Market Transformation

Technical Plan — Production

Applied Research

and Technology Development

Fuel Cell

R&D

Manufacturing R&D Safety, Codes & Standards

Education

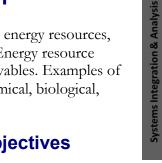
Hydrogen Fuel R&D

Delivery
Storage

3.1 Hydrogen Production

Hydrogen can be produced from diverse energy resources, using a variety of process technologies. Energy resource options include fossil, nuclear, and renewables. Examples of process technologies include thermochemical, biological, electrolytic, and photolytic.

3.1.1 Technical Goal and Objectives



Goal

Research and develop technologies for low-cost, highly efficient hydrogen production from diverse renewable sources.

Objectives

Reduce the cost of hydrogen production to <\$200/gge¹(\$2.00-\$4.00/gge delivered and dispensed^{2,3}). This cost is independent of the technology pathway and takes into consideration a range of assumptions for fuel cell electric vehicles (FCEVs) to be competitive with hybrid electric vehicles (HEVs). Those considerations include a range of gasoline prices and fuel economies. Technologies are being researched to achieve this goal in timeframes appropriate to their current states of development.

- By 2020, reduce the cost of distributed production of hydrogen from biomass-derived renewable liquids to <\$2.30/gge (≤\$4.00 delivered and dispensed).
- By 2020, reduce the cost of distributed production of hydrogen from water electrolysis to <\$2.30/gge (≤\$4.00 delivered and dispensed).
- By 2015, reduce the cost of central production of hydrogen from water electrolysis using renewable power to \$3.00/gge at plant gate. By 2020, reduce the cost of central production of hydrogen from water electrolysis using renewable power to ≤\$2.00/gge at plant gate.
- By 2020, reduce the cost of hydrogen produced from biomass gasification to ≤\$2.00/gge at the plant gate.
- By 2015, verify the potential for solar thermochemical (STCH) cycles for hydrogen production to be competitive in the long term and by 2020, develop this technology to produce hydrogen with a projected cost of \$3.00/gge at the plant gate.

¹ The energy content of a gallon of gasoline and a kilogram of hydrogen are approximately equal on a lower heating value basis; a kilogram of hydrogen is approximately equal to a gallon of gasoline equivalent (gge) on an energy content basis.

² This cost range results in equivalent fuel cost per mile for a hydrogen fuel cell vehicle compared to gasoline hybrid vehicles in 2020. The full explanation and basis can be found in U.S. Department of Energy (DOE) Record 11007 (see www.hydrogen.energy.gov/program_records.html).

³ All costs in this plan are in 2007 dollars to be consistent with EERE planning which uses the energy costs from the 2009 Annual Energy Outlook.

- By 2020, develop advanced renewable photoelectrochemical hydrogen generation technologies to produce hydrogen with a projected cost of \$4.00/gge at the plant gate.
- By 2020, develop advanced biological generation technologies to produce hydrogen with a projected cost of \$10.00/gge at the plant gate.
- By 2017, develop technologies for direct solar-to-hydrogen (STH) production at centralized facilities for ≤\$5.00/gge at the plant gate.
- By 2020, demonstrate plant-scale-compatible photoelectrochemical water-splitting systems to produce hydrogen at solar-to-hydrogen energy conversion efficiencies ≥15%, and plant-scale-compatible photobiological water-splitting systems to produce hydrogen at solar-to-hydrogen energy conversion efficiencies ≥5%.

3.1.2 Technical Approach

Hydrogen production research is focused on meeting the objectives outlined in Section 3.1.1 by conducting Research and Development (R&D) through industry, national laboratory, and university projects. The Hydrogen Production sub-program will continue to develop the technologies to produce hydrogen for transportation and stationary applications. Integrated systems will be validated in the field by the Technology Validation sub-program to obtain real-world data (refer to the Technology Validation section of the Multi Year Research, Development, and Demonstration Plan). Results of validation projects will guide continued Research, Development, and Demonstration (RD&D) efforts.

A portfolio of feedstocks and technologies for hydrogen production will be necessary to address energy security and environmental needs and the geographic variability in feedstock availability and cost. This sub-program addresses multiple feedstock and technology options for hydrogen production for the short and long term. The research focus for the near term is on distributed

reforming of renewable liquid fuels and on electrolysis to meet initial lower volume hydrogen needs with the lowest capital equipment cost. An example of a near term distributed hydrogen production and delivery station is shown in Figure 3.1.1. Both short and long-term research is focused on hydrogen production from renewable feedstocks and energy sources, with an emphasis on centralized options to take advantage of economies of scale when an adequate hydrogen delivery infrastructure is in place. There is collaboration with the U.S. Department of Energy's (DOE's) Office of Fossil Energy (http://fossil.energy.gov/programs/fuels/index.html) to develop centralized production from coal with carbon sequestration, and with DOE's Office of Nuclear Energy (http://www.nuclear.energy.gov/HTGCR/overview.html)



Figure: 3.1.1 Distributed Hydrogen Reforming Station

to develop centralized production from advanced nuclear energy-driven high temperature electrolysis. DOE's Office of Science (<u>http://science.energy.gov</u>) is a collaborator on longer-term technologies such as biological and photoelectrochemical hydrogen production.

The development of a national hydrogen production infrastructure will likely take multiple pathways. Some of these pathways and their roles within the strategy of the Hydrogen Production subprogram are described below.

Distributed Production Pathway

Distributed hydrogen production (i.e., production of hydrogen at the point of use) may be the most viable approach for introducing hydrogen as an energy carrier because it does not require a substantial transport and delivery infrastructure or large capital investments as high as those needed for large central production plants.

Two distributed hydrogen production technologies that have good potential for development are (1) reforming of natural gas or liquid fuels, including bio-derived liquids, such as ethanol and pyrolysis oil; and (2) small-scale water electrolysis. Distributed steam methane reforming technologies exist today for hydrogen to be cost-competitive with gasoline.⁴ Projections based on high-volume production indicate that reforming natural gas at the fueling station can produce hydrogen for a cost close to \$2/gge (See Tables 3.1.1 and 3.1.1.A). As a result, the Department of Energy is no longer funding R&D in natural gas reforming for FCEV fueling, although it is anticipated that industry will continue to make incremental improvements to this technology. Using a renewable resource, high temperature and aqueous phase bio-derived liquids reforming are two possible pathways to produce hydrogen with dramatically lower net greenhouse gas emissions. Reforming of bio-derived liquids is applicable to distributed, semi-central, and central production.

The second focus area is on small-scale electrolyzers for splitting water. Electrolyzers present the opportunity for non-carbon-emitting hydrogen production when a renewable electricity source such as wind or hydropower is used. To be cost competitive, R&D is necessary to reduce electrolysis capital and operating costs and the cost of electricity needs to be less than or equal to half the current average grid price of electricity.

Table 3.1.1 Distributed Forecourt Natural Gas Reforming ^{a, b, c}								
Characteristics Units 2011 Status ^d 2015 Estimate ^e								
Hydrogen Levelized Cost (Production Only) ^f	\$/kg H ₂	2.00	2.10					
Production Equipment Total Capital Investment	\$M	1.5	1.2					
Production Energy Efficiency ⁹	%	71.4	74					
Production Equipment Availability ^c	%	97	97					
Industrial Natural Gas Price ^h	\$/MMBtu	from Annual Energy Outlook (AEO) 2009	from AEO 2009					

⁴ Distributed Hydrogen Production from Natural Gas—Independent Review, National Renewable Energy Laboratory, October 2006, <u>http://www.hydrogen.energy.gov/pdfs/40382.pdf</u>.

Table 3.1.1.A Distributed Natural Gas H2A Example Cost Contributions ^{a, b, c}						
Characteristics	Units	2011 Status ^d	2015 Estimate ^e			
Production Unit Capital Cost Contribution	\$/kg	0.60	0.40			
Feedstock Cost Contribution	\$/kg	1.10	1.30			
Production Fixed Operations and Maintenance (O&M) Cost Contribution	\$/kg	0.20	0.20			
Production Other Variable Cost Contribution	\$/kg	0.10	0.20			
Hydrogen Levelized Cost (Production)	\$/kg	2.00	2.10			
Compression, Storage, and Dispensing (CSD) Levelized Cost ⁱ	\$/kg	2.50	1.70			
Total Hydrogen Levelized Cost (Dispensed)	\$/kg	4.50	3.80			

- ^a The H2A Distributed Production Model 3.0 (<u>www.hydrogen.energy.gov/h2a_production.html</u>) was used to generate the values in the table with the exceptions described in the notes below.
- ^b The H2A Distributed Production Model 3.0 was used with the standard economic assumptions: All values are in 2007 dollars (2007\$), 1.9% inflation rate, 10% After Tax Real Internal Rate of Return, 100% equity financing, 20-year analysis period, 38.9% overall tax rate, and 15% working capital. A MACRS (Modified Accelerated Cost Recovery System) 7-year depreciation schedule was used. The plant design capacity is 1,500 kg/day of hydrogen. It is assumed that Design for Manufacture and Assembly (DFMA) would be employed and that production would have realized economies of scale.
- ^c The plant production equipment availability is 97% including both planned and unplanned outages; ten unplanned outages of 14h duration per year; 1 planned outage of 5 days duration per year. The plant usage factor (defined as the actual yearly production/equipment design production capacity) is 86% based on over sizing of the production equipment to accommodate a summer surge in demand of 10% above the yearly average demand.
- ^d Current technology status based on 01D_Current_Forecourt_Hydrogen_Production_from_Natural_Gas_(1,500_kg_per_day)_version_3.0 <u>http://www.</u> <u>hydrogen.energy.gov/h2a_prod_studies.html</u>
- 2015 Technology projections based on
 02D_Future_Forecourt_Hydrogen_Production_from_Natural_Gas_(1,500_kg_per_day)_version_3.0 http://www.h
 ydrogen.energy.gov/h2a
 prod_studies.html
- ^f The levelized cost is equivalent to the minimum required selling price to achieve a 10% annual rate of return over the life of the plant.
- g Energy efficiency is defined as the energy of the hydrogen out of the production process (lower heating value [LHV]) divided by the sum of the energy into the process from the feedstock (LHV) and all other energy needed for production. Energy used for compression, storage and dispensing (CSD) is not included in the calculation of production energy efficiency.
- ^h Industrial natural gas prices are taken from the U.S. Energy Information Administration (EIA) 2009 AEO reference case projection, in 2007\$. The average price over the modeled life of the plant is \$7.87/MMBtu (LHV) for the current technology case, and \$9.35/MMBtu for the 2015 case. Prices are in \$/MMBtu on a LHV basis, as utilized in the H2A models. Conversion of EIA natural gas price data on a HHV basis to a LHV basis is done with heat content values of 52.2 MJ/kg (HHV) and 47.1 MJ/kg (LHV).
- ⁱ Costs for the forecourt station compression and storage are consistent with the status and targets in the Delivery Multi Year Research, Development and Demonstration (MYRD&D) section. Storage capacity for 1540 kg of hydrogen at the forecourt is included. It is assumed that the hydrogen refueling fill pressure is 5000 psi for 2010/11 and that in 2015 and 2020, the hydrogen refueling fill pressure is 10,000 psi.

Centralized Production Pathway

Large hydrogen production facilities that can take advantage of economies of scale will be needed in the long term to meet increases in hydrogen fuel demand. Central hydrogen production allows management of greenhouse gas emissions through strategies like carbon sequestration. In parallel with the distributed production effort, DOE is pursuing central production of hydrogen from a variety of resources - fossil, nuclear, and renewable.

- Coal and natural gas are possibly the least expensive feedstocks, and carbon sequestration is required to reduce or eliminate greenhouse gas emissions. Centralized natural gas reforming is not being pursued because it is already an established commercial technology.
- Biomass gasification offers the potential of a renewable option and near-zero greenhouse gas emissions.
- Water electrolysis based on renewable power may be a viable approach as the cost of capital equipment is reduced through advanced development providing the cost of electricity is less than or half of the current average grid price.
- DOE's Office of Nuclear Energy has been investigating the feasibility of hydrogen production through high-temperature electrolysis as a potential end-user application under the Next Generation Nuclear Plant project.
- High-temperature thermochemical hydrogen production that uses concentrated solar energy may be viable with the development of efficient water-splitting chemical process cycles and materials.
- Photoelectrochemical and biological hydrogen production are early development technologies to produce hydrogen using sunlight and need long-term research and development to produce hydrogen economically.
 - In photoelectrochemical production, hydrogen is produced directly from water using sunlight and a special class of semiconductor materials. These highly specialized semiconductors absorb sunlight and use the light energy to separate water molecules into hydrogen and oxygen.
 - In biological production, specialized microorganisms produce hydrogen using different feedstock materials and conditions: sunlight drives photolytic production from water and photosynthetic production using organic matter, dark fermentation releases hydrogen from biomass without requiring light, and microbial electrolysis cells use bacterial metabolism to generate a low voltage that, supplemented with a small amount of energy, produces hydrogen gas at a submerged cathode.

Other feedstocks and technologies for hydrogen production that show promise may also be considered. Central production of hydrogen includes a wide diversity of feedstocks, but to be viable, it would require development of a distribution and delivery infrastructure. DOE is pursuing projects to identify a cost-effective, energy-efficient, safe infrastructure for the delivery of hydrogen or hydrogen carriers from centrally located production facilities to the point of use (refer to the Delivery MYRD&D section).

Semi-Central/City-Gate Production Pathway

Another option for hydrogen production is semi-central facilities that could be located, for example, on the edge of urban areas. These would be intermediate in production capacity. They would have limited economies of scale while being located only a short distance from refueling sites and thus reduce the cost and infrastructure needed for hydrogen delivery. Several technologies may be well suited to this scale of production including wind or solar driven electrolysis, reforming of renewable bio-derived liquids, natural gas reforming and photoelectrochemical and biological hydrogen production. Although many of the technologies currently under development are applicable to the semi-central concept, it is not a major focus of the program to emphasize development at the semi-central scale.

Co-Production Pathways

Other production pathways being explored combine production of hydrogen fuel, heat, and electric power. In these scenarios, hydrogen fuel could be produced for use: (1) in stationary fuel cells to produce electricity and heat and (2) as a transportation fuel in fuel cell vehicles or hydrogen internal combustion engine vehicles. This process allows two markets for the hydrogen that could help to initiate the use of hydrogen when hydrogen demand is small. As the demand grows, more of the hydrogen could be produced for vehicle fuel rather than used for power production.

Hydrogen Purification and Enrichment

Hydrogen purification and enrichment are key technology needs that cross-cut hydrogen production options. The quality of the hydrogen produced must meet the hydrogen quality requirements as described in Appendix C. Additional performance requirements for cost, flux rates, hydrogen recovery, and hydrogen purification will be functions of actual system configurations and operation. Going forward, innovations in purification and enrichment of hydrogen will be addressed in pathway specific RD&D.

The DOE Office of Fossil Energy (FE) is developing coal to hydrogen membrane separation systems that will operate in large-scale integrated gasification combined cycle plants to separate hydrogen and to capture and sequester carbon dioxide.

In addition to hydrogen separation membranes, FE is developing oxygen separation membranes. These could be used to replace expensive oxygen cryogenic separation technologies, reducing the cost of hydrogen production from processes that use oxygen such as coal gasification, potentially biomass gasification, or even auto-thermal distributed reforming.

3.1.3 Programmatic Status

Current Activities

Major hydrogen production sub-program activities are listed in Table 3.1.2.

Table 3.1.2 FY 2012 Current Hydrogen Production Program Activities						
Technology Pathway	Approach	FY 2012 Activities				
Distributed reforming of renewable liquid feedstocks	 Improve reforming and separation efficiencies and yields Identify more durable, low cost, reforming catalysts Incorporate breakthrough separations technology Reduce space needed Optimize system operation Intensify and consolidate the number of process steps, unit operations 	 National Renewable Energy Laboratory (NREL): Catalytic steam reforming of biomass pyrolysis-derived bio-oils Pacific Northwest National Laboratory (PNNL): Aqueous phase reforming of biomass liquids such as sugar alcohols and pyrolysis oils 				
Electrolysis	 Reduce electricity costs of hydrogen production by developing new materials and systems to improve efficiency Reduce capital costs of electrolysis system through new designs with lower cost materials and advanced manufacturing methods Develop low-cost hydrogen production from electrolysis using wind and other renewable electricity sources Develop stacks with integral electrochemical compression schemes to produce hydrogen at higher pressures 	 Proton Energy Systems: PEM electrolysis system for reduced cost, improved subsystem/component performance, and increased durability Giner Electrochemical Systems: Lower cost, higher pressure PEM electrolyzer stacks and electrolysis system NREL: Integrated electrolysis with the renewable power source, including power electronics development Avalence: High-efficiency, ultra high-pressure alkaline electrolysis 				
Biomass Gasification	 Develop advanced, lower-cost reforming technologies for hydrogen production from biomass gasification Reduce capital costs of gasification Demonstrate feasibility at pilot scale 	Gas Technology Institute (GTI), National Energy Technology Laboratory, Schott North America , Wah Chang (An Allegheny Company): One step shift separation Membrane reactor for biomass gas reforming for hydrogen production				

Table 3.1.2 FY 2012 Current Hydrogen Production Program Activities (continued)					
Technology Pathway	Approach	FY 2012 Activities			
Solar Thermochemical ⁵	 Utilize the high-temperature energy from concentrated solar power to produce hydrogen through thermochemical cycles Demonstrate feasibility of reaction cycles Demonstrate durability of cycle reaction materials Develop durable materials of construction. Improve solar to hydrogen efficiencies. 	 Science Applications International Corporation: High-temperature water splitting using the sulfur-ammonia reaction cycle for large scale production of hydrogen using solar energy. Sandia National Laboratories, University of Colorado, Boulder: Solar hydrogen production with a metal oxide based thermochemical cycle. Argonne National Laboratory, GTI, Pennsylvania State University of Illinois- Chicago: Membrane/electrolyzer development in the Cu-Cl thermochemical cycle 			
Photoelectrochemical (PEC) ⁶	 Establish standards in theory, synthesis, characterization, and certification for PEC materials, interfaces, devices, and systems Develop durable forms of known PEC materials and devices with limited-lifetime high efficiencies Develop high-efficiency forms of known PEC materials devices with stabilized moderate efficiencies Discover and develop new generation of high-efficiency, high-durability photocatalytic materials and devices Develop cost-effective solar watersplitting reactors based on the best available PEC photoelectrode or photocatalyst materials and devices 	 NREL: III-V crystalline material and device development; Improving stability/durability of the III-V materials; Study corrosion mechanism and validate surface of III-V semiconductors; Theoretical discovery of new PEC materials; Standardization of PEC characterizations and certifications University of Nevada, Las Vegas; Advanced spectroscopic characterizations of PEC materials and interfaces synthesized by PEC Working Group researchers Stanford University: Development of new generation MoS₂ nano-particle photocatalysts with electronic support scaffolds for device integration Lawrence Livermore National Laboratory: Advanced ab initio theoretical modeling of water-splitting and corrosion reactions at the semiconductor/electrolyte interface MV Systems / University of Hawaii at Manoa: development of thin film PEC materials and monolithic integrated devices based on low cost metal oxides, silicon alloys, and copper chalcopyrites Midwest Optoelectronics: Develop combinations of solar cell and catalyst materials for PEC immersion-type devices and systems 			

 ⁵ In collaboration with DOE Office of Nuclear Energy.
 ⁶ In collaboration with DOE's Office of Science (<u>http://science.energy.gov</u>).

Table 3.1.2 FY 2012 Current Hydrogen Production Program Activities (continued)				
Technology Pathway	Approach	FY 2012 Activities		
Biological ⁷	 Develop modifications to green algae, cyanobacteria, dark fermentative microorganisms, and microbial electrolysis systems that will facilitate efficient production of hydrogen Develop biochemical process methods 	 NREL: Develop photobiological and integrated biological systems for large-scale H₂ production using green algae University of California Berkeley: Minimize the chlorophyll antenna size of photosynthesis to maximize solar conversion efficiency in green algae. J. Craig Venter Institute and NREL: Develop an O₂-tolerant cyanobacterial system for continuous light-driven H₂ production from water NREL and Penn State University: Develop direct fermentation technologies to convert renewable lignocellulosic biomass resources to H₂ by bioreactor optimization, improving molar yield, and developing a microbial electrolysis cell system 		
Separation and purification systems (cross-cutting research) ⁸ (ended in 2011)	 Develop separation technology for distributed and central hydrogen production 	 Media and Process Technologies: Carbon molecular sieve membrane in a single-step water-gas shift reactor University of Cincinnati: Zeolite membrane reactor for single-step water-gas shift reaction 		

Table 3.1.2 FY 2012 Current Hydrogen Production Program Activities (continued

3.1.4 Technical Challenges

The overarching technical challenge to providing hydrogen that is cost competitive with other fuels is reducing cost. The production cost component for hydrogen from central natural gas reforming is unlikely to decrease significantly from current projected costs

(See <u>http://hydrogen.energy.gov/h2a_prod_studies.html</u>). As a result, achieving the threshold cost of \$2.00 – \$4.00/gge will depend primarily on technical improvements leading to cost reductions in station compression, storage, and dispensing (CSD).

The capital cost of current water electrolysis systems, along with the high cost of electricity in many regions, limits widespread adoption of electrolysis technology for low cost hydrogen production. Water electrolyzer capital cost reductions and efficiency improvements are required along with the design of utility-scale electrolyzers capable of grid integration and compatible with low-cost, near-zero emission electricity sources. Electrolytic production of hydrogen, where coal is the primary

⁷ In collaboration with DOE's Office of Science (<u>http://science.energy.gov</u>).

⁸ In collaboration with DOE Office of Fossil Energy (<u>http://fossil.energy.gov/programs/fuels/index.html</u>,).

energy resource, will not lead to carbon emission reduction without carbon sequestration technologies.

Hydrogen can be produced from biomass either by reforming of bio-derived liquids or through gasification or pyrolysis of biomass feedstocks. The costs of currently available bio-derived liquids such as ethanol or sugar alcohols (e.g., sorbitol) need to be reduced. Significant improvements in reforming and associated technologies need to be developed for bio-derived liquids to reduce the capital and operating costs for this distributed production option to become competitive. As is the case for electricity, biomass feedstocks costs and availability may vary significantly from region to region. The efficiencies of biomass gasification, pyrolysis, and reforming need to be increased and the capital costs need to be reduced by developing improved technologies and approaches.

High-temperature, solar-driven, thermochemical hydrogen production using water-splitting chemical cycles is in an early stage of research. Research is also needed to cost-effectively couple the thermochemical cycles with advanced concentrated solar energy technology. If these efforts are successful, high-temperature thermochemical processes may provide a clean, efficient, and sustainable route for producing hydrogen from water.

Photoelectrochemical (PEC) hydrogen production based on semiconductor photoelectrodes or photocatalysts is in an early stage of development and requires significant advancements in materials, material systems, and reactor concept development. The primary materials-based research in this area is progressing on three fronts: (1) the study of costly high-efficiency materials to establish performance benchmarks, and to attain a fundamental understanding of PEC hydrogen generation versus corrosion mechanisms; (2) the study of durable lower-quality/lower-cost material systems to improve efficiency by mitigating loss mechanisms; and (3) the development of sophisticated multi-component devices and systems with the potential to achieve efficient PEC water splitting through the effective combination of functionalized materials specifically optimized for light-absorption, charge transport and interfacial catalysis.

Biological hydrogen production is in early- to mid-stage of research and presents many technical challenges, beginning with bioengineering of microorganisms that can efficiently produce hydrogen at high rates. Some of the challenges are related to the need for increased light utilization efficiency, increased rate of hydrogen production, improved continuity of photoproduction, and increased hydrogen molar yield. The advantages of biological hydrogen production are that high-purity water is not required and toxic or polluting by-products are not generated.

Technical Targets

A variety of feedstocks and processes are being researched and developed for producing hydrogen fuel. Each technology is in a different stage of development, and each offers unique opportunities, benefits, and challenges. Economics favor certain technologies more than others in the near term, and other technologies are expected to become economically viable as the technologies mature and market drivers shift.

Tables 3.1.3 through 3.1.12 list the DOE technical targets for hydrogen production from a variety of feedstocks. The targets and timeline for each technology reflect a number of factors, including the expected size/capacity of a production unit, the current stage of technology development, and the costs and characteristics of the feedstock. The current case values in the tables are based on the

status of technologies which have been demonstrated in the laboratory, not on currently available commercial systems. Current cost estimates (2007\$) are based on the projected high volume production of these technologies. Where appropriate, target tables are accompanied by another table that details the estimated cost breakdown as determined using the H2A hydrogen production cost models. The accompanying table is provided as an example only. The cost breakdowns are not targets. For many of the production pathways, achievement of the cost targets will depend on technical breakthroughs (e.g., feedstock processing, heliostat development) beyond the scope of the Hydrogen and Fuel Cells Program. Feedstock costs (including electricity costs) and availability may limit deployments of some pathway technologies.

Out-year targets are RD&D milestones for measuring progress. For hydrogen to become a major energy carrier, the combination of its cost and that of the power system it is used in, must be competitive with the alternatives available in the marketplace. For light duty vehicles, this means that the combination of the hydrogen cost, and its use in a hydrogen fuel cell vehicle, must be competitive with conventional fuels used in advanced vehicles on a cost per mile basis to the consumer. The estimated cost of hydrogen needed to be competitive (with HEVs) is \$2.00 – \$4.00/gge (untaxed) at the dispenser. This estimate will be periodically re-evaluated to reflect projected fuel costs and vehicle power system energy efficiencies on a cost-per-mile basis. The ultimate target for all of the production technologies being researched is a hydrogen cost that will be competitive for transportation on a well-to-wheels basis, regardless of the production method.

The threshold cost goal of 2.00 - 4.00/gge was apportioned between the production and delivery components of the total cost in order for targets, goals, and R&D priorities to be set. A split of the target based on central natural gas reforming as the dominant incumbent technology was used to identify separate threshold targets of <2.00/gge by 2020 for both production and delivery. Somewhat higher costs can be allowed for distributed production since the 2020 targets for CSD result in a levelized cost projection of forecourt costs of < 1.70/gge.

Although not listed in each table, it is understood that the quality of the hydrogen produced by each of these production technologies must meet the hydrogen quality requirements as described in Appendix C. All costs in the following tables are in 2007 dollars to be consistent with DOE Office of Energy Efficiency and Renewable Energy (EERE) planning which uses the energy costs from the 2009 Annual Energy Outlook.

⁹ Record 12001, in preparation

Table 3.1.3 Technical Targets: Distributed Forecourt Production of Hydrogen from Bio-Derived Renewable Liquids – High Temperature Ethanol Reforming ^{a, b, c}						
Characteristics	Units	2011 Status ^d	2015 Target ^d	2020 Target ^e		
Hydrogen Levelized Cost (Production Only) ^f	\$/kg	6.60	5.90	2.30		
Production Equipment Total Capital Investment ^c	\$	1.9M	1.4M ^e	1.2M ^e		
Production Energy Efficiency ^g	%	68	70 ^e	75 ^{e, h}		
Production Equipment Availability ^c	%	97	97	97		
Ethanol Price ^{d,e}	average \$/gal	2.47	2.41	0.85		

Table 3.1.3.A Distributed Bio-Derived Renewable Liquids H2A – High Temperature Ethanol Reforming Example Cost Contributions ^{a, b, c}

Characteristics	Units	2011 Status ^d	2015 ^d	2020 ^e
Production Unit Capital Cost Contribution ^b	\$/kg	0.80	0.70	0.50
Feedstock Cost Contribution ^{d,e}	\$/kg	5.50	5.10	1.60
Production Fixed O&M Cost Contribution	\$/kg	0.20	0.10	0.10
Production Other Variable O&M Cost Contribution ^d	\$/kg	0.10	0.10	0.10
Hydrogen Levelized Cost (Production)	\$/kg	6.60	5.90	2.30
CSD Cost Contribution ⁱ	\$/kg	2.50	1.70	1.70
Total Hydrogen Levelized Cost (Dispensed)	\$/kg	9.10	7.70	4.00

Note: numbers may not sum due to rounding.

- ^a The H2A Distributed Production Model 3.0 (<u>www.hydrogen.energy.gov/h2a_production.html</u>) was used to generate the values in the table with the exceptions described in the notes below. Results are documented in the H2A v3 Current and Future Case studies for Forecourt Hydrogen Production from Ethanol (<u>http://www.hydrogen.energy.gov/h2a_prod_studies.html</u>).
- ^b The H2A Distributed Production Model 3.0 was used with the following standard economic assumptions: All values are in 2007 dollars, 1.9% inflation rate, 10% After Tax Real Internal Rate of Return, 100% Equity Financing, 20-year analysis period, 38.9% overall tax rate, and 15% working capital. The plant design capacity is 1,500 kg/day of hydrogen. It is assumed that Design for Manufacture and Assembly (DFMA) would be employed and that production would have realized economies of scale.
- ^c The plant production equipment availability is 97% including both planned and unplanned outages; ten unplanned outages of 14h duration per year; 1 planned outage of 5 days duration per year. The plant usage factor (defined as

the actual yearly production/equipment design production capacity) is 86% based on over sizing of the production equipment to accommodate a summer surge in demand of 10% above the yearly average demand.

- Ethanol prices for the 2011 status and 2015 target cases are derived from Table B-6: Unit Operation Cost Contribution Estimates (2007 Dollars) and Technical Projections for Thermochemical Conversion to Ethanol Baseline Process Concept. Biomass Multi-Year Program Plan, DOE April 2011. Minimum ethanol price (\$/gal) = 2.77 (2010), 2.15 (2012) for ethanol from corn stover feedstock. An additional cost of \$0.25/gal was added for delivery. The 2012 target price was assumed throughout the remainder of the analysis period. The average delivered ethanol prices shown in Table 3.1.3 were calculated assuming a 20 year facility life starting in 2010 and 2015, respectively. The electricity cost utilized is the EIA AEO 2009 reference case commercial rate.
- ^e The capital cost and energy efficiency of the production unit are based on preliminary analyses and projections for what could be achieved with successful development of this technology (i.e., 2020 target values for conversion process efficiency and equipment cost are assumed to be the same as the 2015 projection for distributed steam methane reforming. The threshold cost goal of <\$4.00/gge dispensed hydrogen cost could be achieved with ethanol reforming if the equipment cost and efficiency targets are met and the cost of ethanol is reduced to <\$.85/gal (40% of the value projected by the Biomass Program).</p>
- ^f The levelized cost is equivalent to the minimum required selling price to achieve a 10% annual rate of return over the life of the plant.
- ^g Energy efficiency is defined as the energy of the hydrogen out of the production process (LHV) divided by the sum of the energy into the process from the feedstock (LHV) and all other energy needed for production. Energy used for CSD is not included in the calculation of production energy efficiency.
- ^h Production unit energy efficiency may vary (as low as 65%) if the capital cost, feedstock costs and other costs associated with alternative process options such as aqueous phase reforming are low enough to still achieve the target of <\$4.00/gge dispensed hydrogen cost.</p>
- ⁱ Costs for the forecourt station compression and storage are consistent with the status and targets in the Delivery MYRD&D Section. Storage capacity for 1540 kg of hydrogen at the forecourt is included. It is assumed that the hydrogen refueling fill pressure is 5000 psi for 2010 and it assumed that in 2015 and 2020, the hydrogen refueling fill pressure is 10,000 psi.

Table 3.1.4 Technical Targets: Distributed Forecourt Water Electrolysis Hydrogen Production ^{a, b, c}									
CharacteristicsUnits201120152020StatusTargetTarget									
Hydrogen Levelized Cost ^d (Production Only)	\$/kg	4.20 ^d	3.90 ^d	2.30 ^d					
Electrolyzer System Capital Cost	\$/kg \$/kW	0.70 430 ^{e, f}	0.50 300 ^f	0.50 300 ^f					
	% (LHV)	67	72	75					
System Energy Efficiency ⁹	kWh/kg	50	46	44					
Stack Energy Efficiency ^h	% (LHV)	74	76	77					
Stack Energy Eniciency	kWh/kg	45	44	43					
Electricity Price	\$/kWh	From AEO 2009 ⁱ	From AEO 2009 ⁱ	0.037 ^j					

Table 3.1.4.A Distributed Electrolysis H2A Example Cost Contributions ^{a, b, c}						
Charact	teristics	Units	2011 Status	2015	2020	
	Cost Contribution ^{a, b, e}	\$/kg H ₂	0.70	0.50	0.50	
Electrolysis System	Production Equipment Availability ^c	%	98	98	98	
Electricity	Cost Contribution	\$/kg H ₂	3.00 ⁱ	3.10 ⁱ	1.60 ^j	
Production Fixed O&M	Cost Contribution	\$/kg H ₂	0.30	0.20	0.20	
Production Other Variable Costs	Cost Contribution	\$/kg H ₂	0.10	0.10	<0.10	
Hydrogen Production	Cost Contribution	\$/kg H ₂	4.10	3.90	2.30	
Compression, Storage, and Dispensing ^k	Cost Contribution	\$/kg H ₂	2.50	1.70	1.70	
Total Hydrogen Levelize	d Cost (Dispensed)	\$/kg H ₂	6.60	5.60	4.00	

^a The H2A Distributed Production Model 3.0 (<u>www.hydrogen.energy.gov/h2a_production.html</u>) used alkaline electrolysis parameters to generate the values in the table with the exceptions described in the notes below. Results are documented in the Current and Future H2A v3 case studies for Forecourt Hydrogen Production from Grid Electrolysis which can be found at <u>http://www.hydrogen.energy.gov/h2a_prod_studies.html</u>.

^b The H2A Distributed Production Model 3.0 was used with the standard economic assumptions: All values are in 2007 dollars, 1.9% inflation rate, 10% After Tax Real Internal Rate of Return, 100% Equity Financing, 20-year analysis period, 38.9% overall tax rate, and 1% working capital (based on independent review input). A MACRS 7-year depreciation schedule was used. The plant design capacity is 1,500 kg/day of hydrogen. It is assumed that

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Design for Manufacture and Assembly (DFMA) would be employed and that production would have realized economies of scale.

- ^c The plant production equipment availability is 98% including both planned and unplanned outages; four unplanned outages of 14h duration per year; 1 planned outage of 5 days duration per year. The plant usage factor (defined as the actual yearly production/equipment design production capacity) is 90% based on over sizing of the production equipment to accommodate a summer surge in demand of 10% above the yearly average demand.
- ^d The levelized cost is equivalent to the minimum required selling price to achieve a 10% annual rate of return over the life of the plant.
- ^e Electrolyzer uninstalled capital costs based on independent review panel results [DOE 2009, Current (2009)] Stateof-the-Art Hydrogen Production Cost Estimate using Water Electrolysis, Independent Review, NREL/BK-6A1-46676, September 2009 (<u>http://www.hydrogen.energy.gov/pdfs/46676.pdf</u>). "Electrolyzer capital costs are expected to fall to \$380/kW for forecourt production." Escalated to 2007 dollars = \$430/kW (purchased equipment cost).
- ^f Electrolyzer cells capital replacement = 25% of total purchased capital every 7 years (DOE, 2009).
- ^g System energy efficiency is defined as the energy in the hydrogen produced by the system (on a LHV basis) divided by the sum of the feedstock energy (LHV) plus all other energy used in the process.
- ^h Stack energy efficiency is defined as the energy in the hydrogen produced by the stack (on a LHV basis) divided by the electricity entering the stack. Additional electricity use for the balance of plant is not included in this calculation. Stack energy efficiency is a guideline and the targets do not need to be met as long as the system energy efficiency meets the targets.
- ⁱ Hydrogen cost is calculated assuming purchase of industrial grid electricity. Electricity prices are taken from the 2009 AEO Reference Case price projections to 2030. Prices beyond 2030 are not available in the 2009 AEO case so they are projected based on the PNNL MiniCAM model output <u>http://www.globalchange.umd.edu/models/gcam/</u>). The average electricity price is \$0.063/kWh (\$0.061/kWh effective) over the modeled life of the plant for the current (2011) case and \$0.070/kWh (\$0.069/kWh effective) for the 2015 case.
- ^j Electricity cost is assumed to be 3.7¢/kWh throughout the analysis period to meet the \$4.00/gge target for dispensed hydrogen.
- ^k Costs for the forecourt station compression and storage are consistent with the status and targets in the Delivery MYRD&D section. Storage capacity for 1579 kg of hydrogen at the forecourt is included. It is assumed that the hydrogen refueling fill pressure is 5000 psi for 2010 and it assumed that in 2015 and 2020, the hydrogen refueling fill pressure is 10,000 psi.

Table 3.1.5 Technical Targets: Central Water Electrolysis Using Green Electricity ^{a,b}								
CharacteristicsUnits201120152020Status °Target dTarget e								
Hydrogen Levelized Cost (Plant Gate) ^f	\$/kg H ₂	4.10	3.00	2.00				
Total Capital Investment ^b	\$M	68	51	40				
System Energy Efficiency ^g	%	67	73	75				
	kWh/kg H ₂	50	46	44.7				
Stack Energy Efficiency ^h	%	74	76	78				
Slack Energy Eniclency	kWh/kg H ₂	45	44	43				
Electricity Price ⁱ	\$/kWh	From AEO '09	\$0.049	\$0.031				

Table 3.1.5.A Central Water Electrolysis H2A Example Cost Contributions ^{a,b}								
CharacteristicsUnits2011 Status c2015 d2020 e								
Capital Cost Contribution	\$/kg	0.60	0.50	0.40				
Feedstock Cost Contribution	\$/kg	3.20	2.30	1.40				
Fixed O&M Cost Contribution	\$/kg	0.20	0.10	0.10				
Other Variable Cost Contribution	\$/kg	0.10	0.10	0.10				
Total Hydrogen Levelized Cost (Plant Gate)	\$/kg	4.10	3.20	2.00				

^a The H2A Central Production Model 3.0 (<u>www.hydrogen.energy.gov/h2a_production.html</u>) assumed alkaline electrolysis was used to generate the values in the table with the exceptions described in the notes below. Results are documented in the Current and Future H2A v3 case studies for Central Hydrogen Production from Grid Electrolysis which can be found at <u>http://www.hydrogen.energy.gov/h2a_prod_studies.html</u>.

^b The H2A Central Production Model 3.0 was used with the standard economic assumptions: All values are in 2007 dollars, 1.9% inflation rate, 10% After Tax Real Internal Rate of Return, 100% Equity Financing, 40-year analysis period, and a 38.9% overall tax rate. A MACRS 20-year depreciation schedule was used. The working capital was set at 5% instead of the standard 15% based on input from the 2009 independent review of the "Current State-of-the-Art Hydrogen Production Cost Estimate Using Water Electrolysis" (<u>http://www.hydrogen.energy.gov/pdfs/46676.pdf</u>). The plant design capacity is 52,300 kg/day of hydrogen. The cell stacks for central electrolyzers are assumed to be replaced regularly at a cost of 25% of the initial capital cost. The replacement period is every 7 years in the 2011 case and every 10 years in the 2020 target case. Power availability of 100% is assumed so the electrolysis capacity factor is 98%. The staffing requirement is 10 full time

equivalents (FTE) in the 2011 case and 4 FTE in the target cases. The plant gate hydrogen pressure is 300 psi.

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- ^c The 2011 status is based on the H2A v3 case study on Current Central Hydrogen Production from Grid Electrolysis (http://www.hydrogen.energy.gov/h2a_prod_studies.html) with modifications as outlined in the other footnotes. The uninstalled equipment cost of the electrolyzer system is \$368/kW (2007\$ equivalent to \$327/kW in 2005\$). They were calculated from the independent review panel's report (http://www.hydrogen.energy.gov/pdfs/46676.pdf). The panel reported a Total Depreciable Capital Cost of \$50M (2005\$) in table 4 (p 22). Using the H2A v2 default indirect costs of 1% for site preparation, 5% for Engineering and Design, 10% for Project Contingency, and 1% for up-front permitting (all percentages of the total direct capital cost), the calculated total direct capital cost is \$43,000,000. Removing the installation factor of 1.2, results in a purchased cost of \$35,700,000. At the panel's design capacity of 52,300 kg/day and electricity usage of 50kWh/kg, the resulting purchased cost is \$327/kW. The estimated system operation is 50 kWh/kg hydrogen resulting in an efficiency of 67%. The startup year is 2010 and the electricity prices over the plant's life are from the 2009 AEO's
- ^d The 2015 targets are intermediate targets between the 2011 status and 2020 targets. Uninstalled cost of the electrolyzer was set at \$300/kW (2007\$ equivalent to \$267/kW in 2005\$), system electricity requirement set at 46 kWh/kg (73% efficiency), and staffing set at 4 FTE. The startup year is 2015 and the electricity price is held constant at \$0.049/kWh.

reference case projections (extrapolated for dates beyond 2030).

- ^e The 2020 target is based on the capital cost and performance (energy efficiency) required to approach the production portion of the \$2-\$4/gge overall delivered hydrogen production cost consistent with the threshold cost and the 2020 delivery cost target of \$2.00/gge. The startup year is set to 2025. Uninstalled cost of the electrolyzer is \$242/kW (2007\$ equivalent to \$215/kW in 2005\$) based on a 50% reduction in the stack cost from the 2010 status and a 20% reduction in the cost of power electronics resulting in an overall reduction of 34% from the 2010 status. Electricity requirement is reduced to 44.7 kWh/kg (75% efficiency). Electricity price was set to \$0.031/kWh (constant over the analysis period) and staffing level was reduced to 4 FTE to achieve the targeted levelized cost of \$2.00/kg.
- ^f The H2A Central Production Model 3.0 (<u>www.hydrogen.energy.gov/h2a_production.html</u>) was used to generate these values at the total invested capital and process energy efficiency indicated in the table.
- ^g System energy efficiency is defined as the energy in the hydrogen produced by the system (on a LHV basis) divided by the sum of the feedstock energy (LHV) plus all other energy used in the process.
- ^h Stack energy efficiency is defined as the energy in the hydrogen produced by the stack (on a LHV basis) divided by the electricity entering the stack. Additional electricity use for the balance of plant is not included in this calculation. Stack energy efficiency is a guideline and the targets do not need to be met as long as the system energy efficiency meets the targets.
- ⁱ Hydrogen cost is calculated assuming purchase of industrial grid electricity. Electricity prices are taken from the 2009 AEO Reference Case price projections to 2030. Prices beyond 2030 are not available in the 2009 AEO case so they are projected based on the PNNL MiniCAM model output (http://www.globalchange.umd.edu/models/gcam/). The average electricity price is \$0.067/kWh (\$0.063/kWh effective) for the modeled life of the plant for the 2011 case. The electricity price for the 2015 target case is held constant over the plant's life at \$0.049/kWh. The electricity price for the 2020 target case is held constant over the plant's life at \$0.049/kWh.

Table 3.1.6 Technical Targets: Biomass Gasification/Pyrolysis Hydrogen Production ^{a,b}							
CharacteristicsUnits2011 Status c,d2015 Target e2020 Target f,g							
Hydrogen Levelized Cost ^h (Plant Gate)	\$/kg	2.20	2.10	2.00			
Total Capital Investment b,i	\$M	180	180	170			
Energy Efficiency ^j	%	46	46	48			

Table 3.1.6.A Biomass Gasification H2A Example Cost Contributions ^{a,b}							
Characteristics	Units	2011 Status ^c	2015	2020 ^d			
Capital Cost Contribution	\$/kg	0.60	0.60	0.60			
Feedstock Cost Contribution	\$/kg	1.00	1.00	0.90			
Fixed O&M Cost Contribution	\$/kg	0.20	0.20	0.20			
Other Variable Cost Contribution	\$/kg	0.40	0.30	0.30			
Total Hydrogen Levelized Cost (Plant Gate)	\$/kg	2.20	2.10	2.00			

^a These costs are based on modeling the cost of hydrogen production utilizing the H2A Central Production Model 3.0. Results are documented in the Current and Future H2Av3 case studies for Central Hydrogen Production via Biomass Gasification (<u>http://www.hydrogen.energy.gov/h2a_prod_studies.html</u>).

- ^b The H2A Central Production Model 3.0 was used with the standard economic assumptions: All values are in 2007 dollars, 1.9% inflation rate, 10% After Tax Return on Investment, 100% Equity Financing, 20-year MACRS straight line depreciation, 40-year analysis period, and 38.9% overall tax rate, 90% capacity factor, and 15% working capital. The plant gate hydrogen pressure is 300 psi. The nominal processing capacity is 2070 and 2000 dry metric tons of biomass per day in the current and 2020 cases, respectively. The specific hydrogen design capacity is 155 metric tons per day for both cases. The current case has a startup year of 2010 and the 2020 case has a startup year of 2020. All feedstock and utility costs are based on their projected costs over the 40-year plant life consistent with the approach used to determine the overall delivered hydrogen threshold cost of \$2-\$4/gge. The biomass feedstock cost varies over time and is \$75/dry short ton in 2010 and \$63/dry short ton in 2017 and following. It is consistent with the EERE Biomass Program estimate for 2012 for woody biomass. The utility costs are based on the 2009 U.S. Energy Information Administration AEO reference projection consistent with the standard H2A methodology.
- ^c The current status is based on the H2A v3 Hydrogen Production via Biomass Gasification Current Case (<u>http://www.hydrogen.energy.gov/h2a_prod_studies.html</u>). No one has actually operated an integrated biomass gasification process designed specifically for hydrogen production at any scale. The H2A analysis is based on pilotscale results of biomass gasification for power generation combined with available information from similar processes for the other components. Performance parameters (e.g., efficiencies) are on individual unit operations hypothetically linked together because integrated performance data are unavailable. Startup year is 2010.
- ^d An independent review panel found the current status of a first-of-a-kind plant to be \$5.40/kg (2009\$) based on a nominal capacity of 500 dry short ton/day with a total capital investment of \$214,000,000 (2009\$). They used a different methodology for estimating capital costs than this analysis as well as different feedstock costs (\$60/dry short ton). Their results are reported at http://www.hydrogen.energy.gov/pdfs/51726.pdf.

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- ^e The 2015 Targets are intermediate targets between the current status and 2020 targets. The capital cost, biomass yield, and natural gas requirement in the current case were used, the startup year was set to 2015, and all other factors are set to the same as the 2020 target case.
- ^f The 2020 Targets are based on the capital cost and performance (energy efficiency) required to approach the production portion of the \$2-\$4/gge overall delivered hydrogen production cost consistent with the threshold cost and the 2020 delivery cost target of \$2.00/gge. The startup year is set to 2025. Capital cost reductions are based on development of a gasification system with internal reforming that produces hydrogen thus making a stand-alone tar reforming system unnecessary. The capital improvements fall within the sensitivity analysis of the H2A Biomass Gasification Future case (2020 technology-readiness, 2025 startup).
- ^g An independent review panel (<u>http://www.hydrogen.energy.gov/pdfs/51726.pdf</u>) projected a levelized cost of \$2.80/kg for an nth plant based on a nominal capacity of 2000 dry ton/day with a total capital investment of \$344,000,000 (2009\$). They used a different methodology for estimating capital costs than this analysis and different feedstock costs (\$80/dry ton).
- ^h The H2A Central Production Model 3.0 (<u>www.hydrogen.energy.gov/h2a_production.html</u>) was used to generate these values at the total invested capital and process energy efficiency indicated in the table. See Record #12007 (in preparation) for more details (<u>www.hydrogen.energy.gov/program_records.html</u>).
- ⁱ All cases assume capital replacement at 0.5%/yr. of total depreciable capital investment.
- ⁱ Energy efficiency is defined as the energy in the hydrogen produced (on a LHV basis) divided by the sum of the feedstock energy (LHV) plus all other energy used in the process.

Table 3.1.7 Technical Targets: Solar-Driven High-Temperature Thermochemical Hydrogen Production ^a							
Characteristics	Units	2011 Status	2015 Target	2020 Target	Ultimate Target		
Solar-Driven High-Temperature Thermochemical Cycle Hydrogen Cost ^b	\$/kg	NA	14.80	3.70	2.00		
Chemical Tower Capital Cost (installed cost) $^{\rm c}$	\$/TPD H ₂	NA	4.1MM	2.3MM	1.1MM		
Annual Reaction Material Cost per TPD H_2^{d}	\$/ yrTPD H ₂	NA	1.47M	89K	11K		
Solar to Hydrogen (STH) Energy Conversion Ratio ^{e,f}	%	NA	10	20	26		
1-Sun Hydrogen Production Rate ^g	kg/s per m²	NA	8.1E-7	1.6E-6	2.1E-6		

- ^a The targets in this table are for research tracking with the Ultimate Target values corresponding to market competitiveness. Targets are based on an initial analysis utilizing the H2A Central Production Model 3.0 with standard H2A economic parameters (<u>http://www.hydrogen.energy.gov/h2a_production.html</u>). Projections assume a ferrite high-temperature cycle with a central production capacity of 100,000 kg H₂/day. Further analysis assumptions may be found in "Support for Cost Analyses on Solar-Driven High Temperature Thermochemical Water-Splitting Cycles, TIAX LLC, Final Report to U.S. Department of Energy, 22 February 2011" (http://www1.eere.energy.gov/hydrogenandfuelcells/pdfs/solar_thermo_h2_cost.pdf).
- ^b Hydrogen cost represents the complete system hydrogen production cost for purified, 300 psi compressed gas. System level losses such as heliostat collector area losses, replacement parts, operation, and maintenance are included in the cost calculations which are documented in the H2A v3 Future Case study for Solar-thermochemical Production of Hydrogen (http://www.hydrogen.energy.gov/h2a_prod_studies.html).
- ^c The chemical tower capital cost is the projected total installed cost for the ferrite cycle conversion of water into hydrogen.
- ^d Reaction material cost is defined as the effective annual cost of the active (ferrite) material within the thermochemical process per metric ton rated hydrogen capacity of the system. The value is calculated as the expected annual purchase price of the material in its usable form (e.g., ferrite coated on a substrate) divided by the material lifetime under expected use condition (i.e., nearly continuous usage during the sunlight hours with an annual capacity factor of 90%); divided by the net rated hydrogen production capacity of the system [in metric tons per day (TPD)] (For example, 100,000 kg H₂/day = 100 TPD). Material cost improvements are expected to result from a combination of decreased material usage, improved cycle time, and increased material lifetime.
- ^e STH energy conversion ratio is defined as the energy of the net hydrogen produced (LHV) divided by full-spectrum solar energy consumed. For systems utilizing solar energy input only, the consumed energy is calculated based on the incident irradiance over the total area of the solar collector. For hybrid systems, all additional non-solar energy sources (e.g., electricity) must be included as equivalent solar energy inputs added to the denominator of the ratio.
- ^f Due to the developmental nature of the technology, the STH energy conversion ratio has not yet been measured for the complete solar to hydrogen reaction. Consequently, STH targets are calculated based on partial laboratory measurements using artificial light sources with extrapolation to overall system performance.
- ^g The hydrogen production rate in kg/s per total area of solar collection under full-spectrum 1-sun incident irradiance $(1,000 \text{ W/m}^2)$. Under ideal conditions, STH can be related to this rate as follows: STH = H₂ Production Rate (kg/s per m²) * 1.23E8 (J/kg) / 1.00E3 (W/m²). Measurements of the 1-sun hydrogen production rate can provide an invaluable diagnostic tool in the evaluation of loss mechanisms contributing to the STH ratio.

Table 3.1.7A contains the values of several cost and performance parameters which, when combined, achieve the DOE performance targets for each target year. The parameters may be traded-off against one another to achieve the overall cost targets (e.g. reaction material cost may be traded-off with replacement lifetime). Consequently, the parameter values are listed merely as examples as there are numerous numerical combinations that meet the DOE targets.

Table 3.1.7.A Example Parameter Values to Meet Cost Targets: Solar-Driven High-Temperature Thermochemical Hydrogen Production							
Characteristics	Units	2011 Status	2015 Target	2020	Ultimate		
Solar to Hydrogen (STH) Energy Conversion Ratio	%	NA	10	20	26		
Cycle Time	minutes/ cycle	NA	5	3	1		
Reaction Material Cost	\$/kg	270	270	270	270		
Reaction Material Replacement Lifetime	years	NA	1	5	10		
Heliostat Capital Cost (installed cost) ^a	\$/m²	200	140	75	75		

^a Heliostat capital costs encompass all capital costs, including installation, with the solar reflector system needed to focus solar energy onto the chemical tower reactor. Cost is stated per square meter of solar capture area. Heliostat capital cost status for 2010 and the capital cost targets for 2015 and 2020 are consistent with the current viewpoint of the EERE Solar Program as reflected in the "Power Tower Technology Roadmap and Cost Reduction Plan" SAND2011-2419, April 2011, (http://prod.sandia.gov/techlib/access-control.cgi/2011/112419.pdf) and the DOE SunShot Vision Study (http://www1.eere.energy.gov/solar/pdfs/47927_chapter5.pdf), respectively.

Table 3.1.8 Technical Targets: Photoelectrochemical Hydrogen Production:Photoelectrode System with Solar Concentration ^a							
Characteristics	Units	2011 Status	2015 Target	2020 Target	Ultimate Target		
Photoelectrochemical Hydrogen Cost ^b	\$/kg	NA	17.30	5.70	2.10		
Capital cost of Concentrator & PEC Receiver (non-installed, no electrode) ^c	\$/m ²	NA	200	124	63		
Annual Electrode Cost per TPD H ₂ ^d	\$/ yr-TPDH ₂	NA	2.0M	255K	14K		
Solar to Hydrogen (STH) Energy Conversion Ratio ^{e, f}	%	4 to 12%	15	20	25		
1-Sun Hydrogen Production Rate ⁹	kg/s per m²	3.3E-7	1.2E-6	1.6E-6	2.0E-6		

- ^a The targets in this table are for research tracking with the Ultimate Target values corresponding to market competitiveness. Targets are based on an initial analysis utilizing the H2A Central Production Model 3.0 with the standard H2A economic parameters (<u>www.hydrogen.energy.gov/h2a_production.html</u>). Targets are based on photoelectrode-type PEC systems wherein a solar trough collector concentrates light onto a PEC receiver assembly. The PEC receiver consists of a flat panel PEC electrode (submerged in an electrolyte bath) and the collection housing and manifolds to collect and separate the evolved hydrogen and oxygen gases. Solar concentration is assumed to be 15:1 for the ultimate target case and 10:1 for all others. Further analysis assumptions may be found in "Technoeconomic Analysis of Photoelectrochemical (PEC) Hydrogen Production", Directed Technologies Inc., Final Report to the Department of Energy, December 2009 (<u>http://www.hydrogen.energy.gov/pdfs/review09/pd_23_james.pdf</u>). Plant assumed capacity is 50,000 kg H₂/day
- for all years. All targets are expressed in 2007 dollars.
 ^b Hydrogen cost represents the complete system hydrogen production cost for purified, 300 psi compressed gas. System level losses and expenses due to solar collection/concentration, window transmittance/refraction, replacement parts, operation, and maintenance are included in the cost calculations which are documented in the H2A v3 Future Case study for Type 4 (Photoelectrode System with Concentration) Photoelectrochemical (PEC) Production of Hydrogen (http://www.hydrogen.energy.gov/h2a_prod_studies.html).
- ^c Capital cost includes solar concentration and associated tracking (if any), the optical window, and the water/electrolyte/gas containment subsystem. The cost of the PEC electrode is not included. All areas refer to total solar capture area. While improvements beyond the current status are needed to meet these cost goals, this area is not presently a research focus of the Fuel Cell Technologies Program.
- ^d Annual electrode cost refers to the annual replacement cost of the PEC photoelectrode panel normalized by the design capacity of the system (in metric tons H₂ per day). Electrode cost includes both the material and manufacturing cost of the PEC electrode used within the reactor.
- ^e STH energy conversion ratio is defined as the energy of the net hydrogen produced (LHV) divided by full-spectrum solar energy consumed. For systems utilizing solar energy input only, the consumed energy is calculated based on the incident irradiance over the total area of the solar collector. For hybrid systems, all additional non-solar energy sources (e.g., electricity) must be included as equivalent solar energy inputs added to the denominator of the ratio.
- ^f The 2011 Status of STH ratio is in the range of 4% and 12% for different semiconductor material systems exhibiting different levels of operational durability. Thin film material systems have been demonstrated with STH > 4% for hundreds of hours (A. Madan, Fuel Cell Technologies Program 2011 Annual Progress Report: <u>http://www.hydrogen.energy.gov/pdfs/progress11/ii g 5 madan 2011.pdf</u>); Crystalline material systems have been demonstrated with STH > 12% for tens of hours. [O. Khaselev, J.A. Turner, Science 280, 425 (1998)].
- ^g The hydrogen production rate in kg/s per total area of solar collection under full-spectrum 1-sun incident irradiance (1,000 W/m²). Under ideal conditions, STH can be related to this rate as follows: STH = H₂ Production Rate (kg/s per m²) * 1.23E8 (J/kg) / 1.00E3 (W/m²). Measurements of the 1-sun hydrogen production rate can provide an invaluable diagnostic tool in the evaluation of loss mechanisms contributing to the STH ratio.

Table 3.1.8A contains the values of several cost and performance parameters which, when combined, achieve the DOE performance targets for each target year. The parameters may be traded-off against one another to achieve the overall cost targets (e.g., electrode cost may be traded-off with replacement lifetime). Consequently, the parameter values are listed merely as examples as there are numerous numerical combinations that meet the DOE targets.

Table 3.1.8.A Example Parameter Values to Meet Cost Targets: Photoelectrochemical Hydrogen Production (Photoelectrode System)							
CharacteristicsUnits2011 Status20152020Ultimate							
Solar to Hydrogen (STH) Energy Conversion Ratio	%	NA	15	20	25		
PEC Electrode cost ^a	\$/m ²	NA	300	200	100		
Electrode Cost per TPD H ₂ ^b	\$/ TPD	NA	1.0M	510K	135K		
Electrode Replacement Lifetime ^c	Years	NA	0.5	2	10		
Balance of Plant Cost per TPD H ₂ ^d	\$/ TPD	NA	420K	380K	310K		

^a PEC photoelectrode cost refers to the material and manufacturing cost of the PEC electrode. Area is based on the actual area of the electrode itself.

^b This parameter is the PEC photoelectrode cost (as defined above) normalized by the metric tons per day of hydrogen design capacity of the electrode.

c Electrode replacement lifetime denotes the projected total duration of the electrode being immersed in electrolyte and under cyclic solar illumination until process energy efficiency drops to 80% of its original values. Thus, a 10 year electrode replacement lifetime refers to 10 years of operation under diurnal cycles and approximately 5 years of actual hydrogen production.

^d This parameter denotes non-electrode, non-concentrator/PEC receiver, non-installation balance of plant costs normalized by the metric tons per day of hydrogen design capacity of the electrode.

Table 3.1.9 Technical Targets: Photoelectrochemical Hydrogen Production:Dual Bed Photocatalyst System ^a							
Characteristics	Units	2011 Status	2015 Target	2020 Target	Ultimate Target		
Photoelectrochemical Hydrogen Cost ^b	\$/kg	NA	28.60	4.60	2.10		
Annual Particle Cost per TPD H_2 ^c	\$/ yr-TPDH ₂	NA	1.4M	71K	4K		
Solar to Hydrogen (STH) Energy Conversion Ratio ^{d,e}	%	NA	1	5	10		
1-Sun Hydrogen Production Rate ^f	kg/s per m ²	NA	8.1E-8	4.1E-7	8.1E-7		

^a The targets in this table are for research tracking with the Ultimate Target values corresponding to market competitiveness. Targets are based on an initial analysis utilizing the H2A-Central Production Model 3.0 with standard H2A economic parameters (<u>www.hydrogen.energy.gov/h2a_production.html</u>). Targets are based on a dual-bed PEC nanoparticle slurry-type system wherein clear thin film polymer bag-style reactors are filled with water and photocatalytically active nanoparticles. The hydrogen evolution half-reaction occurs in one bag reactor section and the oxygen evolution half-reaction occurs in an adjacent reactor section. The reactor sections are connected by a porous ionic bridge which permits ion exchange to complete the electrochemical circuit but prevents gas mixing. Solar energy energizes both reactions. No solar concentration is used. Further analysis assumptions may be found in "Technoeconomic Analysis of Photoelectrochemical (PEC) Hydrogen Production," Directed Technologies Inc., Final Report to the Department of Energy, December 2009 (<u>http://www.hydrogen.energy.gov/pdfs/review09/pd_23_james.pdf</u>). Plant capacity is 50,000 kg H₂/day for all years. All targets are expressed in 2007 dollars.

- ^b Hydrogen cost represents the complete system hydrogen production cost for purified, 300 psi compressed gas.
 System level losses and expenses due to solar window transmittance/refraction, replacement parts, operation, and maintenance are included in the cost calculations which are documented in the H2A v3 Future Case study for Type 2 (PEC Dual Bed Photocatalyst System) Photoelectrochemical Production of Hydrogen (http://www.hydrogen.energy.gov/h2a_prod_studies.html).
- ^c PEC particle cost refers to the annual replacement cost of the PEC nanoparticles normalized by the design capacity of the system (metric tons H₂ per day). Particle cost includes both the material and manufacturing cost of the PEC nanoparticles used within the reactor. Although different chemical reactions occur in the two bed sections, particle cost is combined for purposes of cost reporting.
- ^d STH energy conversion ratio is defined as the energy of the net hydrogen produced (LHV) divided by full-spectrum solar energy consumed. For systems utilizing solar energy input only, the consumed energy is calculated based on the incident irradiance over the total area of the solar collector. For hybrid systems, all additional non-solar energy sources (e.g., electricity) must be included as equivalent solar energy inputs added to the denominator of the ratio. In a dual bed system, this requires two material systems each with half reactions operating at twice the stated net STH energy conversion ratio.
- ^e Dual bed systems are less mature than photoelectrode PEC systems. The current status STH energy conversion ratio is still under investigation.
- ^f The hydrogen production rate in kg/s per total area of solar collection under full-spectrum 1-sun incident irradiance (1,000 W/m²). Under ideal conditions, STH can be related to this rate as follows: STH = H₂ Production Rate (kg/s per m²) * 1.23E8 (J/kg) / 1.00E3 (W/m²). Measurements of the 1-sun hydrogen production rate can provide an invaluable diagnostic tool in the evaluation of loss mechanisms contributing to the STH ratio.

Table 3.1.9A contains the values of several cost and performance parameters which, when combined, achieve the DOE performance targets for each target year. The parameters may be traded-off against one another to achieve the overall cost targets (e.g., particle cost may be traded-off with replacement lifetime). Consequently, the parameter values are listed merely as examples as there are numerous numerical combinations that meet the DOE targets.

Table 3.1.9.A Example Parameter Values to Meet Cost Targets: Photoelectrochemical Hydrogen Production (Dual Bed Photocatalyst)						
Characteristics	Units	2011 Status	2015	2020	Ultimate	
Solar to Hydrogen (STH) Energy Conversion Ratio	%	NA	1	5	10	
PEC particle cost ^a	\$/kg	NA	1000	500	300	
Particle Replacement Lifetime ^b	Years	NA	0.5	1	5	
Capital cost of reactor bed system (excluding installation and PEC particles) ^c	\$/m²	NA	7	7	5	
Balance of Plant Cost per TPD H ₂ ^d	\$/ TPD	NA	6.4M	1.0M	0.6M	

^a PEC particle cost refers to the material and manufacturing cost of the PEC nanoparticles used within the reactor. While different chemical reactions occur in the two bed sections, the particle costs are combined for purposes of cost reporting. Particle mass is based on the total particle mass (including inert substrate if used).

^b Particle replacement lifetime denotes the projected total duration of the nanoparticles being immersed in electrolyte and under cyclic solar illumination until process energy efficiency drops to 80% of its original values. Thus, a 5 year particle replacement lifetime refers to 5 years of operation under diurnal cycles and approximately 2.5 years of actual hydrogen production.

 Reactor system capital cost includes only the high density polyethylene clear plastic film reactor bed assembly and its associated ionic transfer bridges. Installation, fluid piping, and the photocatalytic nanoparticles are not included. All areas refer to total solar capture area.

^d This parameter denotes the non-installed balance of plant costs exclusive of reactor beds and PEC particles. It includes piping, controls, sensors, pumps, and compressors and is normalized by the metric tons per day of hydrogen design capacity of the system.

Table 3.1.10 Technical Targets: Photolytic Biological Hydrogen Production ^a							
Characteristics	Units	2011 Status	2015 Target ^c	2020 Target ^d	Ultimate Target [°]		
Hydrogen Cost ^b	\$/kg	NA	NA	9.20	2.00		
Reactor Cost ^f	\$/m ²	NA	NA	14	11		
Light utilization efficiency (% incident solar energy that is converted into photochemical energy) ^g	%	25 ^h	28	30	54		
Duration of continuous H_2 production at full sunlight intensity i	Time Units	2 min ^j	30 min	4 h	8 h		
Solar to H_2 (STH) Energy Conversion Ratio ^k	%	NA	2%	5%	17%		
1-Sun Hydrogen Production Rate ¹	kg/s per m²	NA	1.6E-7	4.1E-7	1.4E-6		

^a The targets in this table are for research tracking with the Ultimate Target values corresponding to market competitiveness. Targets are based on an initial analysis utilizing the H2A Central Production Model 3.0 with standard H2A economic parameters (**Error! Hyperlink reference not**

valid.www.hydrogen.energy.gov/h2a_production.html.)

- ^b Hydrogen cost represents the complete system hydrogen production cost for purified, 300 psi compressed gas. Projections assume photolytic production of hydrogen gas by genetically engineered organisms (algal or bacterial) suspended in a water solution under solar illumination, modeled as algae, with an O₂-tolerant hydrogenase, grown in large, raceway-type, shallow bed reactors that are covered by a thin, optically transparent film, and provided with nutrients, CO₂, and sunlight. The evolved gas will be collected, purified to 99.999+ hydrogen purity by pressure swing adsorption (PSA), and compressed to 300 psi for hydrogen pipeline transport. Plant capacity is 50,000 kg H₂/day for all years. All targets are expressed in 2007 dollars. Cost calculations are documented in the H2A v3 Future Case Study for Photolytic Biological Production of Hydrogen (http://www.hydrogen.energy.gov/h2a_prod_studies.html). Further analysis assumptions may be found in "Technoeconomic Boundary Analysis of Biological Pathways to Hydrogen Production," Directed Technologies, Inc., Final Report to U.S. Department of Energy, 31 August 2009 (http://www1.eere.energy.gov/hydrogenandfuelcells/pdfs/46674.pdf).
- ^c The 2015 target is based on analysis of the best technologies projected to be available in 2015 and assumes integration into a single, non-hybrid organism. Specifically, the 2015 target is based on a model of a *Chlamydomonas reinhardtii* strain with an O₂-tolerance hydrogenase system and a reduced chlorophyll antennae light harvesting complex (LHC), in which all the improvements listed in the table have been integrated.
- ^d For 2020, all assumptions of the 2015 target system apply (such as reactor system design and organism type) except the organism is assumed to be further improved in the target parameters indicated in the table.
- ^e For the 2015 and 2020 targets, the organism modeled is assumed to be an algal strain with a native photosynthesis system (i.e., with Photosystems I and II). For the Ultimate Target, previous assumptions (such as reactor system design) apply, but the modeled organism is both optimized and has a genetically modified hybrid photosynthetic system combining the native algal Photosystem II with a bacterial Reaction Center, achieving greater hydrogen production rates by extending the light spectrum that can be collected and improving the efficiency of other conversion steps. Fundamental genetic engineering advances are required to reach the hybrid organism's ultimate target efficiency values. If the hybrid organism was not successfully genetically engineered, performance would be limited to a light utilization efficiency of 34%, an STH ratio of 9.8%, and a cost of \$2.6/kg H₂.

- ^f Installed cost per square meter of organism bed reactor equipment includes the containment structure, film covering, and any reactor interior flow control equipment. It does not include cost of complementary equipment such as compressors, PSA, Control Room, etc. Square meters are defined as the solar capture area. Future designs for the reactors will need to address safety measures to deal with the co-production of hydrogen and oxygen (e.g., replacing PSA systems with Temperature Swing Apparatus systems), which may increase costs. Due to the early stage of development, photobioreactor designs and the required organismal characteristics will likely undergo modifications before widespread commercial use to address issues such as temperature, salinity, and pH control.
- ^g The light utilization efficiency is the conversion efficiency of incident solar energy into photochemically available energy and is the product of two values: the light collection efficiency and the photon use efficiency at full sunlight intensity. The first value, light collection efficiency, is the fraction of solar incident light that is within the photosynthetically active radiation (PAR) wavelength band of the organism. For green algae, the light collection efficiency is estimated to be 45% ("Light and photosynthesis in aquatic ecosystems," Kirk, Cambridge University Press, 1994), and is considered fixed for the 2015 and 2020 targets; the hybrid organism modeled for the ultimate target is estimated to have a light collection efficiency of up to 64% ("Integrated biological hydrogen production," Melis and Melnicki, International Journal of Hydrogen Energy, September

2006) http://www.sciencedirect.com/science/article/pii/S0360319906002308). The second value, photon use efficiency, is the efficiency of converting the absorbed photon energy into chemical energy through photosynthesis at full sunlight intensity (2,500 micromol photons per square meter per second). At low-light conditions (i.e., with no light saturation), the average photon use efficiency for algae is 85% ("Absolute absorption cross sections for photosystem II and the minimum quantum requirement for photosynthesis in *Chlorella vulgaris*." Ley and Mauzerall, Biochim. Biophys. Acta 1982). Experimentally, photon use efficiency is determined by measuring the rate of photosynthesis (via oxygen evolution) per photon at different light intensities and comparing the rates at full sunlight and at sub-saturating light levels, with the maximum value set at the 85% efficiency level.

- ^h "Maximizing Light Utilization Efficiency and Hydrogen Production in Microalgal Cultures," Melis, 2008 Annual Progress Report for DOE's Hydrogen Program
- (http://www.hydrogen.energy.gov/pdfs/progress08/ii_f_2_melis.pdf).
- ⁱ For purposes of conversion efficiencies and duration reporting, full sunlight (2,500 micromol photons per square meter per second) conditions are assumed. Since in actual practice light intensity varies diurnally, only 8 hours of continuous duration is needed for a practical system. The duration values assume a system where the enzyme is regenerated at night with respiration scavenging oxygen.
- ^j Brand et al., 1989, Biotechnol. Bioeng.
- ^k STH energy conversion ratio is defined as the energy of the net hydrogen produced (LHV) divided by net fullspectrum solar energy consumed. For systems utilizing solar energy input only, the consumed energy is calculated based on the incident irradiance over the total area of the solar collector. For hybrid systems, all additional nonsolar energy sources (e.g., electricity) must be included as equivalent solar energy inputs added to the denominator of the ratio. For photolytic biological hydrogen production, this can be thought of as the product of three components: $E_0*E_1*E_2$. The maximum potential value is calculated by determining the highest possible conversion efficiencies at three steps: E_0 , the percent of solar energy (at sea level) that is absorbed by the organism; E_1 , the percent of absorbed energy that is utilized for charge separation by the photosystems; and E_2 , the energy for charge separation that is utilized for water splitting. The E_2 value is reduced by 20% to account for the fact that some photon energy will go to other processes, such as cellular maintenance, rather than hydrogen production. The hydrogen cost calculation takes into consideration reductions due to reactor light transmittance (10% loss) and the loss of production over a full production day due to durations less than 8 h. Cost calculations are documented in the H2A v3 Future Case Study for Photolytic Biological Production of Hydrogen (http://www.hydrogen.energy.gov/h2a_prod_studies.html).
- ¹ The hydrogen production rate in kg/s per total area of solar collection under full-spectrum 1-sun incident irradiance $(1,000 \text{ W/m}^2)$. Under ideal conditions, STH can be related to this rate as follows: STH = H₂ Production Rate (kg/s per m²) * 1.23E8 (J/kg) / 1.00E3 (W/m²). Measurements of the 1-sun hydrogen production rate can provide an invaluable diagnostic tool in the evaluation of loss mechanisms contributing to the STH ratio.

Table 3.1.11 Technical Targets: Photosynthetic Bacterial Hydrogen Production ^a						
Characteristics	Units	2011 Status	2015 Target	2020 Target ^b		
Efficiency of Incident Solar Light Energy to H_2 (E0*E1*E2) ^c from organic acids	%	NA	3	4.5		
Molar Yield of Carbon Conversion to H ₂ (depends on nature of organic substrate) E3 ^d	% of maximum	NA	50	65		
Duration of continuous photoproduction ^e	Time	NA	30 days	3 months		

^a The targets in this table are for research tracking. The final targets for this technology are costs that are market competitive. This table will be updated in a future version of this plan to incorporate hydrogen cost target and current technology assumptions.

^b Technology readiness targets (beyond 2020) are 5.5% efficiency of incident solar light energy to H₂ (E0*E1*E2) from organic acids, 80% of maximum molar yield of carbon conversion to H₂ (depends on nature of organic substrate) E3, and 6 months duration of continuous photoproduction. See Figure 3.1.2 for a schematic representation of conversion steps and associated efficiencies.

c E0 reflects the light collection efficiency of the bacteria in the photoreactor and the fact that only a fraction of incident solar light is photosynthetically active (theoretical maximum is 68%, from 400 to 1000 nm). E1*E2 is equivalent to the efficiency of conversion of absorbed light to primary charge separation then to adenosine-5'-triphosphate; both are required for hydrogen production via the nitrogenase enzyme. E0*E1*E2 represents the efficiency of conversion of incident solar light to hydrogen through the nitrogenase enzyme (theoretical maximum is 10% for 4-5 electrons). This efficiency does not take into account the energy used to generate the carbon substrate.

- ^d E3 represents the molar yield of H_2 per carbon substrate (the theoretical maximum is 7 moles per mole carbon in the substrate, based on the average yield of acetate and butyrate).
- ^c Duration reflects continuous production in the light, not necessarily at peak efficiencies. It includes short periods during which ammonia is re-added to maintain the system active.

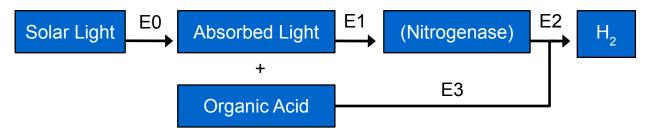


Figure: 3.1.2 Photosynthetic Bacterial System Overview Illustrating E0, E1, E2 and E3 Conversion Processes

Table 3.1.12 Technical Targets: Dark Fermentative Hydrogen Production and Microbial Electrolysis Cells (MECs) ^a							
Characteristics	Units	2011 Status	2015 Target	2020 Target ^b			
Feedstock Cost ^c	cents/lb. sugar	13.5	10	8			
Yield of H ₂ production from glucose by fermentation ^d	mol H₂ /mol glucose	3.2 ^e	4	6			
Yield of H ₂ production from glucose by integrated MEC – fermentation ^f	mol H ₂ /mol glucose	-	6 ^e	9 ^e			
Duration of continuous production (fermentation)	Time	17 days ^g	3 months	6 months			
MEC cost of electrodes	\$/m ²	2,400 ^h	300	50			
MEC production rate	L-H ₂ / L-reactor- day	-	1	4			

- ^a The targets in this table are for research tracking. The final targets for this technology are costs that are market competitive. This table will be updated in a future version of this plan to incorporate hydrogen cost targets and feedstock assumptions.
- $^{\rm b}$ Technology readiness targets (beyond 2020) are 10 molar yield of H₂ production from glucose, 6 cents/lb. sugar feedstock cost, and 12 months duration of continuous production.
- ^c Targets are from the DOE Biomass Program Multi Year Program Plan 2007-2012, August, 2005, for sugar from lignocellulosic biomass. The targets have been shifted 2-5 years in Table 3.1.12 for purposes of FCT planning pending further analysis of this pathway.
- ^d The theoretical maximum from known fermentative pathways is 4, although the H_2 content of 1 mole of glucose and the H_2O required for fermentation is 12. Clearly, in order to achieve molar yields greater than 4, the feasibility of developing new pathways or discovering new microbes needs to be assessed.
- In 2010, NREL reported a H₂ molar yield of 3.2 by supplying limited amounts of cellulose substrate during fermentation (2010 Annual Progress Report DOE Hydrogen Program; (http://www.hydrogen.energy.gov/pdfs/progress10/ii h 3 maness.pdf).
- ^f The yield assumes a system where the effluent from the glucose-fed fermentation system is used as feedstock for an MEC (e.g., in 2015 the target for fermentation is 4 mol H_2/mol glucose while that for MEC is 2 mol H_2/mol glucose, for a total combined target of 6 mol H_2/mol glucose). The goal is for continuous flow operation conditions.
- ^g Van Ginkel, S., Sung, S. 2001. Environ. Sci. Technol. 35: 4726-4730.
- ^h Estimated for replacing Pt with MoS₂, based on Tokash, J.C. and B.E. Logan. 2011. "Electrochemical evaluation of a molybdenum disulfide catalyst for the hydrogen evolution reaction under solution conditions applicable to microbial electrolysis cells." Int. J. Hydrogen Energy. 36(16): 9439-9445.

3.1.5 Technical Barriers

The following sections detail the technical and economic barriers that must be overcome to attain the Hydrogen Production goal and objectives. The barriers are divided into sections depending on the hydrogen production method.

Distributed Hydrogen Production from Renewable Liquid Feedstocks

Reforming of ethanol and other bio-derived liquids is similar to natural gas reforming but presents several unique issues, such as high feedstock costs and catalyst and water requirements. This technology is suitable for application in distributed and semi-central production.

A. Reformer Capital Costs and Efficiency. Current small-scale distributed renewable liquid feedstock reforming technologies have capital costs that are too high to achieve the targeted hydrogen production cost. Multiple-unit operations that entail many process steps in converting bioderived liquids to hydrogen and low energy efficiencies are key contributors to the high capital cost. Improved reforming and water-gas shift catalysts are needed to increase yield and improve performance. Reforming and water-gas shift unit operations also generate considerable costs. Finally, the high purity of hydrogen required for fuel cells puts upward pressure on the capital costs.

B. Operations and Maintenance (O&M). O&M costs for distributed reforming hydrogen production from renewable feedstocks are too high. Robust systems that require little maintenance and that include remote monitoring capability need to be developed. The reliability of balance of plant (BOP) equipment (pumps, compressors, blowers, sensors, etc.) is often the limiting factor in overall system reliability. Increasing the reliability and service life of these components is critical, as is minimizing equipment complexity. For reformer systems, catalyst activity is also critical for reliable and efficient operation.

C. Biomass Feedstock Issues. Feedstock costs for bio-derived liquids are too high, and there is likely to be strong competition for the available resources from other end-use applications (e.g., bio-derived fuels). In addition to cost, biomass feedstock quality and availability may be limited in some areas, or the quality of the feedstock may change throughout the year. Feedstock-flexible reformers are needed to address location-specific feedstock supply issues. Effects of impurities on the system from multiple feedstocks as well as the effects of impurities from variations in single feedstocks need to be addressed in the reformer design.

D. Forecourt Footprint and Storage. To be economically feasible in urban settings, the physical footprint of stations needs to be reduced. Issues may arise regarding the storage of renewable feedstocks on site. Some feedstocks will be relatively benign (e.g., carbohydrates) and will likely require minimal regulation, while others may fit under the regulations now being developed for E85, E100, and bio-diesel. Regulations for still other types of feedstocks may need to be developed. Permitting will need to be addressed.

E. Control and Safety. Control and safety issues are associated with natural gas and renewable feedstock reforming, including on-off cycling. Effective operation control strategies are needed to minimize cost and emissions, maximize efficiency, and enhance safety. Hydrogen leakage is addressed within the Delivery and Safety, Codes & Standards sub-programs.

Hydrogen Generation by Water Electrolysis

F. Capital Cost. The capital costs of water electrolysis systems are prohibitive to widespread adoption of electrolysis technology for low cost hydrogen production. RD&D is needed to develop lower cost materials with improved manufacturing capability to lower capital cost requirements while improving the efficiency and durability of the system. Development of larger systems is also needed to take advantage of economies of scale. Technically viable systems for low-cost manufacturing need to be developed for this technology.

G. System Efficiency and Electricity Cost. Improvements in BOP efficiency and durability are necessary to the commercial viability of electrolysis. Mechanical high-pressure compression technology exhibits low energy efficiency and may introduce impurities while adding significantly to the capital and operating cost. Efficiency gains can be realized through minimized mechanical compression using electrochemical compression in the cell stack. Development is needed for low-cost cell stack optimization addressing efficiency, compression, and durability. Target costs cannot be met unless electricity price is < \$0.04/kWh (see Tables 3.1.4 and 3.1.5).

H. Footprint. Station footprint is dependent on location and the needs of each specific locality. The footprint, in general, will have the same limitations that were described in the distributed hydrogen production from renewable liquid feedstocks section.

I. Grid Electricity Emissions (for distributed). The current grid electricity mix in most locations results in greenhouse gas emissions in large-scale electrolysis systems. Low-cost, carbon-free electricity generation is needed. Electrolysis systems that can produce both hydrogen and electricity need to be evaluated. (Renewable electricity costs are being addressed by the DOE EERE renewable power programs – Solar, Wind, Hydropower, Geothermal, and Biomass.)

J. Renewable Electricity Generation Integration (for central). More efficient integration with renewable electricity generation is needed to reduce costs, improve performance, and increase onstream time (i.e., increase the number of hours per year the renewable electricity is available). Development of integrated renewable electrolysis systems is needed, including optimization of power conversion and other system components from renewable electricity to provide high-efficiency, low-cost integrated renewable hydrogen production.

K. Manufacturing. Currently, the electrolysis units are produced in low volumes. Since development of fabrication technologies is capital intensive, manufacturers must have assurance that there will be high demand for the product in order to produce adequate returns on investments. The cost of water electrolysis systems is driven up by the high cost of BOP, the short lifespan of system components, and site-specific fabrication of system components.

L. Operations and Maintenance. The O&M cost for electrolysis are currently too high. Durability, maintenance, reliability, and demand management are similar to those of the distributed natural gas reforming systems. Operating efficiency, component durability, purification of water, and transients and changes in duty cycles need to be addressed.

M. Control and Safety. Barriers in control and safety include the efficiency of start-up and shutdown processes, turn-down capability, and the capability for rapid on-off cycling. Control and safety costs still remain high due to complex system designs and high-cost sensors. For commercialization of this technology, reliability and safety of these units is a key qualification target.

Biomass Gasification Hydrogen Production

N. Feedstock Cost and Availability. Feedstock costs are high. Improved feedstock/agricultural technologies (higher yields per acre, etc.), lower cost feedstock collection, and improved feedstock preparation are needed. Because biomass feedstocks are seasonal in nature, feedstock-flexible processes and cost-effective feedstock storage are needed. (Tasks to overcome these barriers are the responsibility of the DOE Biomass Program and the U.S. Department of Agriculture.)

O. Capital Cost and Efficiency of Biomass Gasification Technology. The capital cost for biomass gasification/pyrolysis needs to be reduced. Process intensification by combining unit operations can significantly reduce capital costs. For example, combining the current two step water-gas shift and PSA separation to a one step water-gas shift with integrated separation, to integrating gasification, reforming, water-gas shift and separation all in one unit operation. Improved process efficiency and higher hydrogen yields and selectivity's through catalyst research, better heat integration, and alternative gas clean-up approaches are needed. Improved catalysts or engineering approaches for tar cracking are also needed.

P. Emissions Gasification produces significant amounts of greenhouse gases (GHGs) even though emissions are much lower than those from coal plants.

Q. Operations and Maintenance. Operation and maintenance costs are too high. More efficient and durable equipment is needed.

R. Control and Safety. Control and safety issues need to be addressed particularly in biomass and biomass-coal co-gasification. Certification codes and standards should be standardized. Gasification operations should have back-up and fail-safe modes to improve safety and operation.

High Temperature, Solar-Driven Thermochemical Production of Hydrogen

There are over 200 potential thermochemical cycles for water splitting driven by concentrated solar power. These cycles have been evaluated and ranked for their suitability.¹⁰ The most promising cycles will require extensive research and development efforts.

S. High-Temperature Robust Materials. High temperatures are required for these thermochemical systems (500-2000°C). Cost-effective, durable materials are needed that can withstand these high temperatures and the thermal duty cycles present in solar concentrator systems.

T. Coupling Concentrated Solar Energy and Thermochemical Cycles. Coupling concentrated solar energy with thermochemical cycles presents many challenges. Receivers, heat transfer systems, as well as reactors, need to be developed and engineered. Cost effective approaches and systems to deal effectively with the diurnal nature of sunlight need to be researched and developed.

U. Concentrated Solar Energy Capital Cost. Concentrated solar energy collection is currently expensive and requires large areas of land. Improved, lower-cost solar concentrator/collection technology, including materials, is needed.¹⁰

V. Heliostat Development and Cost. Heliostats, a reflective device that tracks the sun to keep the mirrors focused onto a target receiver, are currently too expensive to be economically viable. The

¹⁰ Perret, Robert. (May 2011). "Solar Thermochemical Hydrogen Production Research (STCH)." Technical Report SAND2011-3622, Sandia National Laboratories.

cost needs to be reduced by 50% in order to achieve the targeted $120/m^2$ installed. The high costs are due to lack of standardization in design which is associated with inefficient manufacturing and poor durability of the heliostat.

W. Materials and Catalysts Development. The required temperatures for the cycle reactions are often in excess of 1,000°C. Current materials for the reactor, seals, catalysts, and supports are inefficient and do not meet operating requirements at these temperatures. Materials also need to operate in corrosive and reactive environments, some materials meet a few of the requirements but not all.

X. Chemical Reactor Development and Capital Costs. Reactors will need to be efficient, inexpensive, and entail minimal BOP to meet the cost targets. The high cost of material is due to the requirements for high durability and chemical and thermal stability. Thermal losses must be minimized to achieve an efficient process. There are also high capital costs that are associated with hydrogen separation and purification.

Y. Diurnal Operation. Solar power availability and fluctuations will strongly influence the design, performance, and economic viability of this technology.

Z. Control and Safety. Control and safety issues associated with STCH include optimization of start-up and shut-down processes, improved turn-down capability, activated material and thermal storage integration and control, and the capability for rapid on-off cycling. Costs remain high due to system complexity and sensor count to assure reliability. Operation of this system should occur with minimal manual assistance, which will require attributes such as back-up fail-safe modes, remote monitoring, and sparse maintenance schedules. Gaseous chemicals are used and can be harmful.

AA. Feedstock Issues. Water is the primary feedstock of STCH hydrogen production therefore an adequate amount of water must be available. The water must also be free of contaminants.

AB. Chemical and Thermal Storage. Capturing and storing thermal energy during peak solar times will extend the operational time of the STCH reactor. However, storage will require solar power which will add to complexity and cost to receiver-reactor interface. Molten nitrate salts enable temperatures up to 650°C. Molten carbonates can store higher amounts of thermal energy but are extremely corrosive which can hinder operation. Also, some cycles require higher temperatures (>1,500°C). In these cases molten metals may be an option but are also highly corrosive.

AC. Solar Receiver and Reactor Interface Development. The solar receiver interface with the chemical reactor is an important consideration in the selection of a solar receiver. For directly heated reactors, the receiver and reactor are integrated, enabling solar flux to heat the reactor. Solid particle and volumetric receivers are heated indirectly by the sun. In these reactors, the heat is absorbed by solid particles or molten salts, which then heat the reactors. In addition to interfacing with the receiver, the reactor must also interface with thermal storage, if used.

AD. Operations and Maintenance. All system components must be considered in O&M, including feed pre-conditioning, heliostats, solar receivers, reactor, hydrogen purification, controls, utilities, sensors, compression, storage, and safety. 24/7 operation may be ideal but not feasible due to variability of the power source. Durability, scheduled maintenance, storage, and hydrogen quality monitoring need to be considered when improving O&M and reducing costs.

Photoelectrochemical Hydrogen Production

Photoelectrochemical (PEC) hydrogen production based on semiconductor photoelectrodes or photocatalysts is in an early stage of development and requires significant advancements in materials, material systems, and reactor concept development. The primary materials-based research in this area is progressing on three fronts: (1) the study of costly high-efficiency materials to establish performance benchmarks and to attain a fundamental understanding of PEC hydrogen generation versus corrosion mechanisms; (2) the study of durable lower-quality/ lower-cost material systems to explore the mitigation of loss mechanisms for improving efficiency toward benchmark values; and (3) the development of sophisticated multi-component devices and systems with the potential to achieve efficient PEC water splitting through the effective combination of functionalized materials specifically optimized for light-absorption, charge transport, and interfacial catalysis. As efficient, durable and cost-effective materials systems are developed with the assistance of state-of-the-art methods in materials theory, synthesis, and characterization, further advanced work will be needed on integration schemes into high-performance photoelectrode or photocatalyst devices and reactors. For long-term practicality, cost-effective methods of engineering and manufacturing the best available PEC materials, devices, and systems need to be identified and developed.

Current material systems for PEC photoelectrodes or photocatalysts can be broadly divided into three categories, each with its own characteristics and research challenges. These groupings are:

(I) highly efficient light absorbers typically with limited lifetimes and relatively high cost (e.g., Group III-V crystalline materials),

(II) stable materials typically with lower visible light absorption efficiency and relatively lower cost (e.g., metal- and mixed-metal oxide thin films), and

(III) hybrid and multi-junction systems which combine multiple functionalized materials in multi-photon device schemes.

The group (I) materials studied to date can exhibit high light conversion efficiencies, often better than 60% incident-photon-to-electron conversion (IPEC) throughout the visible spectrum, but have been susceptible to corrosion. The well-known group (II) materials are characterized by high bandgaps and lower integrated IPEC over the solar spectrum, but have demonstrated good stability in some cases. Many of the groups (I) and (II) materials have majority band edge potentials that are insufficient to drive one of the water-splitting half reactions, necessitating the multi-junction approaches in group (III). It is anticipated that the group (III) material systems can exhibit high efficiency and long lifetime, depending on the material set, but these systems can be complicated and expensive to synthesize. Research in all three categories is deemed necessary for developing systems that meet the ultimate targets reflected in the PEC target table. The research in these categories also needs to include the latest development in nanomaterials and nanotechnology for enhancement of bulk and interface properties.

To date, a range of materials and material systems have met individual 2015 targets for efficiency or durability, but no single material/system has simultaneously met the ultimate efficiency, durability, and cost targets, which is the primary research challenge for photoelectrochemical hydrogen production. Drawing on the ongoing lessons learned from the research and development of group (I), (II), and (III) material systems, PEC researchers continue to make the innovative scientific advances needed to converge on systems incorporating the best improvements in efficiency,

durability and cost. The materials-by-design approach facilitated by interactive development of advanced materials theory, synthesis, and characterization methodologies is viewed as an important cornerstone to overcome the barriers in this PEC materials systems research. Specific technical barriers are related to the efficiency, durability and cost of PEC materials, interfaces, devices, systems and reactors. These include:

AE. Materials Efficiency - Bulk and Interface. PEC semiconductor efficiency is limited by light absorption, charge separation, and transport in the bulk, and by energetics and charge transfer at the solid/liquid interface. Semiconductor materials with smaller bandgaps more efficiently utilize the solar spectrum but are often less energetically favorable for hydrogen production because of the bandedge mismatch with respect to either hydrogen or oxygen redox potentials. Large bandgap semiconductors can provide favorable energetics for splitting water at the interface but are poor bulk absorbers of light. Material systems must be developed with

- appropriate bandgap for light absorption,
- bandedges aligned energetically for hydrogen and oxygen evolution,
- low-loss charge separation and transport in the solid state, and
- interfaces kinetically favorable for the photoelectrochemical water-splitting half reactions.

Theory, synthesis, and characterization methods in materials discovery and screening are important tools.

AF. Materials Durability - Bulk and Interface. PEC semiconductor/electrolyte junctions are prone to both dark and light-induced degradation due to corrosion reactions which compete with water-splitting half-reactions at the interfaces, and which can propagate into the bulk. Intrinsically durable materials with the appropriate characteristics for photoelectrochemical hydrogen production that meet the ultimate program goals have not been identified. The high-efficiency materials currently available corrode quickly during operation, and the most durable materials are inefficient for hydrogen production. Discovery of intrinsically stable and efficient materials would be an ideal solution to this barrier, but represents a significant challenge. Promising alternative approaches focus on modification of surfaces through coatings or dispersions to energetically or kinetically stabilize the interface and protect the bulk. The use of theory, synthesis, and characterization methods can facilitate a better understanding of corrosion mechanisms for development of mitigation schemes to enhance durability.

AG. Integrated Device Configurations. Efficient and stable integrated devices combining the best available semiconductors, surface treatments, and auxiliary linking materials are needed for achieving ultimate targets in PEC solar hydrogen production. These can be planar-integrated devices for photoelectrode reactor configurations, or functionalized particle devices for photocatalyst reactor configurations. Hybrid and other device designs that combine functionalized materials specifically optimized for light-absorption, charge transport, and interfacial catalysis could simultaneously address issues of durability and efficiency. Techniques are needed for synthesizing these integrated device configurations which maintain the integrity of each component material. Appropriate manufacturing techniques based on these synthesis routes are needed to scale device configurations to commercial scales.

AH. Reactor Designs. Solar water-splitting reactor system designs incorporating the most promising device configurations, and using cost-effective, hydrogen-impermeable auxiliary materials, are also needed to implement the photolytic production routes, including PEC. Complete systems evaluations need to consider a range of important operational constraints and parameters, including the diurnal operation limitations and the effects of water purity on performance and lifetime. Preliminary technoeconomic analysis

(http://www.hydrogen.energy.gov/pdfs/review09/pd_23_james.pdf) of conceptual reactor types has indicated that the ultimate targets for PEC are most readily achievable in photoelectrode systems with modest concentrations (Type 4 reactors, in the nomenclature of the technoeconomics report) or in dual-bed photocatalysts systems (Type 2 reactors). Both reactor types feature built-in separation of evolved hydrogen and oxygen, and both operate at sufficiently low temperatures to avoid the need for costly high-T materials. Ion transport in the liquid electrolyte, particularly in the Type 2 reactors, can limit the water splitting efficiency, calling for engineering solutions. Type 4 reactors require additional hardware for modest solar concentration. For both reactor types, full engineering options need to be carefully analyzed to minimize capital and operational requirements.

AI. Auxiliary Materials. The functional requirements for auxiliary materials for semiconductorbased PEC hydrogen production must be determined, and the auxiliary materials discovered, developed, and tested to facilitate PEC device and systems development. Auxiliary materials for PEC devices include photoelectrode substrate materials, protective coatings for enhanced durability, catalytic coatings for enhanced interface kinetics, photovoltaic semiconductor under-layers for enhanced energetics, and interface and contact materials. Auxiliary materials for PEC reactors include hydrogen impervious materials, stable and transparent coverings for light transmission and concentration, electrolyte components, and ionic conduits.

AJ. Synthesis and Manufacturing. Synthesis and manufacturing techniques need to be developed for the PEC materials, materials systems, devices, and reactors capable of solar water-splitting at high efficiency, long durability and low cost. For materials and devices, the synthesis techniques need to be scalable and affordable and need to preserve the integrity of all integrated component materials. For the systems and reactors, manufacturing techniques need to be on scales consistent with implementation in commercial installations.

AK. Diurnal Operation Limitations. Photolytic processes are discontinuous because they depend on sunlight, which is unavailable at night and available only at low intensities on cloudy days. This variability results in increased capital costs for larger facilities to accommodate higher short-term production rates and larger hydrogen storage needs. Diurnal operation conditions are explicitly included in the cost estimate analyses.

AL. Operations and Maintenance. Potential costs, including labor, required for PEC hydrogen production could make the technology too costly to compete in the marketplace. Barriers to minimizing these costs will need to be addressed in a number of areas.

AM. Control and Safety. Control issues dealing with PEC hydrogen include optimizing start up and shutdown processes, turn-down capability (for cloudy days), and rapid on-off cycling. The system should be able to operate with minimal manual assistance, which will require a back-up fail-safe mode, remote monitoring, and sparse maintenance schedules.

Biological Hydrogen Production

A number of technologies for biological hydrogen production are available, but they are not mature at present. Technical barriers related to each individual technology must be overcome, integrated models must be developed, and barriers related to an integrated system must be identified. Methods for engineering and manufacturing these systems have not been fully evaluated.

Barriers are listed below for each technology, followed by a model for how these different technologies could be integrated and a list of barriers for the integrated process.

Photolytic Hydrogen Production from Water (green algae or cyanobacteria)

AN. Light Utilization Efficiency. The microorganisms used for photobiological hydrogen production possess large arrays of light-capturing antenna pigment molecules, which absorb more light than can be utilized by the photosynthetic electron transport apparatus, resulting in heat dissipation and loss of up to 80% of the absorbed sunlight. Research is needed to identify ways to increase the light conversion efficiency, including genetic engineering to improve microorganism light utilization mechanisms and the identification of natural strains with better light utilization.

AO. Rate of Hydrogen Production. The current hydrogen production rate from photolytic microorganisms is too low for commercial viability. The low rates have been attributed to (a) the non-dissipation of a proton gradient across the photosynthetic membrane, which is established during electron transport from water to the hydrogenase (the hydrogen producing enzyme) under anaerobic conditions, and (b) the existence of competing metabolic flux pathways for photosynthetic reductant. Genetic means to overcome the restricting metabolic pathways may be used to significantly increase the rate of hydrogen production. Under aerobic conditions, with an oxygen tolerant hydrogenase catalyzing hydrogen production, the competition between carbon dioxide fixation and hydrogenase will have to be addressed.

AP. Oxygen Accumulation. Along with hydrogen, photolytic microorganisms such as algae coproduce oxygen, which inhibits the hydrogenase enzyme activity and can create a safety issue if stoichiometric mixtures of the two gases are reached. Both issues could be addressed by affecting the ratio of photosynthesis to respiration by a variety of means, such that oxygen is consumed as quickly as it is produced and does not accumulate in the medium, while maintaining the quantum yield of photosynthesis and full hydrogenase activity (see details under Integrated System). The inhibition may also be addressed through engineering or identifying a naturally occurring less oxygen sensitive enzyme or separating the oxygen and hydrogen production cycles. Options to address the safety issue may include ensuring ignition sources are not present and/or mechanical separation of the gases.

AQ. Systems Engineering. System requirements for cost-effective implementation of photolytic hydrogen-production technologies have not been adequately evaluated. Analysis and research are needed on inexpensive/transparent materials for hydrogen containment, hydrogen collection systems, continuous bioreactor operation, monoculture maintenance, land area requirements, and capital costs.

AR. Diurnal Operation Limitations. The same issues apply as for photoelectrochemical systems (see Barrier AK).

Photosynthetic Bacterial Hydrogen Production, Required for an Integrated System:

AS. Light Utilization Efficiency. Same issues apply as for photolytic systems (see barrier AN).

AT. Net Hydrogen Production. Metabolic processes in photosynthetic bacteria can reduce net hydrogen production by using the produced hydrogen and through metabolic pathways that compete with hydrogen production for electron donors. Genes controlling these pathways must be inactivated to maximize hydrogen production or alternative metabolic enzymes must be identified or engineered.

AU. Carbon/Nitrogen Ratio. To maximize nitrogenase activity, the proper ratio of carbon to nitrogen (C/N) nutrients must be maintained. The C/N nutrient content in the photo reactor (algal and cyanobacteria) and in the dark fermenter needs to be evaluated to assess whether the media composition is suitable for subsequent photosynthetic bacterial hydrogen production. Enzyme engineering approaches may be needed to alleviate inhibition of nitrogenase by elevated levels of nitrogen nutrient.

AV. Systems Engineering. The same issues apply as for photolytic systems (see barrier AQ), except for the mixture of gases. Photosynthetic bacteria do not co-evolve hydrogen and oxygen but release hydrogen and carbon dioxide. The cost of hydrogen and carbon dioxide separation must be evaluated.

AW. Diurnal Operation Limitation. The same issues apply as for photoelectrochemical systems (see barrier AK).

Dark Fermentative Hydrogen Production:

AX. Hydrogen Molar Yield. Up to 4 moles of hydrogen can theoretically be produced per mole of glucose through the known fermentative pathways. However, various biological limitations such as hydrogen-end-product inhibition, competition with other metabolic pathways for electron donors, and accumulation of waste byproducts such as organic acids limit the molar yield to around 2 moles per mole glucose consumed. Hydrogen molar yields must be increased significantly through metabolic engineering efforts. Waste byproducts may also require subsequent wastewater treatment. Elimination of these by-product generation pathways and/or subsequent by-product processing (such as in an integrated biological hydrogen production system) of the organic acids by photosynthetic bacteria or MECs (see below) is needed to increase hydrogen yields. Potential release of toxins and their inhibition of the subsequent steps in an integrated system will need to be evaluated.

AY. Feedstock Cost. The glucose feedstock is the major cost driver for economic hydrogen production via fermentation. For renewable hydrogen to be cost competitive with traditional transportation fuels, the glucose cost must be around \$0.05 per pound and provide a molar yield of hydrogen approaching 10 (see Barrier AX and Table 3.1.12). Lower-cost methods to use whole biomass are needed including, but not limited to, reducing the cost of conversion to glucose or identifying cellulose-degrading bacteria or consortia that can utilize untreated lignocellulosic biomass directly. Bioprospecting for cellulolytic microbes with a high rate of hydrogen production are also needed to use the cell biomass of the green algal/cyanobacterial and photosynthetic bacterial co-culture (in an integrated biological hydrogen production system).

AZ. Systems Engineering. The same issues apply as in photosynthetic bacterial production (see barrier AQ), plus prevention of methanogen contamination and reduced fermentation time are needed.

Microbial Electrolysis Cell (MEC):

AAA. Electrode Costs. The cost of the cathode materials remains the largest cost in the system. Early systems used very expensive fuel cell carbon cloth, Pt catalysts, and binders (Nafion). These costs must be reduced by discovering or engineering less expensive materials.

AAB. Solution Density (Production Rate). The hydrogen gas production rate per volume of reactor needs to be increased. Solutions include, but are not limited to, building reactors with more dense packing of electrodes. The early work was conducted with small electrode packing, resulting in 0.37 L of hydrogen gas per liter of reactor per day. Advancement must be made to increase electrode packing and therefore reduce the overall tankage and piping needed to produce hydrogen gas.

Integrated Biological Hydrogen Production System (many configurations are possible, Figure 3.1.3):

AAC. Photosynthesis/Respiration Capacity Ratio. Green algae and cyanobacteria become anaerobic when their P/R (photosynthesis/respiration) capacity ratio is 1 or less. Under such anaerobic conditions, photosynthetic water oxidation produces hydrogen (instead of starch), and the oxygen evolved by photosynthesis is consumed by respiration, producing carbon dioxide. Currently, this process is achieved by nutrient deprivation, but this method decreases the quantum yield of photosynthesis. Alternative mechanisms to bring the P/R ratio to 1 need to be investigated, particularly those methods that will not reduce the quantum yield of photosynthesis. Two further issues will need to be investigated under these conditions: (a) rate limitations due to the non-dissipation of the proton gradient and (b) the ability of the culture to take up a variety of exogenous carbon sources under the resulting anaerobic conditions.

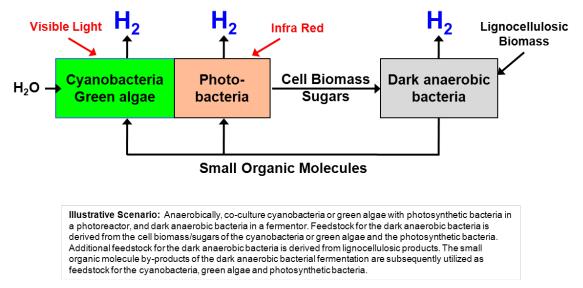


Figure 3.1.3 Integrated Biological System

AAD. Co-Culture Balance. To extend the absorption spectrum of the hydrogen photoproducing cultures into the infrared, the possibility of co-cultivating oxygenic photosynthetic organisms with anoxygenic photosynthetic bacteria should be investigated. Another option to be investigated is further genetic modifications to integrate pigments and the single photosystem from Purple Non-Sulfur (PNS) photobacteria to the oxygenic photosynthetic organisms.

AAE. Concentration/Processing of Cell Biomass. In an integrated system, cell biomass from either green algae/cyanobacteria or photosynthetic bacteria can serve as the substrate for dark fermentation. Pretreatment of cell biomass may be necessary to render it more suitable for dark fermentation. Methods for cell concentration and processing will depend on the type of organism used and how the biological system is integrated.

3.1.6 Technical Task Descriptions

The technical task descriptions and the barriers associated with each task are presented in Table 3.1.13. Concerns regarding safety and environmental effects will be addressed within each task in coordination with the appropriate sub-program.

Table 3.1.13 Technical Task Descriptions		
Task	Description	Barriers
1	 Distributed Reforming of Renewable Liquid Feedstocks Analyze and research options for alternative renewable feedstocks (e.g., ethanol, methanol, sugars, sugar alcohols, bio-oils, bio-based Fischer-Tropsch liquids) for distributed production. Develop catalysts for optimized feedstock utilization and H₂ yield. Utilizing the technology concepts developed for distributed natural gas reforming, develop efficient, integrated, compact, robust process technology for bio-derived liquid feedstocks. Explore novel technology, such as low temperature aqueous phase processing, for reforming bio-derived renewable liquid feedstocks that could result in a cost breakthrough. Verify achievement of 2015 and 2020 cost and efficiency targets through the operation of bench scale, and small (up to 30 kg/day) pilot scale development units respectively, for reforming of a bio-derived liquid. 	A, B, C, D, E
2	 Advanced Electrolysis Technologies Evaluate low cost electrolysis pathways by developing a model for analyzing various options for low cost renewable and nonrenewable electricity and then analyzing distributed and central electrolysis. Reduce distributed electrolyzer capital and operating costs by reducing system cost and increasing system energy efficiency, developing novel compression designs, integrating system components, advanced BOP designs and developing efficient manufacturing process technology. Develop central renewable integrated electrolysis technologies by evaluating viable renewable electricity integration approaches, developing advanced power electronics interface components, developing a stack module pilot scale (250 - 500 kW) electrolysis system suitable for renewable and grid electricity integration, and integrating and verifying feasibility of renewable hydrogen production at pilot scale. 	F, G, H, I, J, K, L, M

	Table 3.1.13 Technical Task Descriptions	
Task	Description	Barriers
	Hydrogen Production from Biomass Gasification	
	 Reduce the cost and increase the feedstock flexibility of biomass feedstock preparation (e.g., handling, size reduction, etc.) (Biomass Program). 	
	 Research and develop more cost-effective, efficient, and robust biomass product gas clean-up technologies for feeding into reforming operations, including hot-gas clean-up, tar cracking, and other related technologies. (This will be coordinated with the Office of Fossil Energy for coal-gasifier product gas clean-up technologies and with the EERE Biomass Program.) 	
	 Investigate opportunities for catalyst and reactor improvement for tar cracking, reforming, and conditioning of gasifier product gases. 	
	 Improve hydrogen yield and selectivity and overall heat integration to improve energy efficiency and reduce cost. 	
3	• Reduce the capital cost by combining/integrating process steps and operations. This integration could include single step water-gas shift with an integrated membrane, combining shift and reforming into one operation, combining gasification, tar cracking, and reforming into one operation, etc. Develop a gasification system with internal reforming that produces hydrogen and makes a stand-alone tar cracking/reforming system unnecessary.	N, O, P, Q, R
	 Investigate and develop alternative biomass gasification technology approaches such as biomass hydrolysis followed by aqueous phase reforming. 	
	 Verify an integrated biomass gasification system for hydrogen production at targeted costs. 	
	 Reduce the cost of emission control systems that handle pollutants from coal and biomass. Also, reduce carbon capture and sequestration mechanism costs, and improving efficiency. 	
	 Improve system durability, robustness, and lifespan to reduce the time needed for maintenance and to lower O&M costs. 	

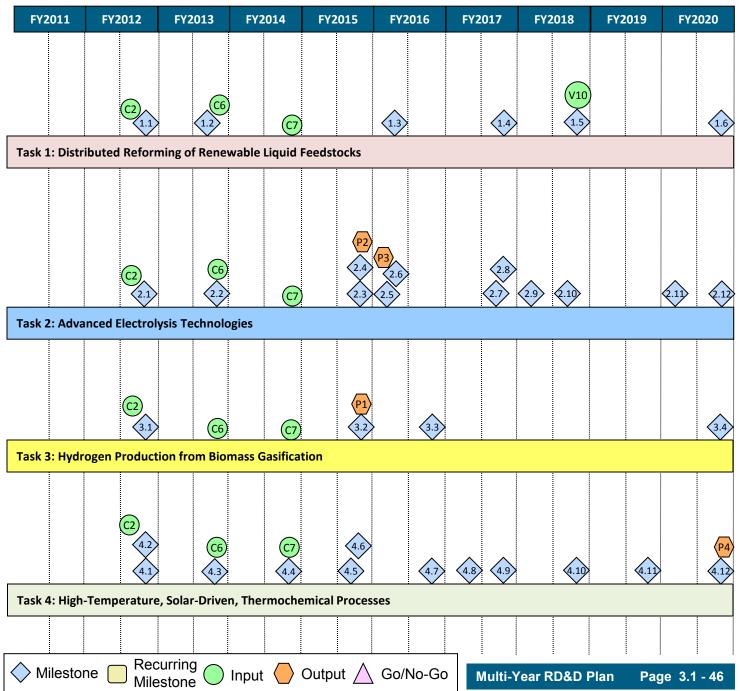
	Table 3.1.13 Technical Task Descriptions	
Task	Description	Barriers
	High-Temperature, Solar-Driven, Thermochemical Processes	
4	 Evaluate and research potential high-temperature, solar driven thermochemical water-splitting cycles and down-select to the most promising cycles. Optimize sub-cycle reactions and verify effective hydrogen production at laboratory scale. Verify stability of reaction materials under extended lab-scale thermochemical cycling Determine active material cost and durability requirements to meet targets. Optimize electrolytic processes, electrode and catalyst materials, and cells. Verify cycle operation and durability of materials of reaction during on-sun tests. Quantify and verify conversion efficiency and kinetics for reaction cycles. Develop lower capital cost solar heliostat, secondary concentrators, and solar tower technology. (This will leverage the efforts in the EERE Solar Program.) Develop cost-effective, high-temperature materials of construction compatible with thermochemical processes. These materials must have minimal hydrogen and heat loss. Develop cost-effective thermal and chemical storage methods. Develop a viable integrated, solar-driven high-temperature thermochemical water-splitting process. Verify an integrated, solar-driven high-temperature thermochemical water-splitting process. Develop a solar field configuration and design to match chemical plant requirements. Identify strategies for full integration of solar thermal energy collection and storage with the chemical reaction cycle for thermochemical water-splitting. Verify performance of a semi-integrated system at small scale (5-100 kW). Verify that a fully-integrated system can achieve 2020 targeted costs and yields. 	S, T, U, V, W, X, Y, Z, AA, AB, AC, AD

Table 3.1.13 Technical Task Descriptions		
Task	Description	Barriers
6	 Biological Hydrogen Production Systems Engineering for All Biological Hydrogen Production Systems Optimize photoreactor material and system designs (including system scale- up and alternative reactor beds and alternative immobilization material systems for photolytic production). Discover and develop cost-effective, transparent, H₂-impermeable materials for biological H₂ production systems. Develop hydrogen collection and gas-separation technologies. Molecular and Physiological Engineering of Organisms for Photolytic Hydrogen Production from Water Generate organisms with O₂-tolerant hydrogenases, that have increased light conversion efficiency, allow more efficient photosynthetic electron transport toward H₂, and eliminate competing pathways for enhanced H₂ production. Eliminate H₂ uptake pathways in cyanobacteria. Research and develop systems in which water photolysis occurs under anaerobic conditions (i.e., in which the ratio of O₂-producing photosynthesis to O₂-consuming respiration (P/R) is ≤1). Test different methods to achieve that ratio without affecting H₂ production. Molecular Engineering of Organisms for Photosynthetic electron transport. Eliminate competitive pathways such as H₂ oxidation and polymer accumulation. Engineer organisms to remove the repression of fixed nitrogen on nitrogenase expression and have a functional nitrogenases. Molecular and Systems Engineering for Dark Fermentative Hydrogen Production Research and develop improved cellulolytic microbes or a consortium with high rates of biomass degradation and H₂ production. Increase rates of H₂ production and eliminate competing pathways for H₂ production. Increase rates of H₂ production and eliminate competing pathways for H₂ production. 	AN, AO, AP, AQ, AR, AS, AT, AU, AV, AW, AX, AY, AZ, AAA, AAB, AAC, AAD, AAE

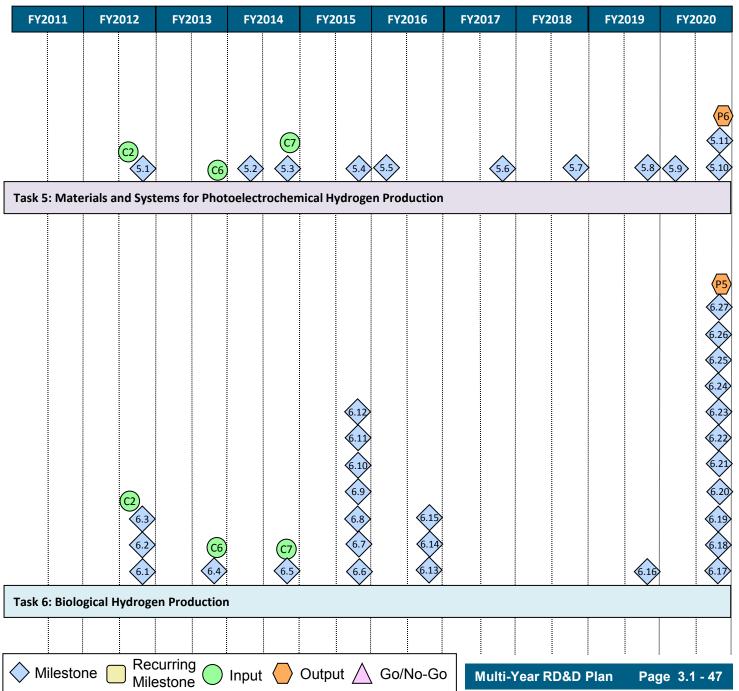
3.1.7 Milestones

The following chart shows the interrelationship of milestones, tasks, supporting inputs from other sub-programs, and technology outputs for the Hydrogen Production sub-program from FY 2012 through FY 2020. The input-output relationships are also summarized in Appendix B.

Production Milestone Chart



Production Milestone Chart



2012

Technical Plan — Production

	Task 1: Distributed Reforming of Renewable Liquid Feedstocks	
1.1	Demonstrate a cumulative 100 hours of catalyst operation in an integrated bench-scale production system. (Q4, 2012)	
1.2	Determine technical and economic feasibility of hydrogen from reforming of pyrolysis oil. (Q3, 2013)	
1.3	Verify 2015 cost and efficiency targets through the operation of a bench scale development unit for reforming of a bio-derived liquid. (Q2, 2016)	
1.4	Select and optimize feedstock, catalyst, and reforming reactor for system integration, construction, and scale up testing. (Q4, 2017)	
1.5	Verify through H2A analysis the feasibility of achieving less than \$4.00/gge (delivered) from bio-derived renewable liquid fuels. (Q4, 2018)	
1.6	Verify 2020 cost and efficiency targets through the operation of a small scale (up to 30 kg/day) pilot scale development unit for reforming of a bio-derived liquid. (Q4, 2020)	

	Task 2: Advanced Electrolysis Technologies
2.1	Verify the capital cost of the electrolyzer stacks against the 2012 target of <\$400/kW projected for high volume. (Q4, 2012)
2.2	Verify the system performance against the 2012 targets for efficiency and production rate. (Q4, 2013)
2.3	Verify the stack and system efficiencies against the 2015 targets. (Q4, 2015)
2.4	Develop technologies for producing hydrogen through electrolysis at centralized facilities using renewable power for a cost ≤\$3.00/gge at the plant gate. (Q4, 2015)
2.5	Verify the total capital investment for a central electrolysis system against the 2015 targets using H2A. (Q1, 2016)
2.6	Verify the total capital investment for a distributed electrolysis system against the 2015 targets using H2A. (Q2, 2016)
2.7	Verify 2015 distributed hydrogen production levelized cost target through pilot scale testing coupled with H2A analysis to project economies of scale cost reduction. (Q3, 2017)
2.8	Verify 2015 central hydrogen production levelized cost target through pilot scale testing coupled with H2A analysis to project economies of scale cost reduction. (Q4, 2017)
2.9	Verify the BOP's ability to meet the 2020 system efficiency targets. (Q1, 2018)
2.10	Create modularized designs for optimized central electrolysis systems projected to meet 2020 capital and hydrogen production cost targets. (Q3, 2018)
2.11	Verify the stack and system efficiencies against the 2020 targets. (Q1, 2020)
2.12	Build an integrated renewable energy source and electrolysis pilot system for target verification and durability testing. (Q4, 2020)

	Task 3: Hydrogen Production from Biomass Gasification	
3.1	Demonstrate that a biomass gasification membrane reactor can achieve a projected high volume $H_2 \cos t$ of <\$2.00/kg based on preliminary process design and H2A cost analysis. (Q4, 2012)	
3.2	Demonstrate that a biomass gasification membrane reactor can achieve the 2015 cost target of \$2.10/gge based on preliminary process design and H2A cost analysis. (Q4, 2015)	
3.3	Verify 2015 cost and energy efficiency targets through the operation of an integrated biomass gasification development unit. (Q4, 2016)	
3.4	Verify techno-economic feasibility for a 2000 dry ton per day plant producing hydrogen at \$2.00/gge. (Q4, 2020)	

	Task 4: High-Temperature, Solar-Driven, Thermochemical Processes
4.1	Demonstrate that a particle reactor has the potential to achieve >30% solar-to- H_2 thermal efficiency based on a theoretical analysis of the particle reactor performance. (Q4, 2012)
4.2	Design a central receiver based hydrogen production system capable of achieving an annual average solar to hydrogen production efficiency in excess of 14%. (Q4, 2012)
4.3	Determine active material cost and durability requirements to meet 2020 and Ultimate targets. Develop a characterization protocol for a standard metric for metal oxide reaction materials. (Q4, 2013)
4.4	Demonstrate electrolyzer performance at required cell potential and current density to meet 2015 targets for hydrogen production. (Q4, 2014)
4.5	Demonstrate 100 hours on-sun hydrogen production for a solar thermochemical reaction cycle. (Q3, 2015)
4.6	Verify the successful on-sun operation of a promising high-temperature solar-driven thermochemical cycle that projects to the 2015 cost and efficiency targets. (Q4, 2015)
4.7	Design and test a "cold" prototype reactor (T _{max} ~200°C). (Q4, 2016)
4.8	Complete thermal reactor/receiver, storage and heat transfer system designs including materials specifications and testing. (Q2, 2017)
4.9	Verify the successful on-sun operation of a promising high-temperature solar-driven thermochemical cycle for direct solar-to-hydrogen production that projects to a cost target of ≤\$5.00/gge at the plant gate for central production. (Q4, 2017)
4.10	Design and test a "warm" prototype reactor (T _{max} ~900°C). (Q4, 2018)
4.11	Design and test a fully operational hydrogen production prototype reactor at the 5kW (thermal input) level (T > 1,200°C). (Q4, 2019)
4.12	Verify 2020 cost and energy efficiency targets for an integrated system. (Q4, 2020)

2012

Task 5: Materials and Systems for Photoelectrochemical Hydrogen Production	
5.1	Identify material systems compatible with photoelectrode reactors demonstrating stabilized STH ≥10%. (Q4, 2012)
5.2	Verify material systems with stabilized STH ≥10% in a photoelectrode configuration. (Q2, 2014)
5.3	Identify material systems compatible with photocatalyst particle reactors demonstrating stabilized STH ≥1%. (Q4, 2014)
5.4	Identify material systems compatible with photoelectrode reactors demonstrating stabilized STH ≥15%. (Q4, 2015)
5.5	Verify material systems with stabilized STH ≥1% in a photocatalyst particle configuration. (Q1, 2016)
5.6	Build a lab-scale PEC system based on best available 2015 technology to validate technoeconomic analysis. (Q4, 2017)
5.7	Identify material systems compatible with photocatalyst particle reactors demonstrating stabilized STH ≥5%. (Q4, 2018)
5.8	Verify material systems compatible with photoelectrode reactors with stabilized STH ≥15%. (Q4, 2019)
5.9	Verify material systems with stabilized STH ≥5% in a photocatalyst particle configuration. (Q1, 2020)
5.10	Identify material system compatible with photoelectrode reactors demonstrating stabilized STH ≥20%. (Q4, 2020)
5.11	Demonstrate plant-scale-compatible photoelectrochemical water-splitting systems to produce hydrogen at solar-to-hydrogen energy conversion efficiencies ≥15%. (Q4, 2020)

Task 6: Biological Hydrogen Production	
6.1	Generate or identify a naturally occurring Fe-hydrogenase with a half-life of 5 min in air for photolytic hydrogen production. (Q4, 2012)
6.2	Characterize an algal strain with 25% primary utilization efficiency of incident solar light energy. (Q4, 2012)
6.3	Increase the duration of H ₂ production by immobilized, sulfur-deprived algal cultures to 2 months. (Q4, 2012)
6.4	Produce one cyanobacterial recombinant evolving H ₂ from water through an O ₂ -tolerant NiFe-hydrogenase. (Q4, 2013)
6.5	Complete research to develop a photosynthetically efficient green algae/cyanobacterial system in which the P/R ratio is \leq 2. (Q4, 2014)
6.6	For photolytic hydrogen production, achieve the 2015 targets for solar-to-hydrogen conversion ratio. (Q4, 2015)

Task 6: Biological Hydrogen Production (continued)	
6.7	Identify or generate a Fe-hydrogenase that achieves 2015 target duration half-life in air for photolytic hydrogen production. (Q4, 2015)
6.8	For photosynthetic bacterial hydrogen production, achieve the 2015 targets for efficiency of incident solar light energy to H_2 (E0*E1*E2) from organic acids, yield of carbon conversion to H_2 , and continuous photoproduction. (Q4, 2015)
6.9	For dark fermentative hydrogen production, achieve 2015 targets for molar yield of H_2 production from glucose and continuous production duration. (Q4, 2015)
6.10	Complete research to determine the efficacy of green algae/cyanobacteria and photosynthetic bacteria to metabolize carbon substrates (C \leq 4) and produce H ₂ in integrated systems, including co-cultivation, immobilized cultures or a single oxygenic photosynthetic organism with genetic modifications to add the pigments and single photosystem from PNS. (Q4, 2015)
6.11	For an MEC system, achieve 2015 targets (Table 3.1.12) for production rates and electrode costs. (Q4, 2015)
6.12	Increase production rate of combined fermentation/MEC system to 2015 targets. (Q4, 2015)
6.13	Complete research to generate photosynthetic bacteria that have 50% smaller (compared to wild-type) Bacteriochlorophyll (Bchl) antenna size and display increased sunlight conversion efficiency. (Q4, 2016)
6.14	Complete research to engineer photosynthetic bacteria with a 30% expression level of a functional nitrogenase/hydrogenase at elevated nitrogen-carbon ratios (expression level is defined relative to that detected at low N:C ratios). (Q4, 2016)
6.15	Complete research to inactivate competitive uptake of H_2 by hydrogenase (also a priority for Dark Fermentative systems). (Q4, 2016)
6.16	Complete research to develop a photosynthetically efficient green algae/cyanobacterial system in which the P/R ratio is ~ 1. (Q4, 2019)
6.17	Demonstrate H ₂ production in air in a cyanobacterial recombinant. (Q4, 2020)
6.18	For photolytic hydrogen production, achieve the 2020 targets for solar-to-hydrogen conversion ratio when averaged over production and growth phases, reactor costs, and H ₂ production costs. Specifically, demonstrate plant-scale compatible photobiological water splitting systems to produce hydrogen at a solar-to-hydrogen energy efficiency of 5%. (Q4, 2020)
6.19	Complete research to generate photosynthetic bacteria that have 70% smaller (compared to wild-type) Bchl antenna size and display increased sunlight conversion efficiency. (Q4, 2020)
6.20	Complete research to engineer photosynthetic bacteria with a nitrogenase/hydrogenase at that is functional at elevated nitrogen-carbon ratios to at least 60% of the expression level at low N:C ratios. (Q4, 2020)
6.21	Complete research to inactivate the photosynthetic bacterial metabolic pathways leading to polymer accumulation that competes with H_2 production. (Q4, 2020)
6.22	For photosynthetic bacterial hydrogen production, achieve the 2020 targets for efficiency of incident solar light energy to H_2 (E0*E1*E2) from organic acids, maximum molar yield of carbon conversion to H_2 , projected hydrogen production cost, and duration of continuous photoproduction. (Q4, 2020)

Task 6: Biological Hydrogen Production (continued)	
6.23	For dark fermentative hydrogen production, achieve 2020 targets for molar yield of H_2 production from glucose, hydrogen production costs, and continuous production duration. (Q4, 2020)
6.24	For an MEC system, achieve 2020 targets (Table 3.1.11) for production rates and electrode costs. (Q4, 2020)
6.25	Increase production rate of combined fermentation/MEC system to 2020 targets. (Q4, 2020).
6.26	Complete research to regulate growth/competition between different organisms in co-cultivation (e.g., to maintain optimal Chl/Bchl ratios). (Q4, 2020)
6.27	Complete research to identify cell-growth inhibitors and eliminate transfer of such compounds from bacterial fermenters to photo reactors. (Q4, 2020)

Outputs

- P1 Output to Technology Validation and Manufacturing: Hydrogen production system based on centralized biomass gasification technology producing hydrogen at a projected cost of \$2.10/kg at the plant gate. (4Q, 2015)
- P2 Output to Technology Validation and Manufacturing: System based on distributed production of hydrogen from electrolysis at a projected cost of \$3.90/kg without compression, storage and dispensing. (4Q, 2015)
- P3 Output to Technology Validation and Manufacturing: Hydrogen production system based on centralized electrolysis technology producing hydrogen at a projected cost of \$3.00/kg at the plant gate. (1Q, 2016)
- P4 Output to Technology Validation: Solar hydrogen production system based on centralized hightemperature thermochemical conversion technology producing hydrogen at a projected cost of \$3.10/kg at the plant gate. (4Q, 2020)
- P5 Output to Technology Validation: Solar hydrogen production system based on photolytic biological hydrogen production from water at a solar to hydrogen conversion efficiency of 5%. (4Q, 2020)
- P6 Output to Technology Validation: Solar hydrogen production system based on photoelectrochemical hydrogen production from water at a solar to hydrogen conversion meeting 2020 targets. (4Q, 2020)

Inputs

- C2 Input from Safety, Codes and Standards: Hydrogen fuel quality standard (SAE J2719). (3Q, 2012)
- C6 Input from Safety, Codes and Standards: Updated materials compatibility technical reference manual. (4Q, 2013)
- C7 Input from Safety, Codes and Standards: Materials reference guide and properties database. (4Q, 2014)
- V10 Input from Technology Validation: Validate distributed production of hydrogen from electrolysis at a projected cost of \$3.90/kg with an added delivery cost of <\$4/gge. (4Q, 2018)