Macro-System Model for Hydrogen Energy Systems Analysis in Transportation

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ABSTRACT

The introduction of hydrogen as an energy carrier for light-duty vehicles involves concomitant technological development of an array of infrastructure elements, such as production, delivery, and dispensing, all associated with energy consumption and emission levels. To analyze these at a system level, the suite of corresponding models developed by the United States Department of Energy and involving several national laboratories is combined in one macro-system model (MSM). The MSM uses a federated simulation framework for consistent data transfer between the component models. The framework is built to suit cross-model as well as cross-platform data exchange and involves features of "over-the-net" computation.

While the MSM can address numerous hydrogen systems analysis aspects, of particular interest is the optimal deployment scenario. Depending on user-defined geographic location and hydrogen demand curve parameters, the cost-optimal succession of production/delivery/dispensing pathways undergoes significant changes (the most important of these being the transition between distributed and central hydrogen production with delivery). Some 'tipping' (break-even) points are identified.

FORMATTING

1.1 Introduction

The Hydrogen Macro System Model (MSM) is a simulation tool that links existing and emerging hydrogen-related models to perform rapid, cross-cutting analysis. It allows analysis of the economics, primary energy-source requirements, and emissions of hydrogen production and delivery pathways. The MSM simulates cost, energy use, and emissions of the entire hydrogen system (including feedstock, conversion, infrastructure, and vehicles) in an integrated fashion, and its analyses and sensitivity runs can provide a basis for decisions regarding research focus.

Furthermore, the MSM tool can help users understand the effects of varying parameters on a pathway's results without requiring expertise in all of its models. The MSM promotes consistency between the methodologies and assumptions of each model by transferring information between models as well as identifying contradictions so they can be corrected.

The MSM was jointly developed by the the National Renewable Energy Laboratory (NREL) and Sandia National Laboratories (SNL). It was designed to act as an overarching system that provides a cross-cutting analysis and simulation capability to the U.S. Department of Energy's (DOE) Hydrogen Program. In addition, MSM may be used to guide the development of other similar simulation tools.

MSM was developed to accomplish the following specific objectives:

- Rapid, cross-cutting analysis in a single location by linking existing applicable models
- Improve consistency of technology representation (i.e., consistency between models)
- Consistent use of hydrogen models without requiring all users to be experts in all models
- Decision support regarding programmatic investments, focus of funding, and research milestones through analyses and sensitivity runs.

1.2 Scope

The macro-system model combines tools and models related to gaseous hydrogen fuel production, delivery and dispensing. Other fuel types (for example, liquid hydrogen or natural gas as vehicular fuels) cannot be analyzed at the same level of detail within the suite of DOE hydrogen models and are outside the scope of this paper.

The MSM <http://h2-msm.ca.sandia.gov/> (Ruth et al. 2009) can currently perform pathway, also known as well-to-wheels (WTW), analysis of hydrogen production and delivery pathways. Spatial and temporal models are added to the MSM to allow users to answer more complex questions regarding the market dynamics and infrastructure needs related to developing a hydrogen economy.

Pathway, or WTW, analysis responds to the need to understand costs, the breakdown of these costs, energy use, and emissions related to different hydrogen production/delivery pathways. The approach is to examine pathways from the extraction of feedstock for hydrogen, through the production, storage, and delivery processes, to the use of hydrogen in vehicles. Through its links to component models such as the H2A Production model (Steward et al. 2008), the Hydrogen Delivery Scenario Analysis Model (HDSAM) (Mintz et al. 2008), and the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model (Wang et al. 2009), the MSM is capable of performing a comprehensive WTW analysis that provides users with details such as the amount and type of feedstock used to produce hydrogen, efficiencies of different technologies, energy use and emissions of various pathways, hydrogen production capacity to meet demand, and cost of hydrogen at the pump achievable under different scenarios.

- HDSAM is a delivery-scenario model that links various hydrogen delivery component costs to develop capacity/flow parameters for a hydrogen delivery infrastructure. This approach allows the model to calculate the full cost of hydrogen delivery and accounts for any tradeoffs between components. The structure provided by this model allows the efficient examination of new technologies, alternative delivery pathways/packaging solutions, and the effect of demand density and scale. HDSAM uses financial calculation methodologies and parameters consistent with H2A Production to provide a “snapshot” of delivery cost results based upon input assumptions.
- The H2A Production model is used to assess the cost of producing hydrogen for central and forecourt (filling station) technologies. Users are permitted to define several characteristics of the production such as process design, capacity, capacity factor, efficiency, feedstock requirements, capital costs, and operating costs. For more customized analyses, users may also manipulate various financial parameters including internal rate of return, plant life, feedstock costs, and tax rate. In the MSM, assumptions and data on several key technologies were also taken from the H2A Production case studies. Hydrogen production from natural gas using molten carbonate or phosphoric acid fuel cell is included in the model as well.
- Created by the Argonne National Laboratory, the GREET model (version 1.2011) allows for the evaluation of various vehicle and fuel combinations on a full fuel-cycle/vehicle-cycle basis. More than 100 fuel production pathways (e.g., corn to ethanol and soybean-based biodiesel) are included in GREET 1.2011 to calculate the consumption of total energy, greenhouse gas emissions (primarily carbon dioxide, methane, and nitrous oxide), and six criteria pollutants. For use in the MSM, energy requirements in H2A Production and HDSAM are converted to standard GREET inputs (yields, shares, distances, etc.).
- The MSM also uses the vehicle cycle portion of GREET (version 2.7) which relates to energy and materials consumption and emissions associated with vehicle production.
- The Cost Per Mile Tool (CPM) helps calculate the cost of ownership of a hydrogen fuel cell vehicle.
- Geo-spatial model HyDRA provides region-specific inputs to and incorporates region-specific results from the MSM
- Hydrogen pathways evolution analysis tool HyPro is also incorporated in the MSM framework.

The ability to compare critical factors such as levelized hydrogen costs at the pump using different hydrogen production/delivery technologies, raw material needs required to meet a city’s potential hydrogen demands, energy use, efficiencies and emissions profile (carbon dioxide, methane, other GHG, VOC, CO, NOx, PM10, SOx) for varying population and hydrogen market penetration levels is a capability that delivers a comprehensive and cross-cutting view of factors related to the development of a hydrogen economy.

The following production and delivery technologies have been included in the MSM:

Central production technologies (involving hydrogen delivery to refueling stations)

- biomass gasification,
- coal gasification (with or without carbon dioxide sequestration),

- natural gas reforming (with or without carbon dioxide sequestration),
- electrolysis using wind generated electricity;

Distributed production technologies (hydrogen is produced at the refueling station site)

- electrolysis,
- natural gas reforming,
- ethanol reforming;

Delivery options

- pipeline delivery of gaseous hydrogen,
- gaseous hydrogen delivery by tube trucks
- liquid hydrogen delivery by trucks
- cryogenic hydrogen delivery (also by trucks)

1.3 Approach

In linking disparate constituent models together, the MSM needs to feature extensibility, distributability and scalability. We were inspired by the example of the federated object model (FOM), as exemplified in the DoD High Level Architecture (HLA) (Dahmann et al. 1997). The FOM approach requires the explicit definition of the messages (objects and interactions) through which the models interact with their environment, providing a common interlingua for the models that is extensible as new models are added. It solves the problem of proliferating interfaces as the number of integrated components grows, which helps keep the model framework scalable. The models in the MSM were in general not designed with federation in mind, so we have had to write specialized code to extract data from them and provide data to them; these modules constitute an implicit statement of the interaction of the models with their environment. There is only one such interface module per model, rather than one for each pair of models. The FOM approach has been a success in the arena of distributed simulation in the defense community, and we apply this approach to link models pertaining to the evolution of the hydrogen economy. The general framework is extensible (accommodates new models with minimal difficulty), distributable (can be used by multiple people in different areas of the country), and scalable to large numbers of participating models.

Web servers and browsers use the HTTP protocol (Fielding et al. 1999) to transport data, and most Internet firewalls allow HTTP traffic to pass through unhindered. Having the MSM use HTTP to communicate with component models allows these models to lie in other security domains without requiring their administrators to reconfigure the firewalls to let MSM traffic through.

The MSM includes the following functional blocks: i) Unifying Framework implemented in the Ruby scripting language; consists of model application programming interfaces (APIs), model control scripts, unit conversion facility, global data storage (GDS), and execution control; ii) Graphical User Interface (GUI) implemented in Java and delivered via Java Web Start and the user's installed browser; iii) Database Management System (DBMS) implemented in MySQL and contains archived jobs and user data; iv) Web Services with some component models being housed in different locations and communicating with the MSM via HTTP.

Through the GUI, the user sets variables such as timeframe, production technology, feedstock, delivery method, city size, and penetration of the technology. The Detailed Inputs section of the GUI renders virtually all parameter inputs available for the user through the Web interface. User input data is initially transferred to the GDS, which holds all data in a consistent set of units. As each component model is run, data from it is transferred to the GDS, and calculations are done by the GDS script. Input data for subsequent models are taken from the GDS. As the capabilities of the MSM are expanded in the future, optimization routines and solution methodology schemes may also be added.

The current MSM version co-locates all back-end resources on a single server (application server) while the future planned version will allow models, their APIs, and their control scripts to be located at the model owner's/developer's site or other location (model server). Representational State Transfer (REST) over HTTP is used to connect the MSM with models physically located in other places.

Delivered hydrogen costs, primary energy requirements, and emissions have been estimated for multiple pathways. Figure 1 shows results for production of hydrogen from woody biomass via gasification in central plants 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 or 1.02 kg 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 hydrogen cost at the pump for this pathway is estimated to be $5.43/kg. MSM produces analogous results for other pathways.

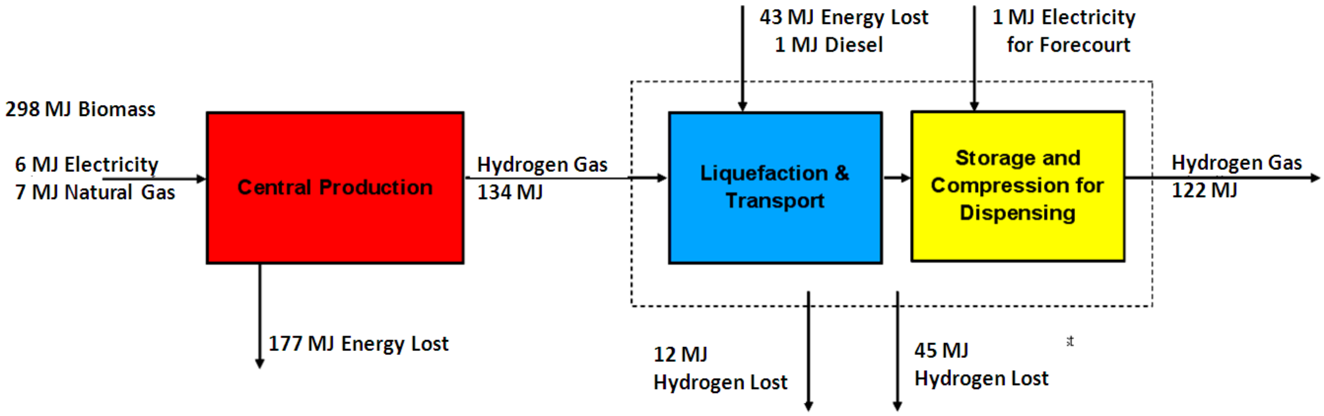

Figure 1. MSM results for hydrogen production from biomass with liquid hydrogen delivery to refueling stations

The MSM results are validated at both component models and integrated levels by industry and hydrogen analysis community experts. MSM is available for hydrogen analysis web-users at http://h2-msm.ca.sandia.gov.

CURRENT DEVELOPMENTS

2.1 Infrastructure evolution technical breakthrough points

In analyzing hydrogen infrastructure evolution scenarios, we choose a set of competing infrastructure technologies (we limit this set by H2A Production and HDSAM options), apply the most recent published inputs for these technologies, and use optimization software designed to select the most cost efficient hydrogen production/delivery/dispensing pathways depending on demand evolution curve. The most important input parameters used in this study are given in Table 1.

Each production technology has two entries: current (labeled 2005) and advanced (2025). Although technological improvements will most certainly occur at different time frames for these technologies, the year of 2025 was selected as the transition year when the advanced technology version is available. In addition, it is assumed that pipeline hydrogen delivery will be available only starting at 2025 (the year when new technologies or pipeline delivery become available will depend on many factors such as location and development efforts; for a generic case study, we assume all new technologies become available at the same time). The upper part of the table shows central production options (i.e. the ones that also require delivery of produced hydrogen), while the lower part presents distributed (forecourt, FC) production options including steam methane reforming (SMR), electrolysis (Elys) and hydrogen production from ethanol (EtOH). Central production options may involve carbon capture and sequestration (CCS), in which case GHG emissions associated with producing one kg of hydrogen are significantly lower. GHG emissions for central electrolysis are set to zero as wind produced electricity is the intended feedstock for hydrogen production in these cases and no life-cycle analysis is included.

We are investigating a generic case when all central production facilities are assumed to be equally distanced from city boundaries. This assumption is subject to change when a geographically specific region is chosen. And for this, more detailed models should be applied, as for example, SERA (Bush et al. 2010). The range of questions that MSM – HyPro tandem is suitable to answer includes i) what is the typical succession of hydrogen pathways that should be expected? ii) what are the major factors that will likely influence this sequence?

For the set of inputs shown in Table 1 and an optimistic user-input hydrogen demand growth rate (NAS 2004 report), the cost-optimal technologies include forecourt SMR production (up to the year 2025) and coal gasification (after 2025).

While there are several possibilities of stimulating the development of cleaner, less GHG emitting technologies (such as cap-and-trade, renewable portfolio standard, or a GHG emissions tax on hydrogen producers), we assume a carbon cost applied in terms of dollars per ton carbon dioxide equivalent of emissions associated with hydrogen production. Then, depending on carbon cost rate, different technologies become cost optimal. The trend, expectedly, shows lower overall GHG emissions with increasing carbon cost (figure 2).

TABLE 1. SCENARIO EVOLUTION PARAMETERS

Production technology	Design capacity ton_hydrogen/yr	$/(kg hydrogen design capacity)	Feedstock cost, $/kg hydrogen produced	GHG emissions kg carbon dioxide / kg hydrogen produced
COAL 2005	103598	4.19	0.29	26.5
COAL 2025	80968	6.17	0.26	24.7
COAL CCS 2005	101071	6.83	0.39	1.98
COAL CCS 2025	80968	8.29	0.27	2.47
NG 2005	124628	1.45	1.04	9.28
NG 2025	124628	1.08	1.01	9.28
NG CCS 2005	124628	2.68	1.08	0.93
NG CCS 2025	124628	2.01	1.04	0.93
Biomass 2005	50908	3.03	0.41	0.44
Biomass 2025	50838	2.85	0.44	0.23
C Elys 2005	18517	5.96	2.87	0
C Elys 2025	18517	2.22	2.51	0
Nuclear HTE	268297	3.68	1.98	0
FC SMR 2005	547.5	2.08	1.07	9.26
FC SMR 2025	547.5	1.62	1.04	8.66
FC Elys 2005	547.5	5.00	2.88	43.4
FC Elys 2025	547.5	2.01	2.52	32.4
FC EtOH 2005	547.5	2.56	3.80	12.5
FC EtOH 2025	547.5	2.19	3.46	11.3

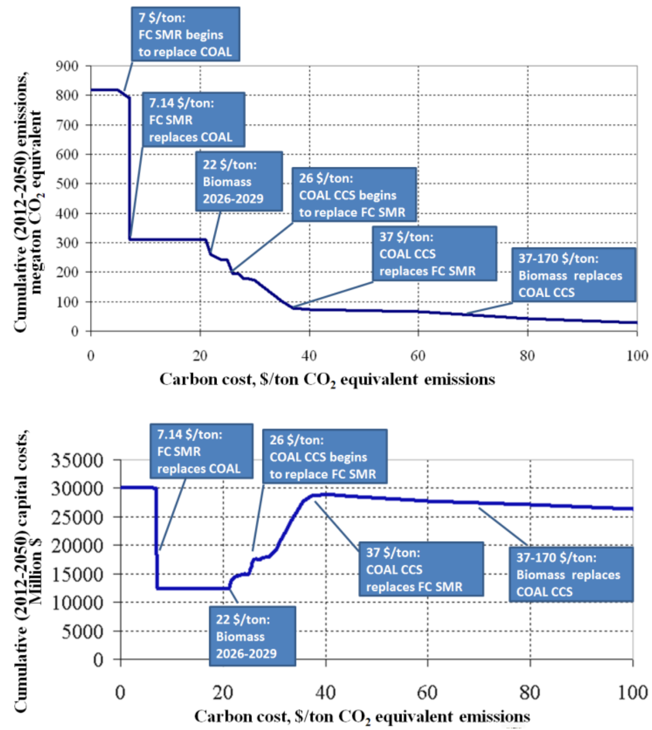

Figure 2. Anticipated carbon cost effect on the overall emissions level (top) and capital costs (bottom chart) for a mega-city with 12 million population

As seen on Figure 2, small carbon cost levels do little towards stimulating cleaner hydrogen production. When carbon cost exceeds $7 per ton GHG, distributed SMR production option becomes more economical than central coal gasification which causes a large decrease in GHG emissions (top graph) and capital costs (bottom graph). FC SMR is gradually replaced by coal gasification with CCS in the tax range between $20 and $40 per ton carbon dioxide equivalent, and at levels above $40/ton COAL CCS is gradually replaced by biomass gasification (contingent on biomass availability, depends on specific location). Interestingly, the largest effect (in terms of overall GHG emissions reduction) is achieved at relatively low carbon cost levels. Finally, higher carbon cost levels tend to decrease total capital costs of building the hydrogen infrastructure, mainly because of lower capital costs for biomass and SMR options.

The above results relate to gaseous hydrogen vehicular fuel. The basis for optimizing production/delivery/dispensing pathways is the hydrogen cost at the pump. Important characteristics (such as GHG emissions) are included in consideration only as they have monetary value (carbon cost).

2.2 CONCLUDING REMARKS

The macro-system model is developed for DOE's Hydrogen, Fuel Cell, and Infrastructure Program to analyze cross-cutting issues. The federated object model structure proved to be efficient for this purpose. The large number of variables involved in the process of combining several models under one framework poses specific challenges, which call for specific solutions in building the user interface.

A wide variety of input parameters is presented to the user in the form of 'branches and leaves' structure which proves to be useful in several ways. First, it provides easy access to the input parameters without overcrowding the screen. Second, the 'branches and leaves' have built-in conditional logic dependent on previous user's choices which eliminates irrelevant branches from the interface screen. Third, for flexibility, the structure is defined separately from the server, which allows for easy modification and addition of input parameters. The approach was expanded to accommodate the display of output parameters as well.

NOMENCLATURE

API – application programming interface

CCS – carbon capture and sequestration

DOD – U.S. Department of defense

DOE – U.S. Department of energy

Elys – electrolysis

EtOH - ethanol

FOM – federated object model

GDS – global data storage

GHG – greenhouse gases

GREET – greenhouse gases, regulated emissions and energy use model

GUI – graphical user interface

HDSAM – hydrogen delivery scenario analysis model

HLA – high level architecture

HTTP – hypertext transfer protocol

HyDRA – hydrogen resource analysis model

HyPro – hydrogen pathways evolution analysis model

MSM – macro systems model

NAS – National academy of science

NREL – National renewable energy laboratory

REST – representation state transfer (a web service access style)

SEPI – systems engineering and process integration

SERA – scenario evaluation, regionalization and analysis

SMR – steam methane reforming

SNL – Sandia national laboratories

VOC – volatile organic compounds

WTW – well-to-wheels.

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