XI.9 Macro-System Model

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- SRA International, Inc., Fairfax, VA

Project Start Date: February 2005
Project End Date: Project continuation and direction determined annually by DOE

Fiscal Year (FY) 2011 Objectives

- Develop a macro-system model (MSM):
  - aimed at performing rapid cross-cutting analysis
  - utilizing and linking other models
  - improving consistency between models
- Support decisions regarding programmatic investments through analyses and sensitivity runs.
- Support estimates of program outputs and outcomes.

Technical Barriers

This project addresses the following technical barriers from the Systems Analysis section (4.0) of the Fuel Cell Technologies Program Multi-Year Research, Development and Demonstration Plan:

(A) Future Market Behavior
(B) Stove-Piped/Siloed Analytical Capability
(C) Inconsistent Data, Assumptions and Guidelines
(D) Suite of Models and Tools

Contribution to Achievement of DOE Systems Analysis Milestones

This project will contribute to achievement of the following DOE milestones from the System Analysis section of the Fuel Cell 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 27**: Complete the 2nd version of the Macro-System Model to include the analytical capabilities to evaluate the electrical infrastructure. (2Q, 2011)

FY 2011 Accomplishments

- Completed Version 1.3 of the MSM and used it for programmatic analysis.
- Created, and (later) updated the MSM User Guide (version 1.3.2).
- 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.
- Enhanced the Web-based user interface so that many members of the analysis community can use the MSM.
- Added stochastic (Monte Carlo) capabilities to the MSM.
- Upgraded the MSM to the latest versions of H2A Production (V.2.1.1-3), HDSAM (V 2.2) and GREET (V 1.8d.1).
- Linked with geospatial model HyDRA to add the spatial dimension to the MSM.
- Linked MSM with the temporal pathway evolution assessment tool HyPro.
- Linked the MSM with vehicle cycle analysis model GREET 2.7.
- Linked the Fuel Cell Power Model (FC Power) in the MSM framework.

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Introduction

At the DOE Fuel Cell Technologies Program's behest, we are developing an MSM 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 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 because 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 a common platform for data exchange necessary to update integrated models when the component models have been updated.

The MSM is being built on a framework inspired by an example of 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 V2.1 [2], HDSAM V2.2 [3], and GREET V1.8d.1 [4]. Within the MSM, hydrogen production and other costs [5] are connected with associated emissions, which is one of the advantages that the MSM provides by linking together different models. Figure 1 shows the levelized hydrogen fuel cost per mile and the well-to-wheels (WTW) greenhouse gas (GHG) emissions for each of the seven pathways assessed

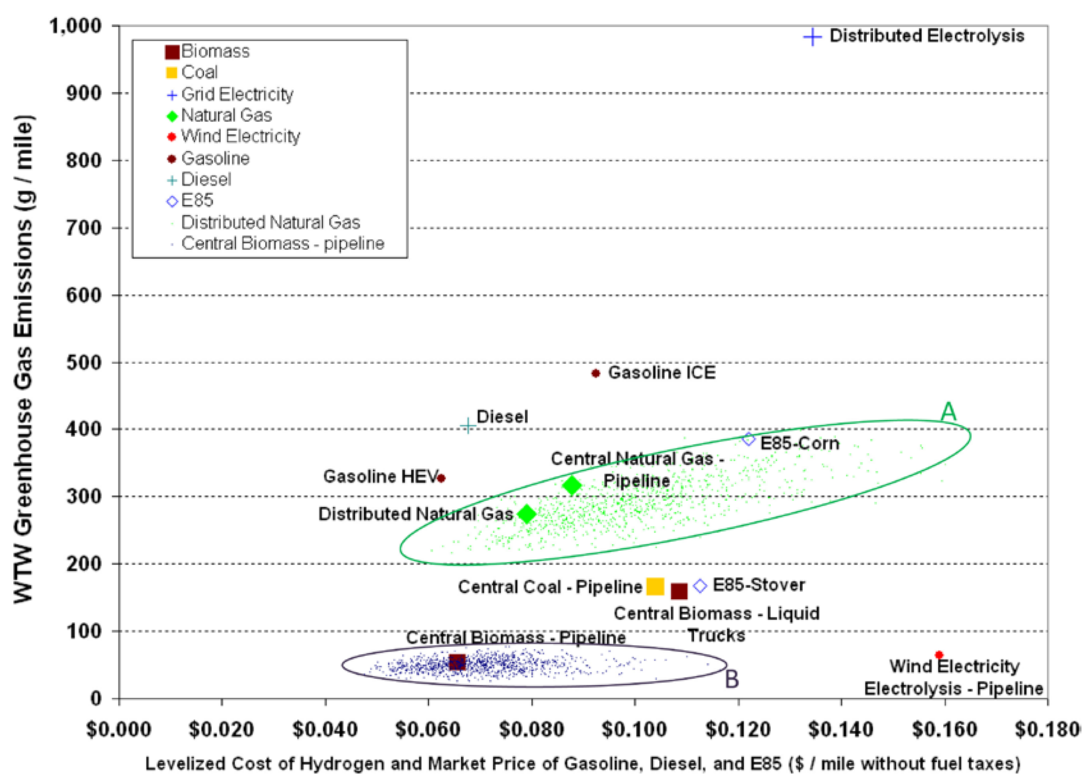

FIGURE 1. Pathways Levelized Costs and GHG Emissions

based on U.S. average fuel costs and fuel cycle energy requirements. For comparison, it also shows the projected 2009 market price per mile (in 2005 dollars) and GHG emissions for gasoline-, diesel-, and E85-fueled vehicles. The levelized fuel cost was put onto a per-mile basis. The projected fuel cost per mile for most of the hydrogen pathways (based on projected, mature fuel cell electric vehicle [FCEV] markets) is similar to that for gasoline in a traditional vehicle and corn ethanol as E85 fuel in a flexible-fuel internal combustion engine (ICE) vehicle. The fuel costs per mile for gasoline in a hybrid electric vehicle (HEV) and diesel in a conventional diesel ICE vehicle are lower.

The dotted green cloud in the figure (surrounded by oval A) represents the stochastic analysis results obtained based on input distributions for the forecourt SMR production option [6]. The dispersion of the data points well surpasses the differences between the central (with pipeline delivery) and distributed SMR production options. This relates to both the per-mile cost of hydrogen and the WTW GHG emissions. Similarly, the blue cloud surrounded by oval B shows the stochastic analysis result for the central biomass case. For the latter, as seen in the figure, the data point distribution is less significant when compared with the differences incurred by switching from pipeline to liquid truck delivery.

As key MSM inputs are sometimes region-specific, it is important to add the geospatial dimension into the range of the MSM features. Bilateral links with the online geospatial tool HyDRA [7] have been developed that allow the MSM user to easily apply regional electricity and natural gas (NG) feedstock data as MSM inputs and, conversely, update the HyDRA database and maps with the latest MSM version outputs.

Naturally, the user can specify input data as needed (it is not required that the inputs are region specific). As an example, Figure 2 shows the results obtained from NREL's FC Power model for a range of electricity grid mixes (ranked along the x-axis based on the level of upstream GHG emissions, the dotted line shows the average U.S. electricity generation mix upstream emissions level). Depending on the region-specific electricity generation mix, the combined heat, hydrogen, and power fuel cell generation can alleviate or aggravate the level of GHG emissions.

As a part of the ongoing enhancement of the user interface, detailed MSM outputs have been made available to the users via the Web. When combined with detailed MSM inputs access (developed earlier, in FY 2010), it makes the remote, Web-generated MSM runs almost as transparent as if the user has the MSM running on their own computer.

The transition to high-market-penetration levels for hydrogen fuel cell vehicles will likely involve several hydrogen production/delivery/dispensing pathways. To facilitate this analysis and to involve the temporal dimension, the temporal pathway evolution assessment tool HyPro [8] was developed in previous years by Directed Technologies, Inc. It is a computational model that simulates industries decisions regarding construction of new hydrogen production facilities, delivery infrastructure, and dispensing given perfect foresight of hydrogen demand. It is linked to the MSM so HyPro inputs are now updated automatically. A wide range of analysis possibilities of infrastructure evolution are now available using the MSM.

One analysis is the potential effect of a constant GHG tax on the cost-optimal succession of hydrogen production/delivery/dispensing pathways. The results of that analysis are presented in Figure 3 where the three graphs show results over a 40-year buildout scenario resulting in over 5,000,000-kg of hydrogen produced daily during the final

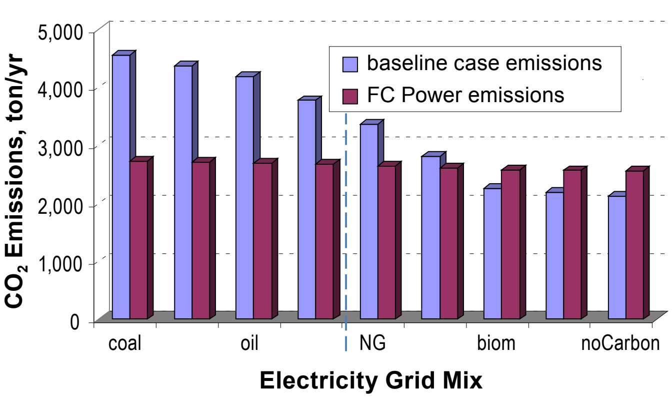

FIGURE 2. Fuel Cell Combined Heat, Hydrogen and Power Generation: Associated Emissions

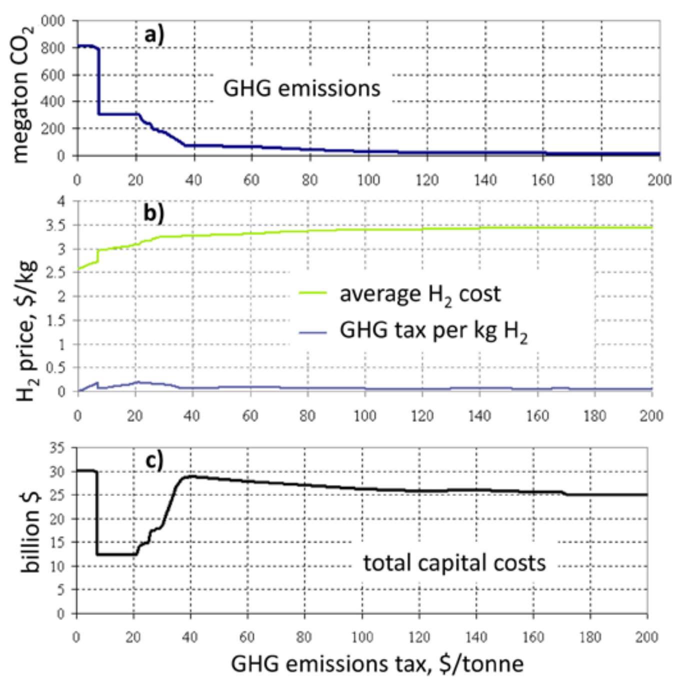

FIGURE 3. GHG Emissions Tax Effect on the Overall Emissions Level (a), Produced H_2 Costs (b) and Capital Costs (c) for a Mega-City with 12 Million Population

year. The x-axis for all graphs is a GHG emissions tax that ranges from $0/metric tonne to $200/metric tonne. Note that the GHG tax is held constant over each buildout scenario. Graph a shows the cumulative GHG emissions over the buildout scenario; graph b shows the average levelized hydrogen cost over the 40 years and the portion of that cost that pays for the GHG tax; graph c shows the cumulative capital investment for infrastructure over the scenario.

When the GHG tax is set to zero, forecourt SMR stations are built initially and those are replaced with central coal gasifiers without CCS and with pipeline delivery of hydrogen once the levelized cost of gasifier/pipeline hydrogen is less than the forecourt SMR cost. When the tax rate is between $7/tonne and $20/tonne, distributed SMR production option becomes more economical than central coal gasification throughout the 40-year buildout scenario so no coal facilities are selected. That choice results in a large decrease in GHG emissions (graph a) because SMR is less carbon intensive than coal gasification and a large decrease in capital costs (graph c) because SMR is less capital intensive. On the other hand, it causes an increase in average levelized cost because large coal facilities have a lower levelized cost than distributed SMR facilities. If the GHG emissions tax is between $20/tonne and $40/tonne, distributed SMR is replaced by coal gasification with CCS. At levels above $40/tonne biomass gasification is the dominant technology. Notably, the largest effect (in terms of overall GHG emissions reduction) is achieved at relatively low tax levels. The penalty (in terms of H_2 cost increase) is significant (up to $1/kg) but not prohibitively high. Only a small fraction of the cost increase is paid as GHG tax (the GHG tax curve on chart b) with most of the cost increase due to technology selection. Finally, higher GHG tax tends to decrease total capital costs of building the H_2 infrastructure.

Conclusions and Future Directions

- By linking production/delivery/dispensing models, the MSM is a tool for rapid cross-cutting comparative analysis of various production/delivery pathways.
- The U.S. region-specific data are readily available as MSM inputs via live MSM/HyDRA links.
- As a result of linking HyPro with the MSM, pathway evolution is examined in a manner consistent with latest versions of H2A and HDSAM.

Future Directions

- Further analyze production, delivery and distribution options, compare pathways to identify strengths of each.
- Analyze hydrogen buildout scenarios.
- Identify potential effects of not meeting targets and ensuing trade-offs.

FY 2011 Publications/Presentations

1. Ruth, M., Diakov, V., Goldsby, M., Sa, T. (2010) Macro-System Model: a Federated Object Model for Cross-Cutting Analysis of Hydrogen Production, Delivery, Consumption and Associated Emissions. In Infraday Conference, 2010.

2. James, B., Diakov, V., Ruth, M., Spisak, A., Perez, J. (2011). Hydrogen Pathway Evolution Analysis within HyPro-MSM modeling Framework. In Fuel Cell and Hydrogen Energy Conference, 2011.

3. Diakov, V., Ruth, M., Goldsby, M., Sa, T. (2011) Macro-System Model for Hydrogen Energy Systems Analysis in Transportation. Accepted for the International Mechanical Engineering Conference and Exhibit, 2011.

References

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. Steward, D., Ramsden, T., and Zuboy, J. (2008, September). *H2A Production Model, Version 2 User Guide*. Golden, CO: National Renewable Energy Laboratory.

3. Mintz, M., Elgowainy, A., and Gillette, J. (2008, September). *H2A Delivery Scenario Analysis Model Version 2.0* (HDSAM 2.0) User's Manual*. Argonne, IL: Argonne National Laboratory.

4. Argonne National Laboratory. (2009, May). *How Does GREET Work?* Retrieved from http://www.transportation.anl.gov/modeling_simulation/GREET/index.html.

5. Ruth, M., Laffen, M., and Timbario, T.A. (2009, September). Hydrogen Pathways: Cost, Well-to-Wheels Energy Use, and Emissions for the Current Technology Status of Seven Hydrogen Production, Delivery, and Distribution Scenarios. Golden, CO: National Renewable Energy Laboratory.

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

7. HyDRA: http://rpm.nrel.gov/.

8. James, B., Schmidt, P., and Perez, J. (2008, December). HyPro: A Financial Tool for Simulating Hydrogen Infrastructure Development (U.S. DOE Contract # DE-FG36-05G01519 Final Report).