VIII.9 Macro-System Model

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Objectives

- Develop a macro-system model (MSM) that will
  - Perform rapid cross-cutting analysis.
    - Utilize and link other models.
    - Improve consistency between models.
  - Support decisions regarding programmatic investments and focus of funding.
  - Support estimates of program outputs and outcomes.
- 2005/2006 objectives
  - Define analysis issues/MSM requirements.
  - Evaluate alternatives for the MSM structure and select an approach for development.
  - Begin initial integration of models.
  - Perform initial analysis – comparison of hydrogen production/delivery pathways.
  - Begin validation of the MSM.

Technical Barriers

This project addresses the following technical barriers from the Systems Analysis section (4.5) of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

(B) Lack of Consistent Data, Assumptions and Guidelines
(C) Lack of a Macro-System Model
(D) Stove-Piped/Siloed Analytical Capabilities

Accomplishments

- Identified the initial issues that the MSM will address based on an evaluation of the analysis issues that the Hydrogen Program needs to address.
- Identified high level architecture (HLA) using the federated object modeling (FOM) method as the means for linking existing models.
- Linked H2A Production cases with the Hydrogen Delivery Scenario Analysis Model (HDSAM) and the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) Model.

Introduction

The Hydrogen Program needs a macro-system model to analyze cross-cutting issues because no existing model sufficiently simulates the entire hydrogen vehicle transportation system including feedstock, conversion, refueling 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 if necessary.

During the past year, we identified issues that Systems Analysis needs to address, selected an approach for developing the MSM, and developed an initial version of the MSM. The initial version of the MSM links H2A Production cases with the HDSAM and the GREET Model. It allows users to compare the economics, primary energy source requirements, and emissions of different hydrogen production/delivery pathways.

Approach

We collected and prioritized analysis issues that the Hydrogen Program needs to address. The initial set of issues was collected from previous analysis meeting minutes and reports about the analysis needs of the Hydrogen Program. Then, we held an analysis workshop to identify additional issues and prioritize all the issues. Finally, we identified several high priority issues which could also be addressed in the early stages of MSM development.

Two approaches could have been used 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 that links or federates existing models together across multiple platforms. We chose 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 necessary expertise to do so was spread among half a dozen DOE laboratories and a dozen or more universities and private contractors. Linking models also 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.

The MSM is based on an FOM framework. That framework links together models and is exemplified by the Department of Defense HLA [1]. The general framework 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).

Results

Figure 1 shows the analysis issues that the Hydrogen Program needs to address organized into the following four categories:

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

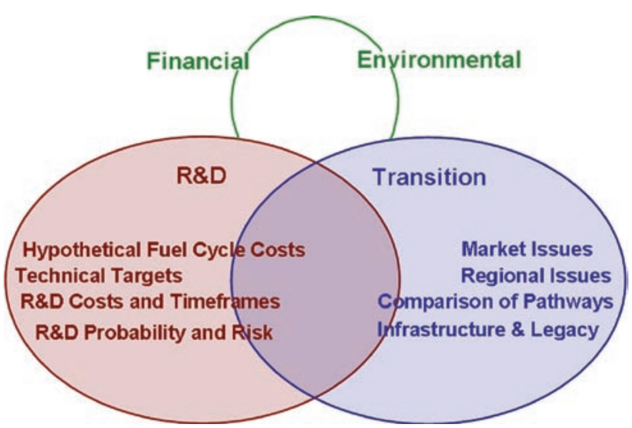

FIGURE 1. Categories of Analysis Issues the Program Needs to Address

- Financial – address corporate and government investment options.
- Environmental – resource requirements and emissions profiles.

We collected issues from previous reports and workshops and added many more at an analysis workshop. Also during the workshop, participants identified the high priority issues. The highest priority issues in each category follow:

- Research and Development
  - Identify critical/risky links in potential hydrogen pathways.
  - Verify that the current technical targets are the best ones and identify their interdependencies.
  - Determine how components and interfaces should be optimized.
- Transition
  - Compare potential transition pathways.
  - Identify stumbling blocks that could affect transition paths and determine whether research and development can overcome them.
  - Identify the impacts competing technologies could have on the transition.
- Financial
  - Identify the effects policy and incentives could have on a transition.
- Environmental
  - Estimate how and how much a hydrogen economy would affect the environment.

Having a list of high priority issues and an approach for developing the MSM, 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 among them."

To analyze that issue, H2A Production models were linked to HDSAM and the GREET model. All three of the models 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.

Three steps were necessary to link those models within the FOM framework: (1) identify the order in which the models would be run; (2) identify the data that needed to be transferred between the models and how they may be different in each model; and (3) write code that publishes data to models, runs the models, and subscribes to each model's results.

In order to carry out the hydrogen production/delivery pathway comparisons, we determined that the MSM had to execute the models in the following order: (1) HDSAM, (2) H2A production, and (3) GREET. HDSAM calculates 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. H2A Production determines 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. GREET calculates primary energy source requirements, well-to-wheels energy requirements, and emission profiles.

We developed an intimate understanding of the three models in order to determine what information needed to be transferred between the models and how it is used differently by different models. Some data transfers were almost trivial and only needed consistent units. Examples of these transfers included mass of hydrogen on trucks, fraction of carbon dioxide that is sequestered during hydrogen production, and vehicles' 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 was calculated using hydrogen throughput, hydrogen losses, and electricity requirements and then was 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 type of data 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 will ever travel 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, the developers of HDSAM, GREET, and the MSM agreed to an algorithm to calculate a single effective pipe length.

The specific framework used to develop the MSM is the enterprise modeling framework (EMF) which was developed by researchers at the Sandia National Laboratories. The EMF uses the HLA standard to exchange data between participating federated models. In the current version of the MSM, the data transferred into and out of each model and the units used for each type of data is specified in a Microsoft Excel worksheet. In future versions of the MSM, we expect to migrate this data transfer specification function from Excel to extensible markup language (XML) because XML allows for more specificity in terms of the operations that can be defined for the model execution and data transfer process. Also, we expect Excel workbooks to get too large and slow for continued use. We wrote the code for the MSM in Java because of increased programmer productivity (over C or C++) and portability to other computing platforms.

Figure 2 shows preliminary results generated by the MSM for hydrogen produced from natural gas in a large, central facility that sequesters carbon dioxide and where the hydrogen is transported to the distribution station as a liquid inside trucks. These results require further validation so should not be considered final; however, they show the type of results that will be calculated using the MSM. For each gallon of gasoline equivalent (GGE – 116,000 Btu of hydrogen) distributed at the fueling station, 127,000 Btu of hydrogen needs to be produced by the central facility. To produce that hydrogen, 172,000 Btu of natural gas and 7,000 Btu of electricity are required. An additional 41,000 Btu electricity and 1,000 Btu diesel fuel are necessary for transport and another 1,000 Btu of electricity are necessary to run the distribution station.

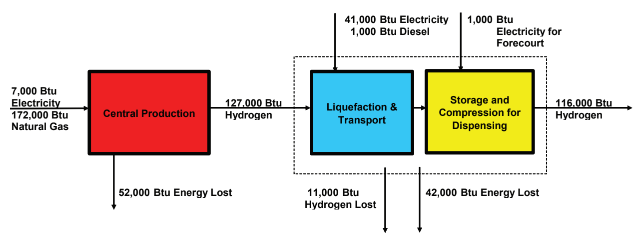

FIGURE 2. Preliminary Pathway Results for Central Hydrogen Production from Natural Gas with Liquefaction and Truck Delivery

Conclusions and Future Directions

During the past year, we have shown that the FOM approach is practical for linking models within the Hydrogen Program. An initial version of the MSM was developed to compare the economics, primary energy source requirements, and emissions of different hydrogen production/delivery pathways. The MSM can help identify which combinations are most likely to be developed and some of the environmental tradeoffs between the pathways. The initial version links H2A Production cases with HDSAM and the GREET Model.

The next steps for the MSM involve:

- Validating the results of the current analysis.

- Developing a user interface and making the MSM available so that more analysts can use it.
- Adding additional models and data sources. These include the Hydrogen Analysis Resource Center (HyARC), a transition model, and material and energy balance and capital cost calculations for at least one production model.

FY 2006 Publications/Presentations

1. An update of this project was presented to the Fuel Pathway Integration Tech Team in October 2005.

2. An update of this project was presented at the Annual Merit Review in May 2006.

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.