



Macro System Model (MSM) User Guide

Version 1.3

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SRA International, Inc.

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List of Acronyms

API	Application programming interface
DBMS	Database management system
DOE	Department of Energy
DTI	Directed Technologies, Inc.
EIA	Energy Information Administration
FCT	Fuel Cell Technologies
GDS	Global data set
GHG	Greenhouse gas
GIS	Geographic Information System
GREET	Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation
GUI	Graphical user interface
HDSAM	H2A Delivery Scenario Analysis Model
HyARC	Hydrogen Analysis Resource Center
JRE	Java Runtime Environment
MSM	Macro System Model
NREL	National Renewable Energy Laboratory
SEPI	Systems Engineering and Project Integration Office
SNL	Sandia National Laboratories
WTW	Well-to-Wheels

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1.0 Guide to MSM User Types

The structure and capabilities of the Macro System Model (MSM) allow it to address the diverse needs of its users. Some users may desire only a “snapshot” of different technologies and pathways while others may wish to investigate options in more detail, searching for answers to specific techno-economic and environmental concerns. This section describes the differing perspectives of end users and the range of approaches to utilizing the MSM. There is some overlap among these perspectives and processes. The end user types may be categorized as:



Basic User



Comprehensive User



Model Developer



Software Architect



System Administrator



1.1 Basic User

The primary value of the MSM is its ability to link existing models across multiple platforms, allowing for consistent cross-cutting analysis. The basic users of the MSM, such as researchers, policymakers, and analysts, will find the tool useful for quickly analyzing a variety of scenarios using industry-accepted assumptions. Section 3 of this manual provides further detail to assist users in navigating the graphical user interface (GUI) of the model.

The MSM has been designed to allow users to analyze the financial, environmental, transitional, geographical, and R&D issues associated with the transition to a hydrogen economy. Basic end users can use the MSM to answer cross-cutting questions that were previously difficult to answer in a consistent and timely manner due to variations in assumptions and methodologies among different models. Examples include the following:

- What is the comparison of hydrogen costs at the pump using different hydrogen production technologies?
- How much fossil fuel versus renewable energy use does a given hydrogen pathway require?
- What is the overall efficiency of the pathway considered versus the efficiency of its components?
- How much hydrogen needs to be produced to supply a given city's demands and what are the raw materials needed to meet those demands? What is the resulting emissions profile if hydrogen is produced to meet a given city's demands?
- How might different locations affect the economics, energy requirements, and emissions of hydrogen pathways?
- Does a specific technology make more sense in one location than another?
- How do potential transition pathways compare and what impacts could competing technologies have on transition?



1.2 Comprehensive User

After exploring the basic user capabilities of the MSM, comprehensive users may find that they need additional functionality. These users can manually edit the input.xml file (see section 4.3) for direct submission to the application server. Although this option affords more flexibility, it is important to note that only minimum error checking takes place on the input file; results obtained by the comprehensive user need careful consideration. It is therefore necessary that comprehensive users have an advanced understanding of the input parameters they are examining. This option enables the user to perform more detailed analyses and to explore different outputs. Details are further explained in section 4.



1.3 Model Developer

Model developers for models such as H2A Production update the MSM scripts and application programming interfaces (APIs) of their own models as the MSM is updated. The MSM scripts and APIs perform the data transfer between the component model and the MSM structure, so the MSM model developers need to identify parameters to transfer between models, explore how their models interact with the MSM framework, and add those parameters to the model scripts and APIs. Model developers do not necessarily need to modify the scripts and APIs but will initially work with the MSM principal investigator to perform these tasks.



1.4 Software Architect

Software architects develop the MSM, including the GUI. As the primary application developers, they understand the file structure and working with the various languages used in the MSM such as Ruby, PHP, MySQL, and Java. Currently, experts at Sandia National Laboratories (SNL) are the exclusive software architects for the MSM and are responsible for the system design and evolution. Domain expertise is provided by the principal investigator and codified by the software architects.



1.5 System Administrator

System administrators maintain computers where the component models, the executable MSM code, Web server, database management system (DBMS), and/or user interface are located. Additionally, they install application updates, perform periodic back-ups of data, and grant user access as authorized by the principal investigator. For example, component models are expected to be housed on servers at host organizations. When the MSM is linked to those models, staff at those organizations will need to become MSM system administrators to enable data transfers between their models and the MSM.

2.0 About the MSM

2.1 Description

The MSM is a simulation tool that links existing and emerging hydrogen-related models to perform rapid, cross-cutting analysis. The current version (version 1.3) of the MSM links several models, as seen in Figure 1. The H2A Production, H2A Delivery Scenario Analysis Model (HDSAM), and Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) models, along with a hydrogen-related database (Hydrogen Analysis Resource Center, HyARC) and risk analysis tools (@risk and DAKOTA), were integrated into the MSM's previous versions. These allowed analysis of the economics, primary energy source requirements, and emissions of hydrogen production and delivery pathways.

Additional capability has been added to the MSM via the integration of the models HyPro, Hydrogen Demand and Resource Analysis (HyDRA), and version 2 of GREET into the MSM. HyDRA brings the spatial component into the analysis, and HyPro allows for temporal evaluations. While the MSM was only able to investigate the fuel cycle before, the addition of version 2 of the GREET model has enabled the vehicle cycle to also be taken into consideration in analyses.

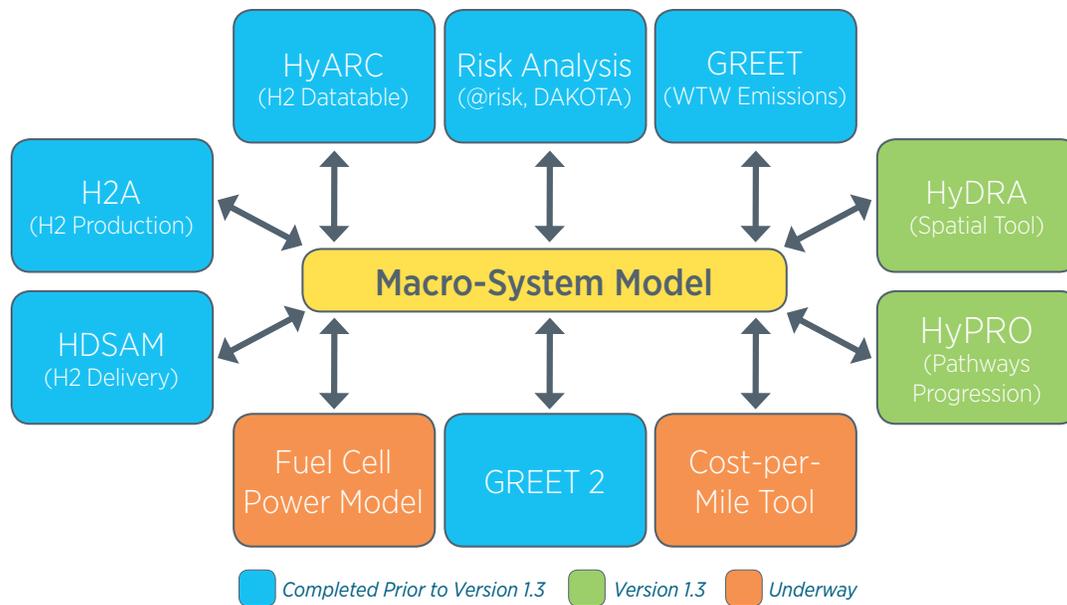


Figure 1. Models and tools integrated into the MSM

The MSM simulates cost, energy use, and emissions of the entire hydrogen system (including feedstock, conversion, infrastructure, and vehicles), and its analyses and sensitivity runs can provide a basis for decisions regarding focus of research needs. The MSM operates as a central hub to guarantee consistency in simulations that involve multiple models. A GUI allows users with minimal understanding of the models to use them. 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. Since the models are linked and data are consistent, the MSM can assist analysts in understanding the effects of changing scenarios (i.e., hydrogen production/delivery options) and parameters (e.g., efficiencies and unit costs) on the pathway costs, well-to-wheels (WTW) energy requirements, and WTW emissions.

The MSM was jointly developed by the Systems Engineering and Project Integration Office (SEPI) at the National Renewable Energy Laboratory (NREL) and SNL. The SEPI provides domain expertise and leads the project; SNL provides computer science expertise.

2.2 Goals and Objectives

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) Fuel Cell Technologies (FCT) Program. In addition, the MSM may be used to guide the development of other similar simulation tools.

The MSM was developed to accomplish the following specific objectives:

- To perform rapid, cross-cutting analysis through a single model 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.

2.3 Scope

The MSM can currently perform pathway, also known as 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.

2.3.1 Pathway/WTW Analysis

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. Pathway analysis 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, 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.

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 following are pathway-defining user inputs:

- Hydrogen production and delivery technology type and size
- Technology year
- Feedstock used
- City size
- Hydrogen vehicle market penetration rate
- Vehicle fuel economy
- Regional resource costs and characteristics

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 (CO₂, CH₄, N₂O, 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 are currently included in the MSM and made available in its GUI:

- Central production technologies¹
 - 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
 - High temperature electrolysis with nuclear reactors (Available in 2015+)
- Distributed production technologies
 - Electrolysis
 - Natural gas reforming
 - Ethanol reforming
- Delivery technologies
 - Piping of gaseous hydrogen
 - Truck transport of liquid hydrogen

1. Production is distributed when hydrogen is produced at refueling stations; central production requires hydrogen delivery from the hydrogen production facility to refueling stations.

2.3.2 Additional Analysis Capability

As additional component models are integrated into the MSM, the structure and components of the MSM allow users to discover answers to more complex questions regarding the market dynamics and infrastructure needs related to transitioning to a hydrogen economy. Work is underway to integrate models related to hydrogen's use for stationary power generation, use of biogas for hydrogen, and vehicle cost.

2.4 Model Structure

The general framework of the model is:

- **Extensible:** Accommodates new models with minimal difficulty
- **Distributable:** Can be used by multiple people in different areas of the country
- **Scalable:** Can be scaled to large numbers of participating models.

Figure 2 illustrates how the MSM software application interconnects the component models:

- **Unifying Framework:** This framework is implemented in the Ruby scripting language and consists of model APIs, model control scripts, unit conversion facility, global data set (GDS), and execution control.
- **Graphical User Interface:** The GUI is implemented in Java and delivered via Java Web Start and the user's installed browser.
- **Database Management System:** The DBMS is implemented in MySQL and contains archived jobs and user data.
- **Web Services:** Some component models are housed in different locations and Web services are used to allow communication via HTTP.

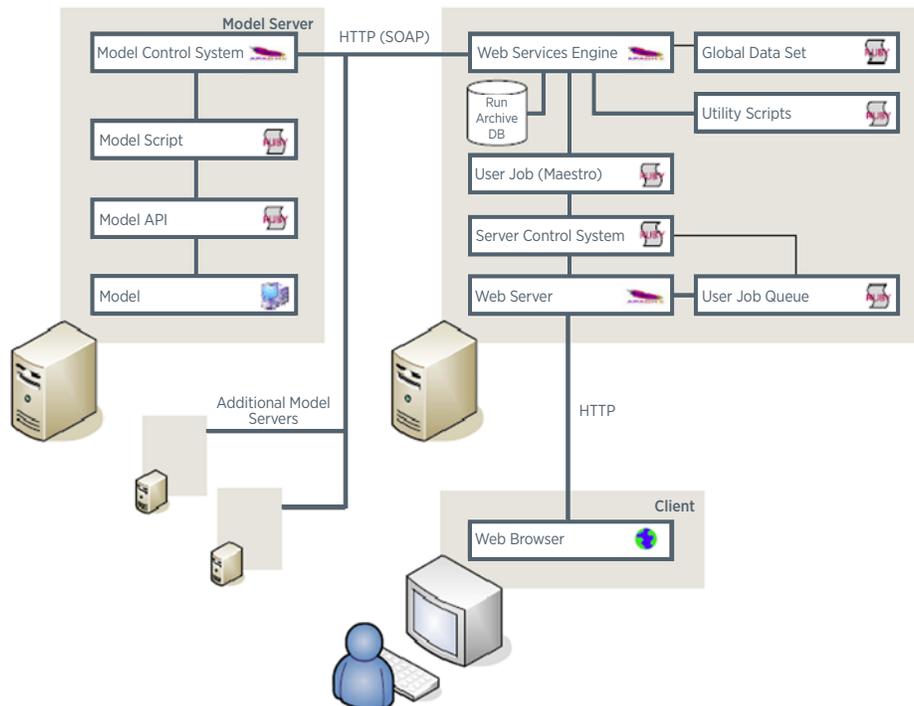


Figure 2. MSM operation process

Through the GUI, the user inputs variables such as timeframe, production technology, feedstock, delivery method, city size, and penetration of the technology. 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 also 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 most of the back-end resources on a single server (application server) while some models and their APIs are located at the model owner's/developer's site or other location (model server).

2.5 Component Models

To date the MSM integrates the following models:

HyARC

<http://hydrogen.pnl.gov/cocoon/morf/hydrogen>

HyARC provides well-documented, reliable physical property information that can serve as a basis for accurate analysis of hydrogen production/delivery costs, markets, policy options, and other key analysis topics. The Resource Center features the Hydrogen Data Book (with a wide range of hydrogen and fuel cell information valuable to infrastructure analysis), links to external data from the Energy Information Administration (EIA) and other government entities specializing in hydrogen and fuel cell analysis, DOE FCT Program analysis guidelines and assumptions, and hydrogen calculation tools. Values from HyARC, including heating values and densities, are transferred to other models in the MSM to ensure consistency.

Version 1.0

HDSAM

http://www.hydrogen.energy.gov/h2a_delivery.html

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.

Version 2.2

H2A Production and Case Studies

http://www.hydrogen.energy.gov/h2a_production.html

http://www.hydrogen.energy.gov/h2a_prod_studies.html

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 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. Case studies were built on the H2A Production model where the process characteristics and parameters are defined for some hydrogen production processes. In the MSM, assumptions and data on several key technologies were taken from those H2A Production case studies.

Versions 2.1.1-2.1.3

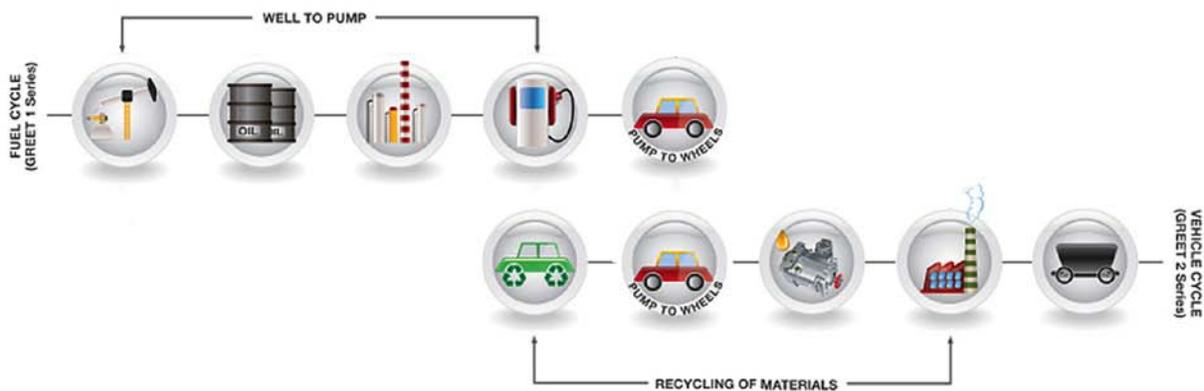


Figure 3. Fuel and vehicle cycles examined in the GREET model

REET

<http://greet.es.anl.gov>

Created by the Argonne National Laboratory, the REET model allows for the evaluation of various vehicle and fuel combinations on a full fuel-cycle/vehicle-cycle basis (Figure 3). For use in the MSM, energy requirements in H2A Production and HDSAM are converted to standard REET inputs (yields, shares, distances, etc.).

REET 1 Series

The MSM uses the REET 1 Series model (version 1.8d.1) to evaluate the fuel-cycle portion of the pathway lifecycle, allowing researchers to evaluate a fuel cycle from the well to the wheels. More than 100 fuel production pathways (e.g., corn to ethanol and soybean-based biodiesel) are included in REET 1.8d.1 to calculate the consumption of total energy, greenhouse gas (GHG) emissions (primarily carbon dioxide, methane, and nitrous oxide), and six criteria pollutants.

Version 1.8d.1

REET 2 Series

The MSM uses the REET 2 Series model (version 2.7) to evaluate the vehicle-cycle portion of the pathway's lifecycle, allowing researchers to evaluate the vehicle cycle from raw materials needed to manufacture the vehicle to its disposal or recycling. REET evaluates more than 80 vehicle/fuel systems, from conventional combustion engine vehicles to hybrids, plug-in hybrids, all-electric vehicles, and fuel cell vehicles.

Version 2.7

The MSM links these individual component models by integrating the various elements of each one that are relevant to hydrogen production, distribution, storage, vehicle technologies, and widespread deployment of a hydrogen fueling infrastructure. Figure 4 demonstrates the hierarchy of data, beginning with physical properties from HyARC feeding into delivery data from HDSAM, followed by production data from H2A Production, and finally accessing vehicle and WTW data from REET (delivery data is generated before production to set the city parameters and will be used to scale production facilities in the future). Data from the most applicable model is used in cases where models may contradict. In such a case, data are taken from the component model that is believed to include the most detail and accuracy. For example, for hydrogen production yield values, H2A Production data are preferred over data from REET, or HDSAM data are preferred over REET data for liquefaction-efficiency values. In some cases, users are able to decide which values to use, such as in the case of vehicle fuel economy, with which the users may opt to use values from HDSAM or REET or enter their own.

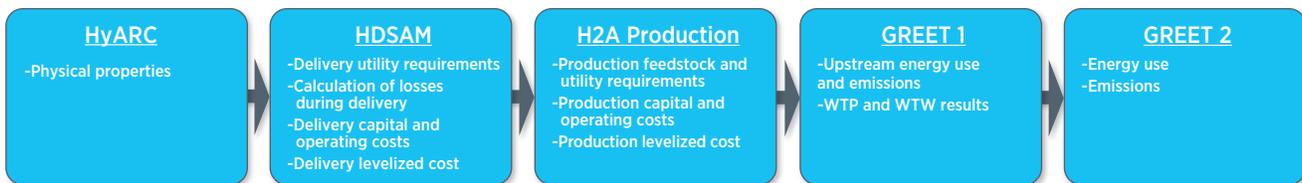


Figure 4. Hierarchy and types of data extracted from the component models to feed into the MSM

Apart from the above models that are fully integrated with the MSM, there are the following auxiliary models:

HyDRA

<http://maps.nrel.gov>

HyDRA is a Web- and geographic information system (GIS)-based spatial model created by NREL. It allows users to view, download, and analyze hydrogen data and how these data vary across the United States on a regional basis. There are currently more than 90 datasets available in the system, including resource cost and availability, hydrogen production potential, hydrogen production cost, resource consumption, hydrogen demand, infrastructure, and results from integration with other hydrogen models. The ability to run the MSM from within the HyDRA application provides access to a significant number of additional datasets and allows for automatic updates of HyDRA datasets that relate to hydrogen production.

HyPro

http://www.hydrogen.energy.gov/pdfs/progress07/viii_1_james.pdf

The HyPro model simulates the build-out of hydrogen production facilities during the transition from gasoline internal combustion engine vehicles to hydrogen fuel cell vehicles. It calculates the expected “pump price” of hydrogen (i.e., the cost of hydrogen ready to be dispensed into a customer’s vehicle at the dispensing station) for a variety of production/delivery/dispensing pathways over a span of years. HyPro postulates the yearly hydrogen demand and calculates which supply infrastructure pathway is expected to provide the cheapest hydrogen in any given year. This results in a prediction of how the infrastructure would be built out over time. This build-out prediction takes into consideration technology changes over time, underutilization of facilities in the early years of a station coming on line, potential stranded assets, feedstock cost differences, economies of scale in the production equipment, and “learning curve” capital cost reductions due to fabrication of multiple systems.

2.6 Restrictions, Assumptions, Constraints

Because individual component models pre-date the MSM in many cases, they have functionality apart from their use in the MSM. Modification of these models to facilitate their incorporation into the MSM is undesirable and should not be necessary. The MSM was designed so that it will be able to accommodate the interaction of models that may be run only remotely from their original institutions. Default assumptions in the MSM are based on assumptions included in the component models.



2.7 Validation Methodology

The MSM developers first consulted with each of the component models’ developers to ensure a full understanding of each model’s purpose, its intended use, and its inputs and outputs, which were incorporated into the MSM before utilizing the model within the MSM. Exhaustive lists of inputs and results were compiled based on these discussions. As the component models were linked to the MSM, terms were defined and calculation methodologies were created. Gaps and additional research needs were identified through this validation process and were fed back to the developers of each individual component model.

Once the component models were linked by the MSM, many comparisons to other analyses were also performed. This involved a meticulous review of inputs and results as well as mapping between results from different analyses, including various production and delivery methods. If differences between the analyses were caused by inputs or outputs omitted by the MSM, they were added to the MSM.

As more members of the hydrogen community use the MSM, interactions will take place to discuss findings and methodologies in more detail and to reach consensus on the MSM approach and defined parameters. Many of the expected users are also developers of component models, and this process is expected to also provide feedback to their modeling efforts. This process will create a continuous information feedback loop between MSM users and developers of both the MSM and component models.

3.0 Operating the MSM as a Basic User

The GUI of the MSM is a convenient and easy-to-use tool to aid those investigating different technology pathways in the transition to a hydrogen economy. This section of the user guide describes steps to follow in navigating this interface, inputting parameters, and obtaining/viewing results.

3.1 Getting Started

To get started, go to the MSM website at <http://h2-msm.ca.sandia.gov/>.



TIP: For any questions related to the model, contact msm@nrel.gov.

If this is your first time accessing the model’s online interface, you will need to request a user name and password. Click on the “new users” button on the left of the page (Figure 5) to email your request. Your user name and password will then be emailed to you.

If you have used the online interface of the model before, click on the “current users” button on the left of the page (Figure 5).



WARNING: The MSM currently does NOT launch automatically from the Google Chrome browser, due to the way the browser interacts with Java Web Start.

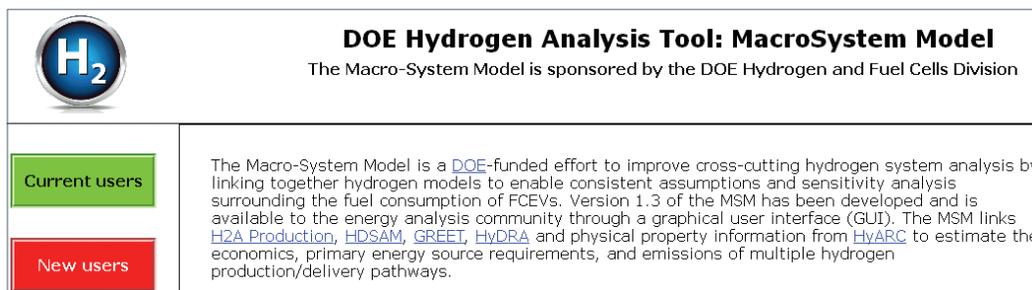


Figure 5. Requesting a new user name and password or logging in to the MSM

When launched, the installed version of the Java Runtime Environment (JRE)² on the user’s computer is automatically checked, and a locally signed Java Application Archive file is presented to the user to accept for downloading. As this is a locally signed file, a warning message will indicate that “the application’s digital signature cannot be verified” (Figure 6). The user may select “Always trust content from this publisher” to avoid seeing this prompt again in the future.



Figure 6. Locally signed Java application archive file



TIP: If Mozilla Firefox is the user’s preferred browser, once Java Web Start is selected, a dialogue box will be displayed. The option “Open with Java Web Start Launcher” should be selected.

A login dialogue box is then displayed (Figure 7), and the user provides the user ID and password. The “Mode” select box allows the user to choose which interface to operate under in inputting data and analyzing.³ After this, the user is able to view the GUI of the model (Figure 8) and start performing simulations.

2. The application is compiled under Java Development Kit (JDK) 6 and thus requires JRE version 6. The application will not start if there is a mismatch with the JRE version on the user’s computer (or if Java is not installed at all). Users should first check that Java is installed on their computer and install version 6 if they have an older version on their computer. If users are unsure, the “Do I have Java” link provided on the Java website (<http://www.java.com>) will check to see if Java is installed. If so, it will indicate the version installed, providing the user with an option to install the latest updates.

3. Currently, the “Interactive” mode is the only option available to the user.



Figure 7. Login dialogue box

Three tabs appear at the top of the GUI (Figure 8):

- **Interactive:** Use this tab to specify inputs or to select values to perform WTW analyses of different cases; more details are provided below.
- **Upload file:** This tab allows users to upload their own set of data to run simulations.
- **Multi-param:** This tab allows for the analysis of additional parameters beyond WTW.

These tabs correspond to the three modes shown in the login dialogue box (Figure 8), allowing users to switch between modes when using the model.

3.2 Defining a Basic Pathway

Upon login, the user is by default taken to the “Interactive” tab. The left-hand pane of this tab allows users to select basic parameters related to factors such as the analysis timeframe, technology options and characteristics, market penetration, and region-specific values to be able to carry out a basic run.

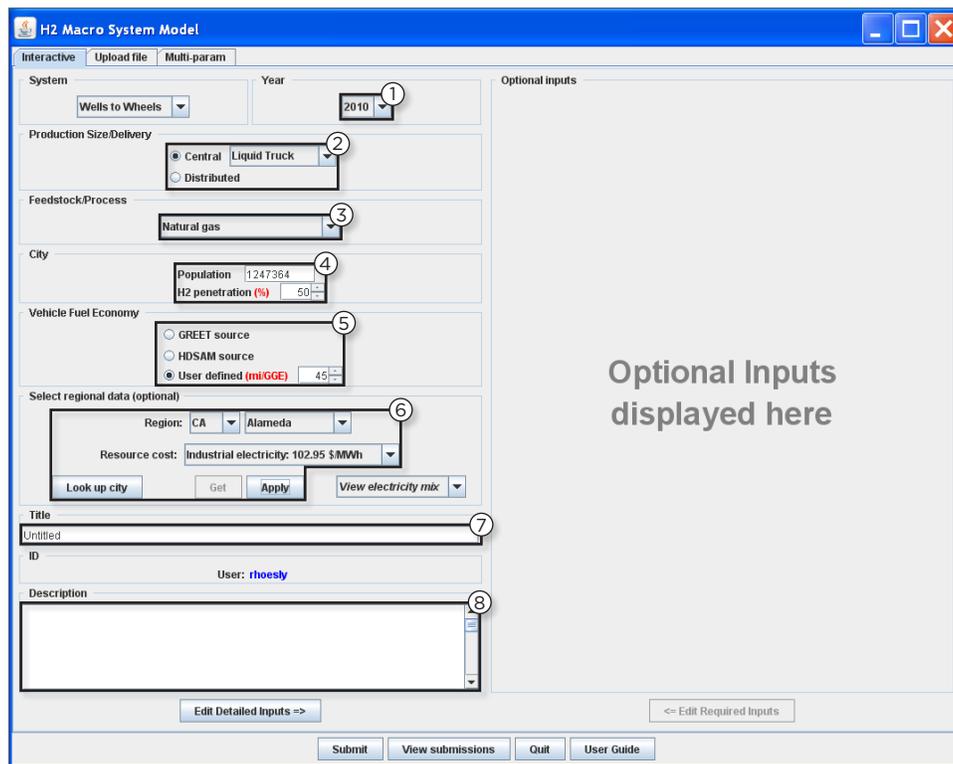


Figure 8. The MSM GUI (required inputs)

1. Select the starting year of the simulated production/delivery scenario.
2. Select the scale/location of hydrogen production (i.e., central or distributed production) and the delivery mode for cases with central production (i.e., gaseous hydrogen via pipelines or liquid hydrogen via trucks).
3. Select the feedstock to be used in generating the hydrogen.
 - a. For “central production”: Coal gasification (with or without carbon sequestration), steam methane reforming (SMR) of natural gas (with or without carbon sequestration), nuclear high temperature electrolysis (for years 2015+), wind electrolysis, and biomass (woody) gasification.
 - b. For “distributed production”: Electrolysis (using grid electricity), ethanol reforming, and on-site SMR of natural gas.
4. Select the city characteristics. Users may select the population and hydrogen market penetration values to be considered. The default range of “50,000 and 20,000,000 inclusive” is given for population, and a minimum of “5%” is given for the hydrogen’s market penetration percentage.
5. Select the vehicle fuel economy. Here, users may either select their own value or allow the MSM to use default values used in GREET or HDSAM.
6. Optional input: Select regional data. This optional input allows the user to be more specific in feedstock and energy prices to be used in the process selected. This regional information is provided by the HyDRA model. As a default, the model uses U.S. average values and characteristics for resources. However, the user has the option here to determine resource values more specific to the region of choice:
 - a. Select the region (state and county). Users may not always be familiar with counties. The “Look up city” button here takes the user to the U.S. Census Bureau website, where users may locate a county name by entering a city/town name or zip code.
 - b. Click the “Get” button. This will activate the “Resource cost” drop down menu, which shows the region-specific costs for utilities. The “electricity mix” option is also activated, where users may view the mix of resources used for electricity production in that region.
 - c. To select utilities, first select an option from the “Resource cost” drop down menu, and then click the “Apply” button to apply the selection to the model run. If more than one selection is desired, the next selection may be made, and again followed by the “Apply” button. Note that the system will not display any notice to acknowledge that the selection has been applied. Users may see the details of their selections when using the “Detailed Inputs” pane (see 3.3 Entering Detailed Inputs).



WARNING! If the “Apply” button is not selected, the model does NOT take the selection shown in the drop down menu into account – it carries out the run with default U.S. average values. The “Apply” button is needed to activate your selection.

7. Optional input: Name your model run in the “Title” field.
8. Optional input: Note any details you wish about the run in the “Description” field.



TIP: It is useful to get into the habit of naming your model runs and even providing a short description, as it is easy to forget the run specifics after a couple runs.

3.3 Entering Detailed Inputs (Optional)

The right-hand pane is an optional input area, which allows users more flexibility and details by enabling the user to view variable values and assumptions, and to view which model is being used to pull data from (or if a variable is using user-defined values). It also allows users to enter their own values in place of the values defined by default. The detailed inputs are listed in the Appendix.

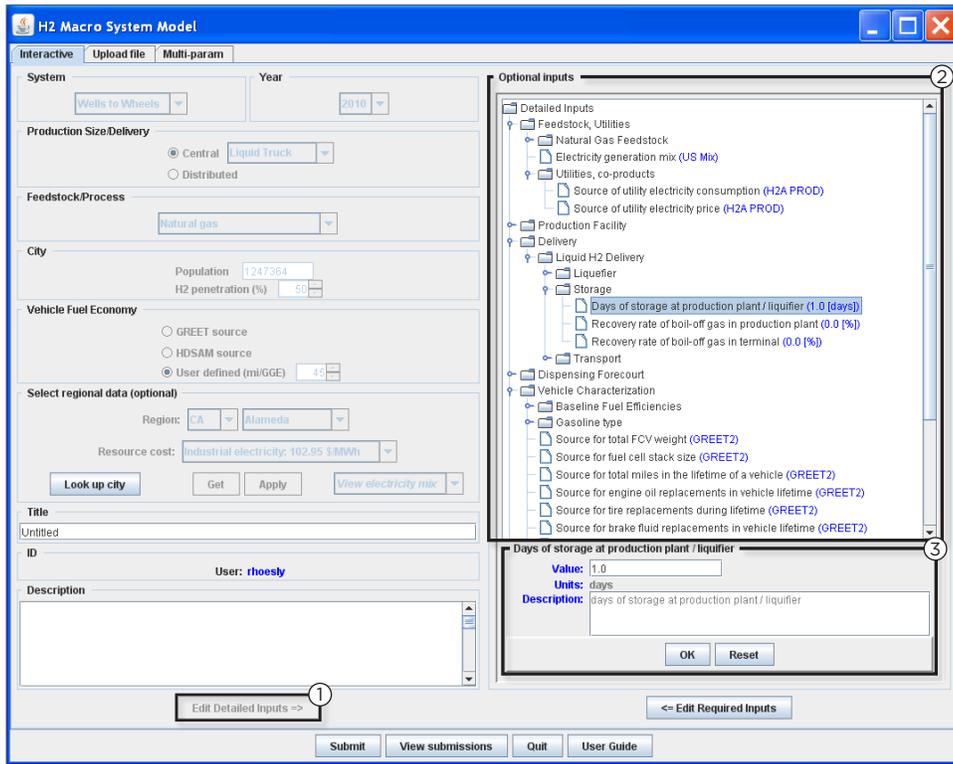


Figure 9. The MSM GUI (optional inputs)

1. Switch to the right-hand pane by clicking the “Edit Detailed Inputs” button.
2. To view details, click on the related variable group and choose the specific variable.
3. The bottom part of the pane will display the variable value, units, and a short description. Here, the user may override the default value and enter a user-defined value.



WARNING! Make sure to click “OK” to apply the user-defined value.

WARNING! Once selections on the right-hand pane are made, if the “Edit Required Inputs” button on the lower part of the pane is selected (to switch to the left-hand pane), all the user-defined values in the right-hand pane are reset to default values. This is because the optional inputs are dependent on the required inputs. If the required inputs are modified, previous values of optional inputs may be rendered invalid. Also, the region-specific resource costs applied on the left-hand pane are lost (the state/county selection remains, but the resource cost values need to be applied again).

3.4 Submitting the MSM Job

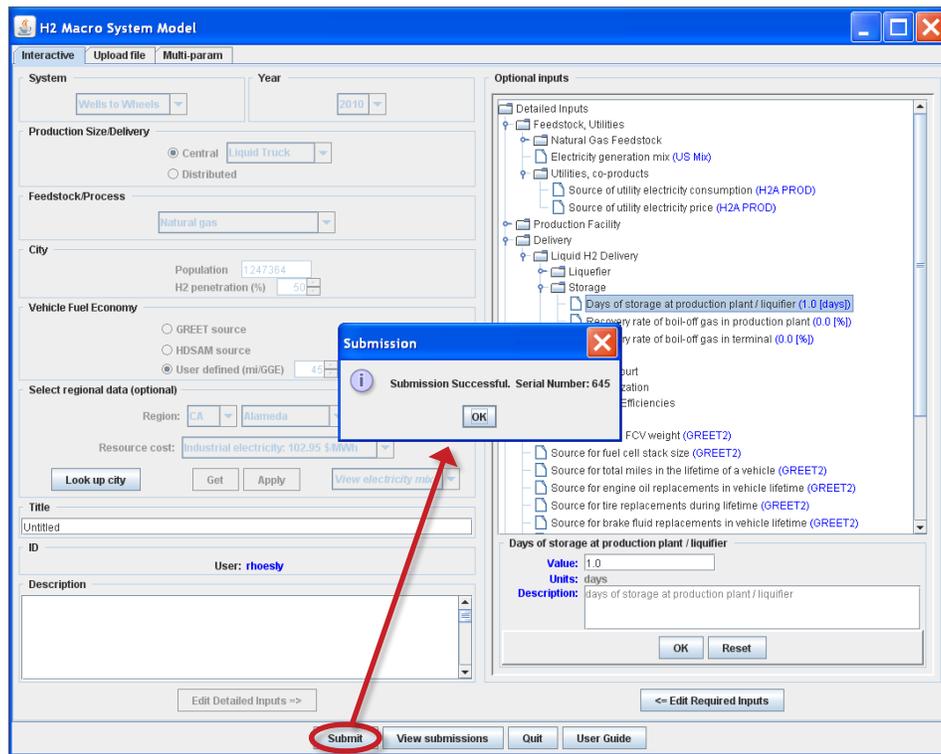


Figure 10. Submissions dialog box

1. WITHOUT clicking the “Edit Required Inputs” button, click the “Submit” button on the lower part of the screen.
2. Now the information about the pathway and detailed input values is sent to the MSM server and an MSM job runs. This takes a few minutes or more, depending on the complexity of the run.
3. A dialogue box appears with a submission notice and run number. If an error message appears instead, a miscommunication between the local computer and the MSM server occurred. In this case, it is recommended that the user close the GUI windows and log in to the MSM website again.
4. When “OK” is clicked, a “Simulations” menu appears. This menu shows that the submitted job is a “new” job. Previously completed runs will show as “complete,” and simulations that ran with errors will show as “error.” When the server finishes running the job, its status will change to “complete.”
 - a. Click the “OK” button and the Simulations menu disappears.
 - b. Click the “View submissions” button and the Simulations menu is back on.
5. When the job is complete, the user will receive an email notification (to the email address provided when first signing up as a user).

3.5 Viewing Results



Figure 11. Simulations menu

1. In the Simulations menu, select the MSM run of interest. (Its status should be “complete.”)
 - a. Clicking the “Get Info” button shows the job description (that the user filled in when defining the job before its submission).

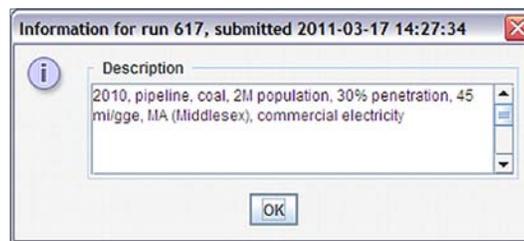


Figure 12. Model description dialogue box

- b. Clicking the “Download results” button will prompt the user to save the output file (run_number.csv) to the location specified by the user. Open the run_number.csv file on your computer. It shows the complete list of parameters acquired in the MSM run.
 - c. Clicking on the “Download input file” button will prompt the user to save the complete list of XML instructions for the MSM. This file can later be uploaded by the user to the server to repeat the same run.
 - d. Clicking on the “View output” button will bring up the Fuel CycleH2 Pathway chart (to view fuel-cycle results) for the selected MSM run. On the bottom right corner of the chart screen, in the drop down view menu, select Vehicle Cycle chart (to view vehicle-cycle results) or select Output Tree (to view the details of both the input and output values).

The Output Tree displays all inputs and outputs through high-level folders (to indicate the pathway components, as well as the overall pathway), and lower level categories under these folders display the detailed values. The most important model inputs are displayed under the high-level folder “Pathway Defining Parameters,” while outputs are shown under the other high-level folders. When an input or output is selected, the bottom part of the screen displays the input or output value, its units, its source, and a short description.



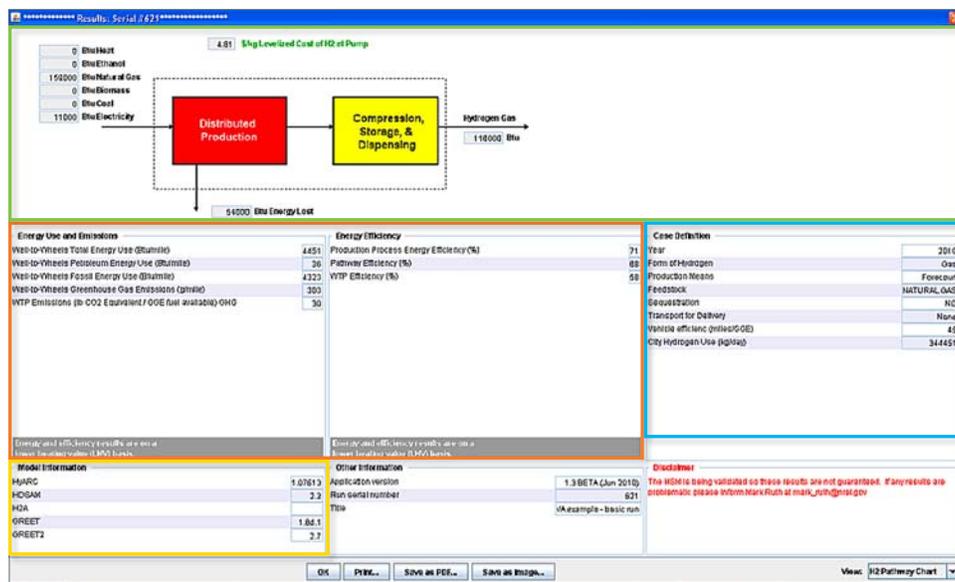
TIP: In the Output Tree, one variable could be seen in more than one place.

In the Fuel Cycle and Vehicle Cycle charts, the top part of the window will display the components and energy flow of the case examined in graphical form. Right below the diagram, the following information will be displayed:

- Levelized Cost of Hydrogen at the Pump (\$/kg)
- Energy Use and Emissions
 - › WTW Total Energy Use (Btu/mile)
 - › WTW Petroleum Energy Use (Btu/mile)
 - › WTW Fossil Energy Use (Btu/mile)
 - › WTW GHG Emissions (g/mile)
 - › Well-to-Pump (WTP) GHG Emissions (lb CO₂-equivalent/gge fuel available)
- Energy Efficiency
 - › Production Process Energy Efficiency (%)
 - › Pathway Efficiency (%)
 - › WTP Efficiency (%)
- Case Definition: The required inputs entered by the user when setting up the simulation are displayed here.
- Model Information: The component models (and their versions) used are displayed here.

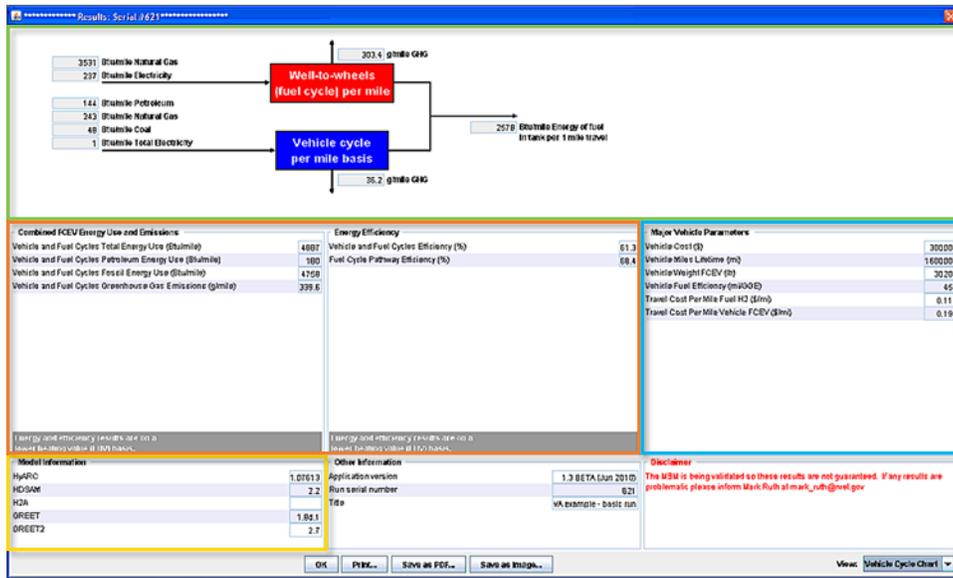
After inspecting the results, the user may then print this results page or save it as a PDF document or as an image by selecting the appropriate buttons. Multiple results may not be viewed at the same time. To compare different cases, the user can either print results or download data to manipulate it according to individual needs.

2. Clicking the “OK” button of the active window closes the graphical display of results and brings the user back to the inputs GUI interface.



- Graphical Output of Results
- Model Outputs
- Model Information
- Model Inputs

Figure 13. Display of results – fuel pathway chart



Graphical Output of Results Model Outputs Model Information Model Inputs

Figure 14. Display of results - vehicle cycle chart

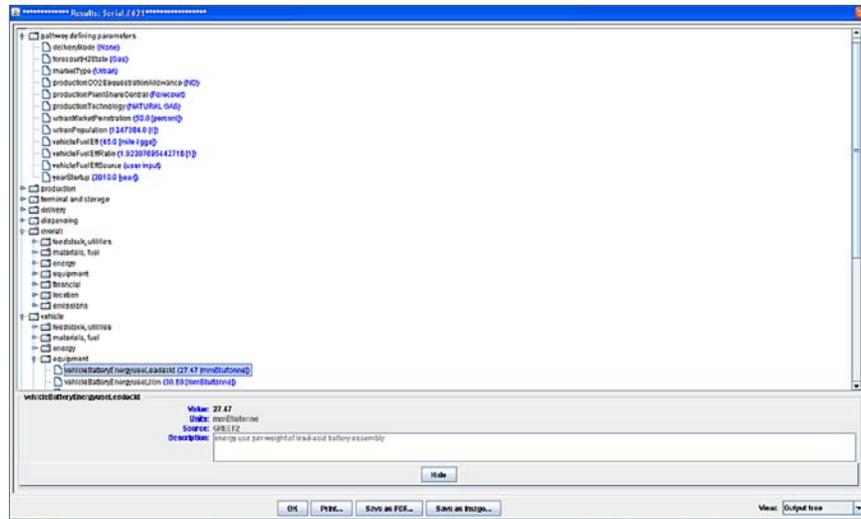


Figure 15. Display of results - output tree

3.6 Viewing Results through the HyDRA Interface

The NREL HyDRA component model gives MSM users the ability to perform spatial analysis of simulations. This is useful for analyzing hydrogen production and delivery costs and emissions as they vary over specified regions. From the MSM GUI, users have the option to add HyDRA data through the “Select regional data” interface (see #6 of section 3.2). For more advanced spatial graphical results, users can run MSM simulations through the HyDRA model. To do this, users first must create a HyDRA account through the website⁴ via the “Create new account” option on the login page, reached after clicking “Launch” as seen in Figure 16. Email confirmation from the HyDRA administrators will activate new accounts.

4. <http://maps.nrel.gov>.

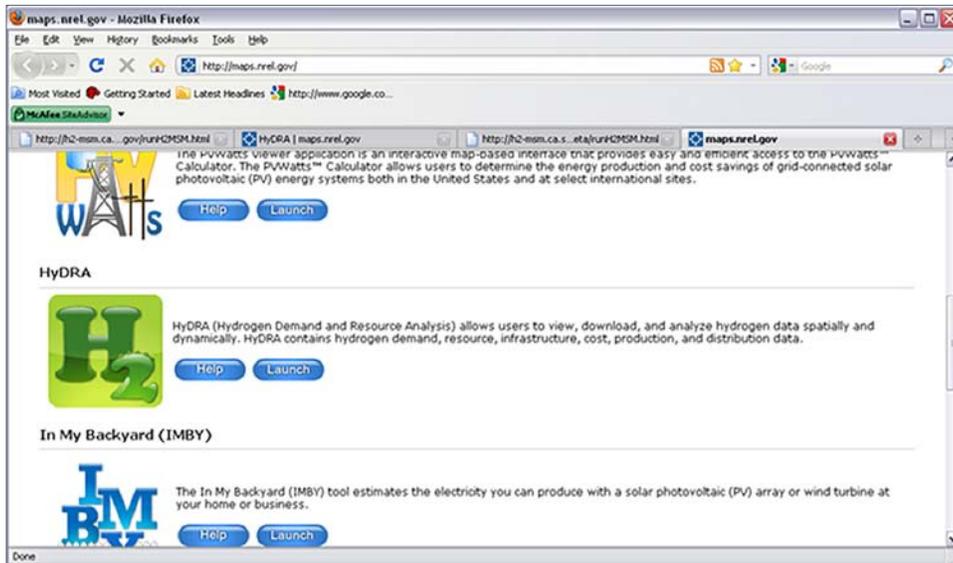


Figure 16. NREL HyDRA website

Upon account activation, users may access HyDRA to perform MSM simulations. As shown in Figure 17, MSM simulations through HyDRA require minimal user inputs. Users can follow the steps below for submitting a simulation:

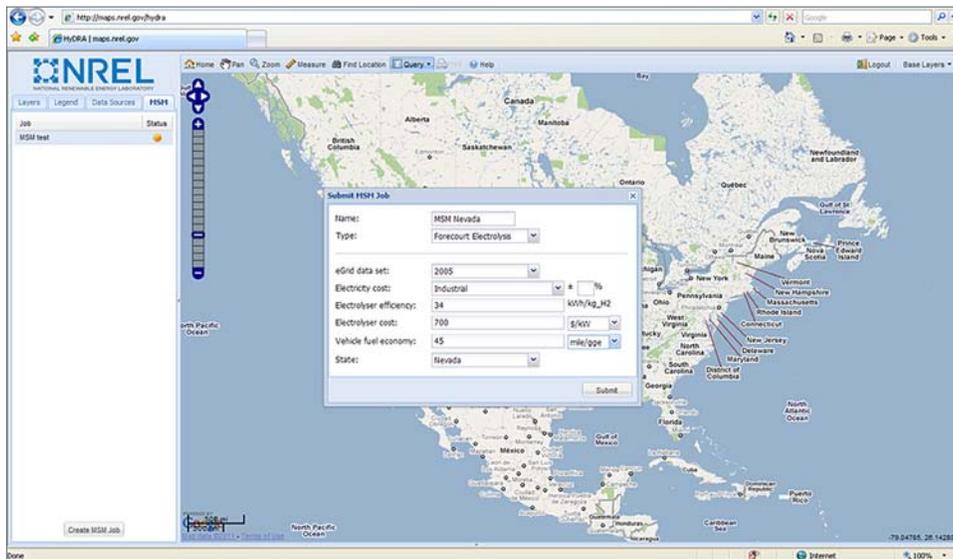


Figure 17. MSM simulations through HyDRA

1. Click “Accept” on the Users Agreement pop-up (not shown) upon logging into HyDRA.
2. Select the “MSM” tab in the pane on the left.
3. To view results of previous submissions, simply click the desired simulation, and a pop-up window will appear listing the status and results of the submission.
4. To create a new submission, click the “Create MSM Job” at the bottom of the left pane.
5. This will open a pop-up, where some limited input data can be entered.
6. To complete the simulation, simply click “Submit.”
7. To view results from a HyDRA submission, click the desired simulation on the MSM tab as seen in Figure 18.

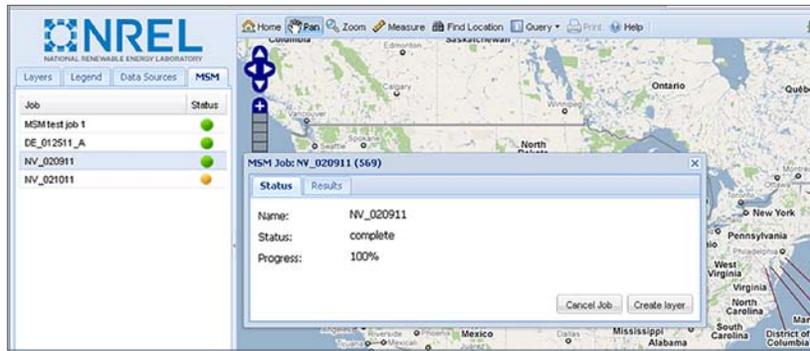


Figure 18. Results of a HyDRA submission

8. Simulations must be completed before viewing; a green circle next to the simulation indicates completion, while a yellow circle indicates a simulation in progress.
9. Once a completed simulation is selected, a pop-up will appear. For graphical results, select “Create layer” from the “Status” tab.
10. A new pop-up will appear indicating successful creation of the map layer.



Figure 19. Pop-up indicating creation of map layer

11. The available map layer results will be listed under the name of the simulation on the “Layers” tab.

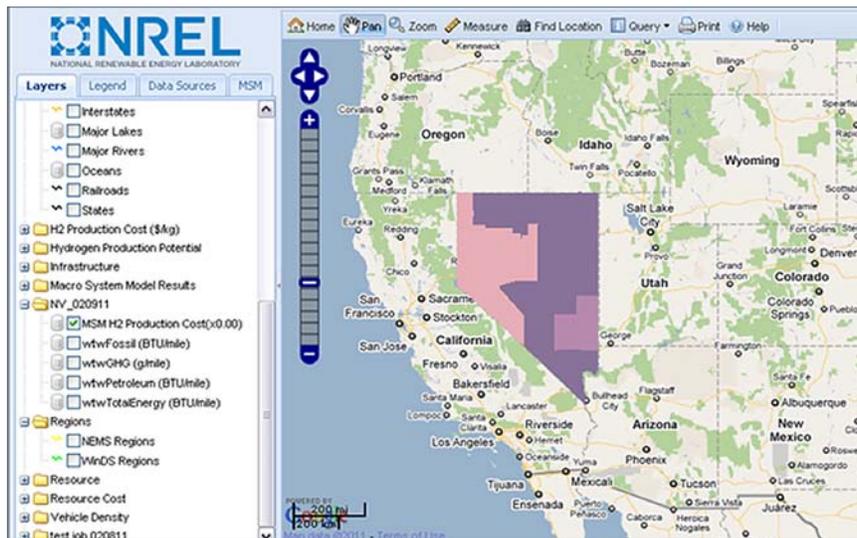


Figure 20. Map showing MSM HyDRA results

12. To view the map showing the MSM HyDRA results, users must check the checkbox corresponding to the simulation results that they wish to view.
13. This will apply the layer to the displayed map.
14. Users may then click the “Legend” tab to interpret the spatial results.

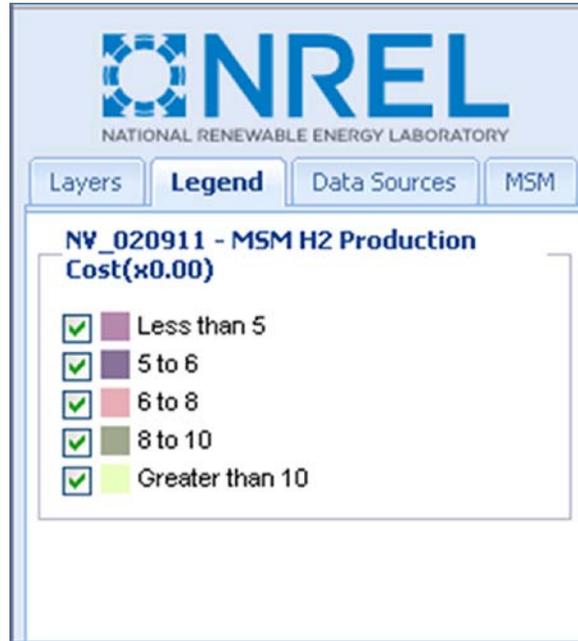


Figure 21. Legend tab output



4.0 Operating the MSM as a Comprehensive User

4.1 Getting Started

Comprehensive users should be familiar with the basic user functions of the MSM before using the comprehensive version. Comprehensive users perform more detailed analysis by running multi-parameter scenarios that allow for comparative analysis of multiple values for specific inputs and by editing the .xml input files through the creation of a comprehensive input file customized by the user.

4.2 Running the Multi-Parameter Option with MSM

The multi-parameter run gives the comprehensive user the option to insert multiple values into the MSM’s various inputs. This is referred to as the parameter schedule. The MSM runs an amount of times that is in accordance with this schedule. This option is often used to give the MSM different distribution values and to probe sensitivities in the system. There are two methods available for preparing a multi-parameter run: using the “Multi-param” tab through the MSM GUI or creating and uploading a .csv multi-parameter schedule file.

Users can input their own sets of values into the schedule file. Often, values will be put in according to Monte Carlo distributions with X sets reflecting X iterations of a simulation. The model would then run the X sets of values through and provide the same number of output sets.

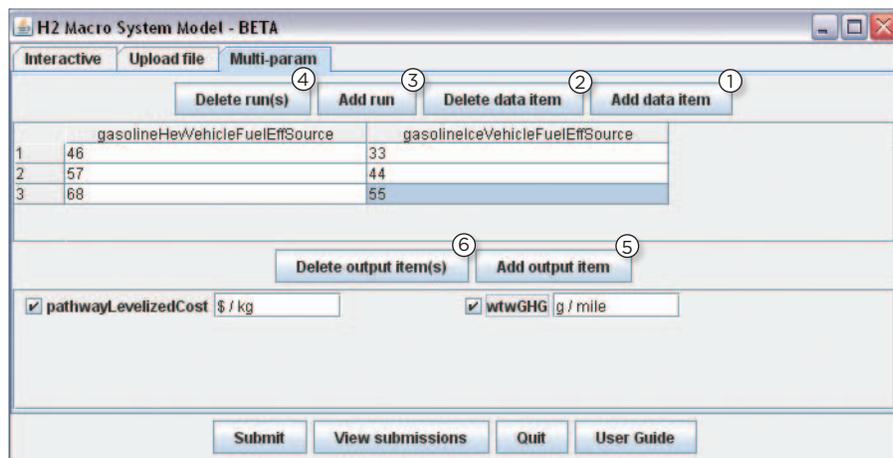


Figure 22. The MSM multi-parameter tab

1. To create a multi-parameter schedule file from the “Multi-param” tab, first select “Add data item.” An “Add data item” pop-up will appear and list all the potentially variable inputs for the simulation. Selecting a data item will create a new input column for the selected variable input data item in the top box of the tab. In this example, two data items were added: gasoline hybrid electric vehicle fuel efficiency (gasolineHevVehicleFuelEffSource) and gasoline internal combustion vehicle fuel efficiency (gasolineIcveVehicleFuelEffSource).
2. The “Delete data item” button will delete the last data item column. In this example, clicking the “Delete data item” button will delete the gasolineIcveVehicleFuelEffSource column. Data item columns can be reordered by the user through “drag-and-drop.”
3. When the variable input data items are first selected, only one data row will be available. The data displayed will reflect the simulation as set up in the “Interactive” tab, and if this data item was not altered in the “Interactive” tab, the value will be a default. These values can be changed by removing the current value and entering a new value. The “Add run” button will add a new row to all of the data items allowing users to specify multiple values for the same data items. In this example, three simulation runs have been specified.
4. The “Delete run(s)” button will delete the entire specified run for all data items. To specify a run for deletion simply select a cell in the row(s) to be deleted and click the “Delete run(s)” button.
5. In order to analyze the effects of the multiple input values from the multi-parameter runs, outputs must be specified. To select outputs, click “Add output item.” This will open an “Add output item” pop-up , which will list the available outputs. The units of the outputs can be altered, although one should take care to enter applicable and logical alternative units.
6. The “Delete output item(s)” button will delete all output items with a check in the checkbox next to the output item.



WARNING! Input data items are dependent on the simulation specified on the interactive tab and potential input items will vary accordingly, e.g., some pipeline data items are only available if “Pipeline” is selected as a delivery method.



TIP: To submit a multi-parameter run, the “Submit” button must be clicked from the “Multi-param” tab.

The other method for running a multi-parameter simulation is to create a .csv parameter schedule input file in Microsoft Excel. Users may choose this option if they prefer to prepare a simulation off-line or wish to run multiple similar simulations over a period of time. Care must be taken to properly format the .csv file as it requires specific formatting and the use of the exact MSM terms for inputs and outputs.

Below is an example of a parameter schedule file with three sets of values. The MSM will run three times with each run using a set (row) of numbers from the schedule. The formatting of the .csv file is very specific.

	A	B	C	D	E	F	G
1	#						
2	# parameter schedule for multiparameter run						
3	#						
4							
5	# names of outputs						
6	pathwayLevelizedCost	wtwGHG					
7							
8	# units of outputs						
9	\$ / kg	g / mile					
10							
11	# names of input parameters						
12	none						
13							
14	# units of input parameters						
15	none						
16							
17	# values of input parameters						
18	none						
19							
20	# names of input variables						
21		gasolineHevVehicleFuelEffSource	gasolineHevVehicleFuelEff	gasolineIceVehicleFuelEffSource	gasolineIceVehicleFuelEff		
22							
23	# units of input variables						
24		none	none	none	none		
25							
26	# values of input variables for each run						
27	run1	User Input		46 User Input		33	
28	run2	User Input		57 User Input		44	
29	run3	User Input		68 User Input		55	

Figure 23. Sample parameter schedule file

The users can input their own sets of values into the schedule file. Often, values will be put in according to Monte Carlo distributions with X sets reflecting X iterations of a simulation. The model would then run the X sets of values through and provide the same number of output sets.

Once created, the .csv input file can be uploaded into the MSM through the “Upload” tab of the GUI. In order to upload a .csv parameter schedule file, users must first upload an .xml input file. Step-by-step instructions for creating an .xml input file are below, and instructions for using the “Upload” tab are given in Figure 28.



WARNING! If there are lengthy multi-parameter runs, the user should contact the MSM team at msm@nrel.gov.

4.3 Editing the .xml Input File

The MSM GUI creates an .xml input file for each simulation run. The input .xml file contains a set of instructions for the MSM back-end process that just runs models and is not the GUI. This file can be downloaded from the “Simulations” window (Figure 24) that opens when the “View Submissions” button is clicked on the MSM GUI.

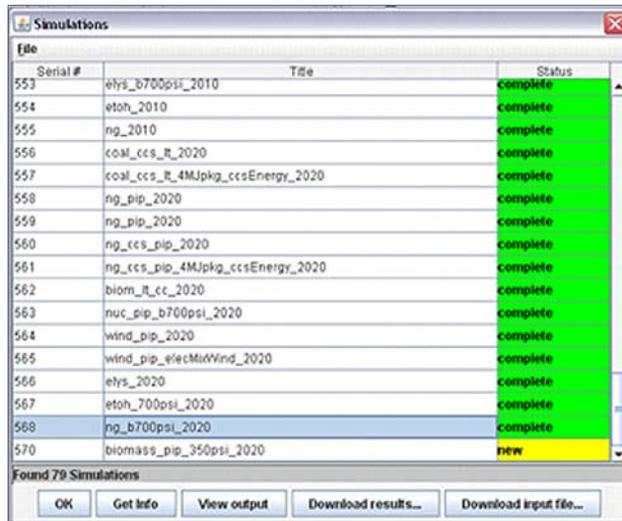


Figure 24. Simulations menu

Clicking “Download input file” will allow users to save the .xml input file from the selected simulation.

To edit the .xml file, users need to open the file in an appropriate editor (typically Microsoft Notepad). Please note that if the .xml file is double-clicked, it will typically open in an Internet browser and will not be editable. The .xml file has several sections. They are arranged as a hierarchy, and the “Required Inputs” portion of the “User Data” section is seen in Figure 25:

```

<?xml version="1.0" encoding="UTF-8"?>

  <appversion>1.3 BETA (Jun 2010)</appversion>
  <requiredinputs>
    <dataitem>
      <name>yearStartup</name>
      <value>2005</value>
      <units>year</units>
      <description>starting year of the simulation</description>
    </dataitem>
    <dataitem>
      <name>productionTechnology</name>
      <value>NATURAL GAS</value>
      <units></units>
      <description>production technology</description>
    </dataitem>
    <dataitem>
      <name>productionCO2SequestrationAllowance</name>
      <value>YES</value>
      <units></units>
      <description>CO2 sequestered in production facilities</description>
    </dataitem>
    <dataitem>
      <name>productionPlantShareCentral</name>
      <value>Central</value>
      <units></units>
      <description>central or forecourt plants</description>
    </dataitem>
    <dataitem>
      <name>deliveryMode</name>
      <value>Liquid Truck</value>
      <units></units>
      <description>how H2 is delivered to forecourt</description>
    </dataitem>
    <dataitem>
      <name>marketType</name>
      <value>urban</value>
      <units></units>
      <description>type of market</description>
    </dataitem>
    <dataitem>
      <name>urbanPopulation</name>
      <value>1247364.0</value>
      <units>1</units>
      <description>population of urban market</description>
    </dataitem>
    <dataitem>
      <name>urbanMarketPenetration</name>
      <value>50.0</value>
      <units>percent</units>
      <description>urban market penetration</description>
    </dataitem>
    <dataitem>
      <name>vehicleFuelEffSource</name>
      <value>user Input</value>
      <units></units>
      <description>source of vehicles' fuel efficiency</description>
    </dataitem>
    <dataitem>
      <name>vehicleFuelEff</name>

```

Figure 25. .xml file sections

- **Required Inputs:** Includes inputs required for hydrogen production, delivery, and dispensing pathways.
- **Optional Inputs:** Includes all of the inputs selectable in the right-hand side of the GUI. The code does not select models based on inputs from here. Instead, the user names the necessary component models in the “Execution Order” section.
- **Default Data:** Contains inputs into the component models that make up the MSM. (Please note that these values are set to specific defaults and no error-checking will be performed by the model to confirm the plausibility of edited inputs in the default data section.)
- **Execution Order:** Shows the order in which the MSM calls the other component models.⁵ This section should be edited only by changing the values (filenames), versions, and descriptions of the component models.

Editable data in the .xml file is arranged in the format of “name,” “value,” “units,” and “description.” Users may edit the “value” and “units” fields of each data entry, although care should be taken to edit only the values between the “> <” symbols. In the example below, the value for “liquidTruckTotalTime” has been changed from 1 (Figure 26) to 14 (Figure 27), and the units were changed from days to hours. This example shows how comprehensive users can edit the model to match their specific situation as opposed to using the model defaults.

```

</dataItem>
<dataItem>
  <name>liquidTruckTotalTime</name>
  <value>1</value>
  <units>days</units>
  <description>time in truck/trailer for transport</description>
</dataItem>

```

Figure 26. Original units for liquidTruckTotalTime

```

</dataItem>
<dataItem>
  <name>liquidTruckTotalTime</name>
  <value>14</value>
  <units>hours</units>
  <description>time in truck/trailer for transport</description>
</dataItem>

```

Figure 27. New units for liquidTruckTotalTime

5. The MSM runs GREET twice. The first instance is to extract some parameters from GREET to use as inputs for H2A production and delivery models, and the second instance is to obtain energy and emissions results from GREET.

The following table shows all the possible unit names accepted by the program.

Unit Type	Unit	Additional Names
Area	square_mile	mile_square, sq_mi, sq_miles, square_miles
	acre	Acre, acres, Acres
	hectare	hectares, ha
	square_feet	feet_square, sq_ft, sq_feet, square_foot
	square_inches	inch_square, sq_in, sq_inch, square_inch
Current	ampere	A, amperes, amp, amps
Coded Mix	coded_mix	Coded_Mix, Coded_mix
Energy	joule	Joule, J, joules, Joules
	megajoule	MJ, megajoules
	gigajoule	GJ, gigajoules
	Btu	BTU, btu, Btus, BTUS, btus, British_thermal_unit, british_thermal_unit, britishthermalunit, British_thermal_units, british_thermal_units, britishthermalunits
	mmBtu	mmBTU, megaBtu, megaBTU
	kWh	kWhr, kWhrs, kWhour, kWhours, kwh, kwhr, kwhrs, kwhour, kwhours, kilowatt_h, kilowatt_hr, kilowatt_hrs, kilowatt_hour, kilowatt_hours
	MWh	MWhr, MWhrs, MWhour, MWhours, mwh, mwhr, mwhrs, mwhour, mwhours, megawatt_h, megawatt_hr, megawatt_hrs, megawatt_hour, megawatt_hours
GGE	gge	GGE
J H2	J_H2	J_h2, joule_h2, joule_H2, Joule_h2, Joule_H2
	MJ_H2	megajoule_h2, megajoule_H2, MJ_h2
	Btu_H2	BTU_H2, BTU_h2, btu_H2, btu_h2, Btus_H2, Btus_h2, BTUS_H2, BTUS_h2, btus_H2, btus_h2
	mmBtu_H2	mmBTU_H2, mmBTU_h2, mmbtu_H2, mmbtu_h2, mmBtus_H2, mmBtus_h2, mmBTUS_H2, mmBTUS_h2, mmbtus_H2, mmbtus_h2
Kg C	Kg_C	
	Kg_CO2	kg_co2, kilogram_CO2, kilogram_co2
	lb_CO2	lbs_CO2, lb_co2, lbs_co2, pound_CO2, pound_co2, pounds_CO2, pounds_co2
Kg H2	kg_H2	kg_h2, kilogram_H2, kilogram_h2, Kilogram_h2, Kilogram_H2
Length	meter	m, meters
	foot	ft, feet
	inch	in, inches
	mile	mi, miles
	km	kilometer, kilometre
	cm	centimeter, centimetre
	mm	millimeter, millimetre
Light	candela	cd, candelas
Mass	kilogram	kg, kilograms
	gram	g, grams, gm, gramme, grammes
	pound	lb, lbs, pounds
	ton	tons, short_ton, short_tons
	metric_ton	mt, metric_tons
Money	dollar	\$, dollars

None	1	
	%	percent, per-cent, per_cent
	mole_fraction	Mole-fraction, mole_frac, mole-frac, mol_fraction, mol-fraction, mol_frac, mol-frac
	fraction	frac, Fraction, Frac
Power	watt	W, Watt, watts, Watts
	kilowatt	kW, kilowatts
Station	station	Station
Substance	lbmol	pound-mole
	kmol	Kmol, kmole, Kmole, kmoles, kilomol, kilomole, kilomoles, Kmoles, Kilomole, Kilomoles
Temperature	kelvin	K
Time	second	s, sec, seconds, secs
	minute	min, minutes
	hour	h, hr, hrs, hours
	day	d, da, days
	year	yr, years, y
Trip	trip	Trip, trips, Trips
	roundtrip	Roundtrip, roundtrips, Roundtrips
Truck	truck	trucks, Truck, Trucks
Truckload	truck load	Truckload, truckloads, Truckloads
Volume	cubic_meter	cubic_m, cubic_meters, m_cubed, meter_cubed, meters_cubed
	cubic_foot	cubic_ft, cubic_feet, ft_cubed, foot_cubed, feet_cubed
	liter	l, L, liters, litre, litres
	gallon	gal, gallons
	normal_cubic_foot	normal_cubic_ft, normal_cubic_feet, normal_ft_cubed, normal_foot_cubed, normal_feet_cubed, Normal_cubic_foot, Normal_cubic_ft, Normal_cubic_feet, Normal_ft_cubed, Normal_foot_cubed, Normal_feet_cubed
	normal_cubic_meter	normal_cubic_m, normal_cubic_meters, normal_m_cubed, normal_meter_cubed, normal_meters_cubed, Normal_cubic_meter, Normal_cubic_m, Normal_cubic_meters, Normal_m_cubed, Normal_meter_cubed, Normal_meters_cubed
	standard_cubic_meter	standard_cubic_m, standard_cubic_meters, standard_m_cubed, standard_meter_cubed, standard_feet_cubed, Standard_cubic_foot, Standard_cubic_ft, Standard_cubic_feet, Standard_ft_cubed, Standard_foot_cubed, Standard_feet_cubed, std_cubic_foot, std_cubic_ft, std_cubic_feet, std_ft_cubed, std_feet_cubed, Std_cubic_foot, Std_cubic_ft, Std_cubic_feet, Std_ft_cubed, Std_foot_cubed, Std_feet_cubed, scf

Table 1. Unit names

When a user is finished changing the MSM model inputs, the file should be saved as filename.xml (“filename” used for example purposes only). It is important that the .xml extension be used here.

4.4 Uploading into the MSM

Once the .xml input file and .csv parameter schedule file are completed, users can upload the files for an MSM simulation through the “Upload file” tab on the MSM GUI as shown in Figure 28.

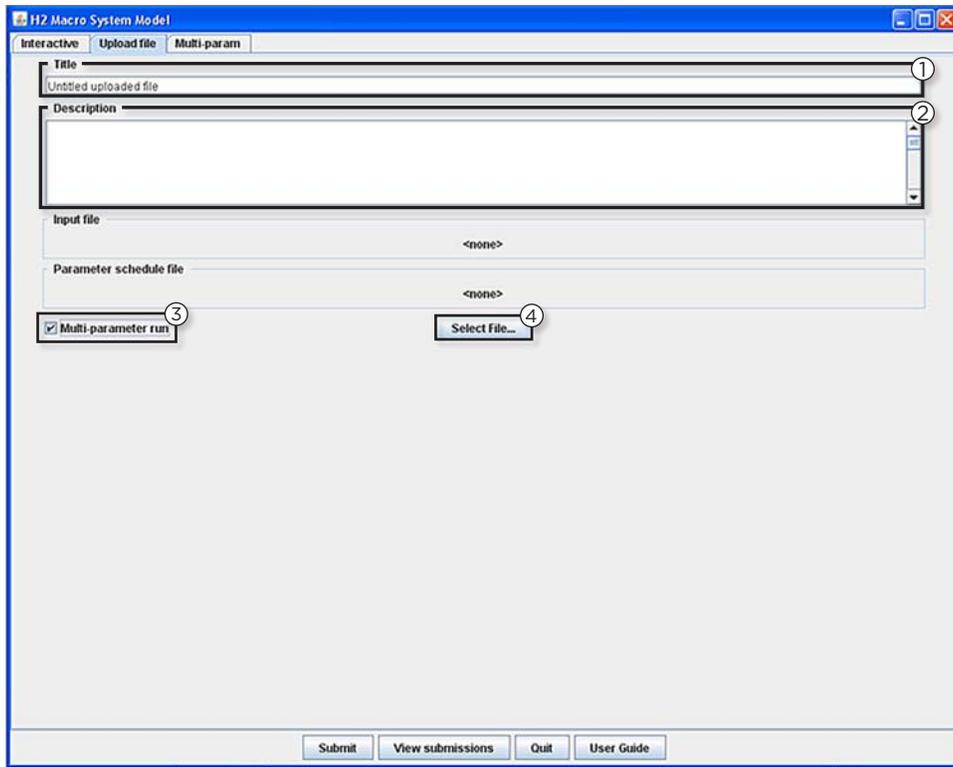


Figure 28. MSM GUI “Upload file” tab

1. The “Title” input box should be used to name the uploaded simulation.
2. The “Description” input box is used for entering a description of the uploaded simulation.
3. If a .csv parameter schedule file has been created, users must check the “Multi-parameter run” checkbox in order to upload the .csv file.
4. To begin uploading, click the “Select File...” button. The first pop-up allows users to select a previously prepared .xml input file. If “Multi-parameter run” is checked, a second pop-up will immediately appear so users can select a previously prepared .csv parameter schedule file. Proper formatting is required for both files; otherwise users will receive an error. For information on proper formatting, see section 4.2 and section 4.3.



WARNING! To upload a .csv parameter schedule file, users must first upload an .xml input file. A simulation cannot be generated with a .csv file only.

WARNING! The “Submit” button is dependent on the active tab, so it must be clicked from the “Upload file” tab in order to run a simulation with the uploaded files.

4.5 Viewing Outputs

As previously stated, details of submitted simulations are viewed in the Simulations menu. The .csv files obtained by clicking the “Download results...” button vary depending on the type of simulation that was run. Shown in Figure 29, typical simulations will output a .csv file detailing all the output results and relevant input values for the simulation. However, a multi-parameter simulation will output a .csv file (Figure 30) showing only the variable multi-parameter inputs and the outputs specified by the multi-parameter run. Outputs can also be viewed in chart format as described in section 3.5; however, users must note that only the final run of a multi-parameter simulation will be displayed in the charts.

1	bituminousCoalLHV	22713095	joule / kilogram	Bituminou	joule / kilogram	HyARC
2	cityH2ProductionRequirement	10568208	kg/yr	City H2 pr	kilogram / year	GDS script
3	cityH2Use	10086131	kilogram / year	City hydr	kilogram / year	HDSAM
4	deliveryDieselUseTotal	212.0751	m^3/yr	diesel use	meter^3 / year	GDS script
5	deliveryDieselUseTotalMass	752147.2	J/kg_H2	diesel use	joule / kg_H2	GDS script
6	deliveryElectricityUseForCompression	0	J/yr	electricity	joule / year	GDS script
7	deliveryElectricityUseForCompressionMass	0	J/kg_h2	electricity	joule / kg_H2	GDS script
8	deliveryElectricityUseForForecourt	9.21E+12	J/yr	electricity	joule / year	GDS script
9	deliveryElectricityUseForForecourtMass	913617.7	J/kg_H2	electricity	joule / kg_H2	GDS script
10	deliveryElectricityUseForLiquefaction	2.48E+14	J/yr	electricity	joule / year	GDS script
11	deliveryElectricityUseForLiquefactionMass	24541180	J/kg_H2	electricity	joule / kg_H2	GDS script
12	deliveryElectricityUseTotal	2.57E+14	J/yr	total elect	joule / year	GDS script
13	deliveryElectricityUseTotalMass	25454798	J/kg_H2	total elect	joule / kg_H2	GDS script
14	deliveryMode	Liquid Truck		how H2 is	delivered to forecourt	User Input
15	deliveryTotalLevelizedCost	3.424677	dollar / kilogram	Total Deli	dollar / kilogram	HDSAM
16	depreciableCapital	4.99E+08	dollar	depreciab	dollar	H2A
17	depreciationLength	20	year	depreciat	year	H2A
18	depreciationTable	[[0.00333		1 Depreciat		1 H2A
19	designCapacity	90026090	kg_H2 / year	design cap	kg_H2 / year	H2A
20	dieselDensity	836.6328	kilogram / meter^3	U.S. Convi	kilogram / meter^3	HyARC
21	dieselLHV	3.58E+10	joule / meter^3	U.S. Convi	joule / meter^3	HyARC
22	dieselLHVperkg	42756576	joule / kilogram	U.S. Convi	joule / kilogram	HyARC
23	distanceTerminalToCity	100000	meter	distance f	meter	HDSAM
24	effectiveIrr	0.1		1 internal r		1 H2A
25	effectiveIrrSource	h2a prod		source of internal rate of return		User Input
26	electricityGenerationMix	US Mix		marginal electricity generation r		User Input
27	electricityGenerationMixUserInputBiomass	0		1 Fraction o		1 User Input
28	electricityGenerationMixUserInputCoal	1		1 Fraction o		1 User Input
29	electricityGenerationMixUserInputNaturalGas	0		1 Fraction o		1 User Input
30	electricityGenerationMixUserInputNoncarbonEmitting	0		1 Fraction o		1 User Input
31	electricityGenerationMixUserInputNuclear	0		1 Fraction o		1 User Input
32	electricityGenerationMixUserInputResidOil	0		1 Fraction o		1 User Input

Figure 29. .csv output of a typical simulation

	A	B	C	D	E	F	G	H	I
1									
2									
3									
4		effectiveIrrSource	effectiveIrr	pipelineTransLengthSource	pipelineTransLength	pathwayLevelizedCost	wtwGHG	pathwayEfficiency	
5		none	1 none		mi	\$ / kg	g / mile	%	
6	run1	User Input	0.1 User Input		30	3.983084406	149.9882	65.42946	
7	run2	User Input	0.12 HDSAM		60	4.387212406	150.0067	65.41726	

Figure 30. .csv output of a multi-parameter simulation

Table 2 includes sample entries from the output.csv file of a typical simulation. The “Variable Name” column shows the name of the variables used by the MSM model. The “Value,” “Units of Output,” and “Proper Units” columns provide the actual values and units resulting from the model scenario set up by the user. The “Variable Description” column displays brief information about each variable. The “Source Model” column shows where each variable’s value is generated. The component models are represented in addition to values specific to the MSM model. The default data entries are variables that are MSM defaults and can be changed only in the .xml input file. The user input entries are variables defined by the user when setting up specific simulations. Finally, the GDS script entries are variables generated by the MSM model run.

Variable Name	Value	Units of Output	Variable Description	Proper Units	Source Model
bituminousCoalLHV	26,100,117	joule / kilogram	Bituminous coal (as received)	joule / kilogram	HyARC
cityH2ProductionRequirement	18,685,863	kg/yr	City hydrogen production required before losses	kilogram / year	GDS script
cityH2Use	18,685,863	kilogram / year	City hydrogen use	kilogram / year	HDSAM
co2SeqBitumCoal	0.9	1	CO2 sequestration in coal case	1	Default data
deliveryMode	None		How hydrogen is delivered to forecourt		User input
productionCapacityFactor	0.7	1	Production capacity factor	1	H2A Production
poplarFarmingEnergyUse	272,812.2	joule / kilogram	Poplar farming energy use	joule / kilogram	GREET

Table 2. Sample entries from output.csv file

5.0 Offline Capabilities

Aside from carrying out analyses through the GUI, users interested in temporal or risk analyses may take advantage of some of the model's offline capabilities.⁶

5.1 MSM-HyPro Links

HyPro is a MatLab-based computer model developed by Directed Technologies, Inc. (DTI) under contract to the U.S. Department of Energy (DOE) for calculation of the expected "pump price" of hydrogen (i.e., the cost of hydrogen ready to be dispensed into a customer's vehicle at the dispensing station) for a variety of production/delivery/dispensing pathways in an area of uniform demand density over a span of years. By postulating the yearly hydrogen demand and calculating which supply infrastructure pathway is expected to provide the least expensive hydrogen in any given year, a prediction can be made of how the infrastructure would be built out over time. This build-out prediction takes into consideration technology changes over time, underutilization of facilities in the early years of a station coming on line, potential stranded assets, feedstock cost differences, economies of scale in the production equipment, and "learning curve" capital cost reductions due to repetitious fabrication of multiple systems.

In order to integrate HyPro into the MSM, a new means was developed for HyPro to obtain the inputs necessary to run the analysis. The data input process built by DTI consists of two related parts: the XML files that store the input data and the M-code that translates the contents of the XML files into HyPro. Data is stored in two XML files: Globals and AllTechs. The global data set is information about the overall analysis, such as annual hydrogen demand, city size, and analysis duration. The remaining inputs are stored in AllTechs.xml and refer to the different components of an infrastructure pathway such as the capital cost, design capacity, and labor requirements for each of the various production, terminal, delivery, and dispensing pathway options.

The original HyPro output consisted of two parts: tables and graphs (shown in Figure 31). However MatLab graphs cannot be readily displayed in the MSM environment. Thus, the output translator was expanded to transfer data from HyPro into an Excel file that will allow recreation of the graphs. The data stored in Excel can then be processed by the MSM.

Currently, the MSM does not allow Web users access to HyPro, but this feature may be added in the future. Those interested in the analysis offered by HyPro with MSM are encouraged to contact msm@nrel.gov for assistance in setting up proper input files and obtaining HyPro results.

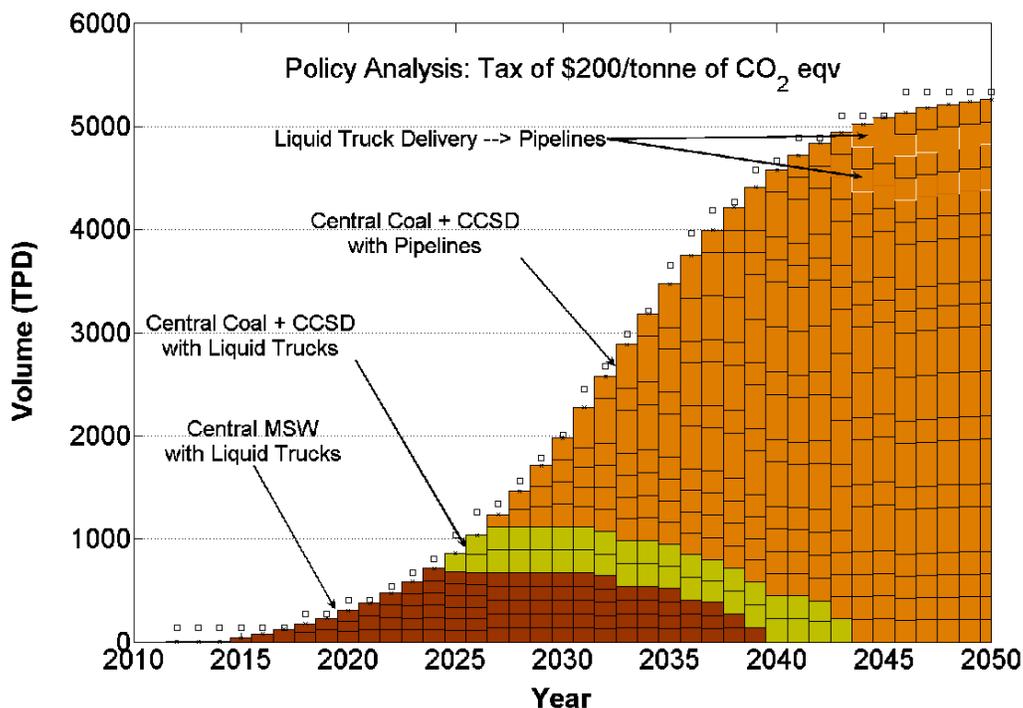


Figure 31. Graph of HyPro output

6. Inquiries about analyses using offline capabilities can be directed to msm@nrel.gov.

5.2 Stochastic Analysis

An important feature available offline for hydrogen analysts is the stochastic analysis of hydrogen production/delivery/dispensing pathways. It allows users to generate randomized sets of MSM inputs in order to get sets of MSM outputs of interest. The approach is similar to multi-parameter runs (section 4.2) with the following differences:

- Input parameter values can follow specific probability distributions.
- The number of input sets can significantly exceed what can reasonably be entered via GUI as described in section 4.2.
- Hence, stochastic analysis runs are not suitable to be generated from the MSM GUI, so they are part of the MSM offline capabilities.

In Figure 32, we present an example of results that can be obtained with MSM stochastic runs.

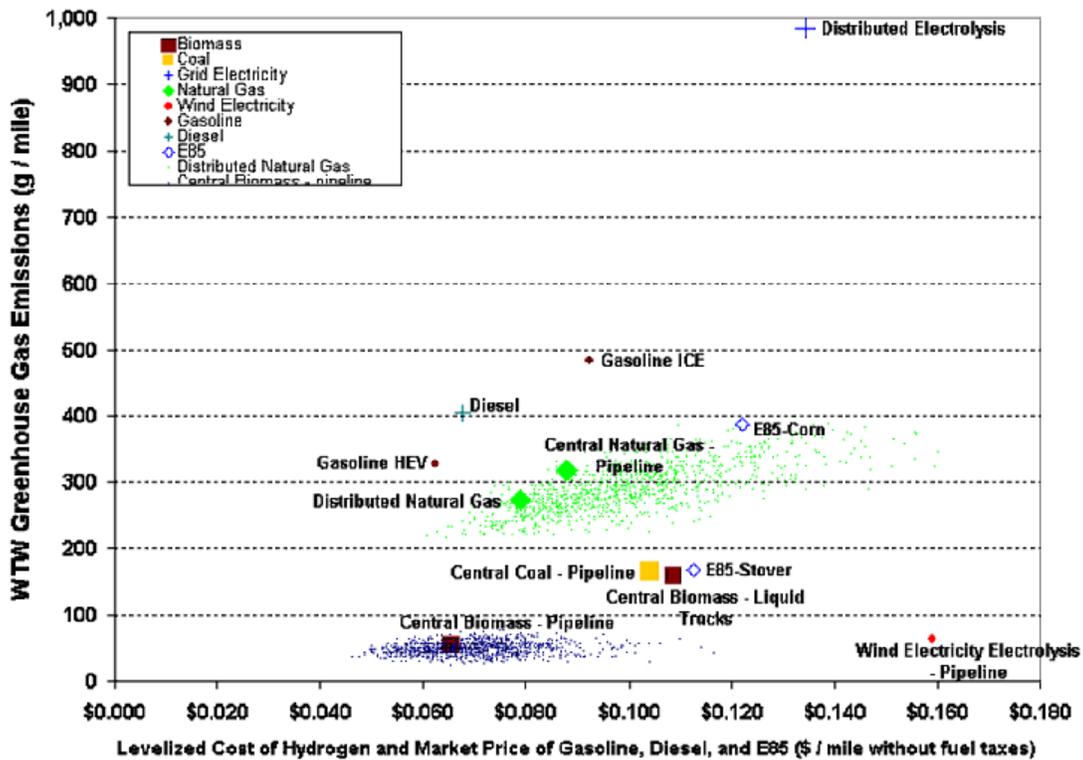


Figure 32. Stochastic (Monte Carlo) results for distributed SMR (green dots) and central biomass pipeline (blue dots) cases mapped on the emissions costs diagram

The distribution of inputs does not need to be stochastic. The prospective users might be interested in having, for example, distributed electrolysis inputs (electricity price and electricity generation grid mix) to correspond to each county in the United States while focusing on well-to-wheels emissions and hydrogen costs (or other MSM outputs). These types of requests can also be accommodated by the MSM team. The prospective users are encouraged to contact msm@nrel.gov for assistance.

6.0 Future Goals and Expanding Model Capabilities

The MSM is a valuable tool that provides an overarching view of different aspects related to the transition to a hydrogen economy. It accomplishes this by linking various detailed models, each offering a unique level of detail and perspective. Future plans regarding expansion and enhancement of the MSM will aid the dialogue among the members of the analysis community and will provide a simplified and integrated tool to better understand the possible pathways to a hydrogen economy.

Developers of the MSM are aiming to give users more flexibility, link to more models, expand to more computers (over the Internet), and use more platforms. Future enhancements in model capabilities include:

- Adding a vehicle cost model.
- Completing links to H2A Power (for analyzing stationary fuel cell systems that generate electricity, heat, and hydrogen).
- Adding a model that simulates vehicle fleet development and related costs, energy use, and GHG emissions.
- Analyzing energy storage options.
- Adding other transition analysis tools.
- Linking HyDRA and GREET2 - 'What if the car is built there?'
- Linking HyDRA and HyPRO - 'How does the deployment scenario change with location?'

Appendix. Detailed Inputs

Feedstock, Utilities	Electricity Generation Mix <i>Combination of various types of power generating methods (coal, nuclear, renewable, etc.) used to create energy for a given region.</i>	CA mix: California NE US mix: Northeast United States US mix: United States Wind only: Power generated exclusively by wind.
	Utilities, Co-products	Source of electricity co-product production: The amount of electricity in kilowatt hours produced per kilogram of hydrogen. Source of electricity co-product cost: The cost in dollars to produce one kilowatt hour of electricity. Source of natural gas consumption: The rate at which natural gas is consumed per mass of hydrogen created. Source of natural gas utility price: The cost of a cubic meter of natural gas. Source of utility electric consumption: The amount of electricity required to generate a kilogram of hydrogen. Source of utility electric price: The cost of one kilowatt hour of electricity.
	Coal	
	Energy Use for Carbon Capture in H2 Central Plants <i>The energy in joules per kilogram of carbon required to sequester carbon particles from exhaust in order to reduce pollution.</i>	
	Natural Gas	Source of natural gas feedstock consumption: The volume of natural gas required to generate one kilogram of hydrogen. Natural gas feedstock price: The cost of a cubic meter of natural gas.
	Electricity Feedstock Use and Cost Characterization	Source of electricity feedstock consumption: The electricity in kilowatt hours required to generate one kilogram of hydrogen. Source of electricity feedstock cost - industrial electricity only: The cost of one kilowatt hour of electricity.
	Nuclear	Source of heat feedstock consumption: The heat in megawatt hours required to generate one kilogram of hydrogen. Feedstock heat price source: The cost of one megawatt of heat.
	Biomass	Source of biomass feedstock consumption: The mass ratio of how much biomass must be consumed in order to produce one kilogram of hydrogen. Source of biomass feedstock cost: The price of a kilogram of biomass. Source of poplar farming energy use: The energy in mega joules required to grow one kilogram of poplar tree.
Production Facility	Source of production total capital investment: Total monetary investment in the production of hydrogen. Source of production capacity factor: The ratio of the projected actual output of a plant over time against its maximum possible output during that time. Source of number of production FTEs: The number of full time employee equivalents. Source of internal rate of return: The average projected annual compound rate of return received by an investor over the life of their investment. This is a key indicator used by institutions in appraising their investments.	

Delivery	Pipeline Delivery	Pipeline Losses	<p>Source of H2 loss in pipeline: The percentage of hydrogen lost in the pipeline delivery system.</p> <p>Source of H2 loss during compression: The percentage of hydrogen lost when it is being compressed.</p>
			Pipeline length from plant to city: Pipeline length for fuel delivery from plant to city.
	Liquid H2 Delivery	Liquefier	<p>Source of liquefier efficiency: The hydrogen liquefied divided by the sum of the hydrogen liquefied plus the energy required for the liquefaction.</p> <p>Electricity generation mix for liquefaction in NG plant.</p> <p>Electricity generation mix for liquefaction in solar plant.</p> <p>Electricity generation mix for liquefaction in nuclear plant.</p> <p>Electricity generation mix for liquefaction in coal plant.</p> <p>Electricity generation mix for liquefaction in biomass plant.</p>
		Storage	<p>Days of storage at production plant/liquefier: The duration of the hydrogen's stay at the plant after being generated.</p> <p>Recovery rate of boil-off gas in production plant: The amount of hydrogen recovered when it escapes as a gas.</p> <p>Recovery rate of boil-off gas in terminal: The percentage of hydrogen recovered when it escapes as a gas.</p>
		Transport	<p>Liquid H2 boil-off rate in transportation from production plant/liquefier to terminal: The percentage of hydrogen that boils off in one day while in the truck tank.</p> <p>Source of liquid H2 truck diesel fuel requirement: The fuel efficiency of liquid hydrogen transportation trucks running on diesel.</p> <p>Source of truck-tank loading losses: The amount of hydrogen lost as a truck tank is loaded.</p> <p>Source of truck-tank boil-off rate losses: The amount of hydrogen that boils off during transportation.</p> <p>Time in truck trailer for transport: The average number of days that the hydrogen will spend in a truck trailer while being transported.</p> <p>Recovery rate of boil-off gas during distributions: The percentage of boil-off gas that is recovered during the distribution process.</p>
Dispensing Forecourt	Forecourt capacity: The amount of hydrogen that can be contained within a distribution center.		
	Gaseous H2 Dispensing		<p>Source of energy efficiency when H2 piped from central plants with electric compressors: Efficiency of the compressor defined as the lower heating value of compressed hydrogen divided by the sum of the lower heating value of hydrogen entering the compressor plus the amount of electricity required for the compression.</p> <p>Source of hydrogen lost at gaseous forecourt station: Hydrogen lost (percent from total) at gaseous forecourt.</p>
	Liquid H2 Dispensing		<p>Time in liquid H2 forecourt stations: The average time hydrogen will spend at a forecourt station from the time it is delivered until it is dispensed.</p> <p>Recovery rate of boil-off in forecourt station: The percentage of hydrogen that is recovered after escaping into the gas phase.</p> <p>Source of liquid forecourt boil-off rate: The percent of the hydrogen stored at a forecourt that boils off every day.</p>
			Time in forecourt storage: The amount of time that hydrogen will spend in forecourt storage from when it is delivered until it is dispensed.

Vehicle Characterization	Baseline Fuel Efficiencies	<p>Source of gasoline internal combustion engine vehicles' fuel efficiency: The value of the assumed average fuel economy achieved by vehicles with gasoline internal combustion engines in miles per gallon of gasoline</p> <p>Source of gasoline hybrid electric vehicles' fuel efficiency: The value of the assumed average fuel economy achieved by vehicles with gasoline hybrid electric engines in miles per gallon of gasoline.</p> <p>Source of E-85 ethanol internal combustion engine vehicles' fuel efficiency: The value of the assumed average fuel economy achieved by vehicles with E-85 ethanol internal combustion engines in miles per gallon of gasoline equivalent.</p>
	Gasoline and Vehicle Type	<p>Vehicle type: This entry has no effect on the model and is used merely to remind the user what is being modeled.</p> <p>Share of RFG in total gasoline use: The percentage of gasoline that has been reformulated and is no longer the conventional mixture.</p> <p>Type of oxygenate in RFG: Type of oxygenate used in the reformulated gasoline.</p> <p>Energy in 1 GGE: The amount of energy in BTUs that is contained within one gallon of gasoline or its equivalent in another substance.</p>
	Source of vehicles per person: The assumed average number of vehicles owned by each person in the population.	
Default Values (Constants) <i>Values being used within the calculations that cannot be altered by the user.</i>	Pipeline Energy Consumption	<p>Share of power generation done by turbine for pipeline compressions stations: Percentage of total power generated by a turbine.</p> <p>Share of power generation done by current NG engine for pipeline compressions stations: Percentage of total power generated by a natural gas engine.</p> <p>Share of power generation done by future NG engine for pipeline compressions stations: Percentage of total power generated by an advanced natural gas engine.</p> <p>Share of diesel fuel for piping: The percentage of energy provided by diesel fuel for piping.</p> <p>Share of NG fuel for piping: The percentage of energy provided by natural gas for piping.</p> <p>Share of residual oil fuel for piping: The percentage of energy provided by residual oil for piping.</p> <p>Share of H2 fuel for piping: The percentage of energy provided by hydrogen for piping.</p> <p>Share of electricity fuel for piping: The percentage of energy provided by diesel fuel for piping.</p>
	Gaseous H2 Dispensing	<p>Natural gas share of process fuels for gaseous H2 compression at central plants: The percentage of energy provided by natural gas for the compression of hydrogen.</p> <p>Electricity share of process fuels for gaseous H2 compression at central plants: The percentage of energy provided by natural gas for the compression of hydrogen.</p>