Macro-System Model
Project #AN011

2010 Annual Merit Review

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Overview

Timeline
Start date: Feb 2005
Completion: Sept 2011
Percent complete: 75%

Budget
Total funding:
- 100% DOE funded
FY09 funding
- $525K NREL/SIO
- $370K Sandia NL
FY10 funding
- $330K NREL/SIO
- $250K Sandia NL

Barriers
Stove-piped/siloed analytical capability (B)
Inconsistent data, assumptions and guidelines (C)
Suite of models and tools (D)

Partners
Sandia National Laboratories
- Computational development
NREL
- H2A Production, HyDRA
Argonne National Laboratory
- HDSAM, GREET
Alliance Technical Services
- Data sourcing and documentation
Directed Technologies, Inc.
- HyPRO
Relevance: Project Objectives

Overall objectives

– Develop a macro-system model (MSM) aimed at
  • Performing rapid cross-cutting analysis
    – Utilizing and linking other models
    – Improving consistency of technology representation (i.e., consistency between models)
  • Supporting decisions regarding programmatic investments through analyses and sensitivity runs
  • Supporting estimates of program outputs and outcomes

2009/2010 objectives

– Increase GUI functionality and capabilities
– Utilize the MSM to compare hydrogen production/delivery/dispensing pathways
– Develop MSM links to the HyDRA spatial data and visualization tool
– Develop MSM links to the HyPRO model to analyze build-out scenarios
– Improve pathway analysis by incorporating vehicle cycle

MSM available to the analysis community at http://h2-msm.ca.sandia.gov/
The MSM is a tool for cross-cutting H2 production pathways analysis – both economics and emissions, which makes it instrumental in assessing technology potential. Analysts can use the levelized cost, energy use, and emissions for sensitivities and comparisons.
Key Assumptions

Pathway assumptions are entered. Other assumptions are embedded in the models being linked but are changed in sensitivity runs.

Production
- Central Biomass
  - Current – 46% conversion efficiency
  - Advanced – 48% conversion efficiency
- Coal Gasification
  - Current – 55% conversion efficiency
  - Advanced – 55% conversion efficiency
- Nuclear HTE
  - Advanced – 83% conversion efficiency
- Distributed SMR
  - Current – 71% conversion efficiency
  - Advanced – 74% conversion efficiency
- Electrolysis
  - Current – 62.5% production efficiency
  - Advanced – 75% production efficiency

Financial
- 10% IRR
- 20 year plant life
- MACRS depreciation where appropriate
- 1.9% inflation

Pathway Assumptions
- Full-deployment scenario
- Urban demand area
- 1,250,000 person city
- 50% H2 penetration
- 1500 kg/day stations
- Mid-size FCV –
  - Current – 45 mi / GGE
  - Advanced – 65 mi / GGE

HDSAM
- Fueling station capacity factor = 0.7
- 62 miles from central production to city
- Liquefier efficiency 77%

GREET
- Gasoline is RFG without oxygenate
- Current technologies use U.S. average grid mix
- Advanced technologies use future grid mix with 85% of CO2 from coal plants sequestered
The MSM provides a central transfer station to guarantee consistency in simulations that involve multiple models. A graphical user interface (GUI) allows users with minimal understanding of the models to use them.
Approach: MSM Development

**Proof of concept / Initial analysis**
- Type of information to transfer
- Define implicit calculations
- Model-linking methodology
- Validate use of models

**Extensible tool**
- Develop & validate extensible & robust structure
- Develop GUI & web interface
- Component model updates (ongoing effort)
- Stochastic capability
- Improved GUI functionality
- Develop run database

**Additional models**
- Revisit analysis issues and MSM requirements
- Select additional models
- Validate use of models
- Develop data-transfer capability

**Analysis community interactions**
- Use MSM for analysis (ongoing effort)
- Update models using the MSM HyPRO
- Pathway report with inputs and pathway results reviewed by industry

**Experience**
- Completed previously
- Completed this year
- Underway
- Future activities
Accomplishment: Increased GUI Functionality

This year, we added some new capabilities for user inputs.

GUI users can download "input" files from previous runs, adjust them, and upload the adjusted files for new runs. Input files are validated against a schema.

GUI users can set up multi-parameter sensitivity runs by selecting the case, setting the variables, and then identifying which should be varied and the values to use.

Default values are from the component models and are pathway-specific.
Accomplishment: Increased GUI Functionality

This year, we added some new capabilities for results.

GUI users can easily see the detailed information entered when the simulation was defined.

GUI users can download results files (in CSV form) to develop their own figures and tables.

GUI users can download input files for record-keeping or to set up additional runs.
Accomplishment: Pathways Report

Report published in September 2009 on the following seven hydrogen production / delivery pathways

<table>
<thead>
<tr>
<th>Scale</th>
<th>Energy Source</th>
<th>CCS</th>
<th>Delivery</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Distributed Natural Gas</td>
<td>No</td>
<td>N/A</td>
</tr>
<tr>
<td>2</td>
<td>Distributed Grid Electricity</td>
<td>No</td>
<td>N/A</td>
</tr>
<tr>
<td>3</td>
<td>Central Biomass</td>
<td>No</td>
<td>Liquid Trucks</td>
</tr>
<tr>
<td>4</td>
<td>Central Biomass</td>
<td>No</td>
<td>Pipelines</td>
</tr>
<tr>
<td>5</td>
<td>Central Natural Gas</td>
<td>No</td>
<td>Pipelines</td>
</tr>
<tr>
<td>6</td>
<td>Central “Green” Electricity</td>
<td>No</td>
<td>Pipelines</td>
</tr>
<tr>
<td>7</td>
<td>Central Coal</td>
<td>Yes</td>
<td>Pipelines</td>
</tr>
</tbody>
</table>

Modeling parameters were reviewed by industrial partners through the Fuel Pathway Integration Technical Team (FPITTT), gaps were identified, and sensitivities were run.

The report provides MSM results for each pathway, broken into supply chain components as shown in these three figures:

- Levelized cost (above)
- Energy input (above-right)
- Well-to-wheel GHG emissions (right)
The report also compares results across pathways and between hydrogen pathways and competing technologies.

Monte Carlo results for distributed SMR and central biomass – pipeline cases are shown here but are not in the report.

Hydrogen results in the figure are based on current technology status scaled to full utilization of production capacity, as represented in H2A and HDSAM. Gasoline and diesel prices are from AEO 2007 high projections for 2009 and do not include fuel taxes.
HyDRA is a spatial database and display tool available at [http://rpm.nrel.gov](http://rpm.nrel.gov). Linking it to the MSM brings spatial data to the MSM and provides a way to display spatial results.

**Use Case 1:**
- **HyDRA**
  - User selects state.
  - Geospatial inputs and some technology parameters are sent to MSM
- **MSM**
  - Batch runs for each county within the selected state
- **HyDRA**
  - Displays levelized pathway cost and WTW results from each county on a map

**Use Case 2:**
- **MSM**
  - User selects county
- **HyDRA**
  - Provides natural gas cost, electricity cost, and grid mix for the county
- **MSM**
  - Allows user to choose natural gas & electricity cost and vary many technical parameters before running a pathway simulation
Accomplishment: HyDRA – Use Case 1

The user selects a state and submits the job. The user is allowed to vary only a few of the technical parameters.
Accomplishment: HyDRA – Use Case 1

The MSM runs cases for each county and results are shown in HyDRA. Levelized production cost is shown.
Many other results are also available. Well-to-wheels greenhouse gas (GHG) emissions are shown.
Accomplishment: HyDRA – Use Case 2

The MSM GUI user selects a county; HyDRA provides feedstock and energy prices and the grid mix for that county. The user can modify many technical parameters.
Accomplishment: Link to HyPRO

HyPRO
- MATLAB-based computer model developed by Directed Technologies Inc. (DTI)
- Calculates the expected levelized “pump price” of hydrogen for a variety of production/delivery/dispensing pathways over a span of years in an area with uniform demand density
- Calculates the ideal infrastructure build-out over time

Inputs to HyPRO:
- i) H2 demand curve projection
- ii) H2 production options and costs (H2A)
- iii) H2 delivery options/costs (HDSAM)

Advantages of linking MSM with HyPRO:
- i) Automatic updates to HyPRO from H2A & HDSAM
- ii) H2A/HDSAM/GREET inputs’ effect on HyPRO can be studied
Accomplishment: HyPRO Upgrades

- Excel input sheets replaced by XML
  - ~ 20x faster data load
  - Validated against use of Excel input
- Revised outputs
  - All pathway costs included
- Pathway components
  - Removed extra production options
  - Added terminal options to make the pathways independent
  - Kept all delivery/dispensing options including those not available in the MSM
- Global variables were added as inputs
  - Demand curve, emissions tax, & feedstock costs were added
    - S-shaped demand curve characterized by three parameters
Accomplishment: HyPRO Results

Baseline production technology buildout

Scenario Assumptions
- 1,125,000 FCVs in 2050
- Average fuel economy: 45 miles / gge
- Average FCV use: 20 mile / day
- City land-area: 1662 square miles
- 1500 kg/day stations

Feedstock is natural gas initially and moves to coal with higher demand
Accomplishment: HyPRO Results

Production buildout with $40/tonne cost of carbon

Feedstock is natural gas throughout buildout
Collaborations

• **Sandia National Laboratories (computational development)**
  – Andy Lutz (MATLAB expertise)
  – Mike Goldsby (MSM architecture)
  – Tim Sa (web server, GUI)

• **NREL**
  – Darlene Steward, Mike Penev (H2A Production, distributed power)
  – Johanna Levene, Chris Helm, Witt Sparks, Chris Culbreth (HyDRA)

• **ANL**
  – Amgad Elgowainy, Michael Wang (HDSAM, GREET)

• **Sentech**
  – Elvin Yuzugullu (documentation)

• **Directed Technologies, Inc.**
  – Brian James, Julie Perez, Andrew Spisak (HyPRO)

• **Indiana University, Kelly School of Business**
  – Ion Diakov (@Risk)

• **Energy companies (pathway analysis and report)**
  – Matt Watkins (Exxon-Mobil)
  – Jonathan Weinert, Bhaskar Balasubramanian (Chevron)
  – Ed Casey (ConocoPhillips)
  – CJ Guo, Karel Kapoun (Shell)

• **Alliance Technical Services (pathway analysis & report)**
  – Melissa Laffen, Tom A. Timbario
## Proposed Future Work

### Analysis Needs & MSM Plans (with planned dates)

| Update the MSM as technical understanding evolves | • Link the MSM to updated component models as they are released (ongoing) |
| Identify the potential effects of not meeting targets and potential tradeoffs | • Add vehicle purchase and maintenance costs to the cost per mile calculation (Sept 2010)  
• Add vehicle production & disposal energy and emissions to the WTW calculation using GREET 2.7 (Sept 2010)  |
| Analyze other production, delivery, and distribution options | • Add combined heat-power-hydrogen as a production option (Dec 2010)  
• Add biogas conversion as a production option (March 2011)  
• Add more delivery and distribution options including cryo-compressed and 700 bar storage and tube trailer delivery (March 2011)  |
| Compare pathways to identify strengths and potential of each | • Complete pathway report focusing on advanced technology status (Sept 2011)  
• Provide support to infrastructure and technical target progress analyses (Sept 2011)  
• Complete a pathway report at various vehicle penetration levels (Sept 2011)  |
| Compare hydrogen build-out scenarios | • Link to a market development model (HyPRO) (complete)  
• Add other transition models to allow for comparisons between methodology while knowing the bases are consistent. (2011 & beyond)  |
Summary

– The MSM is being developed to rapidly perform cross-cutting analysis by linking other models
– It is being used for analyses to understand and compare hydrogen production/delivery/distribution pathways
– This year
  • GUI functionality and capabilities have been improved
  • HyDRA has been linked to provide spatial data and visualization
  • HyPRO has been linked to analyze build-out scenarios
– Future work involves further analysis; adding vehicle cycle costs, energy use, and emissions; and investigating the potential outcomes of technical progress
Supporting Slides
Accomplishment: HyPRO Results

Baseline dispensing buildout

Scenario Assumptions
- 1,125,000 FCVs in 2050
- Average fuel economy: 45 miles / gge
- Average FCV use: 20 mile / day
- City land-area: 1662 square miles
- 1500 kg/day stations

Feedstock is natural gas initially and moves to coal with higher demand
Accomplishment: HyPRO Results

Dispensing buildout with $40/tonne cost of carbon

Feedstock is natural gas throughout buildout