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MACRO-SYSTEM MODEL: A FEDERATED OBJECT MODEL FOR CROSS-CUTTING ANALYSIS OF HYDROGEN PRODUCTION, DELIVERY, CONSUMPTION AND ASSOCIATED EMISSIONS

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ABSTRACT

The introduction of hydrogen as an energy carrier for light-duty vehicles involves concomitant technological progress in several directions, such as production, delivery, consumption and related emissions. To analyze each of these, a suite of corresponding models have been developed by the DOE, involving inputs from several national laboratories. The macro-system model is being developed as a cross-cutting analysis tool which combines a set of hydrogen technology analysis models. Within the macro-system model (MSM), federated simulation framework is used for consistent data transfer between the component models. The framework is built to suit cross-model as well as cross-platform data exchange and will involve features of 'over-the-net' computation.

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 is the first model to simulate cost, energy use, and emissions of the entire hydrogen system (including feedstock, conversion, infrastructure, and vehicles) with the necessary level of technical detail in an integrated fashion, and its analyses and sensitivity runs can provide a basis for decisions regarding focus of research needs.

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 Systems Engineering and Process Integration office (SEPI) at the National Renewable Energy Laboratory (NREL) and the Sandia National Laboratories (SNL). The SEPI provides domain expertise and leads the project; SNL provides computer science expertise.

The MSM 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:

- To perform rapid, cross-cutting analysis in a single location by linking existing applicable models
- To improve consistency of technology representation (i.e., consistency between models)
- To allow for consistent use of hydrogen models without requiring all users to be experts in all models
- To support decisions regarding programmatic investments, focus of funding, and research milestones through analyses and sensitivity runs

2 SCOPE

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. In the future, spatial and temporal models will be 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.

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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. This approach looks at these pathways from the extraction of feedstock for hydrogen, through the production, storage, and delivery processes, and all the way 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.

More detailed description of constituent models incorporated in the MSM follows:

- 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 "snap shot" 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.
- Created by the Argonne National Laboratory, the GREET model allows for the evaluation of various vehicle and fuel combinations on a full fuel-cycle/vehicle-cycle basis. The MSM uses only the fuel-cycle portion of GREET (version 1.8b), which allows researchers to evaluate a fuel cycle from the well to wheels. More than 100 fuel production pathways (e.g., corn to ethanol and soybean-based biodiesel) are included in GREET 1.8b 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.).

With the MSM's ability to integrate multiple variables, the user may modify these variables to observe valuable results highlighting different aspects of various technologies and pathways. The primary variables currently included in the WTW analysis structure of the MSM are technology year, city size and hydrogen fuel penetration, production and delivery technology, and vehicle fuel economy. In some cases, users may also choose whether to use a model's default input values or their own.

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 (CO_2, CH_4, other GHG, VOC, CO, NO_x, PM10, SO_x) of hydrogen use for varying populations and hydrogen 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 carbon dioxide sequestration
    - Coal gasification without carbon dioxide sequestration
    - Natural gas reforming with carbon dioxide sequestration
    - Natural gas reforming without carbon dioxide sequestration
    - Electrolysis using electricity generated with wind turbines
- Distributed production technologies (hydrogen is produced at the refueling station site)
    - Electrolysis
    - Natural gas reforming
    - Ethanol reforming
    - Delivery technologies
    - Piping of gaseous hydrogen

- Truck-transport of liquid hydrogen

As additional component models are integrated into the MSM (such as spatial and temporal models), the structure and components of the MSM will allow users to discover answers to more complex questions regarding the market dynamics and infrastructure needs related to transitioning to a hydrogen economy.

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 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. We achieve scalability because 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, so we expect this approach to work for linking models pertaining to the evolution of the hydrogen economy as well.

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 will allow these models to lie in other security domains without requiring their administrators to reconfigure the firewalls to let MSM traffic through.

Figure 1 illustrates how the MSM software application interconnects the component models.

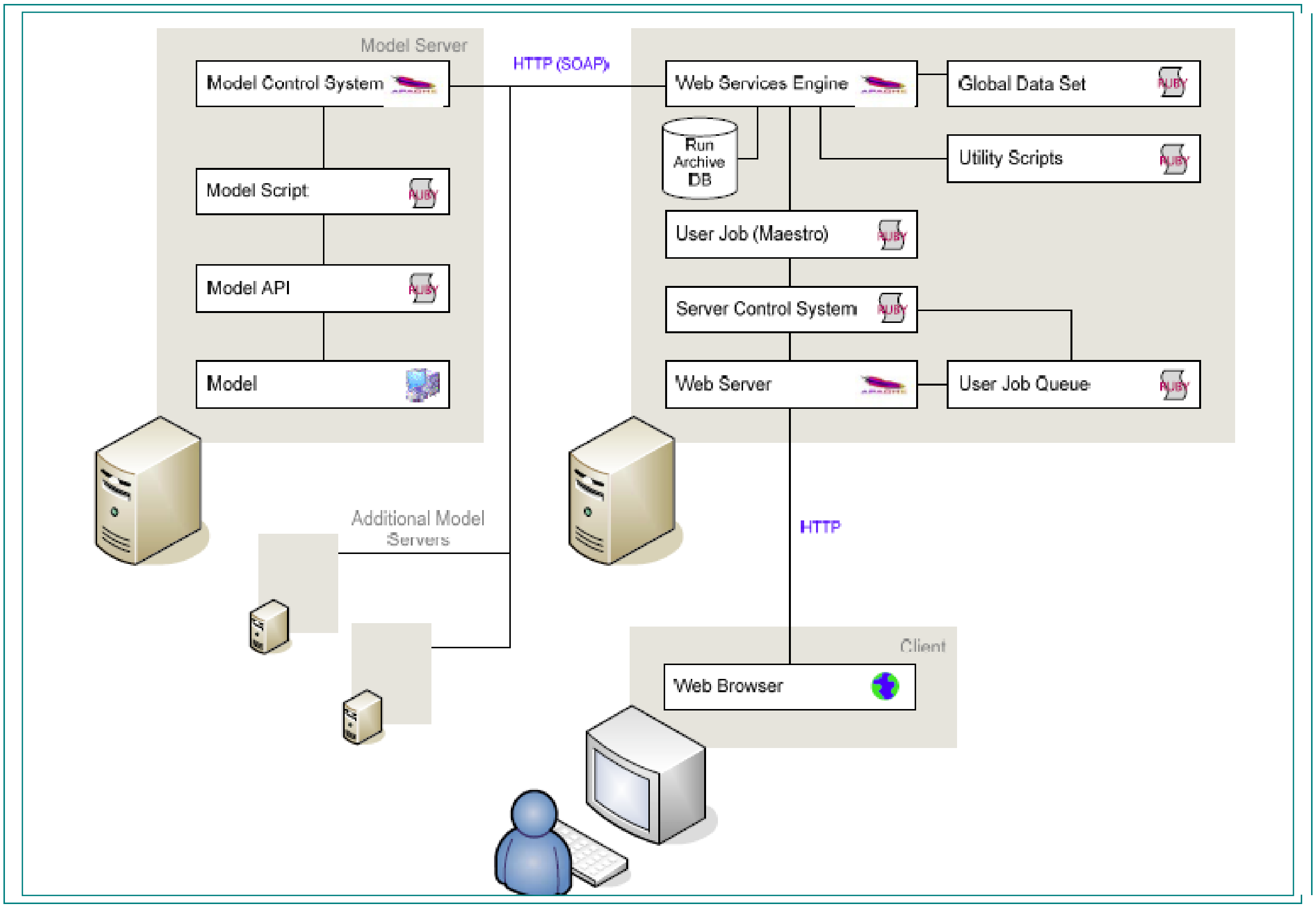


Figure 1: The GUI and the MSM operation process

The interconnects are implemented by the following means:

- *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
- *Graphical User Interface (GUI):* Implemented in Java and delivered via Java Web Start and the user's installed browser
- *Database Management System (DBMS)*: Implemented in MySQL and contains archived jobs and user data
- *Web Services:* Because all the component models are currently housed on a single machine, Web services are not being used. In the near future, component models are expected to be housed in different locations and Web services will be used to allow communication via HTTP.

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.

Through the GUI, the user sets variables such as timeframe, production technology, feedstock, delivery method, city size, and penetration of the technology (Future capabilities of the MSM will involve significantly more 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). Because the models are currently co-located with the unifying framework, SOAP (a simple XML-based protocol that lets applications exchange information over HTTP) is not necessary. This protocol will more likely be used in future versions of the MSM when some models are physically located in other places.

Delivered hydrogen costs, primary energy requirements, and emissions have been estimated for multiple pathways. Figure 2 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 and 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.

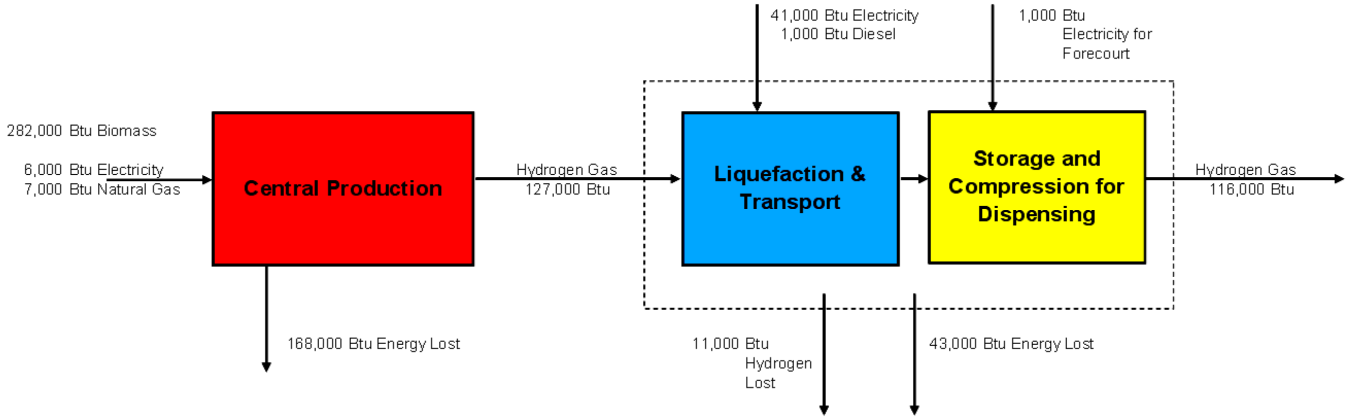


Figure 2: MSM results for hydrogen production from biomass with liquid hydrogen delivery to refueling stations

4 CURRENT DEVELOPMENTS

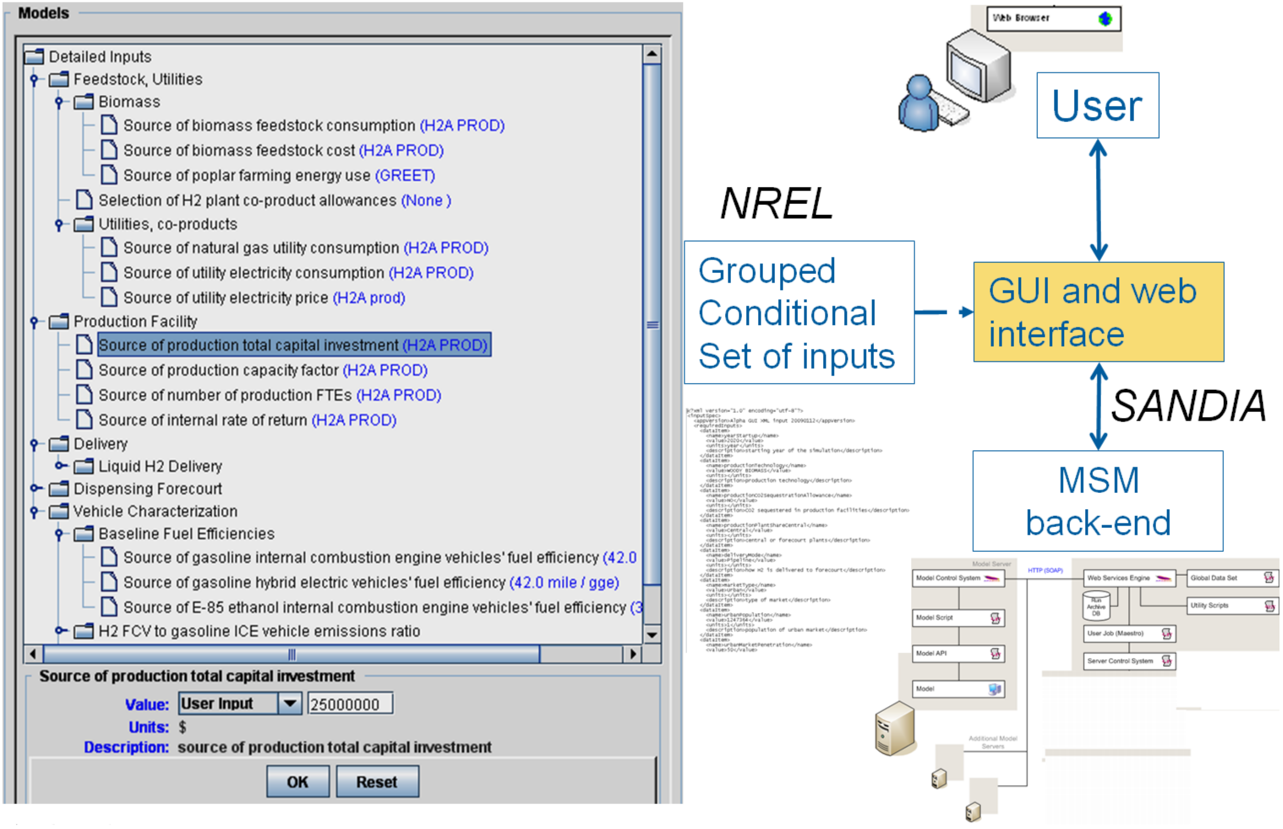
Enhancing the MSM performance involves several paths. First, the component models are being updated on a regular basis to include latest technology improvements; concurrently, the MSM is being updated to account for these changes. Second, the first web-based user interface allowed user access only to the most critical parameters of a pathway to be analyzed, the vast majority of parameters being ‘invisible’ to the user at their default values; this restriction is removed by the new expanded GUI. Third, new models are being added into the MSM to allow new types of analysis; the MSM is being linked with geospatial analysis tool (HyDRA, `<http://rpm.nrel.gov/>`) and technology transition (temporal) model (HyPro).

4.1 Expanding GUI capabilities

MSM being a conjunction of several models, it can potentially involve all variables present in each of the constituent models. Thus the total number of MSM input parameters can significantly exceed that number for an individual model and hence the need for compact ways of accessing large numbers of variables via a friendly user interface. Clearly, just giving the user a long list of variables that might be useful someday is not a very user-friendly solution.

To allow user access to the entire set of MSM input parameters, a ‘branch and leaf’ structure have been adopted. The inputs are grouped into blocks (each block representing a branch containing other blocks or input parameters). One of the challenges encountered while building the expanded GUI is that a compact user interface should exclude user access to parameters that are irrelevant for the hydrogen production/delivery pathway of interest. In other words, the ‘branches and leaves’ structure is conditional upon some basic choices made by the user. For example, when analyzing hydrogen production at refueling stations, we should avoid offering the user to specify hydrogen delivery parameters via pipeline (simply because there is no H_2 delivery involved).

Naturally, all the conditional logic behind the GUI is specified by the domain experts (the NREL side of the project), while the server-based GUI is developed by the computer experts (at the SNL). Further, with upgrading the MSM to newer constituent model versions, the ‘branches and leaves’ structure will be modified almost on a continuous basis. To give us (MSM developers) more flexibility, the GUI server is built in such a way as to take a (complete and extensive) list of instructions (written in XML by the domain experts) and create (according to the conditional logic given in the instructions) a set of grouped input parameters which might be of interest for the user. The schematics of this interaction is shown on the left side of Figure 3, along with an example of ‘branches/leaves’ structure on the left.



Models

- Detailed Inputs
  - Feedstock, Utilities
    - Biomass
      - Source of biomass feedstock consumption (H2A PROD)
      - Source of biomass feedstock cost (H2A PROD)
      - Source of poplar farming energy use (GREET)
    - Selection of H2 plant co-product allowances (None)
    - Utilities, co-products
      - Source of natural gas utility consumption (H2A PROD)
      - Source of utility electricity consumption (H2A PROD)
      - Source of utility electricity price (H2A prod)
  - Production Facility
    - Source of production total capital investment (H2A PROD)
    - Source of production capacity factor (H2A PROD)
    - Source of number of production FTEs (H2A PROD)
    - Source of internal rate of return (H2A PROD)
  - Delivery
    - Liquid H2 Delivery
  - Dispensing Forecourt
  - Vehicle Characterization
    - Baseline Fuel Efficiencies
      - Source of gasoline internal combustion engine vehicles' fuel efficiency (42.0
      - Source of gasoline hybrid electric vehicles' fuel efficiency (42.0 mile / gge)
      - Source of E-85 ethanol internal combustion engine vehicles' fuel efficiency (3
    - H2 FCV to gasoline ICE vehicle emissions ratio

Source of production total capital investment

Value: User Input 25000000
Units: $
Description: source of production total capital investment

Figure 3: Example of ‘branches and leaves’ structure denoting grouped input parameters (left) and the schematics of the user interface (right side of the figure).

NREL domain experts provide the XML list of conditionally grouped input parameters; GUI web-server provides interaction with the user and supplies the MSM back-end with the set of user-specified inputs necessary to start the job. The expanded GUI *both* allows the user to have substantially wider capabilities in controlling MSM runs *and* gives domain experts virtually unlimited flexibility in defining and structuring user access options without altering the web server.

4.2 Adding geo-spatial and temporal capabilities

Economic characteristics of hydrogen production are one of the main types of data being analyzed in the MSM. The reality suggests that these strongly vary with position and with time. Hence, different production/delivery pathways are more advantageous depending on the geographical region and on the time-span of the project, and the analysis has to be geographically and time specific. Evidently, adding geo-spatial and temporal capabilities to MSM is an important task.

To add geo-spatial capabilities, the MSM is being linked with HyDRA. The approach is to use geographically specific data from HyDRA as MSM inputs to generate geographically specific outputs. An example of MSM - HyDRA interaction involves hydrogen production via electrolysis at refueling stations. Geospatial MSM outputs (cost of H2 generated from electrolysis, $/kg, and associated green-house gas emissions, g/mile vehicle distance) are generated using geo-specific HyDRA inputs (county-by-county electricity cost, $/MWh, and electricity mix, state-by-state). The results are visualized using HyDRA. Two areas with both low hydrogen production cost (less than $6/kg) and low associated emissions (not exceeding 550 g per mile vehicle travel) were identified. 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.

It is not surprising that key parameters (such as potential demand, feedstock costs and structure) for hydrogen production/delivery pathways analysis are both geographically and time- dependent. To account for the time variable, MSM is being linked to the HyPRO model by providing production and delivery technical data as inputs for HyPRO. HyPRO analyzes more than 100 production/delivery combinations and finds the optimal succession of production and delivery facilities depending on demand curve.

5 CONCLUSIONS

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. 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.

The 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.

Currently, MSM is developed to include spatial and temporal analysis tools. When using geo-spatial information from HyDRA as inputs for MSM, the output becomes geographically specific and is visualized within HyDRA. ‘Live’ interaction between the models is being developed. HyPRO is linked with MSM as a technology evolution analysis tool.

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