II.0 Hydrogen Production Sub-Program Overview

INTRODUCTION

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 transportation (e.g., specialty vehicles, cars, trucks, and buses), stationary power (e.g., backup power and combined-heat-and-power systems), and portable power. A portfolio of hydrogen production technology pathways utilizing a variety of renewable energy sources and renewable feedstocks is being developed under this sub-program.

Multiple DOE offices are engaged in R&D relevant to hydrogen production, including:

- The Fuel Cell Technologies Office (FCTO), 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) has been 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, utilization, and storage, 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 currently collaborating with EERE on a study of nuclear-renewable hybrid energy systems. Many of the systems being evaluated by this study use hydrogen production as a form of energy storage or as an input to industrial processes. The previous major hydrogen activity in NE, the Nuclear Hydrogen Initiative, was discontinued in Fiscal Year (FY) 2009 after steam electrolysis was chosen as the hydrogen production pathway most compatible with the next generation nuclear power.

GOAL

The goal of the Hydrogen Production sub-program 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 Hydrogen Production sub-program is to reduce the cost of hydrogen dispensed at the pump to a cost that is competitive on a cents-per-mile basis with competing vehicle technologies. Based on current analysis, this translates to a hydrogen threshold cost of <$4 per kg hydrogen (produced, delivered, and dispensed, but untaxed) by 2020,[1] apportioned to <$2/kg for production only.[2] Technologies are being developed 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*.[3] 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% compared with current technology by 2016. The objectives of NE's efforts in hydrogen production have been

[1] *Hydrogen Threshold Cost Calculation*, Program Record (Office of Fuel Cell Technologies) 11007, US Department of Energy, 2012, http://www.hydrogen.energy.gov/pdfs/11007_h2_threshold_costs.pdf

[2] *Hydrogen Production and Delivery Cost Apportionment*, Program Record (Office of Fuel Cell Technologies) 12001, US Department of Energy, 2012, http://hydrogen.energy.gov/pdfs/12001_h2_pd_cost_apportionment.pdf

[3] *Hydrogen from Coal Program Research Development and Demonstration Plan*, Office of Fossil Energy, US Department of Energy, September 2010, http://fossil.energy.gov/programs/fuels/hydrogen/2010_Draft_H2fromCoal_RDD_final.pdf

documented in the *Technology Roadmap for Generation IV Nuclear Energy Systems* (December 2002).[4] They include the development of high-temperature processes for hydrogen production compatible with next generation nuclear plants.

FY 2014 TECHNOLOGY STATUS AND ACCOMPLISHMENTS

In FY 2014, significant progress was made by the Hydrogen Production sub-program on several important fronts. For example:

- A Funding Opportunity Announcement (FOA) was released in November 2013, covering three hydrogen production topics: (1) novel systems using natural gas combined with renewable or low-carbon resources to produce hydrogen with greenhouse gas emissions significantly reduced when compared to traditional steam methane reforming; (2) hydrogen production from bio-derived liquids such as bio-oils, sugars, and alcohols using integrated system technologies for thermochemical conversion; and (3) advanced materials-based systems for direct solar water splitting. Six selected projects were announced in June 2014, as described in the following section.
- A joint solicitation with the National Science Foundation (NSF) was released in November 2013 for applications addressing discovery and development of advanced materials systems and chemical processes for direct photochemical and/or thermochemical water splitting for application in the solar production of hydrogen fuel. The selections were announced in August 2014.
- An Electrolytic Hydrogen Production Workshop was held in February 2014 to identify key R&D needs, and market and manufacturing challenges and opportunities. A report was posted on the website in July 2014, and a Request for Information (RFI) will be released to solicit public input.
- A Biological Hydrogen Production Workshop report was posted to the website in November 2013, and an RFI will be released to solicit public input.
- H2A v3 case studies for polymer electrolyte membrane (PEM) electrolysis were completed and posted,[5] and Hydrogen and Fuel Cells Program Record #14004 was published based on the results of the case studies.[6]

Hydrogen Production Cost Status

Recent and current status for the projected cost of hydrogen production for several of the near- to mid-term pathways is shown in Figure 1.

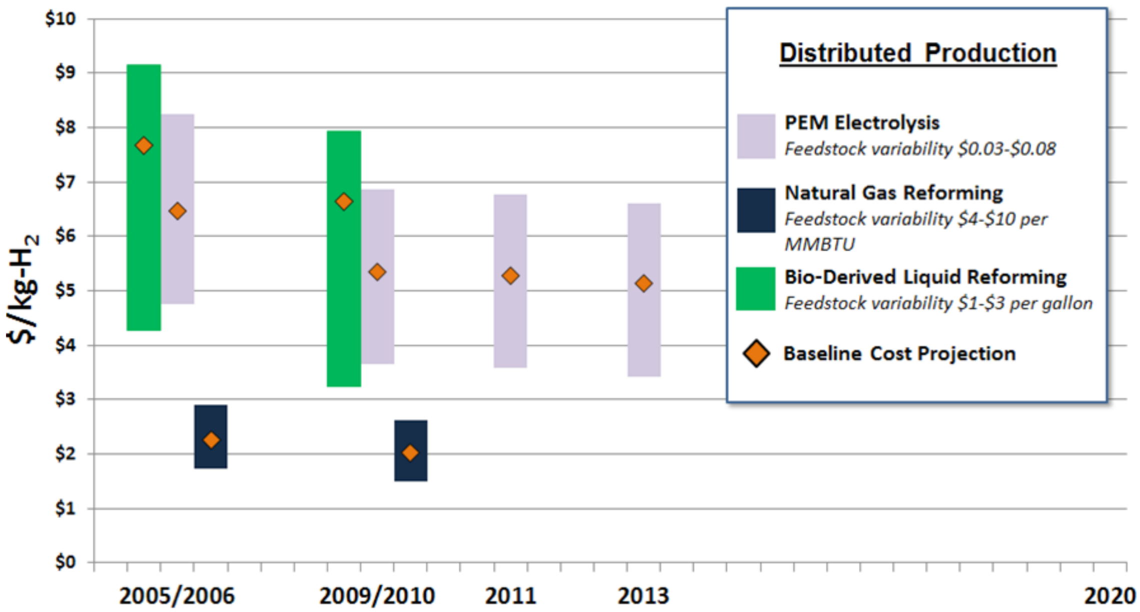
Detailed FY 2014 progress on numerous fronts in the Hydrogen Production sub-program is described in the following.

New Project Selections

In November 2014, a FOA was released to support R&D efforts to address critical challenges and barriers for hydrogen production technology development, and specifically the long-term goal of hydrogen production at <$2/kg hydrogen. Innovative materials, processes, and systems are needed to establish the technical and cost feasibility for renewable and low-carbon hydrogen production. With this FOA, DOE through FCTO sought to fund hydrogen production R&D projects to move technologies towards reaching the hydrogen production cost goal of <$2/kg. The six selected projects, announced at the 2014 Hydrogen and Fuel Cells Program Annual Merit Review and Peer Evaluation Meeting in June 2014, are:

- FuelCell Energy Inc. ($900K), Danbury, Connecticut; *Novel hybrid system for low-cost, low-greenhouse-gas hydrogen production.*
- Pacific Northwest National Laboratory ($2.2M), Richland, Washington; *Scalable, compact piston-type reactor for hydrogen production from bio-derived liquids.*

[4] *A Technology Roadmap for Generation IV Nuclear Energy Systems*, Office of Nuclear Energy, US Department of Energy, December 2002, http://curie.ornl.gov/system/files/documents/167/gen_iv_roadmap.pdf http://curie.ornl.gov/system/files/documents/167/gen_iv_roadmap.pdf
[5] Case studies available at http://www.hydrogen.energy.gov/h2a_prod_studies.html; supporting documents available at http://www.hydrogen.energy.gov/h2a_production_documentation.html
[6] DOE Hydrogen and Fuel Cells Program Record #14004 *Hydrogen Cost from PEM Electrolysis* is available at http://hydrogen.energy.gov/pdfs/14004_h2_production_cost_pem_electrolysis.pdf



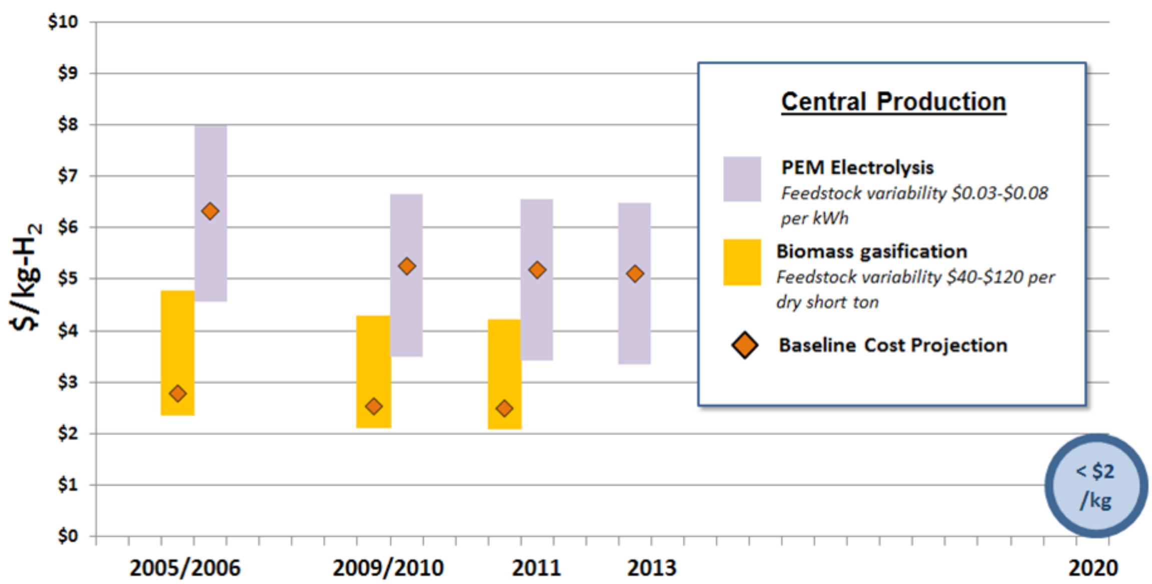


FIGURE 1. Range of hydrogen production costs, untaxed, for near- to mid-term distributed and centralized pathways. The high end of each bar represents a pathway-specific high feedstock cost as well as an escalation of capital cost; while the low end reflects a low end on feedstock costs and no capital escalation. Bars for different years in the same pathway represent improvements in the costs of the specific pathway, based on specific reference data for the appropriate year and pathway. Detailed information is included in the DOE Hydrogen and Fuel Cells Program Record #14005.[7]

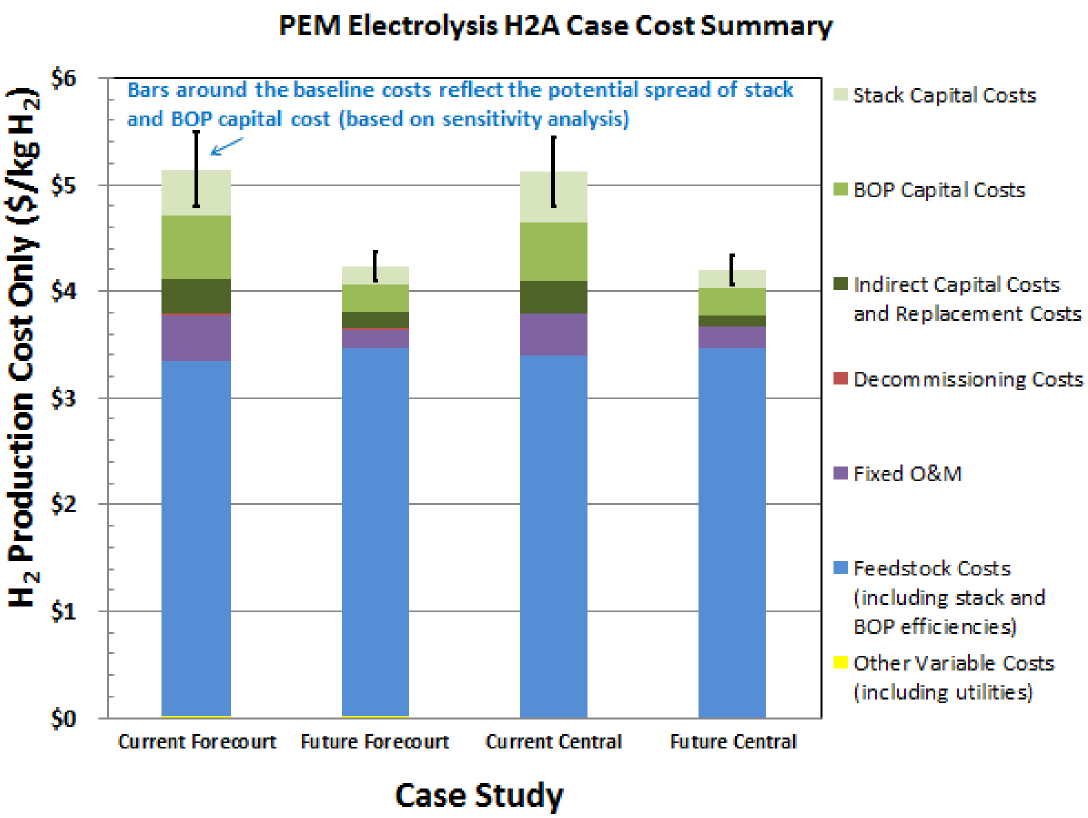
- National Renewable Energy Laboratory (NREL) ($3M), Golden, Colorado; *High-efficiency tandem absorbers based on novel semiconductor materials that can produce hydrogen from water using solar energy.*
- University of Hawaii ($3M), Honolulu, Hawaii; *Photoelectrodes for direct solar water splitting.*
- Sandia National Laboratories (SNL) ($2.2M), Livermore, California; *An innovative high-efficiency solar thermochemical reactor for solar hydrogen production.*
- University of Colorado, Boulder ($2M), Boulder, Colorado; *A novel solar-thermal reactor to split water with concentrated sunlight.*

[7] DOE Hydrogen and Fuel Cells Program Record #14005 *Hydrogen Production Status 2006-2013*, under development.

PEM Electrolysis Case Studies

Industry-vetted case studies of hydrogen production costs via PEM electrolysis were completed and made publically available on the DOE website in FY 2014.[8] These cases modeled representative PEM electrolyzer systems and are based on input from several key industry collaborators with commercial experience. Four cases were analyzed, comprising two technology years, Current (2013) and Future (2025), and two production capacities, Distributed Forecourt (500-1,500 kg/day) and Centralized (50,000 kg/day). The process to evaluate the cases began with soliciting relevant, detailed information from the companies followed by synthesizing and amalgamating the data into base parameters for cases. The base parameters and sensitivity limits were vetted by the companies, and the data was then used to populate the four H2A v3 cases, which were run to project the hydrogen price.

The results of the Distributed and Centralized case studies indicated a current range of projected high-volume untaxed cost of hydrogen production via PEM electrolysis of ~$4.80/kg to $5.50/kg (Figure 2). Key cost drivers were identified and quantified, including electricity cost, electrolyzer efficiency, and capital cost. These results were documented in a DOE Hydrogen and Fuel Cells Program Record.[9]



BOP - balance of plant; O&M - operations and maintenance

FIGURE 2. PEM electrolysis hydrogen production cost contributions (2007$/kg) for four case studies,[10] showing of projected high-volume untaxed costs ranging from ~$4.80 to $5.50/kg, broken down in terms of the major cost contributing factors.

[8] Case studies available at http://www.hydrogen.energy.gov/h2a_prod_studies.html; supporting documents available at http://www.hydrogen.energy.gov/h2a_production_documentation.html.
[9] DOE Hydrogen and Fuel Cells Program Record #14005, Hydrogen Cost from PEM Electrolysis available at http://hydrogen.energy.gov/pdfs/14004_h2_production_cost_pem_electrolysis.pdf
[10] Based on case-dependent electricity prices of 6.12¢/kWh, 6.88¢/kWh, 6.22¢/kWh and 6.89¢/kWh, respectively.

Separation Processes

Membrane separations research, development, and demonstration continued through the Small Business Innovation Research program and FE. Technical progress included:

- A sorbent bed was developed, through a Phase III Small Business Innovation Research project, to operate downstream of a bulk desulfurization system as a polishing bed to provide essentially sulfur-free biogas to a solid oxide fuel cell. In FY 2014, the design of an interface to connect the biogas cleanup skid to a 2-kWe solid oxide fuel cell skid was successfully completed. A field demonstration of the integrated system and an economic assessment of the technology is planned for late FY 2014. (TDA Research, Inc.)
- FE is funding projects to carry out comprehensive engineering design of advanced hydrogen-carbon dioxide Pd and Pd-alloy composite membrane separations for hydrogen production from syngas derived from coal or coal-biomass mixtures. The primary goal is to demonstrate the separation of hydrogen from coal- or coal-biomass-derived syngas via membranes at the pre-engineering/pilot scale to enable the use of coal for hydrogen production with reduced carbon dioxide emissions. The teams evaluated membrane performance based on flux, sulfur tolerance, water-gas shift activity, and hydrogen purity under syngas conditions expected from coal gasification. Five project teams successfully designed, constructed, and tested membranes with operating gasifier and/or simulated syngas mixtures that produced 2 lb/day of hydrogen. A down-select process has resulted in two project teams that were awarded projects to augment successful completion of their designs. The project teams plan to construct membrane separation modules with the capacity to produce up to 50 lbs/day of hydrogen.

Electrolysis Hydrogen Production

The major emphasis of the electrolysis projects was on cost reduction and efficiency improvement through leveraging catalyst development. Work on alkaline membrane electrolysis is showing promise to deliver electrolyzer systems with very low platinum-group metal (PGM) loading. Additional work focused on electrolyzer system cost reductions by minimizing balance-of-plant losses. Technical progress included:

- The manufacture of core shell catalyst technology developed by Brookhaven National Laboratory was successfully transferred to its facility and achieved equivalent cathode performance at $1/10^{th}$ of the cathode PGM loading relative to the 2013 baseline. (Proton OnSite)
- A nano-structured thin film catalyst anode technology was tested under electrolysis conditions and demonstrated comparable performance at $1/16^{th}$ of the anode PGM loading relative to a 2013 baseline. (Giner, Inc. and 3M)
- An improved drying technique was developed with the potential to reduce drying losses in electrolyzers to less than 3.5% (compared with 11-8% in commercial systems) while operating on a variable (wind or solar) stack power profile. Testing is in progress to verify that the new technique meets SAE International Standard J2719 specifications for water content (<5 ppm). (NREL)

Photoelectrochemical Hydrogen Production

The broad focus of projects in this area was on utilizing state-of-the-art theory, synthesis, and characterization tools to develop viable photoelectrochemical material systems and prototypes with improved efficiency and durability. Technical progress included:

- Greater than 300 hours of stability were demonstrated at ~15 mA/cm^2 in III-V semiconductor photoelectrochemical tandem devices, representing a significant improvement over the previous year's 115 hours at 10 mA/cm^2. This result represents an important step forward toward demonstration of stabilized solar-to-hydrogen conversion efficiencies >20% using photoelectrochemical devices. (NREL)
- Joint theoretical/experimental studies were continued on III-V photoelectrochemical electrode surfaces, including the development of a theoretical hydrogen evolution model relevant to photoelectrochemical hydrogen production that incorporates hydrogen diffusion; this resulted in the discovery that a low hydrogen diffusion barrier and low Heyrovsky barrier on a semiconductor surface can activate additional hydrogen evolution reaction channels to improve overall kinetics. (Lawrence Livermore National Laboratory and the NREL Surface Validation Team)
- Midwest Optoelectronics, LLC is working towards commercial-size photoelectrochemical electrodes; achieved 3.3% solar-to-hydrogen conversion efficiency for immersion-type photoelectrochemical cells of 4-inch by 4-inch size using low-cost electroplated Ni hydrogen evolution reaction catalysts. (Midwest Optoelectronics, LLC)

Biological Hydrogen Production

The broad focus of the projects in the biological hydrogen production portfolio addressed key barriers such as oxygen sensitivity and feedstock utilization using molecular biology and genetic engineering techniques along with improved systems engineering. Technical progress included:

- Increased activity of the Chlamydomonas strain was demonstrated expressing the Ca1 hydrogenase from 2% to about 11% of the native hydrogenase, with a duration of 30 minutes or more. (NREL)
- An average hydrogen production rate of 466 mL/L-reactor/day from fermentation of pretreated corn stover (a realistic lignocellulosic feedstock for industrial biofuel production), rather than the pure cellulosic feedstock previously used, was demonstrated with no indication of lignin inhibition. Additionally, a larger, more scalable microbial reverse-electrodialysis cell design demonstrated a 0.9 L/L-reactor/day hydrogen production rate, a 12.5% increase over the 2013 demonstrated rate, using a salinity gradient instead of grid electricity. (NREL)
- The genome of the bacterium Rubrivivax gelatinosus Casa Bonita Strain (CBS) was examined for candidate genes to transfer to the cyanobacteria Synechocystis to improve the expression and activity of the non-native CBS hydrogenase enzyme. The researchers identified slyD, involved in binding and inserting Ni into the hydrogenase active site, as a likely gene as it is present in CBS but absent in Synechocystis. Researchers also improved the Synechocystis expression of the CBS maturation protein HypF, which is involved in assembling the active hydrogenase enzyme, up to nine-fold. (NREL)
- The truncated light-harvesting antenna concept was applied to cyanobacteria, demonstrating that a Δcpc strain of *Synechocystis*, which is missing the phycobilisome portion of the photosynthetic antenna, can reach higher light levels before saturation than the wild type and has 55-60% greater rates of biomass accumulation. (University of California, Berkeley)

Solar-Thermochemical Hydrogen Production

Efforts in these projects were directed toward performance characterization of water splitting by novel, non-volatile metal-oxide based reaction materials and developing new reactor concepts to optimize efficiency of the reaction cycles. Technical progress included:

- A thermodynamic model was developed for Sr- and Mn-doped $LaAlO_3$ perovskite reaction materials that predicts the optimal operating temperature, oxygen pressure, and heat recovery effectiveness required for a solar-to-hydrogen conversion efficiency >20%; and derived performance criteria and thermodynamic properties for an "ideal" non-stoichiometric oxide reaction material. (SNL)
- Over three times improvement in hydrogen production was demonstrated relative to 2013 results of 100 micromole/g for isothermal operation at 1,350ºC for hercynite cycle materials using near-isothermal reduction/oxidation cycling. (University of Colorado, Boulder)
- Integration of major components into a pressurized button cell test facility was completed for the electrolysis step of the Hybrid Sulfur thermochemical cycle that will allow testing of catalysts and membranes at pressures up to 1 MPa and temperatures of 130ºC. The team identified and screened electrocatalysts with the potential to reduce oxidation overpotential by >20 mV versus the state-of-the-art platinum catalyst. Savannah River National Laboratory (SRNL) also tested thin-film electrodes as candidate anode electrocatalysts, including Pt, Pd, Ir, Au, PtAu, and PtV. Au, PtAu and PtV showed 28 mV, 46 mV, and 13 mV reduction, respectively, on the anode polarization versus state-of-the-art Pt catalyst. (SRNL)

Hydrogen Production Pathway Analysis

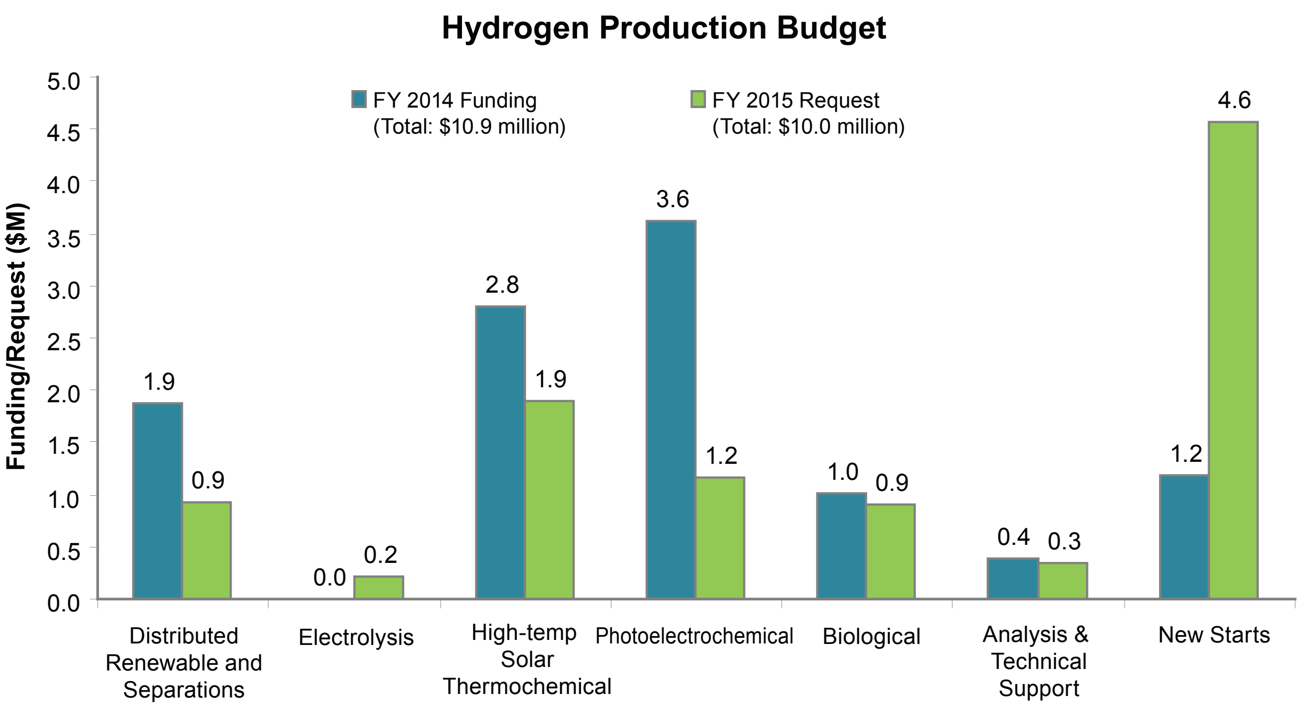
The focus of the analysis efforts was on establishing standardized procedures for hydrogen production pathway technoeconomic case studies utilizing the H2A v3 tool with technical inputs from production pathway experts, applying the procedures toward the completion of a series of PEM electrolysis case studies, and initiating bio-fermentation and high-temperature solid oxide electrolysis case studies. Technical accomplishments included:

- New technoeconomic case studies were completed specifically for the PEM electrolysis production pathway, applying the H2A v3 Production Model to analyze hydrogen costs ($/kg hydrogen) and cost sensitivities. The results of the Distributed and Centralized case studies indicated a current range of projected high-volume untaxed cost of hydrogen production via PEM electrolysis of ~$4.80/kg to $5.50/kg. (Strategic Analysis, Inc., NREL, Argonne National Laboratory, ANL)

- Technical questionnaires were distributed to experts in the fields of bio-fermentation and high-temperature solid oxide electrolysis to initiate the H2A v3 case studies of these pathways. (Strategic Analysis, Inc., NREL, and ANL)

BUDGET

The FY 2014 appropriation for the Hydrogen Production and Hydrogen Delivery sub-programs was $21 million. Funding was distributed approximately evenly between Production and Delivery, representing an increase in funding to Delivery relative to past years, when funding was distributed with approximately two thirds to Production and one third to Delivery. This distribution reflects the current FCTO emphasis on hydrogen infrastructure technology R&D. The request for Production and Delivery in FY 2015 is $21 million. The estimated budget breakdown for Production funding in FY 2014 and FY 2015 is shown in Figure 3. Production has increasingly focused in past years on long-term, renewable pathways such as photoelectrochemical, biological, and solar-thermochemical hydrogen production. This trend generally continued in FY 2014 with several new projects selected from funding opportunities falling into the photoelectrochemical and solar-thermochemical hydrogen categories, supplemented by two newly selected projects in the nearer-term distributed renewable production category. The emphasis on a balanced portfolio of long-term and nearer-term renewable technologies is expected to continue into FY 2015.



* Subject to appropriations, project go/no-go decisions, and competitive selections. Exact amounts will be determined based on research and development progress in each area.

FIGURE 3. Hydrogen Production Budget. Budget amounts for FY 2014 and projected amounts for FY 2015, contingent upon appropriations, are shown broken down by the different production pathways. Exact distribution of funds in FY 2015 will not be defined until funds have been appropriated and new projects selected.

FY 2015 PLANS

General Hydrogen Production sub-program plans for FY 2015 include:

- Demonstrate substantial initial progress in the six new projects selected under the 2014 Hydrogen Production FOA.
- Continue emphasis on materials durability, production efficiency, and process optimization for all pathways, and develop and refine materials characterization protocols and performance metrics for early development technologies.

- Continue to develop and update hydrogen production pathways analyses with the H2A v3 tool developing case studies on bio-fermentation and high-temperature solid oxide electrolysis and establishing cost and performance baselines for new project starts.
- Continue coordination with the Office of Science and NSF, which fund fundamental and use-inspired research related to hydrogen and fuel cell technologies. Leveraging BES and NSF activities improves the understanding of scientific issues related to hydrogen production (particularly in the longer-term R&D areas of photoelectrochemical and biological processes), and can help address the fundamental challenges of hydrogen production. Coordination of FCTO's systems-oriented hydrogen production R&D with the solar-hydrogen-related fundamental research activities in the Office of Science's Solar Fuels Innovation Hub and with the use-inspired projects selected under the joint NSF/EERE solicitation "Renewable Hydrogen Fuel Production via Solar Water Splitting" will remain a high priority.
- Release an RFI inviting further input on the 2014 Electrolytic Hydrogen Production Workshop Report, and prepare and post an Addendum to the Workshop Report based on RFI responses. Outcomes of the workshop and responses to the RFI will be used to inform programmatic planning.

Important pathway-specific milestones planned for FY 2015 in the Hydrogen Production sub-program projects include:

- Demonstrate fermentation of deacetylated corn stover lignocellulose in a sequencing fed-batch bioreactor and obtain a hydrogen production rate of 450 mL H_2/L/d with a total hydrogen output of 80% of that of avicel cellulose based on the same amount of cellulose loading (5 g/L).
- Deliver 100 feet of roll-to-roll produced electrolysis catalyst with a durability of <20 mV drop after 1,000 hours of operation at 1.5 A/cm^2, and with a total PGM loading of less than 0.5 mg/cm^2.
- Demonstrate the viability of stabilized photoelectrochemical systems with >15% solar-to-hydrogen efficiency using advanced tandem devices based on either III-V crystalline semiconductor or chalcopyrite thin-film semiconductor materials.
- Develop a monolith reactor concept for integration of steam reforming reactions with in situ carbon dioxide capture and heat transfer for high-throughput hydrogen production from bio-oils. Identify optimum reforming catalysts and sorbents for >80% of equilibrium hydrogen yield at T <500°C, and >90% carbon dioxide capture under reaction conditions.
- Continue development of conceptual designs for fully integrated solar thermochemical prototype reactors and synthesis and evaluation of perovskite and hercynite reaction materials. Demonstrate the production of spray-dried active materials that produce at least 150 µmol H_2/g total and reduction of at least 1 gram of oxidized spray-dried active materials under vacuum pumping to remove released O_2, and oxidation of at least 1 gram reduced spray-dried active materials with steam to produce hydrogen.
- Completion of H2A v3 case studies for bio-fermentation and high-temperature solid oxide electrolysis hydrogen production pathways.

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