VII.4 Macro-System Model

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Objectives

Develop a macro-system model (MSM) aimed at:

- Performing rapid cross-cutting analysis.
- Utilizing and linking other models.
- Improving consistency of technology representation (i.e., consistency between models).
- Supporting decisions regarding programmatic investments and focus of funding through analyses and sensitivity runs.
- Supporting estimates of program outputs and outcomes.

2008/2009 objectives:

- Improve the structure of the MSM and expand the graphics user interface (GUI).
- Update versions of component models.
- Enhance stochastic analysis capability.
- Validate MSM results.
- Develop interactions between the MSM and spatial and temporal models.

Technical Barriers

This project addresses the following technical barriers from the Systems Analysis section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

(B) Stove-Piped/Siloed Analytical Capabilities
(C) Inconsistent Data, Assumptions, and Guidelines
(D) Suite of Models and Tools

Contribution to Achievement of DOE Systems Analysis Milestones

This project contributes to achievement of the following DOE milestones from the Systems Analysis section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

- **Milestone 5:** Complete analysis and studies of resource/feedstock, production/delivery and existing infrastructure for various hydrogen scenarios. (4Q, 2009)
- **Milestone 6:** Complete analysis of the impact of hydrogen quality on the hydrogen production cost and the fuel cell performance. (4Q, 2010)
- **Milestone 14:** Complete input/output guidelines for the Macro-System Model. (3Q, 2005)
- **Milestone 15:** Select model for analysis and incorporate into Macro-System Model. (4Q, 2005)
- **Milestone 16:** Develop initial model architecture. (4Q, 2005)
- **Milestone 17:** Capture Macro-System Model requirements, description, and usage in a description document. (2Q, 2006)
- **Milestone 18:** Complete a usable "test version" of the Macro-System Model with links to the H2A Production and Delivery models and the ANL GREET model. (2Q, 2006)
- **Milestone 23:** Complete the 1st version of the Macro-System Model for the analysis of the hydrogen fuel infrastructure to support the transportation systems. (4Q, 2008)
- **Milestone 27:** Complete the 2nd version of the Macro-System Model to include the analytical capabilities to evaluate the electrical infrastructure. (2Q, 2011)

Accomplishments

- Completed Version 1.0 of the MSM and used it for programmatic analysis.
- Linked H2A Production cases with the Hydrogen Delivery Scenario Analysis Model (HDSAM), the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) Model, and

physical property information from the Hydrogen Analysis Resource Center (HyARC) and validated the use of those models and the results generated using them.

- Developed a flexible, comprehensive Web-based user interface so that many members of the analysis community can use the MSM.
- Completed a User Guide for the MSM.
- Added stochastic (Monte Carlo) capabilities to the MSM.
- Upgraded the MSM to the latest versions of H2A Production (V.2.1), HDSAM (V 2.0) and GREET (V 1.8b).
- Initiated interaction with the geo-spatial model HyDRA to add the spatial dimension to the MSM. Currently, some of the MSM results are available in HyDRA.

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Introduction

At the DOE Hydrogen Program's behest, we are developing a macro-system model to analyze cross-cutting issues because no existing model sufficiently simulates the entire system including feedstock, conversion, infrastructure, and vehicles with the necessary level of technical detail. In addition, development of the MSM exposes inconsistencies in methodologies and assumptions between different component models so that they can be identified and corrected when necessary.

Version 1.0 of the MSM has been developed and is available to the hydrogen analysis community. It links H2A Production, HDSAM, GREET, and physical property information from HyARC to estimate the economics, primary energy source requirements, and emissions of multiple hydrogen production/delivery pathways. A Web-based user interface has been developed so that many users have access to the MSM; stochastic capabilities have been added to it to provide uncertainty ranges around the results. The MSM has been used for several analyses to compare pathways and to understand the effects of varying parameters on pathway results.

Approach

The MSM is being developed as a tool that links or federates existing models across multiple platforms. This approach was chosen 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 necessary expertise to do so was spread among half a dozen DOE laboratories and a dozen or more universities and private contractors. Linking models allows model users that depend on data from component models to continue using their models while retrieving data from component models in a less labor-intensive manner. In addition, it provides common platform for data exchange necessary to update integrated models when component models have been updated.

The MSM is being built on a framework inspired by the federated object model (FOM). FOMs also link together models and are exemplified by the Department of Defense High Level Architecture (HLA) [1]. The general MSM framework provides a common interlingua that is extensible (accommodates new models with a minimum of difficulty), distributable (can be used by multiple people in different areas of the country), and scalable (to large numbers of participating models). Version 1.0 of the MSM uses Ruby and Ruby interfaces to Microsoft Excel and other platforms to collect, transfer, and calculate data.

Results

Levelized hydrogen costs, primary energy requirements, and emissions have been estimated for multiple pathways using H2A 2.1, HDSAM V2.0, and GREET V1.8b. Figure 1 shows results for production of hydrogen from woody biomass via gasification in central plants using current technology followed by liquefaction and delivery of liquid hydrogen in trucks. To distribute 116,000 Btu of hydrogen (lower heating value – similar to the energy in one gallon of gasoline and 1.02 kg hydrogen), 129,000 Btu of hydrogen need to be produced – 13,000 Btu are lost due to unrecovered boil-off. In addition, 33,000 Btu of electricity are necessary to liquefy the hydrogen; 1,000 Btu of diesel fuel to transport the hydrogen; and 1,000 Btu to compress the hydrogen that has been revaporized so it can be dispensed to vehicles. To produce the necessary hydrogen, energy sources (biomass, electricity, and natural gas) are required as shown in the figure. The levelized cost at the pump for this pathway is estimated to be $5.00/kg. That levelized cost is similar to that reported in the 2006 Hydrogen Posture Plan which was $5.10/kg [2]. The difference is primarily due to liquefaction efficiency as calculated by HDSAM.

Because the MSM is a conjunction of several models, it can potentially involve variables present in each of the constituent models. Thus the total number of MSM input parameters can significantly exceed the number of inputs for an individual model and the user needs a compact and user-friendly way of accessing large number of variables. To fulfill that need, a 'branch and leaf' structure has been adopted. The input variables are grouped into blocks (each block representing a branch containing other blocks or input parameters) as shown in the example in Figure 2. In addition, this compact

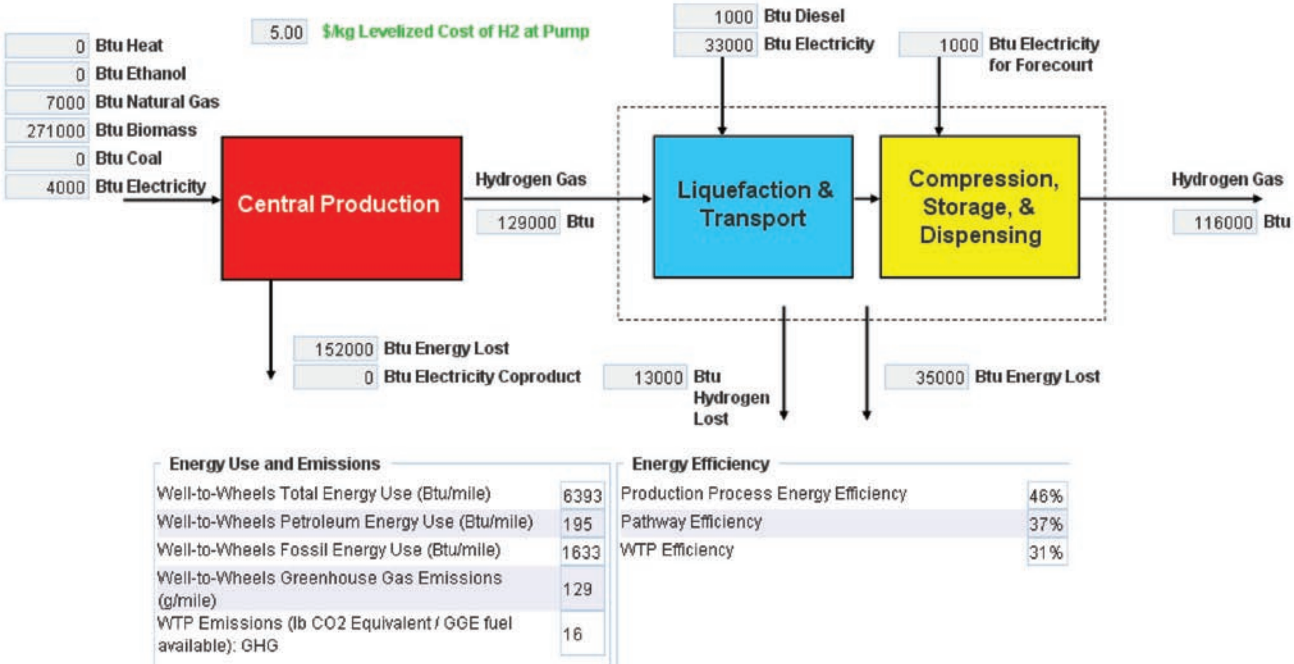

FIGURE 1. Pathway Results for Central Hydrogen Production from Woody Biomass with Liquid Hydrogen Delivered by Trucks

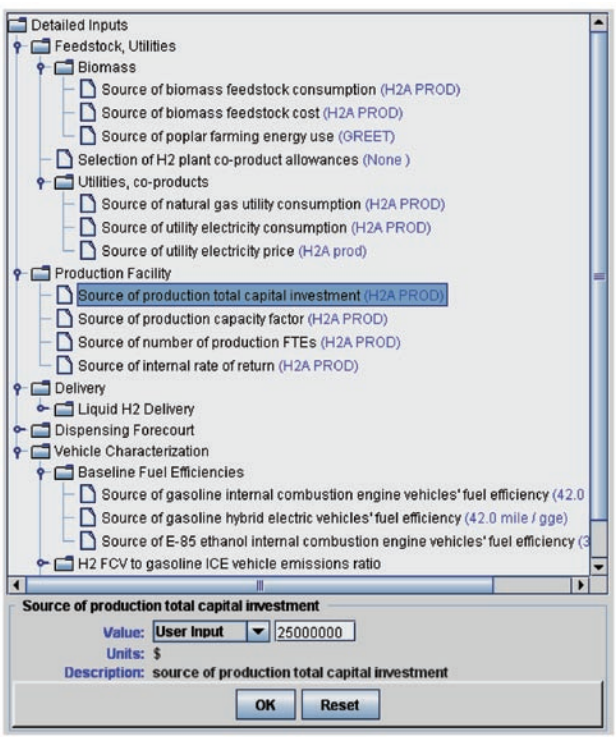

FIGURE 2. Branched structure allows user access to virtually all input MSM parameters. In this example, the user modifies total capital investment for the production facility.

user interface excludes user access to parameters that are irrelevant to the pathway of interest.

Since model estimates have some variability, stochastic modeling capability in the form of Monte Carlo analysis has been added to the MSM. Stochastic tools available in the MSM include the DAKOTA toolbox [3] and @Risk. The latter was used in the MSM to characterize potential impact of green house gas (GHG) emissions from transportation on fuel cost (gasoline vs. hydrogen produced by steam methane reforming at the refueling station). The input distributions (capital investment, operating and maintenance costs, production capacity factor, production unit efficiency) were largely taken from the program's uncertainty analysis [4] with the notable exception of gasoline and natural gas cost distributions which were based on historic data. A GHG emissions tax was applied to both the gasoline and hydrogen fuels at the level of $50 per ton CO_2 equivalent. It increases the per mile cost of each fuel but the increase to gasoline exceeds that of hydrogen on average by a factor of 1.6 and incorporation of the GHG tax increases differentiation between hydrogen and gasoline. The results of this study are presented in Figure 3 in the form of a scatter plot.

Key MSM inputs are sometimes region-specific; therefore, key results are often region-specific as well. For this reason it is important to add the geo-spatial dimension to the MSM so we are linking the MSM to HyDRA - a set of tools for visualization and analysis of geographically distributed data. One example of a HyDRA link is the cost and associated GHG emission distributions for hydrogen produced from electrolysis.

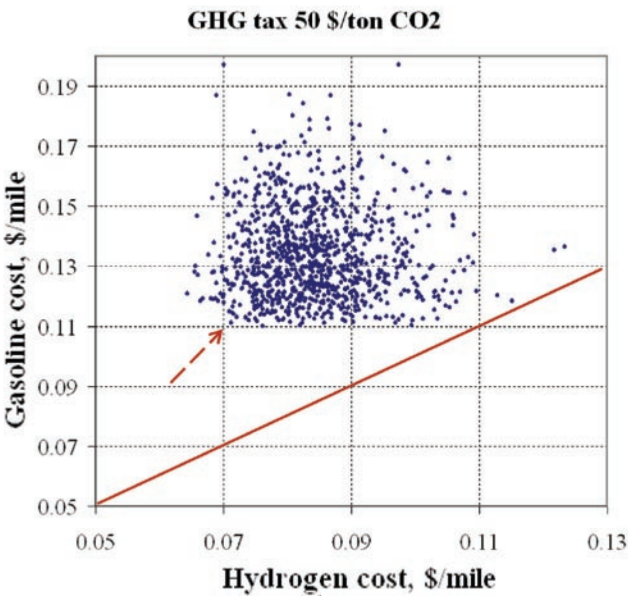

FIGURE 3. Uncertainty analysis: the potential effect of transportation GHG emissions tax on fuel costs. Gasoline and hydrogen costs are shown in $/mile of vehicle travel. The solid red line shows the equivalence level, the arrow denotes typical tax effect on data-point location.

HyDRA databases provided electricity cost and grid mix distributions and the MSM was run to generate levelized hydrogen cost and GHG emissions for each region. Those results identify two areas with both low hydrogen production cost (less than $6/kg) and low associated emissions (not exceeding 550 g per mile vehicle travel). The two areas include a large region covering parts of Idaho, Oregon and Washington and a smaller shore region in Maine. The authors will provide the map imaging these two regions upon request.

Conclusions and Future Directions

Version 1.0 of the MSM has been developed to compare the economics, primary energy source requirements, and emissions of different hydrogen production/delivery pathways and is being used for comparative and sensitivity analyses. The MSM helps identify cost and environmental tradeoffs within and between pathways. Stochastic capability has been incorporated to improve nuance in results and a Web-based GUI has been employed so many members of the hydrogen analysis community can perform their own analyses.

The next steps for the MSM involve:

- Updating the MSM interaction with component models as they are released.
- Establishing direct links between geographical tools and the MSM.
- Linking at least one transition-scenario model to the MSM.
- Using the MSM to update production and delivery information for other models.
- Adding the combined heat, power, and hydrogen production pathway to the MSM.

FY 2009 Publications/Presentations

1. Ruth, M., Diakov, V., Goldsby, M., Sa, T. Macro-System Model: a Federated Object Model for Cross-Cutting Analysis of Hydrogen Production, Delivery, Consumption and Associated Emissions. In Winter Simulation Conference, 2009 (accepted for publication).

2. Ruth, M., Diakov, V., Sa, T., Goldsby, M., Genung, K., Hoseley, R., Smith, A., and Yuzugullu, E. 2009. Hydrogen macro-system model user guide. *Technical Report NREL/TP-6A1-44799*. Available via http://www.nrel.gov/docs/fy09osti/44799.pdf.

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1. Judith S. Dahmann, Richard Fujimoto, and Richard M.Weatherly. The Department of Defense high level architecture. In Winter Simulation Conference, pages 142–149, 1997.

2. Hydrogen Posture Plan: An Integrated Research, Development, and Demonstration Plan. US Department of Energy and US Department of Transportation. December 2006. Available at http://www.hydrogen.energy.gov/pdfs/hydrogen_posture_plan_dec06.pdf

3. DAKOTA (Design Analysis Kit for Optimization and Terascale Applications) for large-scale engineering optimization and uncertainty analysis. http://www.cs.sandia.gov/DAKOTA/index.html

4. Michael Duffy, Marc Melaina, Michael Penev and Mark Ruth. Management Report NREL/MP-150-43250, May 2008. Risk Analysis for Hydrogen, Fuel Cells and Infrastructure Program: Predecisional Report.