Hydrogen Related Analytical Studies

Office of Fossil Energy and National Energy Technology Laboratory

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Charter
Office of Fossil Energy

Describe your group's mission or objectives (group is the part of your org that actually does analysis)

- **Provide guidance for establishing research direction**
  - Define current baseline
    - Centralized production of hydrogen from coal
    - Centralized production of hydrogen from coal with co-production of electric power
    - Centralized production of liquid fuel hydrogen carriers for producing decentralized hydrogen
  - Define advanced configurations, components and the potential for improvement
  - Establish technology cost

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Office of Fossil Energy, cont'd.

Describe your group's mission or objectives (group is the part of your org that actually does analysis)

- Life cycle analysis
- Establish benefits associated with technology development
- Evaluate the potential for individual projects to meet targets

Describe your group's current/past funding sources for analysis projects

FY 2003	FY 2004	FY 2005
$721K	$735K	$750K

Charter
NETL

Describe your organization's mission or objectives

- **NETL Mission (partial)**
  Resolve the environmental, supply, and reliability constraints of producing and using fossil energy resources to provide Americans with a stronger economy, healthier environment, and more secure future.

…continued

Charter – NETL, cont'd.

Describe your group's current/past funding sources for analysis projects

- **FY04 - $450K**
  - Combined funding from Offices of Coal, and Gas and Oil, OFE
  - Does not include personnel costs for NETL Systems Analysis Team

Describe your group's mission or objectives (group is the part of your org that actually does analysis)

- **NETL Systems Analysis Team Mission**
  Develop an in-house systems analysis capability to evaluate new technological concepts that may help resolve energy and environmental issues relevant to the continued use of fossil energy, especially coal.

History - NETL

Describe history of and how long your group has been doing analysis in general

- NETL Systems Analysis Team assembled in June, 2003

List significant past analysis projects (i.e., those no longer being worked on)

- N/A

Describe history and how long you've considered hydrogen in your analyses

- Hydrogen included in analysis since team inception. IGCC with carbon capture plant simulations at NETL since 1999.

History – Parsons

- Parsons (then Gilbert/Commonwealth) started development of modeling of coal conversion systems in the mid-1980's as a Technical Support Contractor for DOE headquarters and what is now NETL. Modeling evolved from spreadsheets to ASPEN. Simulations included production of power, liquids, syngas and hydrogen from coal.

- In the mid-1990s Parsons simulated a series of decarbonized fuel (hydrogen) production plants with design and cost estimating to assess hydrogen production and CO2 capture with advanced membrane systems.

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History – Parsons, cont'd.

- In the early-2000's, Parsons prepared several conceptual designs to produce hydrogen from fossil fuel for EPRI and other private clients. Conceptual designs for hydrogen production from coal were also prepared for the DOE. These designs resulted in published reports and presentations.

- Currently, Parsons is a contributor to the *FutureGen* program and to the H2A study.

History – Mitretek

- In 1980 Mitretek (then Mitre) started development of simulation modeling of coal conversion systems.

- In 1981 simulation models were developed for direct liquefaction of coal including production of coal-derived hydrogen for coal hydroliquefaction.

- In mid 1980s in-house spreadsheet based computer simulation models were developed and these included simulation of coal gasification using Lurgi-dry ash, BGC Lurgi, Westinghouse, Texaco, and Shell gasifiers, Fischer-Tropsch synthesis, SNG production, and synthesis gas production.

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History – Mitretek, cont'd.

- In 1990 models expanded to include use of natural gas, petroleum residues and coke as feed stocks
- In 1999 model expanded to include ionic transport membranes for NG conversion, hydrogen, synthesis gas, and oxygen production
- In 1995 model expanded to include E-gas gasification and simulation of coproduction (polygeneration) plants to produce FT fuels, hydrogen, and electric power

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History – Mitretek, cont'd.

- In 2002 model expanded to include simulation of current and future *FutureGen* plant configurations. Advanced *FutureGen* configurations include membrane separation, advanced gasification, ionic transport membrane air separation, advanced syngas cleaning, advanced gas turbines and solid oxide fuel cells

- In 2004 model expanded to include Noell and Transport gasifiers for syngas production

History – TMS

- Provides program and analytic support to FE RD&D hydrogen and clean fuels programs.
- Developed “well-to-wheel” emissions and energy use models linked to GREET 1.6 for H2 and liquid fuels from coal and natural gas. Models include lifecycle coal and natural gas use and 10+ fuel/vehicle pathways none of which are in GREET.
- Modeled U.S. LD vehicle fleet and H2 market penetration/demand to 2050+.
- Analysis and modeling of petroleum coke use for co-production of fuels/power.

Skill Set – People - NETL

List past analysts that helped develop your group's capabilities

- **N/A**

List current analysts and their primary roles

- **NETL Systems Analysis Team**
  - Peter Balash—Economist—Direct technoeconomic study on alternative scenarios for the Hydrogen Economy through year 2040
  - Dale Keairns—Chemical engineer—Design/evaluate process concepts for producing hydrogen from coal, including *FutureGen*
  - Kenneth Kern—Electrical engineer—Prepare review of principal barriers to widespread use of hydrogen

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Skill Set – People - NETL, cont'd.

List current analysts and their primary roles

- **NETL Systems Analysis Team**
  - Edward Parsons—Mechanical engineer—Prepare review of fossil, nuclear, and renewable energy technologies for producing hydrogen
  - John Ruether—Chemical engineer—Participate in techno-economic study of the Hydrogen Economy; direct ASPEN modeling study of innovative use of ceramic membranes in power generation from coal with carbon capture
  - Larry Ruth—Chemical engineer—team leader
  - John Wimer—Mechanical engineer—Design/evaluate process concepts for producing hydrogen from coal, including *FutureGen*; participate in ASPEN modeling of power systems with ceramic membranes

Skill Set – People - Parsons

List current analysts and their primary roles

- Michael D. Rutkowski—Chemical engineer—Technical analyst and project manager for hydrogen from fossil energy - Production of syngas and hydrogen from coal and natural gas; Manages technical support activity for DOE HQ and NETL; Member of Core H2A Group

Skill Set – People - Mitretek

List current analysts and their primary roles

- David Gray—Chemical engineer—Techno-economic analyses by simulation of coal and NG conversion to hydrogen, FT fuels, SNG, synthesis gas and power.
- Glen Tomlinson—Mechanical engineer—Simulation of coal and NG conversion systems for production of power, FT, SNG, syngas, hydrogen.
- Sal Salerno—Chemical engineer—Energy and environmental engineering studies, equipment design, and modeling of gasification and petroleum refining operations.

Skill Set – People - TMS

List current analysts and their primary roles

- John Anderson—Chemical engineer—Energy and emissions modeling of coal and natural gas fuels on a “well-to-wheel” basis; hydrogen demand scenario analysis; benefits analysis; and refinery linear program modeling.

- Mark Ackiewicz—Chemical engineer—Energy and environmental systems/benefits analysis of fuel/vehicle pathways for H2 and liquids from coal and natural gas; hydrogen demand scenario analysis.

Skill Set – Models - NETL

- **List models that explicitly include hydrogen**

  Model name, dates in use, brief description

  – Extension of NEMS to include a new Market Module for Coal-to-Hydrogen technologies, in progress

  Modeling methodology (e.g., linear programming, thermodynamic, etc.)

  – NEMS: a computable general equilibrium (CGE) economic model. Linear programming with cross economic sector feedback. New module: Cost/performance/efficiency relationships via look-up tables, etc.

  Model platform (e.g., GAMS, ASPEN, etc.)

  – NEMS

  Model limitations

  – (New module): Steady state, simple rules for operation at partial capacity, limited number of process options (e.g. gasifier type, CO2 absorption system)

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Skill Set – Models - NETL, cont'd.

List models that could be adapted to include hydrogen

Model name, dates in use, brief description

- Modeling of process concepts for coal to electricity and/or hydrogen with carbon capture. Case-specific modifications of ASPEN modeling of IGCC systems. Modeling with CO2 capture began in 1999. Principal process variations studied: gasifier type, syn gas cleaning approach, CO2 absorption system type, oxygen supply system type, combustion turbine type.

Modeling methodology (e.g., linear programming, thermodynamic, etc.)

- Steady state chemical process simulation.

Model platform (e.g., GAMS, ASPEN, etc.)

- ASPEN

Model limitations

- Steady state; limited detail in description of individual process units and operations.

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Skill Set – Models - NETL, cont'd.

List models that could be adapted to include hydrogen

Model name, dates in use, brief description

- AMIGA (developed at Argonne National Lab). In use since 1999. A computable general equilibrium (CGE) economic model.

Model platform (e.g., GAMS, ASPEN, etc.)

- AMIGA

Modeling methodology (e.g., linear programming, thermodynamic, etc.)

- Linear programming with cross economic sector feedback

Model limitations

- Limitations inherent in use of CGE models. AMIGA model represents 200 goods and services as well as 200 production process activities.

Skill Set – Models - Parsons

List models that could be adapted to include hydrogen

Model name, dates in use, brief description

- Modeling of process concepts for fossil fuels to power and/or hydrogen with carbon capture. Advanced membrane and gas cleanup technologies. Case-specific modifications of ASPEN modeling of IGCC systems for H2A and *FutureGen* designs. ASPEN expanded to include GE Steam Turbine Procedures.

Modeling methodology (e.g., linear programming, thermodynamic, etc.)

- Steady state chemical process simulation.

Model platform (e.g., GAMS, ASPEN, etc.)

- ASPEN

Model limitations

- Steady state; limited detail in description of individual process units and operations.

Skill Set – Models - Mitretek

- **Spreadsheet based models. Capabilities include:**
  - Coal conversion to SNG, FT fuels, Hydrogen, Synthesis gas, electric power, and combinations of these products (polygeneration or coproduction).
  - Technical and economic analyses for research guidance studies, feasibility analysis
  - Natural gas conversion to hydrogen, FT (GTL)
  - Direct coal hydroliquefaction models and hybrid combinations of direct and indirect coal liquefaction.

Skill Set – Models - TMS

List models that explicitly include hydrogen

Model Name:

– Modified GREET 1.6 Modules with Life Cycle By-Type Fossil Energy Use and Coal-Derived Transportation Fuels

Dates in use:

– 2003-2004

Brief description:

– Modules link 10+ fuel/vehicle pathways with GREET, including central coal to H2/FCV, coal-to-liquids and use in ICEVs, HEVs, and FCVs via distributed H2 production. “Well-to-wheels” lifecycle energy use (coal, nat gas, petroleum, and other); emissions (CO2, NOx, SOx); national costs of fossil energy and impact on U.S. trade deficit; and imported versus domestic lifecycle energy use outputs.

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Skill Set – Models - TMS, cont'd.

Modeling methodology:

- Spreadsheet modeling of techno-economic studies; links to GREET; complex iterations to calculate life cycle energy, including by-type fossil fuels that GREET does not provide.

Model platform:

- Excel

Model limitations:

- Excludes energy use to build infrastructure; some future criteria emissions estimates in GREET are not up-to-date

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Skill Set – Models - TMS, cont'd.

List models that explicitly include hydrogen

Model Name:

– Light duty fleet hydrogen demand model

Dates in use:

– 2002-2004

Brief description:

– Annual U.S. light duty fleet vehicle miles traveled (VMT), sales, and scrapped, plus H2 FCV market penetration scenarios through 2100. Also includes the President's scenario. Output includes annual hydrogen demand.

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Skill Set – Models - TMS, cont'd.

Modeling methodology:

– Spreadsheet modeling with input from AEO for VMT through 2025 and extrapolation thereafter. FCV market penetration option to designate technology "S" shaped curves with user defined initial year and in which year FCVs reach 50% of light duty vehicle fleet or linear growth rates.

Model platform:

– Excel

Model limitations:

– User input required to match recent AEO.

Skill Set – Capabilities Summary

TYPE OF ANALYSIS	RESIDENT CAPABILITY?	STUDIES SPECIFIC TO H_2?	MODELS SPECIFIC TO H_2?
Resource Analysis	Yes	Yes	Yes
Technoeconomic Analysis	Yes	Yes	Yes
Environmental Analysis	Yes	Yes	No
Delivery Analysis	Yes	Yes	No
Infrastructure Development Analysis	Yes	Yes	Yes
Energy Market Analysis	Yes	Yes	Yes

Studies – NETL

List current/planned hydrogen studies

- Review/critique of barriers to extensive use of hydrogen (achieving the “Hydrogen Economy”)
- Review of existing and potential technical approaches for large scale production of hydrogen
- Study of process improvements and innovative technology for generation of hydrogen from coal
- Modeling of improved process for generation of hydrogen from natural gas using ceramic membranes (performed by off-site contractor)
- Modeling of innovative approaches to use of ceramic membranes for oxygen separation in IGCC systems practicing carbon capture

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Studies – NETL, cont'd.

List current/planned hydrogen studies

- Extension of NEMS to include coal-to-hydrogen market module
- Technoeconomic modeling of alternative approaches to use of hydrogen for light duty vehicle transportation through 2040 (with ANL)

Studies - Parsons

List significant past studies that relate to hydrogen

- **Multiple simulations of IGCC process concepts for generation of electricity and/or hydrogen from coal employing carbon capture**
  - Rutkowski, Michael, Hydrogen Production Facilities Plant Performance and Cost Comparisons – Parsons for DOE/NETL, March 2002
  - Rutkowski, Michael, Capital and Operating Cost of Hydrogen Production from Coal Gasification – Parsons for DOE/NETL, April 2003
  - Michael Rutkowski, Parsons - Central Plant Production from Coal and Natural Gas – Provided as input to H2A Study

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Studies – Parsons, cont'd.

List current/planned hydrogen studies

- Parsons - Preparation of Topical Report on FutureGen Alternative Configurations – With and without CO2 Recovery; with and without Hydrogen co-production; alternative coals

Studies - Mitretek

List significant past studies that relate to hydrogen

- Hydrogen from coal: techno-economic analysis of producing hydrogen from coal using current and future technologies. This included production of hydrogen only and coproduction of hydrogen and power. (Presented to the National Academy of Sciences Committee on Alternatives and Strategies for Future Hydrogen Production and Use.)

- Studies of use of petroleum coke for production of hydrogen in the refining industry

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Studies – Mitretek, cont'd.

List significant past studies that could be adapted to hydrogen

- Studies on use of coal for production of SNG and synthesis gas for manufacturing industries and for refineries.
- Conversion of natural gas for production of clean transportation fuels using Gas-to-Liquids technologies
- Coal conversion to FT fuels and electric power using coproduction or polygeneration.

Studies - TMS

List significant past studies that relate to hydrogen

- Review of Public Domain Hydrogen Transportation Demand Assessments: An Analysis of Fuel Cell Vehicle Market Penetration Assessments with Projections Through 2050, TMS, Inc., July, 2003, DRAFT
- Hydrogen from Coal and Natural Gas: A Scoping Analysis of the Benefits of Clean and Secure Transportation Fuel for Fuel Cell Vehicles, TMS, Inc., December 2003

List current/planned hydrogen studies

- Energy and Environmental Benefits of Coal to Liquids and Hydrogen from Coal in the Transportation Sector, TMS, Ongoing (Energy Market Analysis)

Future

If your organization/group has firm plans/commitments to grow or expand your analytical capability (type, people, models, etc.), briefly describe

- **Anticipate expanding into modeling of hybrid fossil energy—renewable energy systems for supply of electricity and transportation fuels with reduced carbon emissions and reduced energy imports.**

Analysis Issues

Open podium – what do you see as the major issues related to analysis of hydrogen systems?

- **Each potential approach to large scale energy supply or use has advantages and disadvantages relative to alternatives. Society continues to weigh and evaluate tradeoffs offered by different energy approaches and the dollar value of achieving improvements of one kind or another. Analysts must strive to evaluate fully and communicate openly the salient features of innovative energy systems they investigate. Here are a number of attributes to consider:**
  - Reduction in petroleum imports and consumption
  - Reduction in GHG emissions

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Analysis Issues, cont'd.

- Reductions in SO2 and NOx emissions
- "Well to Wheels," or life cycle, energy efficiency/resource use
- Land use conflicts/constraints
- Dispatchability of electricity
- Infrastructure systems capital cost
- Consumer/user capital cost
- Consumer/user operating cost
- Consumer safety (excluding threat of terrorism)
- Energy system robustness/safety with respect to terrorism

Backup Slides

Types of Hydrogen Analysis

- **Resource Analysis**
  - Where are the resources to make hydrogen and how much do they cost?
- **Technology Feasibility and Cost Analysis**
  - Which technologies have the greatest potential for economic success?
  - Where should research efforts be focused?
  - What are the impacts of production volume?
- **Environmental Analysis**
  - What are the environmental impacts of hydrogen technologies?
  - What steps can be taken to reduce impacts?
- **Delivery Analysis**
  - What are the most economic options for delivering hydrogen?
- **Infrastructure Development and Financial Analysis**
  - What are the optimal scenarios for developing the hydrogen infrastructure?
  - What will a hydrogen infrastructure cost and what are the financial risks?
- **Energy Market Analysis**
  - What are feasible hydrogen futures?
  - Which technologies are most likely to be a part of the hydrogen future, and what are the interactions between hydrogen and other energy carriers?
  - What are the scenarios for hydrogen use in transportation and stationary markets?
  - What are the impacts, costs, and financial risks?
  - What market penetration pathways are likely?