3.1 Hydrogen Production

Hydrogen can be produced from a diversity of 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

 \overline{a}

Research and develop low-cost, highly efficient hydrogen production technologies from diverse domestic sources, including natural gas and renewable sources.

Objectives

Reduce the cost of hydrogen to $$2.00-\$4.00/gge¹$ (delivered) at the pump.² 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 relative to their current states of development.

- By 2012, reduce the cost of distributed production of hydrogen from biomass-derived renewable liquids to \$3.80/gge (delivered) at the pump. By 2017, reduce the cost of distributed production of hydrogen from biomass-derived renewable liquids to $\langle $3.00/gge$ (delivered) at the pump.
- By 2012, reduce the cost of distributed production of hydrogen from distributed water electrolysis to \$3.70/gge (delivered) at the pump. By 2017, reduce the cost of distributed production of hydrogen from distributed water electrolysis to $\langle 3.00/\text{gge}$ (delivered) at the pump. By 2012, reduce the cost of central production of hydrogen from wind water electrolysis to \$3.10/gge at plant gate (\$4.80/gge delivered). By 2017, reduce the cost of central production of hydrogen from wind water electrolysis to <\$2.00/gge at plant gate (<\$3.00/gge delivered).
- By 2012, reduce the cost of hydrogen produced from biomass gasification to \$1.60/gge at the plant gate (<\$3.30/gge delivered). By 2017, reduce the cost of hydrogen produced from biomass gasification to \$1.10/gge at the plant gate (\$2.10/gge delivered).

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 internal combustion engine and gasoline hybrid vehicles in 2007. The full explanation and basis can be found in DOE Record 11007 (see [www.hydrogen.energy.gov/program_records.html\).](http://www.hydrogen.energy.gov/program_records.html) All costs, in that record are in 2007 dollars. Costs in this document, unless otherwise noted, are in 2005 dollars. Note that the production targets for the specific technologies are being reevaluated and will be updated in the next MYPP update.

- By 2017, develop high-temperature thermochemical cycles driven by concentrated solar energy to produce hydrogen with a projected cost of $$3.00/gge$ at the plant gate (\$4.00/gge delivered) and verify the potential for this technology to be competitive in the long term.³
- Develop advanced renewable photoelectrochemical and biological hydrogen generation technologies. By 2018, verify the feasibility of these technologies to be competitive in the long term.

3.1.2 Technical Approach

Hydrogen production research is focused on meeting the objectives outlined in Section 3.1.1. by conducting R&D through industry, national laboratory, and university projects. The Hydrogen Production Program element will develop the technologies to produce hydrogen for transportation and stationary applications. Integrated systems will be validated in the field by the Technology Validation Program element to obtain real-world data (see Section 3.6 Technology Validation). 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. This program element 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 natural gas and renewable liquid fuels, and on electrolysis to meet initial lower volume hydrogen needs with the least capital equipment costs. For the long-term, research is focused on renewable feedstocks and energy sources, with emphasis on centralized

options to take advantage of economies of scale when an adequate hydrogen delivery infrastructure is in place. There is collaboration with DOE's Office of Fossil Energy

[\(http://fossil.energy.gov/programs/fuels/index.html\)](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

[\(http://www.ne.doe.gov/NHI/neNHI.html\)](http://www.ne.doe.gov/NHI/neNHI.html) to develop centralized production from advanced nuclear energy-driven high-temperature thermochemical cycles and high temperature electrolysis. DOE's Office of Science [\(www.sc.doe.gov/bes/hydrogen.html\)](http://www.sc.doe.gov/bes/hydrogen.html) is a collaborator on longer-term technologies such as biological and photoelectrochemical hydrogen production.

Figure 3.1.1 Distributed hydrogen production facility

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 Program element are described below.

 \overline{a} ³ Collaboration with DOE's Office of Nuclear Energy and the DOE EERE Solar Program.

Distributed Production Pathway

Distributed production of hydrogen may be the most viable approach for introducing hydrogen as an energy carrier. It requires less capital investment for the smaller capacity of hydrogen needed initially, and it does not require a substantial hydrogen transport and delivery infrastructure.

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 bio-oil, and (2) small-scale water electrolysis located at the point of use (i.e., refueling stations or stationary power generation sites). Of these technologies, small-scale natural gas reformers are the closest to meeting the hydrogen production cost targets. Research will focus on applying the latest small-scale natural gas reforming systems to reform renewable liquid feedstocks at a competitive hydrogen cost. Distributed reforming using bio-derived liquids offers dramatically lower net greenhouse gas emissions. The second research focus is on small-scale electrolyzers for splitting water. To be cost competitive the cost of electricity needs to be very low (see Figure 3.1.2). Electrolyzers present the opportunity for non-carbon-emitting hydrogen production when a renewable electricity source such as wind or hydro power is used without grid backup. Additionally, photoelectrochemical hydrogen production has the potential to be used in the long term for distributed hydrogen production.

Technical Plan — Production

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 (DOE Office of Fossil Energy) 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 commercially viable and because there are limited domestic natural gas resources for the long term.
- Biomass gasification offers the potential of a renewable option and near-zero greenhouse gas \bullet emissions.
- Centralized wind-based water electrolysis is a viable approach as the cost of capital equipment is reduced through advanced development.
- DOE's Office of Nuclear Energy ([http://www.ne.doe.gov/NHI/neNHI.html\)](http://www.ne.doe.gov/NHI/neNHI.html) is developing high-temperature electrolysis technology.
- 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 long-term technologies that have the potential to produce hydrogen with sunlight, but they can currently only produce small amounts of hydrogen at high cost.

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 for hydrogen. 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 (see Section 3.2).

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 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 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.

Separations

 \overline{a}

Hydrogen separation is a key technology that cross-cuts hydrogen production options. Both dense metallic and microporous separation membranes are being developed as part of distributed and central hydrogen production systems. Dense metallic and microporous separation membranes have multiple applications that include an array of system configurations. Reducing the cost of membrane materials, achieving higher flux rates, increasing hydrogen recovery, developing durable membranes, and purifying hydrogen to levels similar to that of pressure swing adsorption (PSA) purification will be measured based on analysis of actual system configurations and requirements. Thus, the technology targets presented in Section 3.1.4 are guideposts for membrane developers.

Separations systems that best reduce the cost to produce hydrogen more efficiently from diverse feedstocks will be down-selected. These separations sub-system components must be optimized to achieve the cost and hydrogen quality requirements. In collaboration with the Office of Fossil Energy, Energy Efficiency and Renewable Energy (EERE) sponsored the DOE Workshop on Hydrogen Separations and Purification where input on hydrogen membrane separation performance targets was provided by industry, government researchers, and academia (Report of the DOE Workshop on Hydrogen Separations and Purification, September 8-9, 2004, Arlington, VA, U.S. Department of Energy Office of Hydrogen, Fuel Cells & Infrastructure Technologies)⁴

In addition to hydrogen separation membranes, oxygen separation membranes are being developed by the DOE Office of Fossil Energy [\(http://fossil.energy.gov/programs/fuels/index.html\)](http://fossil.energy.gov/programs/fuels/index.html). 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.

⁴ DOE's Office of Fossil Energy ([http://fossil.energy.gov/programs/fuels/index.html\)](http://fossil.energy.gov/programs/fuels/index.html) is responsible for developing coal to hydrogen membrane separations systems that will operate in large-scale integrated gasification combined cycle plants to separate hydrogen and to capture and sequester carbon dioxide.

3.1.3 Programmatic Status

Current Activities

Major hydrogen production program element activities are listed in Table 3.1.1.

Technical Plan — Production

 \overline{a}

⁵ In collaboration with DOE Office of Nuclear Energy.

⁶ In collaboration with the DOE Office of Science (<u>www.sc.doe.gov/bes/hydrogen.html</u>).
⁷ In collaboration with DOE Office of Fossil Energy (<u>http://fossil.energy.gov/programs/fuels/index.html</u>).

3.1.4 Technical Challenges

 \overline{a}

The overarching technical challenge to hydrogen production is reducing cost. Hydrogen (as of $2003)$ ⁸ costs \$5/gge delivered to a car at a refueling station based on distributed production using natural gas that has a design capacity of 1500 kg/day and is one of 100 production units built per year (see Table 3.1.2). This is significantly higher than the threshold cost of \$2.00-\$4.00/gge (the $\cos t$ in 2006 is estimated to be \$3.00/gge⁹). Estimates of the delivered cost of hydrogen using currently available technology for all production feedstocks is considerably higher than that required for hydrogen to be a cost-competitive primary energy carrier.

The capital costs of current water electrolysis systems, along with the high cost of electricity in many regions, limit widespread adoption of electrolysis technology for 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 energy resource, will not lead to carbon emission reduction without carbon sequestration technologies.

Hydrogen can be produced from biomass either by distributed 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 ethanol reforming and improved technologies need to be developed for other bioderived liquids to reduce the capital and operating costs for this distributed production option to become competitive. 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 hydrogen production (direct water splitting), also in an early stage of development, depends on a breakthrough in materials development and could require large areas of land. Research in this area is progressing on three fronts: (1) the study of high-efficiency materials in order to attain the fundamental understanding needed for improving lower-efficiency lower-cost materials; (2) the study of low-cost durable materials in order to attain the fundamental understanding needed for modifying higher-efficiency lower-durability materials; and (3) the

⁸ This cost for hydrogen in 2003 is based on analysis of distributed production utilizing natural gas reforming technology available in 2003. Details can be found in DOE Record 5030 (see www.hydrogen.energy.gov/program_records.html). A cost of hydrogen of \$3.60/gge has been projected based on 2004 technology for an energy station producing both hydrogen and electricity (U.S. Department of Energy, Hydrogen Program 2004 Annual Progress Report (December 2004), "Research and Development of a PEM Fuel Cell, Hydrogen Reformer, and Vehicle Refueling Facility" (Air Products and Chemicals, Inc.), 701, retrieved September 15, 2005, from http://www.hydrogen.energy.gov/pdfs/progress04/vd5_wait.pdf.

⁹ The 2006 current status of \$3.00/gge was estimated through H2A analysis (see Table 3.1.2) and confirmed by the 2006 Independent Assessment of the Status of Distributed Natural Gas Reforming (http://www.hydrogen.energy.gov/peer_review_production.html).

Technical Plan — Production

development of multijunction devices incorporating multiple material layers to achieve efficient water splitting.

Biological hydrogen production is in an early stage of research and presents many technical challenges, beginning with bioengineering of microorganisms that can produce hydrogen at high rates. Some of the challenges are related to 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, but other technologies are expected to become economically viable as the technologies mature and market drivers shift.

Tables 3.1.2 through 3.1.13 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. 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 breakdown are not targets.

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.

Tables 3.1.6 and 3.1.7 on membrane technology have been included for completeness. The Program has a limited amount of work on membrane materials in support of hydrogen separation processes associated with renewable pathways and is evaluating work being funded by the Office of Fossil Energy [\(http://fossil.energy.gov/programs/fuels/index.html\)](http://fossil.energy.gov/programs/fuels/index.html).

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.

^aThe H2A Forecourt Production Model [\(http://www.hydrogen.energy.gov/h2a_production.html\)](http://www.hydrogen.energy.gov/h2a_production.html) was used for the cost modeling. Economic parameters used were for a production design capacity of 1500 kg/day of hydrogen: 20 yr. analysis period, 10% IRR after taxes, 100% equity financing, 1.9% inflation, 38.9% total tax rate, MACRS 7-year depreciation, and a 70% capacity factor for 2006, 2010, and 2015. The results for 2006, 2010, and 2015 are in 2005 dollars. ^bThe natural gas cost and electricity cost used for 2006, 2010, and 2015 were \$5.24/MMBTU (LHV) and \$0.08/kWhr (commercial rate) respectively based on the EIA 2005 Annual Energy Outlook High A case projection for 2015 in 2005\$. The natural gas cost assumes industrial gas cost is available for distributed production of hydrogen. ^cThe 2003 analysis is based on work first done by TIAX LLC and documented in "Guidance for Transportation Technologies: Fuels Choice for Fuel Cell Vehicles", Phase II Final Report to DOE, February 2002. The results from this analysis were utilized in the H2A Production tool in the fall of 2004 while it was under development. The economic parameters used were: 1500 kg/day of hydrogen, 15-year analysis period, 5% IRR after taxes, 100% equity financing, 1.9% inflation, 38.9% tax rate, and MACRS 7-year depreciation, and a capacity factor of 87% based on the parameters used in the original TIAX analysis. The natural gas cost used was \$4.40/MMBTU (LHV) and the electricity cost was \$.07/kWhr. The results are in 2000 dollars. Further details can be found in DOE Record 5030. ^dFor the 2006, 2010, and 2015 the following assumptions were made: (See Record 6004, www.hydrogen.energy.gov/program_records.html for more details)

- Based on the recommendations made by the 2006 Independent Assessment of the Status of Distributed Natural Gas Reforming [\(www.hydrogen.energy.gov/peer_review_production.html\)](http://www.hydrogen.energy.gov/peer_review_production.html) start-up time was set to 0.5 years, % variable costs in year 1 was set to 50%, and % fixed cost in year 1 was set to 75%.

- It is assumed that Design for Manufacture and Assembly (DFMA) would be employed and that about 500 units per year would be produced.

Technical Plan — Production

- The capital cost for the forecourt station compression and storage are consistent with the status and targets in the Delivery Section 3.2.

^eThe 2006 current status is consistent with the 2006 Independent Assessment of the Status of Distributed Natural Gas Reforming [\(www.hydrogen.energy.gov/peer_review_production.html\)](http://www.hydrogen.energy.gov/peer_review_production.html).

^fEnergy efficiency is defined as the energy of the hydrogen out of the process (LHV) divided by the sum of the energy into the process from the feedstock (LHV) and all other energy needed. The electrical energy utilized does not include the efficiency losses from the production of the electricity.

^gStorage capacity for 1000 kg of hydrogen at the forecourt is included. It is assumed that the hydrogen refueling fill pressure is 5000 psi for 2003, 2006 and 2010. It is assumed that in 2015, the hydrogen refueling fill pressure is 10,000 psi.

Table 3.1.3.A. Distributed Bio-Derived Renewable Liquids H2A Example - Cost Contributions a, b, e,

^aThese costs are based on modeling the cost of distributed bio-derived liquids reforming in the H2A "Forecourt Production Modeling Tool" downloadable from [www.hydrogen.energy.gov/h2a_production.html.](http://www.hydrogen.energy.gov/h2a_production.html) Specific assumptions used to achieve the overall hydrogen cost objectives are documented in Record 6003 [\(www.hydrogen.energy.gov/program_records.html\)](http://www.hydrogen.energy.gov/program_records.html).

^bThe H2A Forecourt Production Model was used with the following standard economic assumptions: All values are in 2005 dollars, 1500 kg/day design capacity, 1.9% inflation rate, 10% After Tax Return on Investment, 100% Equity Financing, 7-year MACRS depreciation, 20-year analysis period, 38.9% overall tax rate, 70% capacity factor, and 15% working capital. It is assumed that Design for Manufacture and Assembly (DFMA) would be employed and that about

500 units per year would be produced. The capital cost for the forecourt station compression and storage are consistent with the status and targets in the Delivery Section 3.2. Based on the recommendations made by the 2006 Independent Assessment of the Status of Distributed Natural Gas Reforming

[\(www.hydrogen.energy.gov/peer_review_production.html\)](http://www.hydrogen.energy.gov/peer_review_production.html) start-up time was set to 0.5 years, % variable costs in year 1 was set to 50%, and percent fixed cost in year 1 was set to 75%.

^cThe 2006 Status and 2012 values are based on the H2A distributed ethanol reforming analyses Current and Advanced cases respectively [\(www.hydrogen.energy.gov/h2a_production.html\)](http://www.hydrogen.energy.gov/h2a_production.html) with respect to the production unit capital and operating efficiency. The cost of ethanol utilized is \$1.07/gal (no tax credit assumed). This is the DOE EERE Biomass Program target for cellulosic based ethanol in 2012. The electricity cost utilized is \$.08/kWh (commercial rate) based on the EIA 2005 Annual Energy Outlook High A case projection for 2015 in 2005\$.

dThe 2017 Target has been set to achieve <\$3.00/gge hydrogen. Aqueous phase reforming of sugars is a technology being researched that has the potential to reach this target and was used as the example H2A Distributed Production case run. The cost of sugar used was \$.07/lb which is consistent with the target cost of cellulosic sugar for ethanol production in 2012 in the DOE EERE Biomass Program. The electricity cost utilized is \$.08/kWh (commercial rate) based on the EIA 2005 Annual Energy Outlook High A case projection for 2015 in 2005\$. 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. (See record 6003, www.hydrogen.energy.gov/program_records.html for more details.) Alternatively, the target of $\langle \$3.00/gge$ could be achieved with ethanol reforming if the cost of ethanol could be reduced to $\langle $.90/gal.$ This ethanol cost is consistent with the longer term (≥ 2015) DOE EERE Biomass Program cost target for cellulosic ethanol.

^eFor the 2006, 2010, and 2015 the following assumptions were made: (See Record 6003, www.hydrogen.energy.gov/program_records.html for more details.)

- Based on the recommendations made by the 2006 Independent Assessment of the Status of Distributed Natural Gas Reforming [\(www.hydrogen.energy.gov/peer_review_production.html\)](http://www.hydrogen.energy.gov/peer_review_production.html) start-up time was set to 0.5 years, % variable costs in year 1 was set to 50%, and % fixed cost in year 1 was set to 75%.
- It is assumed that Design for Manufacture and Assembly (DFMA) would be employed and that on the order of 500 units per year would be produced.
- The capital cost for the forecourt station compression and storage are consistent with the status and targets in the Delivery Section 3.2.

^fEnergy efficiency is defined as the energy in the hydrogen produced (on a LHV basis) divided the sum of the feedstock energy (LHV) plus all other energy used in the process.

^gProduction unit energy efficiency may vary (as low as 65%) as the capital cost, feedstock costs and other costs associated with aqueous phase reforming are low enough to still achieve the target of <\$3.00/gge hydrogen cost. hStorage capacity for 1000 kg of hydrogen at the forecourt is included. It is assumed that the hydrogen refueling fill pressure is 5000 psi for 2006 and 2012. It is assumed that in 2017, the hydrogen refueling fill pressure is 10,000 psi.

Technical Plan — Production

^aThe H2A Forecourt Production Model [\(www.hydrogen.energy.gov/h2a_production.html\)](http://www.hydrogen.energy.gov/h2a_production.html) was used to generate the values in the table with the exceptions described in the notes below. See Record #6002 for more details [\(www.hydrogen.energy.gov/program_records.html\)](http://www.hydrogen.energy.gov/program_records.html).

^bThe H2A Forecourt Production Model was used with the standard economic assumptions: All values are in 2005 dollars, 1.9% inflation rate, 10% After Tax Real Internal Rate of Return, 100% Equity Financing, 7-year MACRS depreciation schedule, 20-year analysis period, 38.9% overall tax rate, and 15% working capital. The electrolyzer design capacity is 1500 kg/day of hydrogen. The cell stack for forecourt electrolyzers is assumed to be replaced every 7 years at a cost of 30% of the initial capital cost.

^cThe 2006 Status is based on the H2A Current Forecourt Electrolysis Hydrogen Production Case [\(www.hydrogen.energy.gov/h2a_production.html\)](http://www.hydrogen.energy.gov/h2a_production.html) with modifications as outlined in the notes. See Record #6002 [\(www.hydrogen.energy.gov/program_records.html\)](http://www.hydrogen.energy.gov/program_records.html) for more details.

^dElectrolyzer capital costs assume high volume annual production of 1,000 units for all purposes and markets. See "The Hydrogen Economy: Opportunities, Costs, Barriers and R&D Needs," by the National Research Council and National Academy of Engineering, pg. 182 for \$125/kW for the electrolyzer.

^eThe capacity factor for the electrolyzer is assumed to be 70%.

^fElectrolyzer systems (including all auxiliaries other than compression) are assumed to operate at 53.4 kWh/kg, 62% efficient LHV or 73% efficient HHV in 2006; 47.9 kWh/kg, 69% efficient LHV or 81% efficient HHV in 2012; and, 46.9 kWh/kg, 71% efficient LHV or 83% efficient HHV in 2017.

^gIn 2006 and 2012, compressors are assumed to operate at 2.2 kWh/kg of hydrogen.

hIn 2017, hydrogen is produced from the electrolyzer at 1000 psi, and electricity cost contribution is lowered by $$0.09/kg$ as a result of a stage reduction due to electrolyzer producing hydrogen at 1000 psi. (From estimate resulting from a run

of the H2A Delivery Components Model [\[www.hydrogen.energy.gov/h2a_production.html\]](http://www.hydrogen.energy.gov/h2a_production.html) that shows if hydrogen is produced in the electrolyzer at 1000psi it reduces the number of stages in the compressor by one.)

ⁱDispensers must be replaced every 10 years at 100% of initial capital cost. Dispenser costs are based on 3 dispensers, each at \$22,400.

 j Compressor costs are based on $$4580/(kg/hr)$ in 2006, $$4000/(kg/hr)$ in 2012, and $$3000/(kg/hr)$ in 2017 for 1500kgH2/day size compressor which are consistent with Delivery (Section 3.2) status and cost targets.

^kStorage costs based on \$820/kg at 6250psi in 2006, \$500/kg at 6250psi in 2012 and \$300/kg H₂ at 10,000 psi in 2017 which are consistent with the Delivery (Section 3.2) status and cost targets. Storage capacity for 1000 kg of hydrogen at the forecourt is included. It is assumed that the hydrogen refueling fill pressure is 5000 psi for 2003, 2006 and 2012. It is assumed that in 2017, the hydrogen refueling fill pressure is 10,000 psi.

^LElectricity costs are \$0.039/kWh. Electricity costs are based on the lowest average industrial grid electricity price 25% of the population paid from 2000-2005, according to EIA.

^mStandard H2A assumptions "Start Up Time" changed from 1 yr. to 0.5 yrs., "Percent Variable Costs During Start-up" changed from 100% to 50%, and "Fixed Costs During Start-up" changed from 100% to 75% based on the recommendations from the 2006 Independent Assessment of the Status of Distributed Natural Gas Reforming [\(www.hydrogen.energy.gov/peer_review_production.html\)](http://www.hydrogen.energy.gov/peer_review_production.html).

Table 3.1.5.A. Central Wind Electrolysis H2A Example Cost Contributions a, b (Technical targets are being reevaluated and will be updated in the next release)

^aThe H2A Central Production Model [\(www.hydrogen.energy.gov/h2a_production.html\)](http://www.hydrogen.energy.gov/h2a_production.html) was used to generate the values in the table with the exceptions described in the notes below. See Record #6002 for more details [\(www.hydrogen.energy.gov/program_records.html\)](http://www.hydrogen.energy.gov/program_records.html).

^bThe H2A Central Production Model was used with the standard economic assumptions: All values are in 2005 dollars, 1.9% inflation rate, 10% After Tax Real Internal Rate of Return, 100% Equity Financing, 40-year analysis period, 38.9% overall tax rate, and 15% working capital. A MACRS 15-year depreciation schedule was used. The plant design capacity

Technical Plan — Production

is 50,000 kg/day of hydrogen. The plant gate hydrogen pressure is 300 psi. The cell stacks for central electrolyzers are assumed to be replaced every 10 years at a cost of 30% of the initial capital cost. Assumes no grid assistance. ^cThe 2006 Status is based on the H2A Current Central Hydrogen Production from Wind Electrolysis Case [\(www.hydrogen.energy.gov/h2a_production.html\)](http://www.hydrogen.energy.gov/h2a_production.html) with modifications as outlined in the other footnotes. See Record #6002 for more details [\(www.hydrogen.energy.gov/program_records.html\)](http://www.hydrogen.energy.gov/program_records.html).

^dElectrolyzer capital costs assume high volume annual production of 1,000 units for all purposes and markets. The 2012 electrolyzer capital costs assume a 12.5% savings on a standard H2A assumption for advanced electrolyzer cost of \$400/kW (see "Modeling the Market Potential of Hydrogen from Wind and Competing Sources," by W. Short, N. Blair, and D. Heimiller, p. 6 for 12.5% reduction of electrolyzer cost for combined wind/electrolyzer electronic controls). 2017 electrolyzer capital costs assume a 12.5% savings on a \$125/kW system (see "The Hydrogen Economy: Opportunities, Costs, Barriers and R&D Needs," by the National Research Council and National Academy of Engineering, pg. 182 for \$125/kW for the electrolyzer).

^eElectrolyzer systems (including all auxiliaries other than compression) are assumed to operate at 53.4 kWh/kg, 62% efficient LHV or 73% efficient HHV in 2006; 47.9 kWh/kg, 69% efficient LHV or 81% efficient HHV in 2012; and, 44.7 kWh/kg, 74% efficient LHV or 87% efficient HHV in 2017.

^fWind farm is 303 MW in the 2006 case, 276 MW in the 2012 case, and 423 MW in the 2017 case. Sizes are based on optimization as outlined in WindPOWER report, "An Economic Analysis of Hydrogen Production from Wind" by J. Levene. Wind capital costs are assumed to be \$873/kW installed in 2006, \$754/kW in 2012, and \$706/kW in 2017. The wind capacity factor is 0.41 in 2006, 0.50 in 2012, and 0.54 in 2017 based on class 6 wind regimes. The wind farm cost contribution (\$/gge) increases in 2017 to accommodate an increase in the capacity factor of the electrolyzer unit. The increase in capacity factor requires a higher capacity wind farm, but lowers the overall hydrogen cost due to the value of the electricity not needed by the electrolyzer. It is assumed the wind turbine rotor will need to be replaced after 20 years at 20% of initial investment.

^gIn the 2006 case, a production tax credit (PTC) of \$0.018/kWh is applied to the by-product electricity produced for the first 10 years.

 h In 2006, 10% of the electricity produced is sold as a by product; in 2012, 27% of the electricity produced is sold as a byproduct; in 2017, 59% of the electricity produced is sold as a by-product.

^aBased on membrane water-gas shift reactor with syngas.

^bFlux at 20 psi hydrogen partial pressure differential with a minimum permeate side total pressure of 15 psig, preferably >50 psi and 400°C.

^cAlthough the cost of Pd does not present a significant cost barrier due to the small amount used, the equipment and labor associated with depositing the material (Pd), welding the Pd support, rolling foils or drawing tubes account for the majority of membrane module costs. The \$1,500 cost status is based on emerging membrane manufacturing techniques achieved by our partners and is approximately \$500 below commercially available units used in the microelectronics industry.

^dIntervals between membrane replacements.

^eDelta P operating capability is application dependent. There are many applications that may only require 400 psi or less. For coal gasification 1000 psi is the target.

^fIt is understood that the resultant hydrogen quality must meet the hydrogen quality requirements as described in Appendix C. These membranes are under development to achieve that quality. Membranes must also be tolerant to impurities. This will be application specific. Common impurities include sulfur and carbon monoxide.

^aBased on membrane water-gas shift reactor with syngas

^bFlux at 20 psi hydrogen partial pressure differential with a minimum permeate side total pressure of 15 psi, preferably >50 psi and 400°C.

^cThe membrane support structure cost is approximately three times more than membrane material costs.

^dIntervals between membrane replacement.

^eDelta P operating capability is application dependent. There are many applications that may require 400 psi or less. For coal gasification 1000 psi is the target.

^fIt is understood that the hydrogen quality produced by production technologies must meet the hydrogen quality requirements as described in Appendix C. These membranes are under development to achieve that quality. Membranes must also be tolerant to impurities. This will be application specific. Common impurities include sulfur and carbon monoxide.

^aThese costs are based on modeling the cost of hydrogen production utilizing the H2A Central Production Model and the results of the H2A Biomass Gasification analyses [\(www.hydrogen.energy.gov/h2a_production.html\)](http://www.hydrogen.energy.gov/h2a_production.html). Record 6001 [\(www.hydrogen.energy.gov/program_records.html\)](http://www.hydrogen.energy.gov/program_records.html) provides additional details.

^bThe H2A Central Production Model was used with the standard economic assumptions: All values are in 2005 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 plant is designed for a nominal processing capacity of 2000 dry metric tons of biomass per day. The specific hydrogen design capacities are 155 and 194 metric tons per day for 2005 and 2017, respectively, based on the plant efficiencies shown in the table. All feedstock and utility costs are based on their projected costs in 2015 consistent with approach used to determine the overall delivered hydrogen production cost objective of \$2-\$3/gge. The biomass feedstock cost used is \$41/dry metric ton consistent with the EERE Biomass Program estimate for 2012. The utility costs are based on the 2005 AEO High A projection for 2015 consistent with the standard H2A methodology.

^cThe 2005 Status is based on the H2A Biomass Gasification Current Case

[\(www.hydrogen.energy.gov/h2a_production.html\)](http://www.hydrogen.energy.gov/h2a_production.html) with some modification. No one has actually operated an integrated biomass gasification process designed specifically for hydrogen production at any scale. The H2A analysis is based on actual results of biomass gasification for power generation and available information from other similar processes for the rest of the process to yield hydrogen. As a result, a more conservative approach is taken for this status column by increasing the capital cost, reducing the process efficiency, and increasing the labor to the limits of the sensitivity analysis in the H2A Biomass Gasification Current Case. See Record #6001 [\(www.hydrogen.energy.gov/program_records.html\)](http://www.hydrogen.energy.gov/program_records.html) for more details. The 2012 Target is based on verifying the H2A Biomass Gasification Current Case estimate with actual data from a fully integrated biomass gasification unit designed to produce hydrogen.

^dThe 2017 Targets are based on the capital cost and performance (energy efficiency) required to approach the low end of the \$2-\$3/gge overall delivered hydrogen production cost consistent with the 2017 delivery cost target of \$1.00/gge. This falls within the sensitivity analysis of the H2A Biomass Gasification Longer-term case. See Record #6001 [\(www.hydrogen.energy.gov/program_records.html\)](http://www.hydrogen.energy.gov/program_records.html) for more details.

^eThe H2A Central Production Model [\(www.hydrogen.energy.gov/h2a_production.html\)](http://www.hydrogen.energy.gov/h2a_production.html) was used to generate these values at the total invested capital and process energy efficiency indicated in the table. See Record #6001 [\(www.hydrogen.energy.gov/program_records.html\)](http://www.hydrogen.energy.gov/program_records.html) for more details.

^fAll cases assume capital replacement at 0.5%/yr of total depreciable capital investment.

^gEnergy 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.

^aBased on initial analysis utilizing the H2A production analysis approach and standard H2A economic parameters [\(www.hydrogen.energy.gov/h2a_production.html\)](http://www.hydrogen.energy.gov/h2a_production.html). Two potential high-temperature cycles were examined: the Westinghouse modified sulfur cycle with electrolysis and a zinc oxide cycle. The capacity basis was central production of 100,000 kg/day of hydrogen. All targets are expressed in 2005 dollars. These costs are at the plant gate. The cost target for delivery of hydrogen from the plant gate to the point of refueling at a refueling station in 2017 is \$1.00/gge (See Section 3.2)

^bThese capital cost targets are consistent with the current viewpoint of the EERE Solar Program. The Solar Program is in the process of updating their targets in this area.

^cThe process energy efficiency is defined as the energy of the hydrogen produced (LHV) divided by the sum of the energy from the solar concentrator system plus any other net energy required for the process.

^aThe targets in this table are for research tracking. The final targets for this technology are costs that are market competitive.

^bTechnology readiness targets (beyond 2015) are 16% plant solar-to-hydrogen (STH) efficiency and 15,000 hours plant durability.

^cThe bandgap of the interface semiconductor establishes the photon absorption limits. Useable bandgaps correspond to systems with adequate stability, photon absorption and charge collection characteristics for meeting efficiency, durability and cost targets.

^dEC reflects the process efficiency with which a semiconductor system can convert the energy of absorbed photons to chemical energy [based on air mass 1.5 insolation] and is a function of the bandgap, IPEC and electronic transport properties. A multiple junction device may be used to reach these targets.

^eSolar-to-hydrogen (STH) is the projected plant-gate solar-to-hydrogen conversion efficiency based on AM (Air Mass) 1.5 insolation. Both EC and STH represent peak efficiencies, with the assumption that the material systems are adequately stable.

fDurability reflects projected duration of continuous photoproduction, not necessarily at peak efficiencies.

^aThe targets in this table are for research tracking. The final targets for this technology are costs that are market competitive.

^b2013 target is based on analysis of best technologies available, theoretically integrated into a single organism. ^c2018 targets are based on analysis of best technologies available, actually integrated into a single organism. dTechnology readiness targets (beyond 2018) are 25% utilization efficiency of incident solar light energy (E0*E1), 10% efficiency of incident light energy to H₂ from water (E0*E1*E2), ≥12h (O₂ tolerant) duration of continuous photoproduction, and 6h O2-tolerance (half-life in air).

^eE0 reflects the light collection efficiency of the photoreactor and the fact that only a fraction of solar incident light is photosynthetically active (theoretical maximum is 45%). E1 is the efficiency with which algae convert the energy of absorbed photons to chemical energy (i.e., chemical potential; theoretical maximum is 71%). E0*E1 represents the efficiency of conversion of incident solar light to chemical potential (theoretical maximum is 32%).

^fE2 reflects the efficiency with which the chemical potential generated by the absorbed photons is converted to hydrogen (theoretical maximum is 41%). E0*E1*E2 represents the efficiency of conversion of incident solar light to H₂ (theoretical maximum is 13% when water is the substrate); only peak efficiencies are meant.

^gDuration reflects continuous production in the light, not necessarily at peak efficiencies. Targets reflect oxygen tolerant system.

^aThe targets in this table are for research tracking. The final targets for this technology are costs that are market competitive.

^bTechnology readiness targets (beyond 2018) 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 H_2 (depends on nature of organic substrate) E3, and 6 months duration of continuous photoproduction.

^cE0 reflects the light collection efficiency of 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 ATP; 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.

^dAverage from data presented by Akkerman, I., M. Janssen, J. Rocha, and R. H. Wijffels. 2002. Intl. J. Hydrogen Energy 27: 1195-1208.

 e E3 represents the molar yield of H₂ per carbon substrate (the theoretical maximum is 7 moles per mole carbon in the substrate, in the case of acetate and butyrate). Average of data presented by Koku, H., I. Eroglu, U. Gunduz, M. Yucel, and L. Turker. 2002. Intl. J. Hydrogen Energy 27: 1315-1329.

^fDuration 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.

^gAverage from data presented by Koku, H., I. Eroglu, U. Gunduz, M. Yucel, and L. Turker. 2002. Intl. J. Hydrogen Energy 27: 1315-1329.

^aThe targets in this table are for research tracking. The final targets for this technology are costs that are market competitive.

 $bTechnology$ readiness targets (beyond 2018) are 10 molar yield of H₂ production from glucose, 6 cents/lb sugar feedstock cost, and 12 months duration of continuous production.

The theoretical maximum from known fermentative pathways is 4, although the H_2 content of 1 mole of glucose 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.

^dDOE Workshop on Hydrogen Production via Direct Fermentation (June 2004) [www1.eere.energy.gov/hydrogenandfuelcells/pdfs/fermentation_wkshp.pdf a](http://www1.eere.energy.gov/hydrogenandfuelcells/pdfs/fermentation_wkshp.pdf)nd Boundary Analysis for H2 Production

by Fermentation, T. Eggeman, www.nrel.gov/docs/fy05osti/36129.pdf

^eTargets set by the DOE Biomass Program for glucose from lignocellulosic biomass. NREL Report TP-510-32438, [www.nrel.gov/docs/fy02osti/32438.p](http://www.nrel.gov/docs/fy02osti/32438)df; NREL E Milestone #586, May 2004. ^fVan Ginkel, S., and S. Sung. 2001. Environ. Sci. Technol. 35: 4726-4730.

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 Natural Gas or Renewable Liquid Feedstocks

A. Reformer Capital Costs. Current small-scale distributed natural gas and renewable liquid feedstock reforming technologies have capital costs that are too high to achieve the targeted hydrogen production cost. Multiple-unit operations 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. Water-gas shift and hydrogen separation and purification costs need to be reduced. Process intensification by combining unit operations could significantly reduce costs. For example, combining the current two step water-gas shift reactor and pressure swing adsorption (PSA) separation into a single unit operation could significantly reduce capital costs.

Technical Plan — Production

B. Reformer Manufacturing. Distributed reforming units are currently designed and built one at a time. Efforts such as Design for Manufacture and Assembly (DFMA) need to be applied to develop more compact, skid mounted units that can be produced using currently available low-cost, highthroughput manufacturing methods (see the Manufacturing section of this plan).

C. Operation and Maintenance (O&M). O&M costs for distributed reforming hydrogen production from natural gas and renewable feedstocks are too high. Robust systems that require little maintenance and that include remote monitoring capability need to be developed.

D. Feedstock Issues. Availability of some feedstocks is limited in certain areas. 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.

E. Greenhouse Gas Emissions. Distributed natural gas reformers emit greenhouse gases. Feedstocks and/or technologies that can approach near zero net greenhouse gas emissions are needed.

F. 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 Program elements.

Hydrogen Generation by Water Electrolysis

G. Capital Cost. The capital costs of water electrolysis systems are prohibitive to widespread adoption of electrolysis technology for hydrogen production. RD&D is needed to develop lower cost materials with improved manufacturing capability to lower capital 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 (see the Manufacturing section of this plan).

H. System Efficiency. New membrane, electrode and system designs are needed to improve system efficiency and durability. 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 using compression in the cell stack. Development is needed for low-cost cell stack optimization addressing efficiency, compression, and durability.

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, carbonfree 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 and improve performance. 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.

Hydrogen Separations

There are a number of technology options available that can be used to separate and purify hydrogen. The following is a set of broad, cross-cutting barriers that must be overcome to reduce the cost and increase the efficiency of these separation technologies. This plan currently focuses on hydrogen separation technologies for thermochemical processes including distributed reforming and biomass gasification. In the future, additional separations technologies may be necessary for other production technologies.

K. Durability. Hydrogen embrittlement can reduce the durability and effectiveness of metallic membrane systems. Thermal cycling can cause failure, reducing durability and operating life. This is especially problematic in distributed applications that may be subject to frequent start-up and shutdown cycles. Support structures with more uniform pore sizes and less surface roughness are needed to avoid membrane defects. Interactions between membrane and support structure materials need to be better understood. Materials science research is needed to understand microstructural evolution during operation and its effect on membrane permeability, selectivity, and failure modes. Combinatorial methods are needed for rapid testing and evaluation of novel materials and alloys.

L. Impurities. The presence of trace contaminants as well as CO , water, and $CO₂$ in the product stream from a gasifier or reformer can reduce the hydrogen flux across different types of membranes. It is not understood whether these effects are caused by competitive adsorption, poisoning, or compositional changes on the membrane surface. Additionally, some membranes exhibit poor thermochemical stability in carbon dioxide environments, resulting in the conversion of membrane materials into carbonates.

M. Membrane Defects. Oxidizing gas mixtures (oxygen, steam, and carbon oxides) have been observed to cause metallic membranes to rearrange their atomic structure at temperatures greater than 450ºC. This results in the formation of permanent defects that reduce membrane selectivity for hydrogen. High-temperature and high-pressure seals can be an issue with membrane systems. Seals and joints are a weak link in membrane module construction and one of the most common points of membrane system failure. The chemical deposition of thin palladium or palladium-alloy membranes onto support structures is also an important technical challenge.

N. Hydrogen Selectivity. The hydrogen selectivity of microporous membranes is lower than desired for cost-effective use, especially for zeolite-supported membranes where selectivity decreases with increasing temperature (inadequate above 150ºC). Process stream temperatures typically are greater than 300ºC in various applications.

O. Operating Temperature. Membrane modules that can be designed to operate at or near process conditions, without the need for cooling and/or re-heating, will be more efficient. For example, dense ceramic proton hydrogen separation membranes currently operate only at high temperatures (~900ºC).

P. Flux. Flux rates for membranes need to be improved to reduce the membrane size and lower overall cost of hydrogen separation and purification systems.

Q. Testing and Analysis. Better information is needed to guide researchers and membrane technology developers towards performance targets that are application specific. Standard methods for evaluating and screening membrane materials and modules are needed to provide a solid basis

Technical Plan — Production

for comparison of alternatives and to conduct needed tests such as accelerated durability tests. Testing under real-world operating conditions is needed to demonstrate durability and robust, reliable performance. Additionally, there is currently a lack of understanding of tradeoffs between different system configurations and operating parameters. Operation at higher temperatures and partial pressure differentials can increase flux rates but results in more expensive membrane modules. Very thin membranes increase flux but they are harder to fabricate defect-free. Analysis is also needed to understand options and tradeoffs for process intensification in different applications.

R. Cost. In addition to precious metals, membrane materials and support structures are costly. Fabrication of high quality (ultra-thin) membranes dominates membrane systems cost.

Biomass Gasification/Pyrolysis Hydrogen Production

S. Feedstock Cost and Availability. Feedstock costs are high. Improved feedstock/agriculture technology (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.)

T. Capital Cost and Efficiency of Biomass Gasification/Pyrolysis Technology. The capital cost for biomass gasification/pyrolysis needs to be reduced. Process intensification by combining unit operations can significantly reduce capital costs. This could range from 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 selectivities 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.

High-Temperature Thermochemical, Solar-Driven Production of Hydrogen 10

U. High-Temperature Thermochemical Technology. There are over 200 potential thermochemical cycles for solar-driven water splitting. These cycles have been evaluated and ranked for their suitability. The most promising cycles need to be fully explored and verified to down select to a few cycles. The most promising cycles will require extensive research and development efforts.

V. 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.

W. 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. 11

 \overline{a}

¹⁰ DOE's Office of Nuclear Energy has the lead responsibility for hydrogen production utilizing nuclear energy for hightemperature (700°-1000°C) thermochemical water-splitting chemical cycles. The Office of Hydrogen, Fuel Cells & Infrastructure Technologies will collaborate with Nuclear Energy on the thermochemical hydrogen production R&D activities.

¹¹ The Hydrogen Program will rely on and collaborate with the DOE EERE Solar Program for the advancement of concentrated solar energy technology.

X. Coupling Concentrated Solar Energy and Thermochemical Cycles. Coupling concentrated solar energy with thermochemical cycles presents many challenges. Receivers, heat transfer and 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.

Photoelectrochemical Hydrogen Production

Photoelectrochemical hydrogen production is in an early stage of development and requires breakthroughs in materials development. The primary research in this area is progressing on three fronts: (1) the study of high-efficiency materials to attain the fundamental understanding needed for improving lower-efficiency, low-cost materials; (2) the study of low-cost durable materials to attain the fundamental understanding needed for modifying higher-efficiency, lower-durability materials; and (3) the development of multijunction devices incorporating multiple material layers to achieve efficient water splitting. Methods of engineering and manufacturing these systems need to be developed in conjunction with the materials and device research (see the Manufacturing section of this plan).

Current materials for photoelectrochemical hydrogen production can be broadly divided into three categories, each with its own characteristics and research challenges. These groupings are: (i) stable materials with low visible light absorption efficiency (e.g., oxides), (ii) highly efficient light absorbers with low lifetimes (e.g., Group III-Vs), and (iii) hybrid and multijunction systems which combine multiple materials in multi-photon devices. The group (i) materials are characterized by high bandgaps and low integrated incident-photon-to-electron conversion (IPEC) over the solar spectrum; the group (ii) materials have very high IPEC (better than 90% throughout the visible spectra), but have low corrosion resistance and poor energetics; and the group (iii) systems can have very high efficiency and long lifetime, depending on the material set, but can be complicated and expensive to build. Research in all three categories is necessary for developing systems that meet the targets reflected in the PEC target table. To date, a range of materials and material systems have met individual 2010 targets of chemical efficiency or durability, but no single material/system has simultaneously met efficiency, durability and cost targets. This is the primary research challenge for photoelectrochemical hydrogen production.

Y. Materials Efficiency. 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. Materials with appropriate bandedge and bandgap for hydrogen production must be developed.

Z. Materials Durability. Durable materials with the appropriate characteristics for photoelectrochemical hydrogen production that meet the program goals have not been identified. The high-efficiency materials currently available corrode quickly during operation, and the most durable materials are very inefficient for hydrogen production.

AA. PEC Device and System Auxiliary Material. The functional requirements for auxiliary materials must be determined and materials discovered, developed, and tested to facilitate PEC device and systems development. The auxiliary materials may include protective coatings, catalytic coatings, photoelectrode substrates, hydrogen impervious materials, and photovoltaic layer materials.

AB. Bulk Materials Synthesis. Fabrication techniques for materials identified to have potential for high efficiency, durability and low cost need to be developed on scales consistent with implementation in commercial reactors.

AC. Device Configuration Designs. Hybrid and other device designs that combine multiple layers of materials could address issues of durability and efficiency. Techniques are needed for manufacturing appropriate photoelectrochemical materials in these device configurations at commercial scales (see the Manufacturing section of this plan).

AD. Systems Design and Evaluation. System designs incorporating the most promising device configurations, and using cost-effective, hydrogen-impermeable, transparent materials are also needed to implement photolytic production routes. The complete systems evaluation will 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. Engineering options need to be carefully analyzed to minimize capital requirements.

AE. 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 results in increased capital costs for larger facilities to accommodate higher short-term production rates and larger hydrogen storage needs.

Biological Hydrogen Production

A number of technologies for biological H_2 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 before economic barriers can be meaningfully considered. Methods for engineering and manufacturing these systems have not been fully evaluated.

AF. Lack of Naturally Occurring Microorganism Characterization. Only a small fraction of the world's microorganisms have been discovered and functionally characterized. Research is needed to discover naturally occurring microorganisms with characteristics necessary for biological hydrogen production.

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 H2 Production from Water (green algae or cyanobacteria):

AG. Light Utilization Efficiency. The microorganisms used for photobiological H₂ production possess large arrays of light-capturing antenna pigment molecules. Under bright sunlight, pigment antennae absorb much 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 the identification of better and/or modified photosynthetic organisms for H_2 production.

AH. Rate of Hydrogen Production. The current H_2 production rate from photosynthetic 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 H₂-producing enzyme) under anaerobic conditions, and (b) the existence of competing metabolic flux pathways for reductant. Genetic means to overcome the restricting metabolic pathways, such as the insertion of a proton channel across the thylakoid membrane, must be used to significantly increase the rate of H_2 production. Under aerobic conditions, with an O_2 -tolerant hydrogenase catalyzing H_2 production, the competition between $CO₂$ fixation and hydrogenase will have to be addressed.

AI. Continuity of Photoproduction. Hydrogen-producing algae co-produce oxygen, which inhibits the hydrogenase enzyme activity. This inhibition needs to be alleviated, possibly by (a) identifying or engineering a less O₂-sensitive enzyme; (b) separating the oxygen and hydrogen production cycles; or (c) affecting the ratio of photosynthesis to respiration by a variety of means, such that O_2 does not accumulate in the medium, the quantum yield of photosynthesis is maintained, and full hydrogenase activity is achieved (see details under Integrated System).

AJ. 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 H_2 containment, H_2 collection systems, prevention of the build-up of H_2/O_2 gas mixtures, separation of co-produced H_2 and O_2 gases, continuous bioreactor operation, monoculture maintenance, land area requirements and capital costs.

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

Photosynthetic Bacterial Hydrogen Production, Required for an Integrated System:

AL. Light Utilization Efficiency. Same issues apply as for photolytic systems (see Barrier X).

AM. Rate of Hydrogen Production. Photosynthetic bacteria can metabolize a variety of organic substrates that are waste by-products of various fermentative processes. However, the metabolism of acetic and lactic acids to H₂ also generates by-products such as the polymer polyhydroxyalkanoate (PHA) . Synthesis of PHA competes with $H₂$ production for the same source of electron donors. Genes controlling PHA synthesis and perhaps other pathways must be inactivated to maximize H_2 production. Alternative types of nitrogenase are needed to produce larger stoichiometric amounts of $H₂/ammonia.$

AN. Hydrogen Re-oxidation. Most photosynthetic bacteria contain an H₂-oxidation pathway catalyzed by an uptake hydrogenase enzyme. This enzyme will recycle the H_2 produced by the nitrogenase to support cell growth. Uptake hydrogenase enzyme(s) must be inactivated to ensure net H₂ accumulation by photosynthetic bacteria.

AO. 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 photoreactor (algal and cyanobacteria) and in the dark fermentor 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.

AP. Systems Engineering. The same issues apply as for photolytic systems (see above), except for the mixture of gases. Photosynthetic bacteria do not co-evolve H_2 and O_2 but release H_2 and CO_2 . The cost of H_2 and CO_2 separation must be evaluated.

AQ. Diurnal Operation Limitation. The same issues apply as for photolytic systems (see Barrier AE).

Dark Fermentative Hydrogen Production, Required for an Integrated System:

AR. H_2 **Molar Yield.** Up to 4 moles of H_2 can theoretically be produced per mole of glucose through the known fermentative pathways. However, various biological limitations such as H₂-endproduct inhibition and waste-acid and solvent accumulation limit the molar yield to around 2 moles per mole glucose consumed. Hydrogen molar yields must be increased significantly through metabolic engineering efforts. New pathways must be discovered to directly take full advantage of the 12 moles of H_2 available in a mole of glucose.

AS. Waste Acid Accumulation. Organic acids such as acetic and butyric acids are waste byproducts of the fermentation process. The production of these acids poses several challenges such as lowering the molar yield of $H₂$ by diverting the metabolic pathway toward solvent production and requiring subsequent wastewater treatment. Elimination of this pathway or subsequent processing (such as in an integrated biological hydrogen production system) of the organic acids by photosynthetic bacteria is needed to increase hydrogen yields. Potential release of toxins during dark fermentation and their inhibition of the subsequent steps (such as in an integrated system) will need to be evaluated.

AT. Feedstock Cost. The glucose feedstock is the major cost driver for economic H₂ production via fermentation. For renewable H_2 to be cost competitive with traditional transportation fuels, the glucose cost must be around \$0.05 per pound and provide a molar yield of H_2 approaching 10 (see Barrier AI and Target Table 3.1.9). Lower-cost methods for producing glucose from whole biomass are needed. Cellulolytic microbes with a high rate of H_2 production are also needed to use the cell biomass of the green algal/cyanobacterial and photosythetic bacterial co-culture (in an integrated biological H_2 production system).

AU. Systems Engineering. The same issues apply as above, plus prevention of methanogen contamination is needed.

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

AV. 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 \rm{H}_{2} (instead of starch), and the \rm{O}_{2} evolved by photosynthesis is consumed by respiration, producing $CO₂$. Currently, this process is achieved by nutrient deprivation, with the drawback that the resulting $P/R \le 1$ ratio is achieved by partially decreasing the quantum yield of photosynthesis. Alternative mechanisms to bring the P/R ratio to 1 need to be investigated, particularly those methods that focus on achieving a P/R ratio of 1 without changing 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.

organic molecule by-products of the dark anaerobic bacterial fermentation are subsequently utilized as feedstock for the cyanobacteria, green algae and photosynthetic bacteria.

Figure 3.1.3. Integrated Biological System

AW. Co-Culture Balance. To extend the absorption spectrum of the H₂-photoproducing cultures to the infrared (700-900 nm), the possibility of co-cultivating oxygenic photosynthetic organisms with anoxygenic photosynthetic bacteria should be investigated. However, in addition to light in the infrared region, photosynthetic bacteria also absorb light in the visible (400 to 600 nm), thus potentially competing with green algae for these latter wavelengths. Strategies need to be devised to either maintain the appropriate biomass ratio of the two organisms as suspensions in the same reactor, or to physically separate them in the same photoreactor via immobilization of one or both cultures. The competition for organic carbon substrates between two organisms in the same medium also needs to be investigated.

AX. 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. The green algal and cyanobacterial cell walls are made mostly of glycoproteins, which are rich in arabinose, mannose, galactose and glucose. Purple photosynthetic bacterial cell walls contain peptidoglycans (carbohydrate polymers cross-linked by protein, and other polymers made of carbohydrate protein and lipid). 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.

3.1.5 Technical Task Descriptions

The technical task descriptions and the barriers associated with each task are presented in Table 3.1.14. Concerns regarding safety and environmental effects will be addressed within each task in coordination with the appropriate Program element.

 \overline{a}

¹² The Hydrogen Program will rely on and collaborate with the DOE EERE Solar Program for the advancement of concentrated solar energy technology

Technical Plan — Production

3.1.6 Milestones

The following chart shows the interrelationship of milestones, tasks, supporting inputs from other Program elements, and technology outputs for the Hydrogen Production Program element from FY 2006 through FY 2018. The input-output relationships are also summarized in Appendix B.

Hydrogen Production Milestone Chart

Hydrogen Production Milestone Chart

Hydrogen Production Milestone Chart

Task 17: Systems Engineering for Dark Fermentative Hydrogen Production

57 For dark fermentative hydrogen production, achieve 6 molar yield of H_2 production from glucose at a projected hydrogen production cost of less than \$4/kg, with projected research improvements that will achieve costs that are competitive with traditional fuels for transportation applications and with other non-biological technologies for central hydrogen production. (4Q, 2018)

Outputs

- P1 Output to Technology Validation: Hydrogen production technology for distributed systems using natural gas with projected cost of \$3.00/gge hydrogen at the pump, untaxed, assuming 500 units of production per year. (4Q, 2005)
- P2 Output to Delivery, Storage, Fuel Cells, and Technology Validation: Assessment of H₂ quality cost and issues relating to hydrogen production. (4Q, 2006)
- P3 Output to Technology Validation and Systems Integration: Impact of hydrogen quality on cost and performance. (3Q, 2007)
- P4 Output to Technology Validation and Manufacturing: Hydrogen production technologies for distributed systems using natural gas with projected cost of \$2.50/gge hydrogen at the pump, untaxed, assuming 500 manufactured units per year. (4Q, 2010)
- P5 Output to Technology Validation and Systems Integration: Hydrogen production technologies for distributed systems using natural gas with projected cost of \$2.00/gge hydrogen at the pump, untaxed, assuming 500 manufactured units per year. (4Q, 2015)
- P6 Output to Technology Validation and Manufacturing: Hydrogen production technologies for distributed systems using renewable liquids with projected cost of \$3.80/gge hydrogen at the pump, untaxed, assuming 500 manufactured units per year. (4Q, 2012)
- P7 Output to Technology Validation and Manufacturing: System making hydrogen for \$3.70/gge (delivered) from distributed electrolysis. (4Q, 2012)
- P8 Output to Technology Validation: System making hydrogen for \$3.10/gge (plant gate) from central wind electrolysis. (4Q, 2012)
- P9 Output to Technology Validation: Hydrogen production system making hydrogen for \$1.60/gge from biomass at the plant gate. (4Q, 2012)

Inputs

- C1 Input from Codes and Standards: Hydrogen fuel quality standard as ISO Technical Specification. (3Q, 2006)
- C8 Input from Codes and Standards: Final hydrogen fuel quality standard as ISO Standard. (2Q, 2010)
- F1 Input from Fuel Cells: Reformer results of advanced reformer development. (4Q, 2007)
- V9 Input from Technology Validation: Final report on safety and O&M of three refueling stations. (4Q, 2007)
- A0 Input from Systems Analysis: Initial recommended hydrogen quality at each point in the system. (4Q, 2007)
- A1 Input from Systems Analysis: Complete techno-economic analysis on production and delivery technologies currently being researched to meet overall program hydrogen fuel objective. (4Q, 2007)
- M4 Input from Manufacturing: Report on manufacturing of distributed reforming of natural gas system to achieve \$2.00/gge (delivered). (4Q, 2015)
- M5 Input from Manufacturing: Report on manufacturing distributed reforming of bio-derived renewable liquid fuels system to achieve \$3.00/gge (delivered). (4Q, 2017)
- M6 Input from Manufacturing: Report on high-volume manufacturing processes for electrolysis membrane assemblies. (4Q, 2011)