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The Hydrogen Futures Simulation Model (H_2Sim) User's Guide

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ABSTRACT

The Hydrogen Futures Simulation Model (H_2Sim) is a high level, internally consistent, strategic tool for exploring the options of a hydrogen economy. Once the user understands how to use the basic functions, H_2Sim can be used to examine a wide variety of scenarios, such as testing different options for the hydrogen pathway, altering key assumptions regarding hydrogen production, storage, transportation, and end use costs, and determining the effectiveness of various options on carbon mitigation. This User's Guide explains how to run the model for the first time user.

Acknowledgements

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Introduction

The Hydrogen Futures Simulation Model (H_2Sim) allows the user to explore options for producing, distributing, and using hydrogen. The model provides answers to questions about economic viability and environmental and energy security consequences associated with various hydrogen pathways by allowing the user to quickly change key assumptions. This guide is intended for the first time user. It demonstrates use of the model, including running reference cases and altering key assumptions. Several examples step the user through illustrative scenarios.

System Requirements

H_2Sim will run on all Pentium class computers. It is best viewed with display resolutions set to 1024x768, large fonts. It will also run satisfactorily with the display set to 800x600, small fonts. The user can change the display settings by opening the display icon in the control panel, accessible from the START menu in Windows. For systems running Windows XP, the font selection is on the settings tab under "advanced." The model is written in Powersim Studio 2001, a dynamic simulation modeling language.[1]

Starting the Model and Running a Base Case

The CD includes the necessary Powersim Studio 2001 software to run H_2Sim. To install the Powersim software, follow these steps:

1. PLACE the CD in the appropriate computer drive on the target computer, locate and open the file "**PS2001**" on the CD.

2. FOLLOW the installation instructions for Powersim Studio 2001.

3. ENTER the long serial number listed on the CD cover when prompted on the Customer Information page.

4. ACCEPT the license agreement to use the software.

5. CHOOSE the Complete installation option.

6. CLICK install.

H_2Sim runs directly from the CD. Double click on the file "**H2Sim.sip**" to open the model. To open the model while the Powersim Studio software is running, choose files of type ".sip" in the "Open" window. Locate the file "**H2Sim.sip**" on the CD and click "Open" to run the model.

[1] More information about Powersim is available at their website: www.powersim.com

The model opens on the license agreement page. Accepting the terms of use takes the user to the title page, Figure 1. The user advances from this point by clicking on the large arrow labeled **Model** in the lower right hand corner of the screen. The next screen is a pictorial representation of the hydrogen pathway, followed by the third screen, labeled **Sectional Overview**. The **Sectional Overview** screen explains the four main components of H_2Sim (Production, Carbon Pathway, Storage and Delivery, and End Use), Figure 2. Clicking on any of the four areas takes the user directly to that section of H_2Sim. From that point, the user is ready to run the model.

In the bottom, right hand corner of the Sectional Overview screen, there is a link to H_2Sim's legend, which explains the user controls associated with H_2Sim. Key model controls are summarized below.

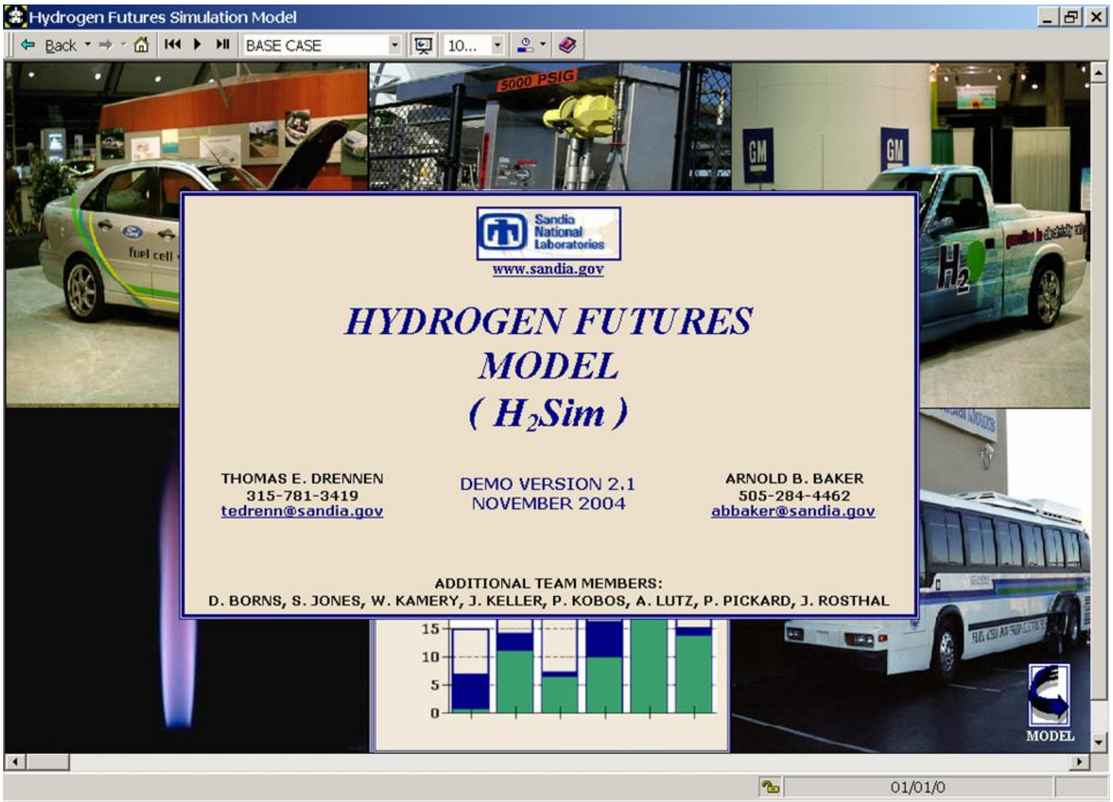

Figure 1. H_2Sim's Title Page

Figure 2. Sectional Overview Screen

Model Operation

PLAY — Click to start model simulation or click during simulation to stop.

REWIND — Click to reset simulation.

PLAY/PAUSE — Click to advance the model one step.

Model Navigation

MAIN TOOLBAR – Click on desired model section (PRODUCTION, CARBON PATHWAY, STORAGE AND DELIVERY, USE) to navigate there.

HYPERLINK – Any underlined word acts as a hyperlink. Click on any hyperlink to navigate to the specified location.

BACK - Back — Click to return to previously visited screen.

LEGEND - Click on the compass icon at any time to go to the legend page for a more detailed description of model control and navigation options.

Select **Production** to start at the beginning of the hydrogen pathway.

Production

H_2Sim generates output based on the dynamic variable, capital cost. To start the model at the beginning of the simulation, press **Rewind** ( ). Rewinding the model at any time will restore all assumptions to their default values. To run the model without pause, press **Play** ( ). To run the model one step forward, use the **Run/Pause** button ( ). Each model step in H_2Sim corresponds to a 10 \$/kW-H_2 increase in assumed capital costs[2] for the various technology options, from a capital cost of zero \$/kW-H_2 to 2000 \$/kW-H_2. The model pauses automatically at 670 \$/kW-H_2 – the highest assumed 2020 capital cost for any of the production technologies (thermochemical nuclear). If the user sets capital costs at higher values, the model would then automatically pause at that user set capital cost. The capital cost for which the model is currently calculating costs, is always depicted on the right hand side of the title bar, towards the top of the page.

The results change as the model runs. To change the displayed units, click on the hyperlinks on the left hand side of each graph (**$/Kg** or $/**GJ).** To view the results in tabular form, click on the **Table** hyperlink.

Within the **Production** section, there are hyperlinks to detailed analyses of the six hydrogen production options included in H_2Sim. Figure 3 illustrates the natural gas reformation option. This screen also illustrates the default model results. Key assumptions on each production page include capital, O&M, and fuel costs, thermal efficiency of the process, interest and discount rates, construction time, plant life, and capacity factor. While some of the assumptions are specific to that production option, changes to assumed interest or discount rates apply to the entire model. Any shaded boxes, such as capital recovery factor, cannot be changed by the user, but will change as other variables (in this case discount rate) change. With the exception of capital cost, these variables may be changed at any point during the simulation via a slider (Thermal Efficiency, Figure 3) or a white number box (Interest Rate, Figure 3). Since the model runs on capital cost, this assumption must be changed prior to running the model (see the shaded box which follows for an example of changing the capital costs).

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[2] Economists typically discuss capital costs in terms of dollars per unit or output. This per unit capital cost is usually dependent on the facility size. A larger unit may have lower per unit capital costs than a smaller unit, due to economies of scale. Total capital costs for a facility would then be the per unit capital costs times the assumed output. For example, a hydrogen plant costing 500.9 \$/kW – H_2 that produces 100,000 kg/day of hydrogen would cost approximately 69.5 million \$: 500.9 \$/kW – H_2 *kW/1000W* W/J/s *10^6J/MJ*120 MJ/kg – H_2*hr/3600s *day/24hr*100,000 kg – H_2/day.

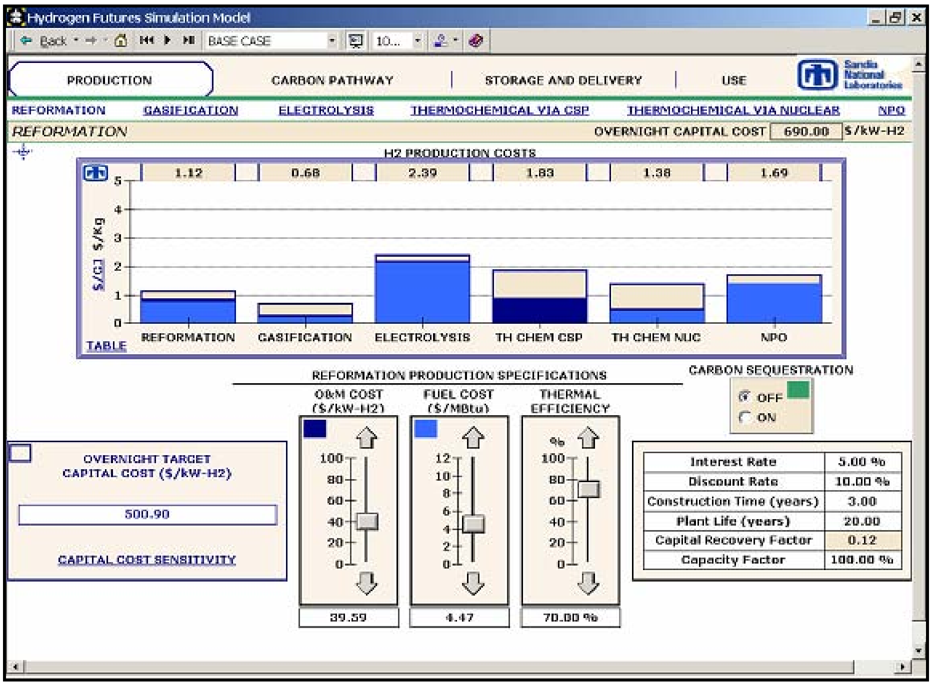

Figure 3. Reformation Production Sensitivity Screen

Illustrative Example of Defining a Custom Overnight Target Capital Cost

The default capital cost for natural gas reformation is 500.90 \$/kW-H_2, based on the estimated costs for a 100,000 kg/day facility built in 2020. Smaller reformation plants will likely have a higher per unit capital cost. One estimate suggests that a smaller, fueling station sized reformer may cost in the range of 1800 \$/kW – H_2. This example illustrates how to change the assumed target overnight capital cost from 500 to 1800 \$/kW-H_2.

Step 1: Reset the model with the **Rewind** icon (⏮).

Step 2: Click in the number box labeled **Overnight Target Capital Cost** and change the value to 1800 \$/kW-H_2.

Step 3: Press the **Play** icon (▶).

H_2Sim now stops at 1800 \$/kW-H_2 as the model always stops at the highest specified capital cost of any technology. Based on this increased capital cost, hydrogen production costs, via natural gas reformation, increase 0.64 \$/kg to 1.76 \$/kg.

Capital Cost Sensitivity

The **Capital Cost Sensitivity** link, located below the edit boxes for all hydrogen production facilities, takes the user to a summary of projected hydrogen production costs for all capital costs, Figure 4. While on this page, one can rerun or change any of the assumptions about a production option; the new scenario will appear as a thin line, while the default scenario will appear as the thick line. Figure 4 illustrates this concept by running H_2Sim to its default stop (670 \$/kW – H_2); at this point, the price of natural gas was increased to \$6/MBtu. The new production costs are shown as the thin green line. This change can be made at beginning of a model run, as shown in Figure 3, or during a model run. Clicking on the magnifying glass icon, , will take the user to an enlarged view of this graph. Clicking on the **Table** hyperlink in the bottom corner of the graph will take the user to a table summarizing the same information. Arrows on the tabular page indicate the default target capital cost of each production option. From here, one can explore other production options or move on to other parts of the model. With the exception of the electrolysis option, the other production screens are similar to the reformation screen. The electrolysis options are discussed next.

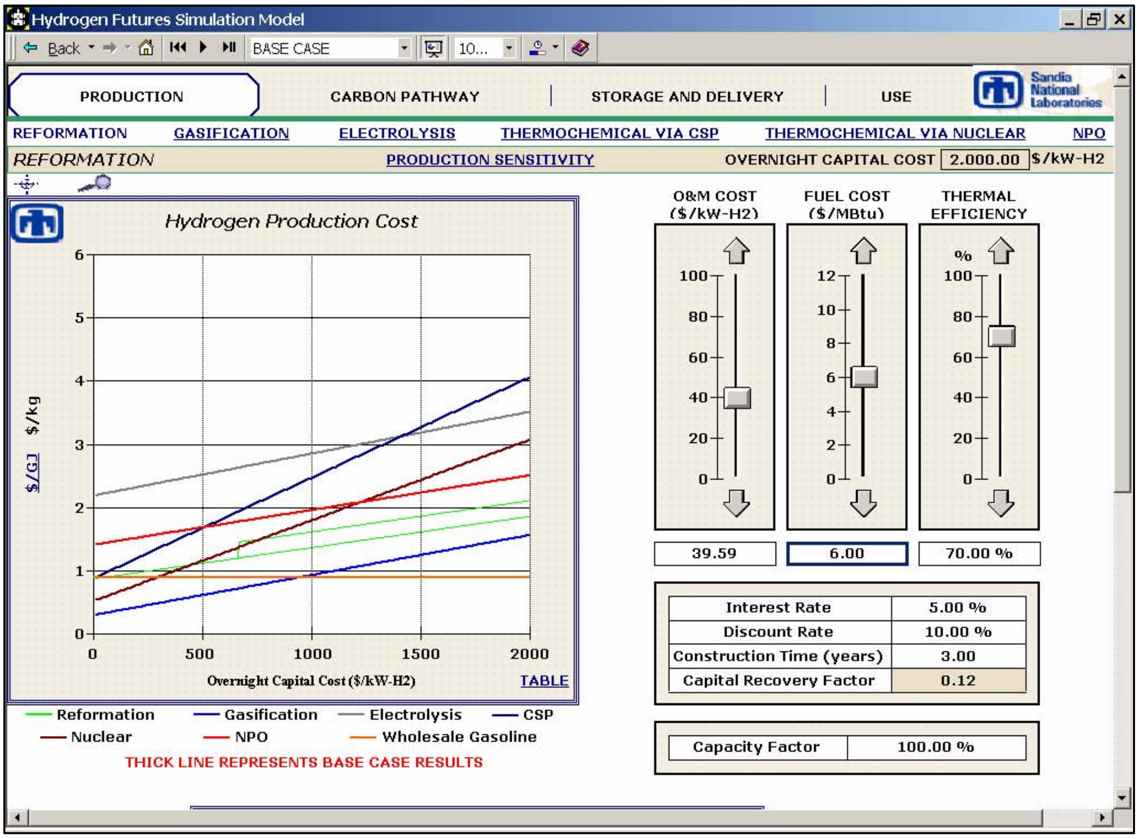

Figure 4. Capital Cost Sensitivity Screen

Electrolysis

The production sensitivity and capital cost sensitivity for electrolysis allow the user to alter the source of the electricity. The default electricity option assumes electricity is produced using gas combined cycle technology (GasCC). The user may also directly set a price (**User Set** option). The electricity costs are calculated at the plant gate and do not include transmission and distribution (T&D) costs. T&D costs may be added by the user (**Electricity Transmission and Distribution** box).

Basic assumptions about the electricity generation in H_2Sim, can be changed by clicking on the **Electricity Generation Sensitivity** hyperlink. This section of the model allows the user to alter basic assumptions about each electricity production option, including capital costs, fuel prices, and construction time. Figure 5 illustrates the options for a GasCC facility. All of the variables on this screen are unique to the electricity generation option, with the exception of the discount rate, which carries over throughout the model. The user must select this **Box to allow alterations** prior to making changes on this screen. By checking this box, the user is selecting the electricity generation type that the electrolysis production process will use. The electricity generation sensitivity screen also shows a comparison of different production options allowing the user to examine the competitiveness of hydrogen produced via electrolysis as they change generating facility assumptions.

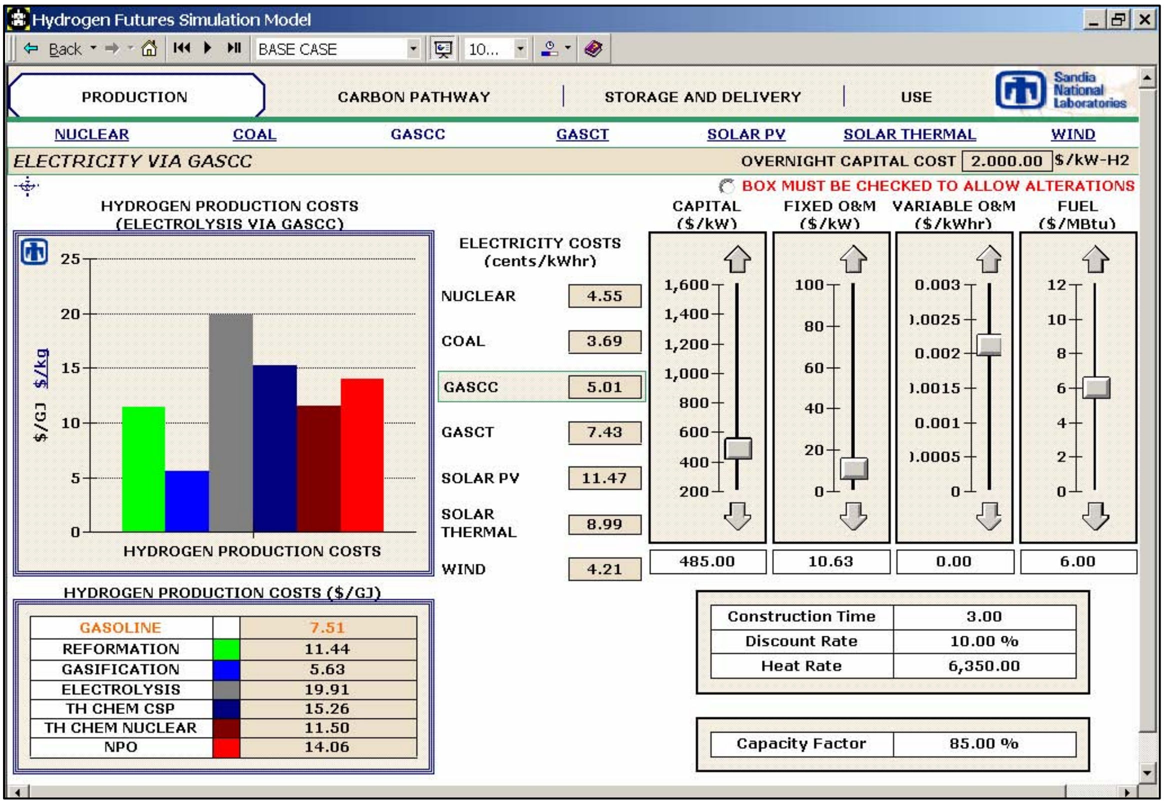

Figure 5. Electricity Generation Sensitivity Analysis Screen

At what price would hydrogen produced from electrolysis be competitive with other options?

This example demonstrates the "what if?" capabilities of H_2Sim. Using the default assumptions, the cheapest production option for hydrogen is coal gasification (0.68 $/kg), followed by natural gas reformation (1.12 $/kg). Hydrogen produced from electrolysis is considerably more expensive (2.15 $/kg). This example demonstrates how H_2Sim can be used to find the electricity price at which the electrolysis option is competitive.

Step 1: Run the model to its default stopping point (670 $/kW-H2).

Step 2. Click the **Electrolysis** hyperlink at the top of the production summary screen.

Step 3: Click on the **User Set** option in the plant gate electricity cost **Source** box.

Step 4: Experiment with electricity prices until find the price at which the electrolysis option is competitive with coal gasification. The user will find that electricity must cost less than one cent/kWhr.

Carbon Pathway

Both the reformation and gasification options would release significant quantities of carbon during the production process. H_2Sim allows the user to explore the options for carbon capture, sequestration, and its impact on overall economic competitiveness. Figure 6 illustrates the carbon sequestration screen for the coal gasification option. From this screen, the user can specify the additional capital and O&M costs associated with the carbon capture, the percentage of carbon removed (default is 87%), and the efficiency penalty associated with carbon capture in terms of the hydrogen production process (default is 2.6%). This screen also contains basic assumptions about the distance and rate of carbon transport and the depth of the disposal wells.

For the example illustrated in Figure 6, carbon capture and transport adds 0.14 $/kg to the price of hydrogen produced from coal gasification; as with most graphs in H_2Sim, the results are color coded to show the composition of costs. Clicking on the **Table** hyperlink provides additional detail. From the table, the default assumptions suggest that 0.09$/kg of the cost is associated with carbon capture (capital, variable O&M, fuel), while the remaining cost of 0.05 $/kg is for the sequestration (pipeline, disposal well). The results in this section are also available in units of $/tC (to view, click on the specific unit along the vertical axis).

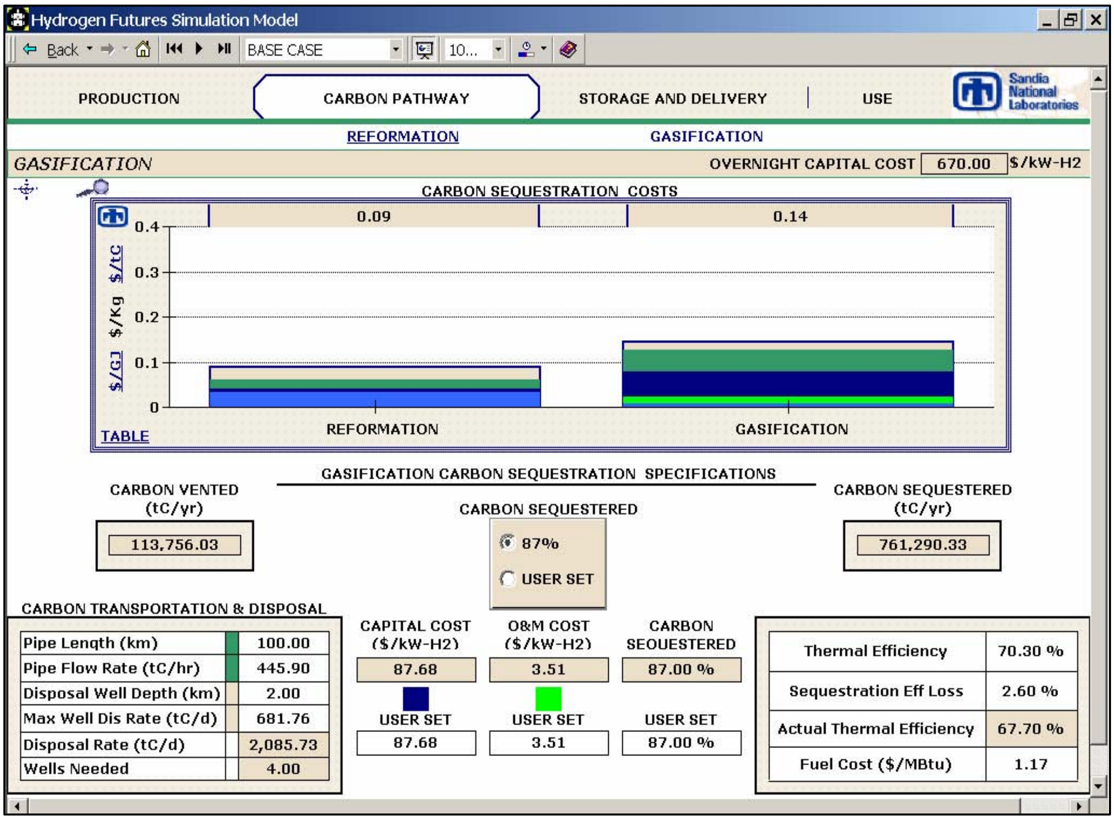

Figure 6. Carbon Pathway Screen for Coal Gasification Option

Storage and Delivery

Clicking on the **Storage and Delivery** tab at the top of the screen advances the user to the screen shown in Figure 7. H_2Sim provides nine options for storing and distributing the hydrogen, Table 1. Each of the nine options, illustrated by a column in Figure 7, includes four steps: storage on site prior to transport (if necessary), primary transport method, secondary transport method, and fuel station costs.

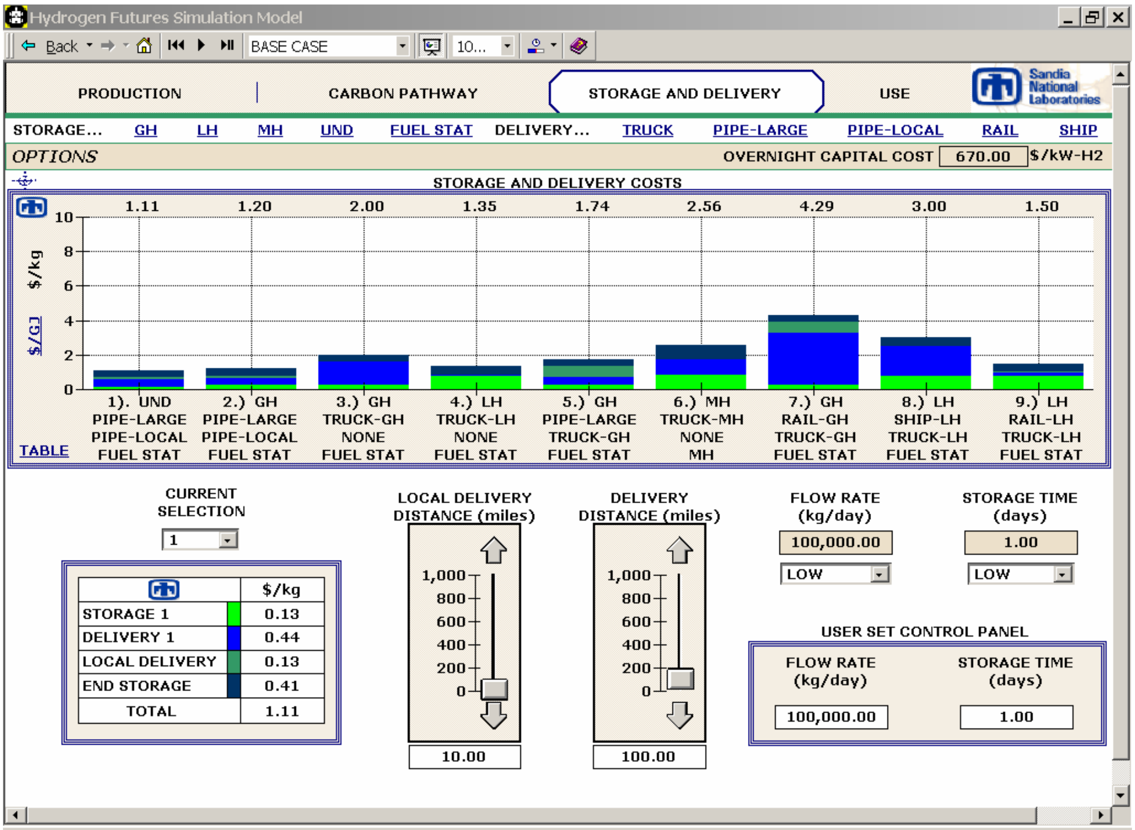

Figure 7. Storage and Delivery Screen

Table 1. Distribution Options in H_2Sim

Option	Storage	Transport 1	Transport 2	Fueling Station
1	Underground, Gaseous	Pipeline, Large	Pipeline, Local	Gaseous
2	Tanks, Gaseous	Pipeline, Large	Pipeline, Local	Gaseous
3	Tanks, Gaseous	Truck, Gaseous	None	Gaseous
4	Tanks, Liquefied	Truck, Liquid	None	Liquefied
5	Tanks, Gaseous	Pipeline, Large	Truck, Gaseous	Gaseous
6	Metal Hydride	Truck, Metal Hydride	None	Metal Hydride
7	Tanks, Gaseous	Rail, Gaseous	Truck, Gaseous	Gaseous
8	Tanks, Liquefied	Ship, Liquid	Truck, Liquid	Gaseous
9	Tanks, Liquefied	Rail, Liquid	Truck, Liquid	Gaseous

While this screen, Figure 7, shows the costs for all nine options, the user must specify which option to use as the basis for calculating total costs of delivered hydrogen. Option 1 is the default scenario (underground, gaseous storage, transport by large pipeline connected to smaller, local pipelines, and storage at the fueling station in gaseous form). To select one of the other options, use the pull down menu on the left hand side of the screen, labeled **Current Selection.** The table located below this pull down menu reports the costs associated with the selection made.

In addition to selecting the mode of storage and transport, the **Storage and Delivery** screen allows for considerable sensitivity analysis of the key variables affecting distribution, including distance (both primary and secondary), production flow rate, and storage time. Clicking specific storage or delivery modes along the top of the screen provides access to additional assumptions. For example, clicking on the **Large Pipeline** link allows one to change assumptions about flow rate, pipe size, delivery pressure, compressor efficiency, and electricity price, Figure 8.

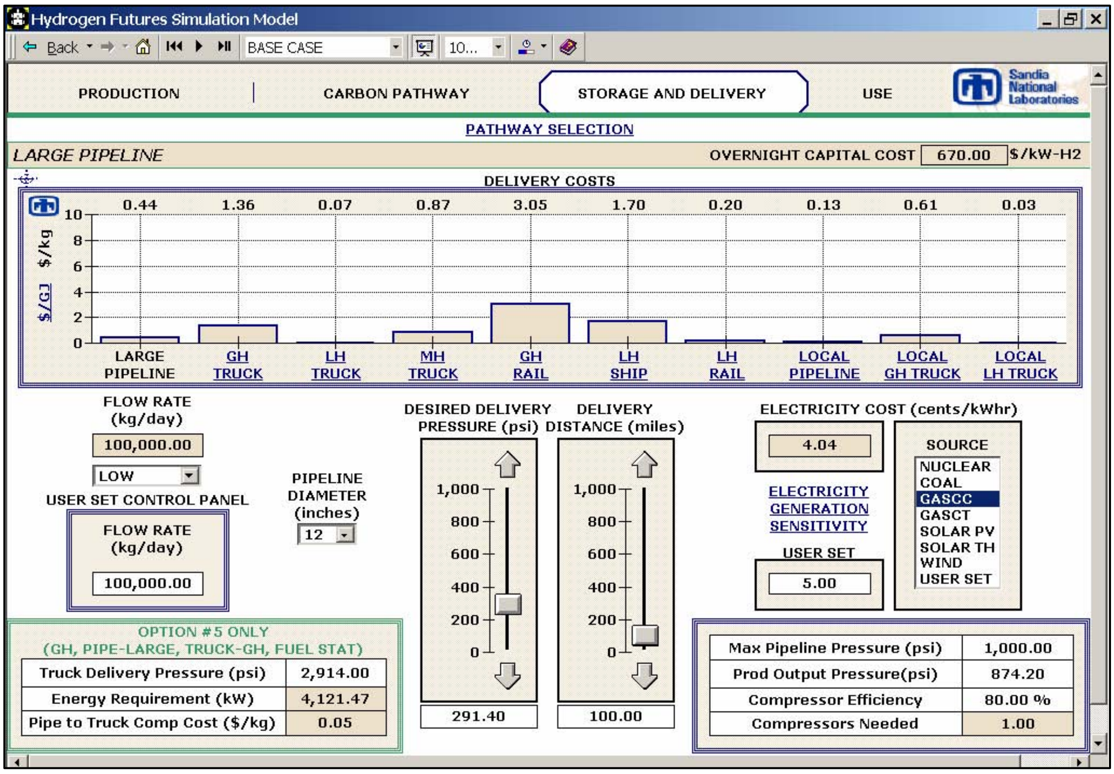

Figure 8. Hydrogen Pathway Sensitivity Screen (Large Pipeline Screen)

End Use

The final section of the model is the End Use section. This version of H_2Sim allows the user to compare the economics and carbon emissions from a variety of existing vehicle technologies (internal combustion engine (ICE) vehicles, hybrids, and electric vehicles) with projected 2020 vehicle technologies (fuel cell vehicle (FVC), fuel cell vehicle with onboard reformation (FCV OB), and direct combustion hydrogen hybrid (H_2Hybrid). While hydrogen may be used for commercial and residential stationary applications as well, these options are not included in this version of H_2Sim.

Figure 9 illustrates the FCV screen in the End Use section. There are separate screens for each vehicle type. The current technology options are on the left hand side of the **Total Vehicle Costs** graph (yellow background); future technologies are on the right hand side (gray background). Vehicle costs, initially displayed in terms of cents per mile to operate, include capital, operating (maintenance, license, and insurance), and fuel costs. The costs are broken down and color-coded by category. To view annual results, click on the **$1000/year** hyperlink on that graph.

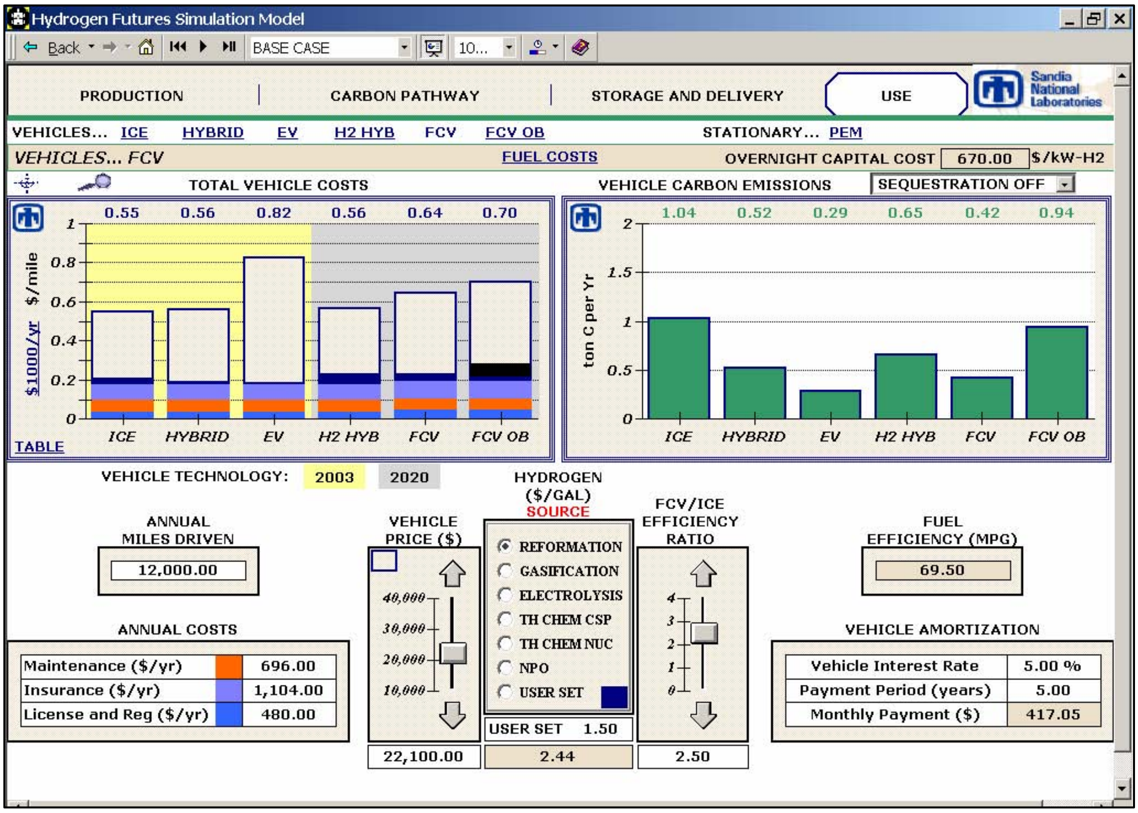

Figure 9. End Use Screen (Fuel Cell Vehicle Sensitivity Screen)

Each of the end use screens shows basic assumptions about annual maintenance, insurance, license and registration costs, vehicle price, efficiency relative to the ICE vehicle (default ICE efficiency is 27.5 mpg), interest rates, amortization period, and annual miles driven. For ICE, hybrid vehicles, and FCV with onboard reformation of gasoline, wholesale gasoline price (before taxes) is also displayed. For the hydrogen vehicles, the user selects the source of hydrogen production. The resulting delivered cost of hydrogen is shown below the **Hydrogen Source** box. For example, in Figure 9, reformation is selected, along with option 1 for storage and delivery (gaseous storage with large regional pipelines connected to smaller pipelines and gaseous fueling stations), selected in the **Storage and Delivery** section of the model. This example also assumes no carbon capture and storage (upper right corner of screen via pull down menu). The user may also set the delivered hydrogen cost directly on this page with the **User Set** option. Finally, the graph on the upper right displays the projected carbon emissions for each vehicle type for the selected assumptions. Because each hydrogen production option has a different carbon profile, projected carbon emissions will vary as the user clicks on different hydrogen options. For example, selecting the thermochemical options for hydrogen production results in zero carbon emissions.

There are other slight variations between end use options. The FCV OB screen contains an additional slider for the reformer cost. The EV screen includes detail about the electricity generation source, allowing the user to select the electricity source. As with other parts of the model, this screen has a hyper link to the **Electricity Generation Sensitivity** section of the model. Changing the electricity source will also impact carbon emissions.

At what gasoline price could fuel cell vehicles using hydrogen from coal gasification compete with current technology ICE vehicles?

The base case results suggest FCVs will have a difficult time competing with current technology ICE vehicles; the FCV would cost about 9 cents per mile more to drive. One option for making the FCV more attractive would be if gasoline prices were higher, either due to market forces or as a result of government action. This example provides a step by step guide to finding the necessary gasoline price at which FCVs could compete.

Step 1: Reset and run the model to its default stopping point (670 \$/kW-H2).

Step 2: Go to the **FCV** screen within the **End Use** section.

Step 3. Select **Gasification** as the hydrogen source.

Step 4. Go to **ICE** screen within the **End Use** section. Using the slider, increase the price of gasoline, observing the affect on ICE vehicle costs. Once the top of the slider is reached, continue increasing the assumed gasoline costs by 25 cents per gallon by typing numbers in the box below the slider until the ICE vehicle costs are equal to the FCV costs (3.50 \$/gallon). This result implies wholesale gasoline prices would have to increase by about \$2.50 per gallon for the FCV to compete with the ICE technology.

Step 5. Return the price of gasoline to \$0.99/gallon and experiment with other key assumptions that could make the FCVs competitive (efficiency, vehicle price, hydrogen price).

Conclusion

The H_2Sim User's Guide provides the first time user with the basic information required to run H_2Sim, change key assumptions, and use more advanced options. Details about the model structure and assumptions are available in the technical report, SAND2004-4937[3]. Once the user understands how to use the basic functions, H_2Sim can be used to explore a wide variety of scenarios.

References

T. Drennen, A. Baker, S. Jones, W. Kamery and J. Rosthal. Sandia National Laboratories, SAND2004-4937, *The Hydrogen Futures Simulation Model (H_2Sim) Technical Description*, October 2004.

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[3] Sandia National Laboratories, SAND2004-4937, *The Hydrogen Futures Simulation Model (H_2Sim) Technical Description*, October 2004.