

Use of Federated Object Modeling to Develop a Macro-System Model for the U.S. Department of Energy's Hydrogen Program

Preprint

Mark F. Ruth
National Renewable Energy Laboratory

Keith B. Vanderveen and Timothy J. Sa
Sandia National Laboratories

*To be presented at the 2006 Winter Simulation Conference
Monterey, California
December 3–6, 2006*

Conference Paper
NREL/CP-150-40222
July 2006

NREL is operated by Midwest Research Institute • Battelle Contract No. DE-AC36-99-GO10337



NOTICE

The submitted manuscript has been offered by an employee of the Midwest Research Institute (MRI), a contractor of the US Government under Contract No. DE-AC36-99GO10337. Accordingly, the US Government and MRI retain a nonexclusive royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for US Government purposes.

This report was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or any agency thereof.

Available electronically at <http://www.osti.gov/bridge>

Available for a processing fee to U.S. Department of Energy and its contractors, in paper, from:

U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831-0062
phone: 865.576.8401
fax: 865.576.5728
email: <mailto:reports@adonis.osti.gov>

Available for sale to the public, in paper, from:

U.S. Department of Commerce
National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
phone: 800.553.6847
fax: 703.605.6900
email: orders@ntis.fedworld.gov
online ordering: <http://www.ntis.gov/ordering.htm>



USE OF FEDERATED OBJECT MODELING TO DEVELOP A MACRO-SYSTEM MODEL FOR THE U.S. DEPARTMENT OF ENERGY'S HYDROGEN PROGRAM*

Mark F. Ruth

National Renewable Energy Laboratory
1617 Cole Blvd
Golden, CO 80401, U.S.A.

Keith B. Vanderveen
Timothy J. Sa

Sandia National Laboratories
7011 East Avenue
Livermore, CA 94550, U.S.A.

ABSTRACT

The U.S. Department of Energy (DOE) is working on changing our transportation fuel from gasoline to hydrogen. To assist in that effort, we are developing a macro-system model (MSM) that will link existing or developmental component models together to analyze crosscutting hydrogen issues. The MSM uses a federated simulation framework that extends the High Level Architecture (HLA). In this initial phase, three existing models have been linked to analyze two primary issues. The first issue we will examine will be the combined price of hydrogen production and delivery and the second will be a comparison of energy requirements and air emissions for multiple hydrogen production / delivery pathways (i.e., hydrogen produced from different feedstocks and transported via different means). Future work will involve linking other models to allow us to better analyze transition issues and making the MSM available to the hydrogen analysis community.

1 INTRODUCTION

Concerns about the availability of fossil fuels and the impact of carbon dioxide (CO₂) emissions on the environment and human health have caused an increasing interest in the use of hydrogen as an energy carrier. Using hydrogen instead of hydrocarbons for transportation has the potential to reduce or virtually eliminate vehicular emissions of most pollutants including CO₂ although it could just displace those emissions to the hydrogen production facilities. Additionally, the distributed nature of hydrogen production

* This work has been authored by an employee of the Midwest Research Institute under Contract No. DE-AC36-99GO10337 with the U.S. Department of Energy. The United States Government retains and the publisher, by accepting the article for publication, acknowledges that the United States Government retains a non-exclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for United States Government purposes.

promises to greatly improve national energy security. For these reasons, during his 2003 State of the Union Address, President Bush launched the Hydrogen Fuel Initiative with the objective of replacing petroleum-based transportation fuels with hydrogen (U.S. Department of Energy 2005).

As a result of the State of the Union Address, the National Research Council (NRC) convened a committee to study the opportunities, costs, barriers, and research and development needs for the hydrogen economy. Their recommendations have helped direct work within the Hydrogen Fuel Initiative. In the NRC's 2004 report, they recommended that a systems analysis function be formed within the Hydrogen Fuel Initiative 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 (NRC 2004).

The Systems Analysis function recognized that the Hydrogen Initiative had already developed or has begun developing many models covering different aspects of a possible hydrogen economy. Those models fall into the following categories:

- Models that estimate the cost and resources necessary to produce hydrogen through various pathways,
- Models that simulate the methods, costs, and resources necessary to deliver and distribute hydrogen to vehicles,
- Models that simulate vehicle performance;
- Both spatial and non-spatial models that estimate development and costs to deploy the necessary vehicle-fueling infrastructure, and
- Models that simulate market transition from today's petroleum economy to a future hydrogen economy.

The Systems Analysis function determined that a macro-system model (MSM) would be necessary for analyzing cross-cutting issues because no existing model en-

compasses 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.

We could have followed either of two approaches to develop the MSM: (1) develop a new model on a single platform that included techniques and information from all other models, or (2) develop a tool to link or federate existing models together across multiple platforms. We selected the second approach because the task of building a single monolithic model incorporating all of the relevant information in the existing models would have been overwhelming, as the expertise necessary to do so was spread among half a dozen DOE laboratories and a dozen or more universities and private contractors.

Linking models should allow us to generate consistent, valid results by publishing consistent values to integrated models. Currently, developers of integrated models get data from different sources. Some of those sources are easy to trace, others are more obscure. The data coming from most of the sources changes frequently, causing difficulties in tracking the timing of the data used in particular model runs.

For example, transition models require projected future hydrogen production costs. Without the MSM, those costs are entered by the modeler and may be based on the modeler's insights, other models, or other calculations. Historically, different modelers used different future hydrogen production costs as inputs and, therefore, obtained inconsistent results. Using the MSM, hydrogen production costs can be calculated by production models and transferred directly to the transition models. This technique provides the same data for all transition models and updates that data with minimal effort from the modelers, resulting in greater consistency between analysis projects.

2 MACRO-SYSTEM MODEL REQUIREMENTS

We are designing the MSM to be used only by analysts within the hydrogen community who understand the available models and how they work. Those analysts also helped identify the issues that the MSM needs to address. The issues the MSM needs to address fall into the following four categories:

- Research and Development – hypothetical fuel cycle costs (i.e., what is the full cost per mile driven and how it might evolve over time) and the suitability of technical targets for the Hydrogen Initiative and their relationships to each other.

- Transition – potential hydrogen infrastructures and how they might compete with the current petroleum infrastructure. Market issues and regional differences, different pathways, and legacy costs of retired infrastructure are included.
- Financial – corporate and government investment options.
- Environmental – resource requirements and emissions profiles.

Other requirements for the MSM include extensibility to multiple platforms, dynamic time-steps, and modeling spatial issues associated with the build-out of hydrogen infrastructure. Multiple platforms are used for models within the hydrogen analysis community; therefore, the MSM will need to link models together across those different platforms including Microsoft Excel, the Generalized Algebraic Modeling System, MatLab, and programs written in C, Java, and FORTRAN.

Some of the models are static in time, while others are dynamic. Among the dynamic models, some run in a time-stepped fashion while others take a time period (e.g. fifty years) and attempt to compute an optimum transition strategy over the entire period. One of the challenges the MSM needs to address is to provide a coordinated view of time for all of the different models. Likewise, some of the models take into account spatial information (e.g. existing centers of population or location of resources), while others are non-spatial, so the MSM must somehow integrate these two types of models in a harmonious fashion.

In addition, because the population of possible component models is growing as new models are developed to address different aspects of a hydrogen economy or transition to such an economy, the MSM framework must accommodate new models with a minimum of difficulty (i.e., be extensible). Furthermore, because model developers and analysts within the hydrogen community are widely dispersed across the United States and throughout the world, it is essential that the MSM framework support distributed operation, preferably over the Internet. Finally, because the number of models eventually incorporated into the MSM (or instantiations of the MSM) could be quite large for some simulations, it is essential that the MSM framework be scalable to large numbers of participating simulations.

3 APPROACH

Because of the need for extensibility, distributability, and scalability, we chose to use a federated object model (FOM) framework on which to base the MSM, as exemplified by the DOD High Level Architecture (HLA) which was described by Dahmann et al. (1997). The FOM approach uses a common interlingua and is extensible, allowing new models to be integrated easily provided they can interface with the objects being exchanged by other models

in the federated simulation. It also solves the problem of proliferating interfaces as the number of integrated component models grows which helps to keep the model framework scalable. The FOM approach has been successfully applied to the problem of distributed discrete event simulation in the defense community, so the System Analysis function expected this approach to work for linking models pertaining to the evolution of a hydrogen economy as well.

The framework used to develop the MSM is the Enterprise Modeling Framework (EMF), which was developed by researchers at Sandia National Laboratories. The EMF uses the HLA standard to exchange data between participating federated models. In addition to HLA, EMF provides support for modular, composable graphical user interfaces (GUIs) for each federate (i.e. each federate carries its own GUI code, which provides a run-time interface to the federate's outputs, inputs, and configurable parameters). The EMF also provides support for distributed role-based access control, which means that each federate can subscribe to only that information to which it is authorized through run-time set up. Web servers and browsers use http to transport data, and hence most Internet firewalls allow http traffic to pass through unhindered whereas firewalls would typically block HLA traffic. Having the MSM use http to communicate with component models would allow these models to sit behind different firewalls without having to ask network security administrators to reconfigure firewalls to let MSM traffic through.

One framework we are examining is IDSim, which was developed by researchers at Georgia Tech and Sandia National Laboratories (Fitzgibbons and Fujimoto 2004). IDSim uses http and XML to exchange data between participating federated models, but is otherwise similar to HLA, which has been used successfully by the defense modeling and simulation community for many years.

Despite the common need for extensibility, distributability, and scalability in a modeling framework, the Hydrogen Initiative faces challenges not encountered by the defense community in its efforts to link together disparate models. For example, different models have different notions of time. Some models, such as the H2A Production models (Mann 2005), do not change internal state as a function of time, but act as calculators which return answers given some set of inputs. The H2A Production models will return the cost of producing hydrogen for a wide variety of production methods, given parameters such as the cost of feedstock, the size of the plant and technology used, and the discount rate to use for capital investments. Other models, such as HyDS (Short 2005), use relatively small timesteps (2 years) to compute the infrastructure required to produce and distribute hydrogen to meet demand which is input as a parameter at each timestep. Still other models, such as HyTrans (Greene 2005), analyze infrastructure over a much longer period (30 or more years) assuming perfect foresight. They require a full set of inputs

before beginning a simulation but cannot use new inputs or provide outputs to other models during the simulation.

There are similar challenges when integrating models with different levels of awareness of spatial issues, e.g. how to best lay out a pipeline system or a truck route for distributing hydrogen.

4 INITIAL DEVELOPMENT STEPS

Having a list of high priority issues, we selected the first issue that the MSM would address: "Compare the economics, primary energy source requirements, and emissions of different hydrogen production / delivery pathways to help choose which are most likely to be developed and determine some of the environmental tradeoffs between them." This comparison will provide insights into two of the categories: research and development (e.g., \$ / kg H₂ for the fuel cycle) and environmental (e.g., resource requirement and CO₂ emissions).

To analyze that issue, we linked H2A production models to the Hydrogen Delivery Scenario Analysis Model (HDSAM) and the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model. We selected these models because all three are built in Microsoft Excel® and they all have static timeframes. Because they are on the same platform and dynamics did not need to be considered, the combination was considered an achievable first step and a useful proof-of-concept for the MSM's development approach.

This MSM analysis will allow decision-makers to make comparisons between hydrogen production/delivery pathways and current and future petroleum pathways with confidence that different results are not caused by different parameters. Future additions to the MSM will be necessary to analyze additional research and development, transition, financial, and environmental issues.

4.1 H2A PRODUCTION

The H2A production models are the result of an effort to standardize production economic calculations. They are a set of spreadsheets with vetted resource requirements and capital cost inputs that use the discounted cash flow rate of return (DCFRROR) method to solve for a profited cost of hydrogen at the plant gate, including operating costs, capital payback, and return on capital investment (Mann 2005). Many different hydrogen production technologies have been input into the H2A production models. The technologies include both large, central production plants from which the hydrogen needs to be transported to distribution facilities that are similar in size to today's gas stations, and small, distributed forecourt stations which also are similar in size to today's gas stations and produce the hydrogen on site. Modeled technologies include the following:

- Production from natural gas in central plants via steam methane reforming,
- Production from coal in central plants via gasification and steam methane reforming (both with and without sequestration),
- Production from biomass in central plants via gasification and steam methane reforming,
- Production in nuclear plants via thermochemical cycles,
- Production in central plants via electrolysis,
- Production at forecourt stations via steam methane reforming, and
- Production at forecourt stations via electrolysis (U.S. Department of Energy 2006a).

4.2 HDSAM

HDSAM estimates the hydrogen requirements of a given city and cost and resource requirements for delivering and distributing that hydrogen. The user selects the city, market penetration of hydrogen in the transportation fuels market, and the method used for delivering hydrogen to the distribution stations. Three methods of delivery are available: compressed gas trucks, liquid hydrogen trucks, and pipelines. The model estimates the amount of hydrogen required annually, the number of distribution stations in the city, and the profited cost of delivering and distributing the hydrogen (Mintz 2005).

4.3 GREET

The GREET model analyzes energy use and emissions from complete vehicle/fuel cycles – commonly termed well-to-wheels (WTW) analysis. It includes energy use and emissions associated with both fuel production and vehicle operation activities. For the fuel production activity, GREET reports total amounts of energy resources (petroleum, natural gas, coal, and biomass) consumed. It also reports the emissions profile including greenhouse gases (GHG) and criteria pollutants (volatile organic compounds, carbon monoxide, nitrogen oxides, particulate matter, and sulfur oxides) emitted during fuel production, delivery, distribution, and utilization (Wang 2005).

4.4 Building the MSM

Three steps were necessary to link these three models within the FOM framework: (1) identify the order in which the models will be run; (2) identify the data that need to be transferred between the models and how they may be different in each model; and (3) publish data to models, run the models, and subscribe to each model's results.

We selected the following order for hydrogen production / delivery pathway comparisons: HDSAM followed by H2A production and, finally, GREET. HDSAM calcu-

lates the profited cost of hydrogen delivery and distribution and the quantity of hydrogen necessary to supply a selected community. HDSAM estimates losses during delivery when a central facility produces the hydrogen as well as energy requirements and form (e.g., diesel for trucks, electricity for liquefaction and/or compression) for delivery and distribution. The H2A production models then determine the profited cost of hydrogen at the plant gate and the energy requirements and form for hydrogen production. The energy requirements, yields, distances, and losses calculated by HDSAM and H2A production are published to GREET, which then calculates primary energy source requirements, WTW energy requirements, and emission profiles.

We developed an intimate understanding of the three models to determine what information needed to be transferred between the models and how the information is used by different models. Some data transfers were almost trivial and only needed consistent units. Examples of those transfers include mass of hydrogen on trucks, fraction of CO₂ that is captured during hydrogen production, and vehicle fuel efficiency.

Other transfers required data to be calculated from previous models' results. One example of that type of data is the efficiency of a hydrogen liquefier. It is calculated using data published by HDSAM (hydrogen throughput, hydrogen losses, and electricity requirements) and then is published to GREET.

Some data need additional thought before determining what values should be transferred because different models are based on different philosophies. One example of this issue is pipe length. GREET requires a pipe length to calculate energy used for hydrogen transport (pipe length multiplied by energy required per unit length). HDSAM calculates lengths of multiple types of pipe: transmission, trunk, and service lines and uses each length for capital cost estimation. No molecule of hydrogen travels the total length of each type because the trunks are circular and each service line transports only a fraction of the total hydrogen entering a city. In this case, an algorithm to calculate a single length was agreed upon by the developers of HDSAM, GREET, and the MSM.

The first set of models integrated into the MSM were implemented using Microsoft Excel. Having chosen Java as our development platform, our initial task was to find a means to manipulate and link the Excel models from within a running Java application. An open source solution, Jakarta POI, allowed us to read and write Excel files using Java. However, POI did not allow us to interact with a running Excel process, which we needed to do in order to call macros contained in the files. Because of this need, our current prototype employs a commercial third-party product (Intrinsyc J-Integra for COM) that provides a complete Java-COM bridge (future prototypes may use a Java-.NET bridge). J-Integra has proven to be a reasonably robust

product and allows us to focus our development efforts on other areas.

In order to permit external manipulation of the Excel models via macros and still provide the model owners with the security of protecting their Visual Basic for Applications (VBA) projects, we requested that the owners create public functions and macros for our use. Where the model developer has tied these functions and macros to VBA GUI elements, we can programmatically interact with a model's GUI and expose its functionality to the larger system. This, coupled with our ability to directly read and write cells and formulae, gives us the necessary access and behavior for integration with non-Excel models.

Remote (i.e. web browser) access to the MSM application will likely be enabled using Java Server Pages (JSP) and a more mature version or our existing code base. Our initial implementation will place all models and integrating framework on the web server. Future versions will allow model developers to host their models at the location of their choosing. Typical access control and user authentication mechanisms will be phased in prior to release for general use.

5 PRELIMINARY RESULTS

The initial phase of the MSM focused on making economic and environmental comparisons between different hydrogen production / delivery pathways; therefore, the H2A production models were linked to HDSAM and the GREET model. With these models linked the user can generate information on each pathway.

Figure 1 shows results from one production / delivery pathway. The analysis is for hydrogen production from natural gas using current steam-methane reforming technology and capturing 90% of the generated CO₂. In this analysis the hydrogen is produced in a large (approximately 125-million-kg annually) facility which is located at the edge of the city where the hydrogen would be used. Two options are available for delivery: pipeline and trucks carrying liquid hydrogen. In this analysis the liquid-hydrogen truck option is chosen so the hydrogen will be liquefied at the production plant, transported to distribution stations via semi, and gasified and pressurized at the distribution station for fueling automobiles.

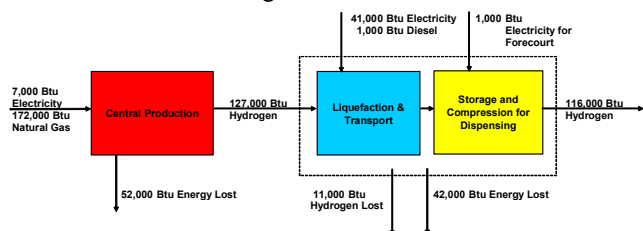


Figure 1. Preliminary Pathway Results for Central Hydrogen Production from Natural Gas with Carbon Sequestration and Using Liquefaction and Truck Delivery

The basis for the analysis shown in Figure 1 is 116,000 Btu of hydrogen gas (lower heating value) which is essentially equivalent to 1-kg of hydrogen. That basis was chosen because it is the average amount of energy available in 1 gal of unleaded gasoline; it is commonly referred to as 1 gal of gasoline equivalent (GGE). The figure shows that 11,000 Btu of hydrogen are lost during liquefaction, transport, storage, and compression. Those losses are due to boil off while the hydrogen is in liquid form and leaks while the hydrogen is in gaseous form. Because of those losses, the production facility needs to produce 127,000 Btu of hydrogen gas for every GGE distributed. In addition to the losses, 42,000 Btu (12 kW hr) of electricity and 1,000 Btu (0.01 gal) of diesel fuel are required for liquefaction, transportation, storage, and compression for dispensing. That energy is lost to kinetic energy, heat, and unusable energy in pressure.

For each 127,000 Btu of hydrogen the production facility will produce, it will require 172,000-Btu natural gas (180 Normal ft³) and 7,000-Btu (2.0 KW hr) of electricity. That energy is required to produce the hydrogen and sequester 90% of the CO₂ generated during the production process.

Table 1 shows energy efficiencies for the process shown in Figure 1. Energy efficiencies are defined as energy available in the hydrogen divided by all energy sources. The production process energy efficiency covers only the central plant that produces hydrogen from natural gas. The pathway energy efficiency includes production, liquefaction, transportation, storage, and compression. Well-to-pump (WTP) efficiency includes every step in the pathway as well as the energy required for supplying natural gas, electricity, and diesel (e.g., drilling for and refining natural gas, mining coal and using it generate electricity, and drilling, refining, and transport for diesel).

Table 1. Energy Efficiencies for Hydrogen Production from Natural Gas with Liquefaction and Truck Delivery

Production Process	71%
Pathway	52%
Well-to-Pump	41%

WTW energy requirements and emissions include energy use and emissions associated with both fuel production and vehicle operation activities. In this case, the vehicle is assumed to be 2.5 times more efficient than today's gasoline-powered automobile because it uses a fuel cell instead of today's internal combustion engine (i.e., the hydrogen-powered fuel cell vehicle is expected to get 57.5 mile/GGE and today's gasoline-powered internal combustion engine gets 23.1 mile/gal gasoline, on average). The total energy required to power the vehicle for one mile is estimated at 4900 Btu; that energy includes not only the coal, electricity, and diesel to produce and distribute the hydrogen, but also the energy included in the WTP calcula-

tion. The total energy requirement is almost 2.5 times greater than the 2000 Btu of hydrogen necessary for vehicle operation due to losses in the process and energy necessary to mine and refine the primary energy sources.

In this case, the petroleum energy use for a hydrogen powered vehicle is much lower than that for the standard vehicle driven today (35 Btu/mile compared to over 5,500 Btu/mile for the baseline vehicle). This supports the Hydrogen Initiative’s claim of reducing the need for petroleum. Likewise, the GHG emissions of 205 g CO₂ equivalent/mile are lower than those of today’s vehicles used for a baseline (485 g/mil). The profited cost at the pump is estimated at \$5.36/GGE. That is the production cost including a 10% after-tax discounted cash flow rate of return over a 20 year equipment life. It includes both federal and state income taxes but does not include the gasoline tax. It also includes the cost to capture CO₂ for sequestration but not the cost of sequestering it.

To date, we have analyzed four central hydrogen production technologies in addition to production from natural gas with carbon capture as reported above. Those technologies include production from natural gas without sequestration, production from coal with and without sequestration, and production from biomass. Table 2 shows resulting profited costs for the full pathway (production, liquefaction, delivery, and distribution) and can be used to compare the technologies. The analysis methodology is recognized as having possible error bars of 30% on capital investment because of potential issues like unexpected catalyst problems; therefore, within the capability of this analysis all five technologies have the same profited cost.

Table 2. Profited Costs of Hydrogen Production/Delivery Pathways for Five Production Technologies

Natural Gas with Sequestration	\$5.36 / GGE
Natural Gas without Sequestration	\$5.15 / GGE
Coal with Sequestration	\$5.30 / GGE
Coal without Sequestration	\$4.98 / GGE
Woody Biomass without Sequestration	\$5.23 / GGE

Profited cost is not the only parameter that we are comparing between technologies. The DOE is also interested in reducing petroleum imports; a primary driver of that reduction could be reduced use of petroleum. Table 3 shows the WTW petroleum energy use for the five technologies. For comparison, over 5400 Btu/mil are necessary to operate today’s average gasoline-powered vehicle. WTW petroleum consumption includes not only petroleum required for production and delivery but also drilling, mining, and/or growing. Biomass requires more petroleum than the other technologies because modern tractors run on diesel. The differences between coal and natural gas are primarily due to the assumption that if hydrogen is made from coal the necessary electricity will be as well; likewise, if hydrogen is made from natural gas the necessary

electricity will be as well. Coal mining requires much more petroleum than natural gas drilling and refining.

Table 3. Well-to-Wheels Petroleum Energy Consumption for Five Hydrogen Production Technologies

Natural Gas with Sequestration	35 Btu/mil
Natural Gas without Sequestration	34 Btu/mil
Coal with Sequestration	67 Btu/mil
Coal without Sequestration	24 Btu/mil
Woody Biomass without Sequestration	216 Btu/mil

GHG emissions are also an issue that many people are interested in. Table 4 shows a comparison of GHG emissions for the five hydrogen production technologies. For comparison, GREET estimates that today’s gasoline vehicles emit approximately 485 g CO₂ equivalent / mile traveled on a WTW basis. Biomass has extremely low emissions because plants remove more CO₂ from the air (and sequester some of it in the ground in the form of roots) than is generated producing hydrogen. Note that coal without sequestration has particularly high GHG emissions because the ratio of CO₂ to energy available in coal is low.

Table 4. Well-to-Wheels Greenhouse Gas Emissions for Five Hydrogen Production Technologies (all on g CO₂ equivalent basis)

Natural Gas with Sequestration	205 g / mil
Natural Gas without Sequestration	312 g / mil
Coal with Sequestration	255 g / mil
Coal without Sequestration	613 g / mil
Woody Biomass without Sequestration	8 g / mil

Other parameters also need to be compared to make qualitative decisions on technology selection. Those parameters include feedstock sources and availability in the region in question; since the MSM does not yet have a spatial aspect. Another set of parameters that should be considered is criteria pollutants. Those are calculated in the pathway analyses and will be considered by decision makers.

All of the results reported here are preliminary and require additional validation; however, they are good examples of the analysis results we expect to get from the MSM.

6 FUTURE WORK

The next steps for the MSM involve completing pathway analysis for additional technologies, adding more models to the framework, making the MSM available to the hydrogen analysis community, and adding stochastic calculations. We are working to complete additional pathway analyses, like the ones reported above. To do that work, additional H₂A production models will be added to the MSM and changes to other models (HDSAM and GREET) will be incorporated into the MSM structure. H₂A produc-

tion models that might be added to the MSM include electrolysis from the grid, electrolysis coinciding with wind turbines, and high-temperature thermo-chemical processes for use at nuclear plants. Models using research and development targets will also be added to compare potential improvements.

We will also address the cross-cutting issue of hydrogen quality. Hydrogen quality is the purity of the hydrogen and the concentration of specific impurities. It is an important cross-cutting issue because low quality hydrogen will affect the performance and lifetime of fuel cells; however, increasing quality increases production expense and energy use and impurities may be introduced during delivery and distribution of the hydrogen. To analyze that issue, models that calculate the material and energy balances for hydrogen production as well as their capital costs will be linked within the MSM. Vehicle performance will be included in the MSM by linking fuel cell performance models that are being modified to include performance loss due to low quality hydrogen.

The three models that have been linked thus far have static timeframes and are essentially location independent. Their results are useful for comparing technologies and making initial estimates regarding profited cost and emissions. They are not useful, however, for location-dependent results or for developing strategies that might overcome issues in the transition from today's petroleum economy to a future, hydrogen economy (one of the major issues identified as requiring analysis within the Hydrogen Initiative). Instead, other models exist that use different techniques to understand those spatial and temporal issues. Those models will be linked using the MSM framework so that modeling changes in hydrogen production, delivery, and emissions can be propagated to the spatial/temporal models. That propagation is necessary to verify that the current technical targets are sufficient to result in a system that can compete in the transportation sector of the economy.

To further improve consistency between models, the Hydrogen Analysis Resource Center (HyARC) will be linked to the MSM. HyARC is being developed to standardize parameters for all modeling for the Hydrogen Initiative because different models have been using different parameters (U.S. Department of Energy 2006b). Linking the MSM to HyARC will allow changes to HyARC to be easily transferred to other models.

The MSM will be made available to hydrogen analysts via a password-protected website. We are developing a GUI for that site with the intent that analysts will be able to access the website, design the desired analysis using the GUI, and run the MSM to get results. The website will also be designed to allow model-developers to update the MSM to link to their updated models as they become available.

MSM will need to be able to make stochastic calculations because very few of the parameters in any of the component models are well known. Once that capability is added, users will be able to select probability distribution parameters and the MSM will calculate probability distributions for the results. The Monte Carlo method is the most likely technique for calculating the resulting probability distributions.

7 CONCLUSIONS

We are developing a macro-system model for DOE's Hydrogen, Fuel Cell, and Infrastructure Program to analyze cross-cutting issues. We have found the FOM framework to link other models effective for this purpose. To date, we have linked three existing models and are comparing economic and environmental parameters between different production and delivery pathways. In the future, we will involve dynamic models to analyze infrastructure development and spatial tools to study regional issues. We also intend to make the MSM available to the hydrogen analysis community via a password protected website.

ACKNOWLEDGEMENTS

The authors wish to thank Dale Gardner, Johanna Levene, Margaret Mann, Margo Melendez, and Matthew Ringer of the National Renewable Energy Laboratory; Jerry Gillette, Marianne Mintz, and Michael Wang of Argonne National Laboratory; Amgad Elgowainy of Tennessee State University; and Jay Keller and Jason Arnold of Sandia National Laboratory for technical assistance. This work has been supported by the Hydrogen, Fuel Cell and Infrastructure Technology Program of the US Department of Energy.

REFERENCES

- Bush, G.W. 2003. State of the Union Address, Washington, DC.
- Committee on Alternatives and Strategies for Future Hydrogen Production and Use, National Research Council, National Academy of Engineering. 2004. The hydrogen economy: Opportunities, costs, barriers, and R&D needs. Washington, DC: The National Academies Press: 9-4 – 9-5.
- Dahmann, J. S., R. Fujimoto, and R. M. Weatherly. 1997. The department of defense high level architecture. In *Proceedings of the 1997 Winter Simulation Conference*: 142–149.
- Fitzgibbons, J. and R. Fujimoto. 2004. IDSim: An extensible framework for interoperable distributed simulation. In *Proceedings of the International Conference on Web Services*. San Diego, CA.

- Greene, D.L. 2005. HyTrans model development. *2005 Annual Progress Report – DOE Hydrogen Program*. Available via http://www.hydrogen.energy.gov/pdfs/progress05/iii_3_greene.pdf. [accessed July 5, 2006]
- Mann, M.; J. Levene, B. James, S. Lasher, D. Mears, M. Placet, M. Ringer, M. Rutkowski, M. Wang. 2005. Moving toward consistent analysis in the HFC&IT Program: H2A. *2005 Annual Progress Report – DOE Hydrogen Program*. Available via http://www.hydrogen.energy.gov/pdfs/progress05/iii_2_mann.pdf. [accessed July 5, 2006]
- Mintz, M. 2005. Hydrogen delivery analysis chapter V.F.1. *2005 Annual Progress Report – DOE Hydrogen Program*. Available via http://www.hydrogen.energy.gov/pdfs/progress05/v_f_1_Mintz.pdf. [accessed July 5, 2006]
- Short, W. 2005. Energy systems analysis: Hydrogen deployment system modeling. *2005 Annual Progress Report–DOE Hydrogen Program*. Available via http://www.hydrogen.energy.gov/pdfs/progress05/iii_4_short.pdf. [accessed July 5, 2006]
- U. S. Department of Energy. 2005. Hydrogen, Fuel Cells & Infrastructure Technologies Program multi-year research, development and demonstration plan – Planned program activities for 2003-2010. DOE/GO-102005-1741. Golden, CO: The US Department of Energy Golden Field Office.
- U.S. Department of Energy. 2006 (a). *DOE H2A Production Analysis*. Available via http://www.hydrogen.energy.gov/h2a_production.html [accessed July 3, 2006].
- U.S. Department of Energy. 2006 (b). *Hydrogen Analysis Resource Center*. Available via http://hydrogen.energy.gov/resource_center.html [accessed July 3, 2006].
- Wang, M.Q. 2001. Development and use of GREET 1.6 fuel-cycle model for transportation fuels and vehicle technologies. Technical report ANL/ESD/TM-163, Argonne National Laboratory, Argonne, IL. Available via <http://www.transportation.anl.gov/pdfs/TA/153.pdf>. [accessed July 5, 2006]

AUTHOR BIOGRAPHIES

MARK F. RUTH is the Macro-System Model Engineer in the Systems Integration Office at the National Renewable Energy Laboratory. He moved into that position in 2005 after over 10 years as an engineer researching biomass conversion to ethanol, other fuels, and other chemicals. Mark's primary research interests are in using models to understand progress in research and development and in analysis to prioritize research. His e-mail address is mark_ruth@nrel.gov.

KEITH B. VANDERVEEN is a Principal Member of Technical Staff at Sandia National Laboratories in Livermore, California. He has eight years of experience in networking, network management, and distributed systems assessment and development. As a member of Sandia's Homeland Security Systems and Development Center, he has participated in numerous modeling and simulation projects, technical assessments, and development of software and hardware systems for homeland security and other national security domains. His e-mail address is kbvande@sandia.gov.

TIMOTHY J. SA is a Distinguished Technologist at Sandia National Laboratories in Livermore, California. He has over ten years of experience in Java software development and specializes in GUI design and graphics. As a member of the Exploratory Computer and Software Engineering Department he has been involved in various proof-of-concept projects as well as creating applications and simulations to support systems analysis and decision making. His e-mail address is tjsa@sandia.gov.

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

The public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing the burden, to Department of Defense, Executive Services and Communications Directorate (0704-0188). Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.

PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ORGANIZATION.

1. REPORT DATE (DD-MM-YYYY) July 2006		2. REPORT TYPE Conference Paper		3. DATES COVERED (From - To)	
4. TITLE AND SUBTITLE Use of Federated Object Modeling to Develop a Macro-System Model for the U.S. Department of Energy's Hydrogen Program; Preprint				5a. CONTRACT NUMBER DE-AC36-99-GO10337	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) M.F. Ruth, K.B. Vanderveen and T.J. Sa				5d. PROJECT NUMBER NREL/CP-150-40222	
				5e. TASK NUMBER HS061003	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) National Renewable Energy Laboratory 1617 Cole Blvd. Golden, CO 80401-3393				8. PERFORMING ORGANIZATION REPORT NUMBER NREL/CP-150-40222	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)				10. SPONSOR/MONITOR'S ACRONYM(S) NREL	
				11. SPONSORING/MONITORING AGENCY REPORT NUMBER	
12. DISTRIBUTION AVAILABILITY STATEMENT National Technical Information Service U.S. Department of Commerce 5285 Port Royal Road Springfield, VA 22161					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT (Maximum 200 Words) The U.S. Department of Energy is working on changing transportation fuel from gasoline to hydrogen. To assist in that effort, we are developing a macro-system model that will link existing or developmental component models together to analyze crosscutting hydrogen issues.					
15. SUBJECT TERMS MSM; macro-system; HLA; high-level architecture; systems analysis					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT UL	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified			19b. TELEPHONE NUMBER (Include area code)

Standard Form 298 (Rev. 8/98)
Prescribed by ANSI Std. Z39.18