# X.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
- 2007/2008 objectives:
  - Improve the structure of the MSM and develop a graphics user interface (GUI)
  - Update versions of component models
  - Add stochastic analysis capability
  - Validate MSM results
  - Begin developing 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 (this plan can be accessed at http://www1.eere.energy.gov/hydrogenandfuelcells/mypp/):

(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 will contribute 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 Argonne National Laboratory Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (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

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 Web-based user interface so that many members of the analysis community can use the MSM.
- Added stochastic (Monte Carlo) capability to the MSM.
- Completed a draft User Guide for the MSM.

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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 and 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 pathways' 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 to provide data necessary to update integrated models when component models have been updated.

The MSM is being built on a federated object model framework. That framework links together models and is exemplified by the Department of Defense High Level Architecture [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). Version 1.0 of the MSM uses Ruby and Ruby interfaces to Microsoft Excel to collect, transfer, and calculate data.

## Results

Levelized hydrogen costs, primary energy requirements, and emissions have been estimated for multiple pathways using H2A V1.0.9, HDSAM V1.0, and GREET V1.7. 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

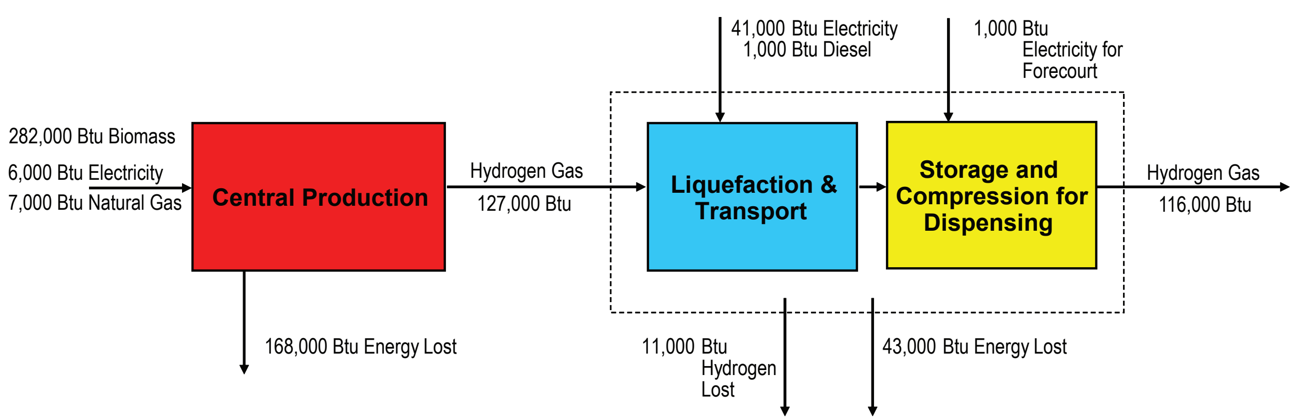


**FIGURE 1.** Pathway Results for Central Hydrogen Production from Woody Biomass with Liquid Hydrogen Delivered via Trucks

hydrogen), 127,000 Btu of hydrogen need to be produced – 11,000 Btu are lost due to unrecovered boil-off. In addition, 41,000 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 $5.43/kg. That levelized cost is higher than the levelized cost reported in the 2006 Hydrogen Posture Plan which was $5.10/kg [2]. The difference is primarily due to boil-off losses that were not included in the calculations used for the Posture Plan. Likewise, the overall production energy efficiency and pathway efficiency were lower than that reported in the Posture Plan (43% vs. 45% and 34% vs. 40%) due to boil-off losses, and inclusion of electricity and natural gas in the efficiency calculations.

In addition to pathway energy requirements, levelized cost, and efficiency, the MSM utilizes GREET to estimate well-to-wheels (WTW) energy use and emissions. The MSM reported a WTW total energy use of 7,400 Btu/mile for this pathway as compared to 6,600 Btu/mile reported in the Posture Plan. The MSM also reported a WTW petroleum use of 240 Btu/mile and a WTW greenhouse gas emissions level of 180 Btu/mile. Those differed from the Posture Plan because the MSM set GREET to use woody biomass to match H2A instead of herbaceous biomass and the MSM transferred the liquefaction efficiency from HDSAM to GREET to make them consistent.

One of the primary factors for comparing pathways is levelized cost (including operating costs and capital costs with a 10% discounted cash flow rate of return). Figure 2 compares the levelized hydrogen costs of multiple pathways using H2A V1.0.9 and HDSAM V1.0. The results for many of the pathways include both current and future technologies and the pathways with central production have results of both liquid hydrogen delivered in trucks and gaseous hydrogen delivered via pipeline. The levelized cost for each pathway is broken into the production cost, the cost of producing extra hydrogen that is lost due to leaks, and the cost of delivery and distribution.

Since all of modeled estimates have some variability, stochastic modeling capability in the form of Monte Carlo analysis has been added to the MSM. The DAKOTA toolbox [3] was used because it not only gives the MSM the capability of running a Monte Carlo analysis now but can be used for optimization runs in the future. Figure 3 shows the range of levelized costs for hydrogen from woody biomass via gasification in central plants using current technology followed by liquefaction and delivery of liquid hydrogen in trucks.

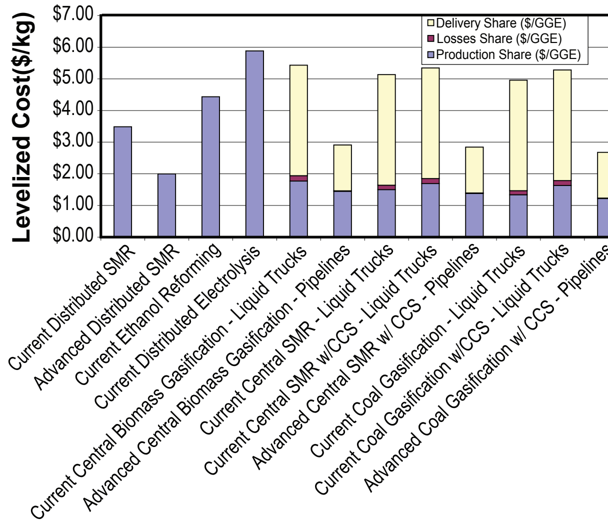


**FIGURE 2.** Comparison of Levelized Costs for Multiple Pathways

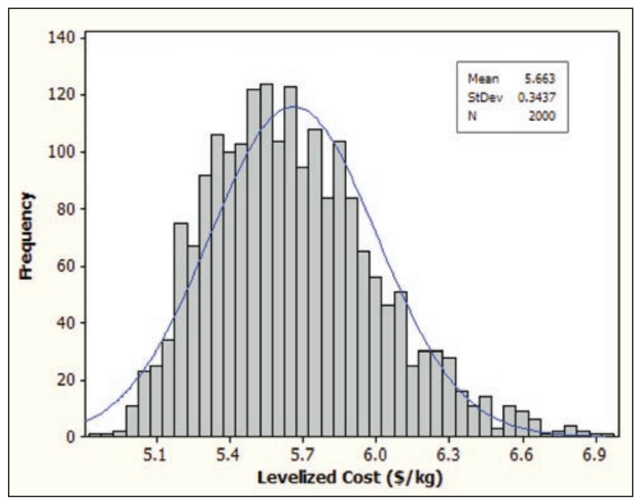


**FIGURE 3.** Uncertainty in Levelized Cost of Hydrogen Produced from Woody Biomass in Central Plants with Liquid Hydrogen Delivered via Trucks

Other results are important to compare as well. Figure 4 shows the estimated levelized cost of hydrogen (on a per mile basis) for many pathways plotted against each pathway's estimated well-to-wheels greenhouse gas emissions. The biomass pathways have the lowest greenhouse gas emissions but may be expensive. In all the cases shown, pipeline delivery is less expensive and has lower greenhouse gas emissions than delivery of liquid hydrogen in trucks (250,000 person city with 50% hydrogen penetration).

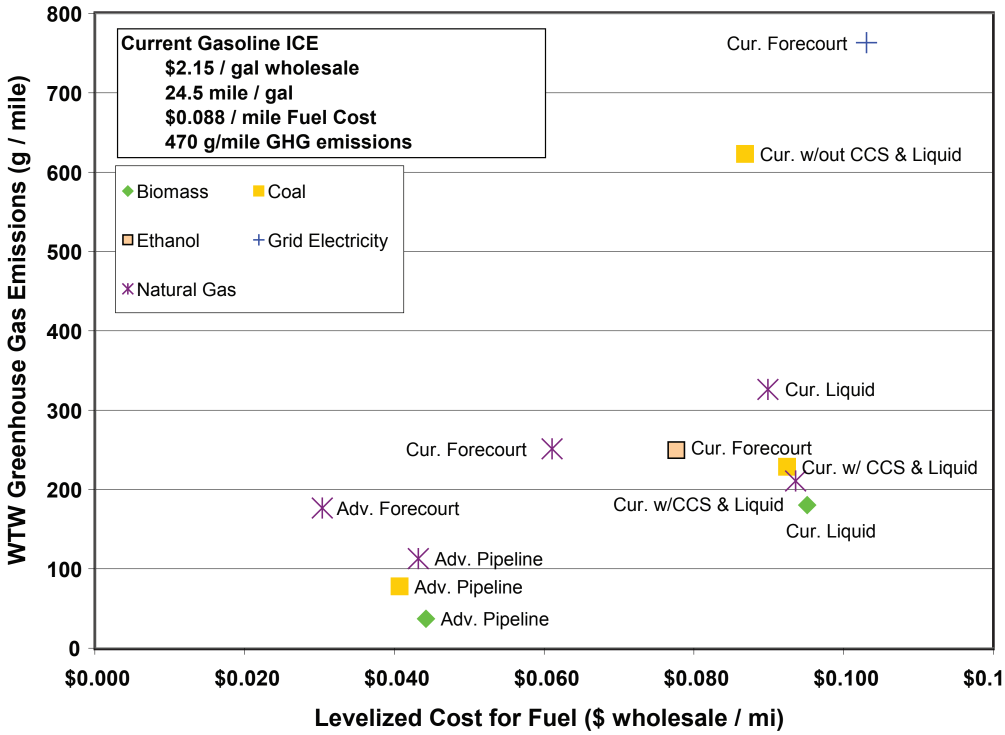


**FIGURE 4.** Levelized Cost and GHG Emissions for Multiple Hydrogen Pathways

## 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 can help identify which combinations are most likely to be developed and some of the environmental tradeoffs between the pathways. Stochastic capability and a Web-based GUI have also been created for the MSM.

The next steps for the MSM involve:

- Updating the MSM's interaction with component models as they are released.
- Linking geographical tools to the MSM.
- Linking at least one transition-scenario model to the MSM.
- Using the MSM to update production and delivery information for other models.

## 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.** 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