Pacific Northwest National Laboratory’s Hydrogen Analysis Capabilities

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Charter

- PNNL Energy Science and Technology Directorate’s Energy Mission:
  Secure, clean, and affordable energy systems in a carbon constrained world.

- PNNL Analysis Objectives/Principles:
  - Development of state-of-the-art analysis tools for critical policy issues (e.g., climate change, electricity grid issues)
  - Use of tools appropriate to the need
  - Objectivity; analysis based on best available, un-biased data and assumptions

- Analysis Funding Sources:
  - DOE/EERE (including HFCIT, FreedomCar, Biomass, IT, BT, DEER, PBA)
  - DOE/SC (integrated assessment modeling)
  - DOE/NA (nuclear hydrogen production study)
  - DOE/OETD (GridWise modeling)
  - DoD – e.g., Army, DARPA
  - Private Sector (integrated assessment modeling, and special studies for private companies)
  - LDRD (PNNL has initiatives in hydrogen, carbon management, and energy systems transformation [GridWise])
History

- Long history of analysis work at PNNL: ~25+ yrs
- Past analysis projects in cost analysis, lifecycle analysis, market analysis, decision analysis, systems optimization, systems comparison for a variety of technologies (see backup slides)
- Hydrogen has been included in PNNL integrated assessment models for 10 years or so
PNNL Tools
Across the Scale and Scope Spectrum

Scale: Components → Technology Systems → Global Energy, Economic, Environmental System

Scope: Energy/Materials
Environment
Economics
PNNL Tools
Across the Scale and Scope Spectrum

Scale: Components ➔ Technology Systems ➔ Global Energy, Economic, Environmental System

Scope:
- Energy/Materials
- Environment
- Economics

Computational mechanics and fluid-dynamics modeling
Chem-CAD modeling
PNNL Tools
Across the Scale and Scope Spectrum

**Scale:**
- Components
- Technology Systems
- Global Energy, Economic, Environmental System

**Scope:**
- Energy/Materials
- Environment
- Economics

- FEDS
- LCAAdvantage™
- TEAM
PNNL Tools
Across the Scale and Scope Spectrum

<table>
<thead>
<tr>
<th>Scale:</th>
<th>Components</th>
<th>Technology Systems</th>
<th>Global Energy, Economic, Environmental System</th>
</tr>
</thead>
</table>

**Scope:**
- Energy/Materials
- Environment
- Economics

- GRIDLAB-D and -T
- Integrated Assessment Models:
  - SGM
  - MiniCAM
  - ObjECTS
PNNL Tools
Across the Scale and Scope Spectrum

Scope:
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Scale:
- Components
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Tools:
- Chem-CAD modeling
- Computational mechanics and fluid-dynamics modeling
- GRIDLAB-D and -T
- Integrated Assessment Models: SGM, MiniCAM, ObjECTS
- LCAdvantage™
- TEAM
- FEDS
<table>
<thead>
<tr>
<th>People</th>
<th>Group or Initiative</th>
<th>Capabilities</th>
</tr>
</thead>
<tbody>
<tr>
<td>George Muntean et al.</td>
<td>Computational Mechanics and Material Behavior Group</td>
<td>Materials components modeling using ANSYS, ABACUS and other commercial codes (H₂ Storage)</td>
</tr>
<tr>
<td>Don Stevens, Todd Werpy, et al.</td>
<td>Chemical and Biological Process Group</td>
<td>Chemical process modeling, e.g., biomass systems (mostly using Chem-CAD)</td>
</tr>
<tr>
<td>Daryl Brown, Jim Dirks, Mark Weimar et al.</td>
<td>Technology Systems Analysis Group; TPD Group</td>
<td>Technology assessment; lifecycle costing; TEAM, FEDS</td>
</tr>
<tr>
<td>Marylynn Placet et al.</td>
<td>Energy Policy and Planning Group (DC)</td>
<td>Financial analysis, strategic planning, program benefits assessment</td>
</tr>
<tr>
<td>Jae Edmonds et al. Charlette Geffen Ken Humphreys</td>
<td>Joint Global Change Research Center (DC); Carbon Management Initiative</td>
<td>Integrated assessment modeling: SGM, MiniCAM, ObjECTS</td>
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Skill Set – Models that Currently Include Hydrogen (1)

- **SGM - MiniCAM - ObjECTS**
  - SGM, MiniCAM and ObjECTS currently in use; ObjECTS is a new framework developed in 2004
  - Global/partial equilibrium model of the economy, with emphasis on the energy sector. Makes 50 to 100-year projections of energy patterns, emissions, costs
  - Part of integrated assessment modeling system targeted toward understanding global climate issues
  - Versions under development are using object-oriented modeling approach (C++); we do not use a commercial modeling platform
  - **Limitations:** Hydrogen infrastructure costs included but infrastructure constraints not modeled. Currently expanding detail on end-use building services to better address hydrogen technologies in buildings.
From the NAE Study to ObjECTS/MiniCAM

- Introduced the NAE technological assumptions into the new ObjECTS/MiniCAM modeling system.
  - Long-term, global integrated assessment model of energy, economy and climate change
  - 14 global regions,
  - Time horizon of 2095

- Took the NAE engineering data as assumptions

- Used the ObjECTS/MiniCAM to analyze market competition and energy-economy interactions.
  - H₂ in transportation, stationary applications, interactions with other energy supply and transformation technologies.
Going Beyond the NAE Study

Four Cases Selected to Frame an Initial Assessment

Two Technology States of the World
- Reference technology (Ref 2100)
- Advanced (NAE) technology (Adv 2100)

Two Policy States of the World
- No explicit climate policy imposed (no constraints)
- Climate policy where concentrations are constrained to 550 parts per million volume (ppmv)
Initial Findings

Climate change policy alone does not necessarily create a market for hydrogen—the technology has to be market competitive without climate policy.

Reference Case, End-use Energy

Reference Case Technology, End-use Energy—550 ppm CO₂
Initial Findings

The introduction of a carbon constraint may actually reduce the deployment of hydrogen, although $H_2$ maintains relative market share.

H$_2$ and CCS Technology Case, End-use Energy—No Climate Policy

H$_2$ & CCS Technology Case End-use Energy—550 ppm CO$_2$
Initial Findings

Hydrocarbons may be the most attractive hydrogen feedstocks. The composition shifts toward bio-fuels in a climate-constrained world.

H$_2$ and CCS Technology Case, End-use Energy—**No Climate Policy**

H$_2$ & CCS Technology Case End-use Energy—**550 ppm CO$_2$**
Skill Set – Models that Currently Include Hydrogen (2)

- **LCAdvantage™**
  - Developed in mid-1990s; won R&D100 award
  - Life-cycle inventory tool with economic accounting capability. Characterizes the energy, economic, and environmental impacts of products and processes over their full cradle-to-grave life cycles.
  - Self-contained, written in C++, runs on any Windows computer
  - Modest LDRD effort directed toward introducing hydrogen technologies
  - **Limitations:** Model produces a snapshot in time for a system, and is not a dynamic simulation.
Potential Application of LCAdvantage™ to Hydro-Produced Hydrogen

Stages in the Hydrogen-Powered and Conventional Vehicle Energy Cycles

- Hydropower Production
- Electrolysis
- Hydrogen Storage
- Hydrogen Distribution
- Hydrogen Vehicle Operation
- Crude Oil Production and Transport
- RFG Production (Refining)
- RFG Storage
- RFG Distribution
- Conventional Vehicle Operation
- Vehicle and Fuel Cell Manufacture

Characterize energy flows, lifecycle costs and environmental impacts for:

- each individual technology in the pathway
- the full energy cycle

17
Skill Set – Models that Could Potentially be Adapted to Include Hydrogen (1)

- **TEAM – “The” Economic Analysis Model**

Could be used to conduct lifecycle cost analysis of a wide range of hydrogen components, technologies, systems

- Flexible, EXCEL-based lifecycle cost analysis tool that generates year-by-year cash flow streams; calculates paybacks, discounted paybacks, IRR, profitability ratios, levelized costs

- Originally developed in 1987 in support of DOE Thermal Energy Storage Program, but developed in a technology-neutral format.

- Considers initial capital, interim capital, O&M, revenue, operating life, property tax rate, income tax rate, discount rate, inflation rate

- **Limitations:** Not completely “user friendly”
Skill Set – Models that Could Potentially be Adapted to Include Hydrogen (2)

- FEDS – Federal Energy Decision System

  Could be used to examine the economics of hydrogen use in building applications

  • Model development and use began in 1990 and continues to date.
  • Fuel-neutral, technology independent, comprehensive method for quickly and objectively identifying building energy technology improvements that offer maximum life-cycle cost savings
  • Hourly building simulation using typical day, hot day, and cold day for each month and day type (weekday, Saturday, and Sunday). FEDS uses a sequential iterative optimization approach to determine the minimum life-cycle cost for building technologies.
  • Model developed in C and C++ with a Visual Basic user interface and Access databases
  • Limitations: Has not been applied to fuels cells or other hydrogen-using technologies
Skill Set – Models that Could Potentially be Adapted to Include Hydrogen (3)

- **GRIDLAB-D (operational) and GRIDLAB-T (under development)**
  - Could be adapted to simulation of hydrogen distribution/delivery systems

- Tool for simulating the combined system performance and operation of the power grid's: (1) electric infrastructure; (2) electric loads at the end-use level including consumer behavior (3) new distributed resource technologies such as distributed generation, storage, and peak load demand response technologies for consumers, (4) wholesale and retail markets, contracts, and trading, including agent-based decision making on the part of buyers, sellers, and consumers

- GridWise-D: scope ranges from the distribution substation and retail markets to individual appliances cycling on and off in populations of ten's of thousands of individual buildings.

- GridWise-T: scope ranges from the substation load (feeder level) up to the transmission system and power plants, including operation of wholesale markets.

- Uses thermodynamic and behavioral/statistical models of end-use loads; partial differential power flow equations and grid control operations; agent-based models of human actors in markets and consumers. Coded in C++ (windows and linux) with MatLab Power Systems Toolkit (GridLab-D); Areva T&D Dispatch Training Simulator (GridLab-T)

- **Limitations**: Presently a research tool -- primitive user interface. It is still under development for public domain use. The simulation includes fuel-based end-uses but not fuel infrastructure or markets (yet).
Skill Set – Models that Could Potentially be Adapted to Include Hydrogen (4)

- Process Engineering Tools
  Could be applied by PNNL for engineering simulation and techno-economic analysis in PNNL technical specialty areas such as:
  - \( \text{H}_2 \) storage materials/systems
  - Microtechnology components in hydrogen systems
  - Bio-processes
  - Solid-oxide fuel cells
## Skill Set – Capabilities Summary

<table>
<thead>
<tr>
<th>TYPE OF ANALYSIS</th>
<th>RESIDENT CAPABILITY?</th>
<th>STUDIES SPECIFIC TO H₂?</th>
<th>MODELS SPECIFIC TO H₂?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resource Analysis</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Technoeconomic Analysis</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Environmental Analysis</td>
<td>Yes</td>
<td>Yes, esp. for carbon emissions</td>
<td>Yes</td>
</tr>
<tr>
<td>Delivery Analysis</td>
<td>Yes, for electricity</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>Infrastructure Development Analysis</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>Energy Market Analysis</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
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</table>
Hydrogen-Specific Studies

- Weimar et al. 2004. “Using a High-Temperature Hydrogen Co-Generation Reactor to Optimize both Economic and Environmental Performance” (Study conducted for DOE/NA; paper presented at NHA)

- Several JGCRI hydrogen papers, e.g.:
Future

Plans for the further development of PNNL’s integrated assessment models include in-depth study of hydrogen technology/infrastructure for improvement of the model’s treatment of hydrogen production, delivery and end use.
Analysis Issues

- What are the best end uses for hydrogen (is it mainly a solution for transportation, or does it make sense for distributed generation, buildings, etc.)? When and where does the hydrogen market develop?

- How much will delivered hydrogen cost? Can it compete with future alternatives? How will regional differences affect the cost?

- What sources will supply the hydrogen, and how does hydrogen production impact existing energy markets?

- What production and delivery scenarios make sense in each US region? When and where does central production make sense? What is the role for forecourt production (is it just a transition approach or does it make sense in the long-run)?
Analysis Issues (cont’d)

- What is the role of storage? Can production and storage be optimized to reduce overall costs, given a range of available production and storage technologies?
- How much will it cost to develop a hydrogen economy? What are the financing options?
- How will hydrogen markets develop outside the United States? How will such developments impact the hydrogen transition, prices, and technologies used in the US?
- To what extent does the availability of hydrogen lower carbon emissions from the transportation (and other) sectors? How would a carbon tax or other carbon policies impact hydrogen markets and hydrogen technology choice?
- What other kinds of policies might encourage hydrogen?
Backup Slides
Component Modeling
Computational Mechanics and Material Behavior Group

- Development of state-of-the-art simulation and modeling solutions to the industrial challenges in manufacturing lightweight vehicles and structures, vehicular air pollutant formation and controls, and energy and fuel storage devices.
- Work has focused primarily on materials that are critical to the development of lightweight, fuel-efficient cars and trucks:
  - Aluminum, Magnesium, Titanium
  - Glass
  - Thermoplastic composites
- Actively supporting research in:
  - new methods for joining dissimilar materials
  - hydroforming, superplastic forming, electromagnetic forming
- Baseline capabilities include
  - High performance computing
  - Collaborative tools
  - Engineering, materials/chemical sciences
- Applications
  - Manufacturing and materials
  - Emission control
  - Fuel cells & fuel storage

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System Modeling Of Hydride Hydrogen Storage Cells

- Simulating this system will require a coupled field Structural/Thermal/Fluid-Dynamics analysis
  - May be doable entirely in ANSYS Multiphysics or may need to be split between ANSYS and StarCD as it is currently done in fuel cell analyses
- H₂ and hydride interaction is a key element of the analysis, and could be handled in a Fortran or C++ model
- System modeling could provide a great advantage when evaluating the suitability of new hydrides other storage methods by estimating:
  - Containment structure (size, materials, mass)
  - Energy requirements (external heating and cooling to drive the reactions)
  - System efficiency
Chemical and Biological Process Group

Chemcad flowsheets used as basis for equipment sizing and costing and/or for flow estimation

Recent activities:

• Prepared relative cost comparison between conventional technology and novel microtechnology reactor to produce Fischer-Tropsch fuels from biomass derived syngas (2003)
• Updating Techno-Economic Analysis for pyrolysis oil upgrading via hydrotreating (2004)
Example of Recent Chemcad Analysis:
Microtech reactors to upgrade biomass-derived syngas to Fischer-Tropsch fuels
Cost comparisons

Breakdown of Investment Costs for 1000 TPD Biomass Plant producing 1100 BPD FT Fuels (Micro-channel contact time 0.06s)

- **CO2 removal**
- **Hydrocracker**
- **Conventional FT**
- **Micro-channel FT**
- **HX, Separators, etc.**

**Capital Investment, millions $**

- **Once through conventional FT, CO2 removal**
- **Micro-channel FT**
- **Micro-channel FT, small Hydrocracker**
- **Micro-channel FT, no CO2 removal**
- **Micro-channel FT, no CO2 removal, small hydrocracker, High CO conversion**

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Technology Systems Modeling
Facility Energy Decision System (FEDS)

An easy to use, yet powerful & flexible tool for quickly and objectively identifying building energy technology improvements

- Accepts generic or very detailed inputs and provides intelligent inferences for missing data
- Evaluates the cost and performance of thousands of building energy retrofit technologies, estimating energy consumption and electric demand (peak & coincident) for all energy systems
- Determines the minimum life-cycle-cost retrofits to systems within a facility and on an installation, considering all interactive effects

- Building Shell
- Advanced HVAC Options
  - Ground-coupled heat pumps
  - Dual-fuel heat pumps
  - Gas engine chillers
  - Absorption chillers
- Advanced Lighting Technologies
- Motors
- Refrigeration Equipment
- Plug Loads
- Central Energy Plants (coming soon)
Facility Energy Decision System (FEDS)

- Examines single buildings to large multi-building installations
- Tracks emissions impacts
- Conducts alternative financing analyses
- Allows users to modify cost data & optimization parameters
- Models 16 civilian & 28 military building types
- Provides detailed output

www.pnl.gov/FEDS
Integrated Assessment Modeling
An integrated assessment approach enables evaluation of the dynamics of technology evolution and change

- Economics-based analysis of price and market share of new technologies under various future scenarios, and their greenhouse gas emissions
- Understand timelines and potential pathways for evolution of hydrogen energy systems
- Global framework for analysis, accounting for regional differences
- Context for evaluating the magnitude of infrastructure investment required by region
Core Elements of MiniCAM Energy Markets

- Regional Fertility & Survival Rates
- Regional Labor Force
- Regional GDP
- Energy Technologies
- Regional Energy Demand
- Regional Prices
- Regional Energy Supply
- World Prices and Quantities
- GHG Emissions
- Regional Resource Bases
- Regional Energy Supply Technologies
Alternative production pathways for hydrogen represented in the MiniCAM

- Oil Production
- Biomass Production
- Coal Production
- N. Gas Production
- Wind
- Nuclear/Fusion
- Hydro
- Solar/SPS
- Synfuel Conversion
- Synfuel Conversion
- Gas Processing
- Liquids Refining
- Electricity Market
- Hydrogen Market
- Coal Market
- Biomass Market
- Natural Gas Market
- Liquids Market
Energy supply pathway options in MiniCAM

- Residential Technologies
- Commercial Technologies
- Industrial Technologies
- Transport Technologies

- Residential Sector
- Commercial Sector
- Industrial Sector
- Transport Sector

- Liquids Market
- Biomass Market
- Coal Market
- Natural Gas Market
- Hydrogen Market
- Electricity Market
Transportation sector detail in MiniCAM

Transport Technologies

Passenger Transport
- Bus
- Rail
- Air
- Motor Cycles
- Water

Freight Transport
- Truck
- Rail
- Air
- Water
- Pipeline

Trucks

Automobile

Gasoline
- Diesel
- Kerosene
- Other Liquids
- Natural Gas
- H2
- Solids
- Electricity
The National Academy of Engineering Study

• Focus on transportation
• Two primary pathways
  • Central H₂ production with pipeline distribution
    – Natural Gas (with or without CO₂ Capture & Storage)
    – Coal (with or without CO₂ Capture & Storage)
    – Nuclear (Wind and Solar also included in MiniCAM)
  • Distributed H₂ production with on site production
    – Electrolysis
    – Natural Gas (CO₂ emissions)
• Detailed estimates of technology options and associated costs

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From the NAE Study to ObjECTS/MiniCAM

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Modeling Insights from ObjECTS.MiniCAM (Preliminary)

- The introduction of NAE optimistic cost estimates into ObjECTS.MiniCAM was consistent with rapid penetration of H₂ into both stationary and mobile transport markets after 2015 (when the NAE assumed these technologies might become available).
  - Total global market H₂ consumption in 2035 exceeds 10 EJ/year.
  - Half of global automobile transportation by 2050 was provided by H₂.
- Given the NAE cost estimates both central station and distributed H₂ production coexist in ObjECTS.MiniCAM runs.
- But, central station earns the larger market share in ObjECTS.MiniCAM under NAE cost and performance assumptions, due at least in part to its advantages in stationary fuel cell applications.
- The development of a H₂ economy in ObjECTS.MiniCAM has:
  - A depressing effect on oil demand.
  - Modest effect on global CO₂ emissions (20% reductions) absent policy.
- Climate policy has only a modest influence on market penetration.
Additional Insights (Preliminary)

- Climate policy will not create a hydrogen economy, the technology must be able to compete in a non-climate constrained world.
- Even if technical hurdles are overcome and hydrogen technology is competitive, a hydrogen economy may not reduce net carbon emissions without a carbon constraint.
- The addition of a climate constraint may actually reduce hydrogen production.
- Hydrocarbon feedstocks (natural gas, coal, and biomass) look particularly attractive as a source of hydrogen.
- Initial deployments may occur in stationary applications.
- Massive deployment in the transportation sector will take time.
Initial Findings

Climate change policy alone does not necessarily create a market for hydrogen—the technology has to be market competitive without climate policy.

Reference Case, End-use Energy

Reference Case Technology, End-use Energy—550 ppm CO$_2$
Initial Findings

- The carbon value penalizes hydrogen too!
- Where did the $H_2$ come from?
  - Hydrocarbons (natural gas and coal), or
  - Electricity (which in turn came from power production using fossil fuels).
Initial Findings

The emergence of a hydrogen economy does not necessarily imply reductions in carbon emissions.

H₂ and CCS Technology Case, End-use Energy—No Climate Policy

A reference case with advanced technology development of carbon capture and H₂, but no climate policy.

A reference case with continued technology development, and no climate policy.

Emissions path that stabilizes CO₂ concentrations at 550 ppm.
Initial Findings

The introduction of a carbon constraint may actually reduce the deployment of hydrogen, although $H_2$ maintains relative market share.

H$_2$ and CCS Technology Case, End-use Energy—No Climate Policy

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Hydrocarbons may be the most attractive hydrogen feedstocks. The composition shifts toward bio-fuels in a climate-constrained world.

H₂ and CCS Technology Case, End-use Energy—No Climate Policy

H₂ & CCS Technology Case End-use Energy—550 ppm CO₂
Initial Findings

Significant deployment of hydrogen in transportation systems will take time with or without climate policy.

H₂ and CCS Technology Case, End-use Energy—No Climate Policy

H₂ & CCS Technology Case End-use Energy—550 ppm CO₂
Acknowledgements

- Much of PNNL’s integrated assessment modeling work is supported by the Global Energy Technology Strategy Program (GTSP), an international public-private collaboration focused on assessing the role that technology can play in addressing the long-term risks of climate change.

- Additional information on the GTSP and a listing of sponsors and collaborators can be found at www.battelle.org/gtsp
Past Systems Analysis Studies
PNNL analysis strengths are based on a history of application to complex energy challenges

- Advanced systems and emerging technologies, where data and experience is less well developed
- New system configurations or applications that must interface with existing subsystems and/or infrastructure
- Requirements to understand and evaluate energy, environmental and economic impacts – in a way that allows effective comparison among technology options
- From design to development to deployment – the need to identify and address institutional and socioeconomic challenges
Technology Characterizations and Market Assessments

Selected examples:

- Fuel Cells: Performance and Market Assessment (Client: Portland General Electric)
- Review of Methods for Forecasting the Market Penetration of New Technologies (Client: US DOE)
- Identification and Evaluation of Technologies for CO₂ Control at Fossil-Fuel Power Plants (Client: Tokyo Electric Power)
- Site-Specific Economic Assessment of Distributed Generation Technologies (Client: Toyota Motor Sales, USA)
- Competitive Intelligence of Battelle’s MicroTechnology: Transportable Energy Applications of Proton Exchange Membrane (PEM) Fuel Cells (Internal PNNL study)
Energy Systems Analysis

**Selected examples:**

- Total Energy Cycle Assessment of Electric and Conventional Vehicles: An Energy and Environmental Analysis (with NREL, ANL)
- Lifecycle Assessment of Building Technologies
- Fuel Cycle Evaluations of Biomass-Ethanol and Reformulated Gasoline (with NREL, ORNL)
- Life-cycle Assessment of 1,4-Butanediol Produced from Petroleum Feedstocks Versus Bio-Derived Feedstocks
- Cost and Energy Consumption Estimates for the Aluminum-Air Battery Anode Fuel Cycle