II.0 Hydrogen Production Sub-Program Overview

The Hydrogen Production sub-program supports research and development (R&D) of technologies that will enable the long-term viability of hydrogen as an energy carrier for a diverse range of end-use applications including stationary power (e.g., backup power and combined-heat-and-power systems), transportation (e.g., specialty vehicles, cars, trucks, and buses), and portable power. A variety of feedstocks and technologies are being pursued.

Three DOE offices are engaged in R&D relevant to hydrogen production:

- The Fuel Cell Technologies Program, within the Office of Energy Efficiency and Renewable Energy (EERE), is developing technologies for distributed and centralized renewable production of hydrogen. Distributed production options under development include reforming of bio-derived renewable liquids and electrolysis of water. Centralized renewable production options include water electrolysis integrated with renewable power generation (e.g., wind, solar, hydroelectric, and geothermal power), biomass gasification, solar-driven high-temperature thermochemical water splitting, direct photoelectrochemical water splitting, and biological processes.

- The Office of Fossil Energy (FE) is advancing the technologies needed to produce hydrogen from coal-derived synthesis gas, including co-production of hydrogen and electricity. Separate from the Hydrogen and Fuel Cells Program, FE is also developing technologies for carbon capture and sequestration, which will ultimately enable hydrogen production from coal to be a near-zero-emissions pathway.

- The Office of Science’s Basic Energy Sciences (BES) program conducts research to expand the fundamental understanding of biological and biomimetic hydrogen production, photoelectrochemical water splitting, catalysis, and membranes for gas separation.

- The Office of Nuclear Energy (NE) is conducting efforts in development of high-temperature electrolysis, under the Next Generation Nuclear Plant (NGNP) project, which also includes evaluations of other end-user applications and energy transport systems. The Nuclear Hydrogen Initiative was discontinued as a separate program in Fiscal Year (FY) 2009 after the selection of steam electrolysis as the hydrogen production pathway most compatible with the NGNP.

Goal

The goal of the Hydrogen Production sub-program’s portfolio is to develop low-cost, highly efficient hydrogen production technologies that utilize diverse domestic sources of energy, including renewable resources (EERE), coal with sequestration (FE), and nuclear power (NE).

Objectives

The objective of the EERE hydrogen production portfolio is to reduce the cost of hydrogen dispensed at the pump to a cost that is competitive with gasoline, on a cents-per-mile basis (based on current analysis, this translates to a hydrogen threshold cost of $2-4 per gallon gasoline equivalent [gge]). Technologies are being researched to achieve this goal in timeframes appropriate to their current stages of development.

The objectives of FE’s efforts in hydrogen production are documented in the Hydrogen from Coal Program Research, Development and Demonstration Plan (September 2009). They include proving the feasibility of a near-zero emissions, high-efficiency plant that will produce both hydrogen and electricity from coal and reduce the cost of hydrogen from coal by 25 percent compared with current technology, by 2016.

FY 2011 Technology Status

The current projected cost of hydrogen from several production pathways is shown in Figure 1. The current status of cost and performance for several other hydrogen production pathways, as determined by independent reviews, are shown in Table 1. These reviews, along with cost projections from the Hydrogen

1Note: Targets and milestones are under revision; therefore, individual progress reports may reference prior targets.
Analysis (H2A) model, were also used in the development of the Hydrogen Production sub-program’s chapter of the Multi-Year Research, Development and Demonstration Plan (MYRD&D Plan), where they were used as the basis for establishing the status of the different technologies and for determining appropriate pathway-independent targets. The 2006 report Distributed Hydrogen Production from Natural Gas\textsuperscript{2} provided the basis for DOE to discontinue R&D of steam methane reforming for hydrogen production—verifying that the use of existing steam methane reforming technologies in distributed hydrogen production could meet the cost target at high-volume production. Targets for hydrogen production efforts in FE, along with information on the status of the technologies, are documented separately in the Hydrogen from Coal Program Research Development and Demonstration Plan (2009).

II. Hydrogen Production / Overview

TABLE 1. Recent Independent Reviews of Production Pathway Costs

<table>
<thead>
<tr>
<th>Pathway</th>
<th>Report</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steam Methane Reforming²</td>
<td>Distributed Hydrogen Production from Natural Gas, NREL, October 2006</td>
<td>$2.75–$3.05/gge</td>
</tr>
<tr>
<td>Photoelectrochemical (PEC) Production⁴</td>
<td>Technoeconomic Analysis of Photoelectrochemical (PEC) Hydrogen Production, Directed Technologies Inc., December 2009</td>
<td>$4–$10/gge (projected cost assuming technology reaches technology readiness); promising PEC materials identified, but durability issues remain</td>
</tr>
<tr>
<td>Biological Production⁴</td>
<td>Technoeconomic Boundary Analysis of Biological Pathways to Hydrogen Production, Directed Technologies Inc., September 2009</td>
<td>$3–$12/gge (projected cost assuming technology readiness) 15% solar-to-chemical energy efficiency by microalgae</td>
</tr>
<tr>
<td>Biomass Gasification</td>
<td>Hydrogen Production Cost Estimate Using Biomass Gasification, Independent Panel Review [DRAFT], NREL, April 2011</td>
<td>Preliminary results: feedstock costs, capital costs, and financing structure are primary influences on overall cost.</td>
</tr>
</tbody>
</table>

¹ Based on H2A V.2.1 using 2005$ inputs for costs, with the exception of the 2011 Solar Thermochemical Production study which used 2007$ inputs.

This year an updated version of H2A (H2A version 3) was published with updated economic data and assumptions; this version also converts all costs to 2007 dollars. Updated economic and cost-sensitivity analyses are currently being performed using H2A version 3, incorporating the most up-to-date information on pathway technologies and technology-readiness projections. These analyses will serve as the basis for updating the status information in Table 1 and will be used to revise pathway-specific targets in an updated version of the MYRD&D Plan.

FY 2011 Accomplishments

Biomass Gasification

- The National Renewable Energy Laboratory (NREL) completed the initial draft of an independent panel review of costs for hydrogen production from biomass gasification and performed an analysis of near-term markets for hydrogen from biomass gasification.
- The United Technologies Research Center (UTRC) demonstrated a novel slurry-based fuel-flexible and carbon-neutral biomass reforming process that exceeded 2012 targets in both projected cost and plant efficiency (current status: $1.54/gge and 51.1% efficiency, respectively).
- The Gas Technology Institute completed a membrane design for a one-step, shift-separation membrane reactor for close-coupling with a biomass gasifier. The module demonstrated a flux rate of 80+ standard cubic feet per hour (SCFH)/ft² and is capable of 125 SCFH/ft². Economic analysis indicates that the technology can meet the production threshold cost target of <$2.00/gge.
Bio-Derived Liquid Pathways

- In the area of autothermal reforming of bio-derived liquids, NREL replaced their catalyst with a better-performing commercial catalyst and reduced the amount of hydrogen oxidized to $\text{H}_2\text{O}$ during reforming, resulting in increased yield from 7.4 g hydrogen to 10.1 g hydrogen per 100 g bio-oil during short-term, bench-scale tests of catalytic steam reforming at $\sim 650^\circ\text{C}$, and increased process efficiency from 47% to 62%.
- Pacific Northwest National Laboratory (PNNL) evaluated the feasibility of aqueous phase reforming (APR) of pyrolysis oil and demonstrated successful reforming of most oil components, but also identified key challenges in reforming the acetic acid component. H2A analysis indicated APR of bio-oil is economically feasible only with complete reforming of all oil components.
- Argonne National Laboratory (ANL) demonstrated a more-than-threefold increase in hydrogen production rate by using a Rh-based catalyst coating on an $\text{BaFe}_{0.9}\text{Zr}_{0.1}\text{O}_x$ (BFZ1) oxygen transport membrane (OTM) compared to that of a lanthanum strontium cobalt iron oxide (LSCF) OTM tube with a $\text{BaFe}_{0.9}\text{Zr}_{0.1}\text{O}_x$ (BFZ1).

Separation Processes

- Pall Corporation demonstrated durable, high-performance palladium alloy membranes for hydrogen separation and purification, achieving 270 SCFH/ft$^2$ flux in pure $\text{H}_2$/N$_2$, 400 pounds per square inch operation, 88% hydrogen recovery, 99.99% hydrogen permeate quality, and a projected cost of <$1,000/ft$^2$, meeting or exceeding the 2012 targets for dense metallic membranes.
- Media and Process Technologies developed hydrogen-selective membranes/modules based on thin-film palladium for use as reactors/separators for distributed hydrogen production, with field tests demonstrating >99% CO conversion, >99.9% hydrogen purity and >83% hydrogen recovery, meeting or exceeding the 2012 targets for dense metallic membranes.
- The University of Cincinnati developed methods and techniques to prepare zeolite membranes for water gas-shift reactions for hydrogen production. High hydrogen permeance ($1.26 \times 10^{-7}$ mol m$^{-2}$ s$^{-1}$ Pa$^{-1}$) and $\text{H}_2/\text{CO}_2$ separation factor improvements from 4.95 to 25.3 were observed for bilayer membranes modified to include a yttria-stablized zirconia intermediate diffusion barrier layer.

Electrolysis Hydrogen Production

- Giner Electrochemical Systems (GES) demonstrated a proton exchange membrane (PEM) electrolyzer incorporating advanced low-cost membrane electrode assemblies using dimensionally stable membranes with chemically etched supports, which exhibited lifetimes over 1,000 hours operating at 80°C. GES additionally demonstrated significantly reduced hydrogen embrittlement in C/Ti cell separators, indicating expected lifetimes of more than 60,000 hours. Projected stack capital costs of <$0.70/gge based on these improvements meets a critical Program milestone.
- Proton Onsite (formerly Proton Energy Systems) demonstrated new catalyst application techniques for lower-cost hydrogen production, with 55% reduction of catalyst loading on the anode and >90% reduction of catalyst loading on the cathode, with negligible effect on stack performance. Projected stack capital costs of <$0.70/gge based on these improvements meets a critical Program milestone.
- NREL completed more than 2,000 hours of testing on a PEM electrolysis system. The system generated 15 kg of hydrogen per day, running continuously, with full stack-monitoring capabilities and with stacks operating on wind power for stack-decay analysis.

Photoelectrochemical (PEC) Hydrogen Production

- Stanford University demonstrated exceptional stability in their quantum-confined 1.8 eV $\text{MoS}_2$ nanoparticle photocatalysts for PEC hydrogen production, showing stable operations over 10,000 voltage cycles of accelerated lifetime testing. Stanford also developed a high-surface-area macroporous scaffold, which is transparent and conducting, as an efficient electrode substrate for the $\text{MoS}_2$ photocatalysts and other PEC materials.
• NREL validated new benchmark levels of solar-to-hydrogen (STH) conversion efficiency in the 16%–18% range in optimized photoelectrode systems using high-quality III-V semiconductor materials in multi-junction configurations.

• Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), the University of Nevada, Las Vegas (UNLV), and NREL worked collaboratively to complete the initial phase of a “III-V Surface Validation Study” to optimize STH performance and enhance lifetime of III-V semiconductor PEC interfaces in aqueous solutions. Ab initio quantum molecular dynamic models of the interface were created by LLNL, and the initial phase of model validation was completed using materials synthesized by NREL/LANL and characterized by UNLV using state-of-the-art spectroscopic facilities.

• MV Systems with the University of Hawaii at Manoa demonstrated 4.3% STH efficiency and device lifetimes exceeding 250 hours in multi-junction devices based on thin-film copper-gallium-diselenide semiconductors, representing a new benchmark in this low-cost class of PEC photoelectrode devices, and representing progress toward the 2010 Program target of stabilized 10% STH.

• The Midwest Optoelectronic Company accelerated development of efficient low-cost substrate-type PEC systems based on multi-junction thin film Si photoelectrodes; they also supplied multi-junction thin-film silicon devices for integration with novel Suncatalytix thin-film catalysts into solar water-splitting demonstration systems. This project demonstrates effective coordination between EERE and Advanced Research Projects Agency-Energy activities.

Biological Hydrogen Production

• University of California, Berkeley successfully characterized the function of a gene that regulates antenna size in chlorophyll (Tla2), and cloned another for further analysis (Tla3). These findings will be applied to reducing chlorophyll antenna size to increase the utilization efficiency of incident solar light energy.

• NREL—through their collaboration with the University of Manitoba, Canada—used a custom-designed plasmid, along with improved transformation protocols, to obtain two mutant lines of C. thermocellum. These lines will serve as the foundation for future genetic engineering efforts with C. thermocellum for fermentative hydrogen production.

• The J. Craig Venter Institute, in collaboration with NREL, successfully expressed and purified a stable recombinant hydrogenase. This is a significant step in transferring a more oxygen-tolerant hydrogenase from photosynthetic bacteria into hydrogen producing cyanobacteria.

• NREL used computational methods to understand the geometries and energies of the gas diffusion barrier protecting the hydrogen cluster in two hydrogenases. This information guided mutagenesis techniques to randomize the amino acid residues around the diffusion barriers with the aim of reducing the oxygen sensitivity of hydrogenase.

Solar-Thermochemical Hydrogen Production

• The University of Colorado demonstrated atomic layer deposition thin-film ferrite-based materials with a peak production rate 100 times faster than that in the bulk material, with the thin-film materials remaining active for up to 30 water splitting cycles, with no signs of deactivation.

• Sandia National Laboratories developed a reactor system concept capable of annual average STH production efficiency in excess of 20% with a heat-to-hydrogen conversion efficiency of 40%, predicting through system models that annual average STH efficiency could reach 23%.

• ANL identified two membranes for the electrolysis step of the hybrid Cu-Cl cycle that are chemically and thermally stable at 80°C for over 36 hours, addressing the key barrier to this cycle.

• SAIC reduced the voltage of their electrolysis cell at 80°C to levels similar to those previously demonstrated at 130°C in order to optimize the electrolysis step in their hybrid sulfur-ammonia cycle; they also demonstrated the feasibility of molten salt storage for continuous operation.

• TIAX LLC completed a report analyzing the costs of solar-driven high temperature thermochemical water-splitting cycles and identifying the key cost drivers for the reaction cycles.
II. Hydrogen Production / Overview

Fossil Energy—Hydrogen from Coal

In FY 2011, the first $H_2/CO_2$ separation membranes were exposed to coal derived syngas under gasification conditions.

- The National Energy Technology Laboratory’s Office of Research and Development in collaboration with Worcester Polytechnic Institute (WPI) and UTRC have obtained over 1800 hours of membrane coupon exposures at the National Carbon Capture Center (NCCC). Preliminary analysis indicates a stable body-centered-cubic Pd-alloy phase under gasification conditions.
- WPI has completed over 750 hours of membrane tests at the NCCC. Tests have demonstrated stable hydrogen flux levels and hydrogen purity in excess of 99.9%.
- UTRC has completed over 500 hours of membrane tests on the TRIG (transport gasifier) at the Energy & Environmental Research Center. Tests have demonstrated stable hydrogen flux levels and hydrogen purity in excess of 99.9%.
- The Colorado School of Mines has demonstrated reasonable flux and moderate selectivity using a non-precious metal membrane under laboratory conditions.

Budget

The FY 2011 DOE appropriation provided $20.9 million for continued R&D efforts in hydrogen production. EERE received $10.9 million, providing $6.4 million for R&D of centralized renewable hydrogen production and $4.5 million for R&D of distributed renewable hydrogen production; FE received $10.0 million for R&D of hydrogen production from coal.

The President’s FY 2012 budget request for EERE provides $11.7 million for hydrogen production, with an emphasis on materials and processes for hydrogen from renewable resources.

FY 2012 Plans

- Continue emphasis on addressing major challenges in hydrogen production. Performance and durability enhancements in materials and systems will remain a priority, and cost reductions will be achieved through process optimization for all production pathways and technologies. Additional efforts will also address reducing the cost of materials and capital equipment.
- Continue EERE coordination with the Office of Science, which plans approximately $50 million in basic research related to hydrogen and fuel cell technologies. Through Basic Science activities, a fundamental understanding of issues related to hydrogen production—particularly in the longer-term R&D areas of PEC.
and biological processes—can help address the challenges of hydrogen production. Coordination of the PEC-related fundamental research activities in the Office of Science's Solar Fuels Innovation Hub with the hydrogen production systems-oriented PEC R&D in EERE will be a high priority.

- Complete fabrication of a prototype alkaline electrolyzer unit capable of providing 30 kg of hydrogen per day at 6,500 psi; complete field testing of a prototype PEM electrolyzer capable of providing 12 kg of hydrogen per day at 300-400 psi; and initiate transition of electrolysis production pathways to the “technology validation” stage.
- Complete lifetime measurements of GaInP$_2$/GaAs devices for PEC production of hydrogen and determine the durability benchmarked against the target of a 100-hour operational lifetime at 10% efficiency.
- Demonstrate 100 hours of total catalyst operation in an integrated bench-scale system for production of pure hydrogen from steam reforming of pyrolysis oil at a rate of 100 liters per hour and with a yield of 10 g of hydrogen from 100 g of bio-oil.
- Operate a microalgae system continuously for two months, with the culture being induced to anaerobiosis with prolonged hydrogen production through use of a physiological switch activated by sulfur deprivation.
- Demonstrate—on-sun, using the NREL High Flux Solar Furnace—the cobalt ferrite/alumina “hercynite” thermochemical reaction cycle with 1,300°C reduction/1,000°C oxidation thermochemical redox cycling to split water, with hydrogen production of >100 micromoles per gram of active material.
- Continue coordination with deployment projects funded by American Recovery and Reinvestment Act to gain lessons learned related to hydrogen production technologies.

Sara Dillich
Hydrogen Production & Delivery Team Lead (Acting)
Fuel Cell Technologies Program
Department of Energy
1000 Independence Ave., SW
Washington, D.C. 20585-0121
Phone: (202) 586-7925
E-mail: Sara.Dillich@ee.doe.gov