PFCS Designs with Low Greenhouse Gas Emissions fueled by Biogas			
Complete initial 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		