DRIVING RESEARCH AND INNOVATION FOR
VEHICLE EFFICIENCY AND ENERGY SUSTAINABILITY

Hydrogen Production Tech Team Roadmap

November 2017

This roadmap is a document of the U.S. DRIVE Partnership. U.S. DRIVE (Driving Research and Innovation for Vehicle efficiency and Energy sustainability) is a voluntary, non-binding, and nonlegal partnership among the U.S. Department of Energy; USCAR, representing FCA US LLC, Ford Motor Company, and General Motors; five energy companies – BP America, Chevron Corporation, Phillips 66 Company, ExxonMobil Corporation, and Shell Oil Products US; two utilities – Southern California Edison and DTE Energy; and the Electric Power Research Institute (EPRI).

The Hydrogen Production Tech Team is one of 13 U.S. DRIVE technical teams that work to accelerate the development of pre-competitive and innovative technologies to enable a full range of efficient and clean advanced light-duty vehicles, as well as related energy infrastructure.

For more information about U.S. DRIVE, please see the U.S. DRIVE Partnership Plan, at www.vehicles.energy.gov/about/partnerships/usdrive.html or www.uscar.org.

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EXECUTIVE SUMMARY

The Hydrogen Production Tech Team (HPTT), one of U.S. DRIVE's 13 Technology Teams, works to support the widespread adoption of hydrogen production technologies by providing a platform for industry to review and provide insight to the Department of Energy's Hydrogen Production research and development (R&D) portfolio. The HPTT interfaces regularly with the Hydrogen Delivery Tech Team, the Fuel Pathways Integration Tech Team, the Hydrogen Storage Tech Team and the Codes and Standards Tech Team to make sure efforts across the hydrogen fuel portfolio are coordinated. The major focus for the HPTT is on hydrogen for light duty fuel cell electric vehicles (FCEVs), but hydrogen production for other applications is also of interest, as hydrogen plays a significant role in the chemical industry and has great potential for important electricity grid services in the future.

Currently, hydrogen is predominately produced via steam methane reforming (SMR) at a cost that can meet the DOE cost goal of < $2/gallon gas equivalent (gge) of hydrogen (for production only, excluding delivery, storage, dispensing, and untaxed). However, long-term, domestically diverse and sustainable hydrogen production pathways, such as direct water splitting (e.g., low- and high-temperature electrolysis as well as direct solar thermochemical and photoelectrochemical water splitting) and hydrogen from biomass (e.g., biogas reforming, bio-waste fermentation, or other biological or hybrid methods), are promising and have the potential to increase our energy security, resiliency, and economic opportunities while also offering environmental benefits.

This Roadmap discusses the current status of hydrogen production pathways and assesses the status and R&D needs of commercial and emerging technologies for hydrogen production from fossil, biomass, and water resources. As these technologies are developed it will be critical to evaluate simultaneously their potential to meet the cost goal, diversify the domestic energy portfolio (positively impacting energy security and the economy), while also ensuring sustainability and environmental benefits, in order to understand the full potential of each hydrogen production pathway.

Moving forward, DOE will continue to effectively leverage the world-class scientific resources at our National Laboratories through the Energy Material Network[1] Consortia (such as the HydroGEN[2] Consortium on Advanced Water Splitting Materials) and the H2@Scale[3] initiative to accelerate progress in promising hydrogen and fuel cell technologies development; and the U.S. DRIVE Tech Teams will play a critical role in providing feedback and insight to the value that the R&D efforts are having on technology development.

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[1] The U.S. Department of Energy's Energy Materials Network website: https://energy.gov/eere/energy-materials-network/energy-materials-network

[2] The U.S. Department of Energy's HydroGEN Consortium website: https://www.h2awsm.org/

[3] The U.S. Department of Energy's H2@Scale website: https://energy.gov/eere/fuelcells/h2-scale

SCOPE AND OBJECTIVES

The mission of the Hydrogen Production Technical Team (HPTT) is to enable the widespread adoption of technologies that leverage the United States' diverse and abundant natural resources for secure, clean, sustainable, large-scale, and low-cost hydrogen production, primarily for transportation applications. A specific DOE cost goal for as-produced, delivered, and dispensed hydrogen fuel is < $4 per gasoline gallon equivalent (gge) of hydrogen. One gge is equivalent to 1 kg of hydrogen based on energy content. This aim supports the U.S. DRIVE (Driving Research and Innovation for Vehicle efficiency and Energy sustainability) Partnership Goal 2, which is to enable reliable fuel cell electric vehicles (FCEVs) with performance, safety, and costs comparable to or better than advanced conventional vehicle technologies, supported by viable hydrogen storage options and the widespread availability of hydrogen fuel. The HPTT facilitates pre-competitive technical information exchange in the area of hydrogen production among experts who interact as equal partners to discuss R&D needs, develop joint goals and technology roadmaps, and evaluate R&D progress.

Because of the already large and increasing demand for hydrogen in the industrial and energy sectors, enabling hydrogen production technologies becomes even more critical when the emerging and growing market for hydrogen in the transportation sector is considered. With over 15 quads of petroleum[4] per year going to light-duty highway transportation, there is a significant opportunity to leverage our other diverse, sustainable, domestic resources to meet the U.S. transportation sector's high energy demand by enabling the development of hydrogen powered FCEVs. With unwanted emissions and criteria pollutants associated with petroleum use, FCEVs using renewable, clean hydrogen can play an important role in our energy future.

Although hydrogen and fuel cell technologies are not yet widespread in the transportation sector, hydrogen is a well-established chemical commodity used at large scale in various industrial sectors, such as oil refining and ammonia/fertilizer production. The petroleum, fertilizer and industrial gas industries have produced and used hydrogen for decades, and global demand is increasing with a current worldwide hydrogen consumption at approximately 23 million tonnes per year[5]. Of this, the United States currently produces and consumes almost 10 million tonnes annually. This production volume, which is predominately from fossil fuels, is equivalent to just over 1 quadrillion BTUs per year (1% of U.S. energy consumption)—and, for reference, represents the hydrogen-fuel production that would be needed to power approximately 40 million FCEVs or approximately 15% of the current U.S. light duty vehicle fleet.

To meet the increased demand from the emerging FCEV market for hydrogen produced from clean, sustainable resources, a broad portfolio of hydrogen production pathway technologies is being considered[6]. Enabling the widespread commercialization of FCEVs will require the development of cost competitive hydrogen production technologies that together offer sustainable, high volume production of hydrogen from a variety of domestic resources; and, in addition, will support job creation, energy security and offer significant environmental benefits. The development of these pathways requires consideration of a wide range of factors including

- feedstock cost and availability,
- life cycle greenhouse emissions, criteria pollutant and other harmful emissions,
- high hydrogen purity requirements for FCEVs,

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[4] Quadrennial Technology Review 2015. Chapter 7: Advancing Systems and Technologies to Produce Cleaner Fuels, Hydrogen Production and Delivery. https://energy.gov/sites/prod/files/2015/11/f27/QTR2015-7D-Hydrogen-Production-and-Delivery.pdf

[5] U.S. Department of Energy, Fuel Cell Technologies Office Program Record #12014, "Current U.S. Hydrogen Production," http://www.hydrogen.energy.gov/pdfs/12014_current_us_hydrogen_production.pdf

[6] Quadrennial Technology Review 2015. Chapter 7: Advancing Systems and Technologies to Produce Cleaner Fuels, Hydrogen Production and Delivery. https://energy.gov/sites/prod/files/2015/11/f27/QTR2015-7D-Hydrogen-Production-and-Delivery.pdf

- the capital costs of the production facilities, and
- the efficiency of the production pathways.

The goal of this roadmap is to identify research pathways leading to industrial technologies that produce hydrogen from domestic, diverse, regionally distributed (Figure 1) [7], and sustainable energy resources with minimal adverse impact on the environment.

This document outlines the benefits, challenges and research and development needs of three major classes of resources for viable, large-scale production of hydrogen, including:

1. fossil-based resources,
2. biological and waste resources, and
3. direct water splitting resources.

The production methods and feedstocks associated with each of these resource classes are discussed in detail in the sections that follow; with additional potential production methods briefly cited.

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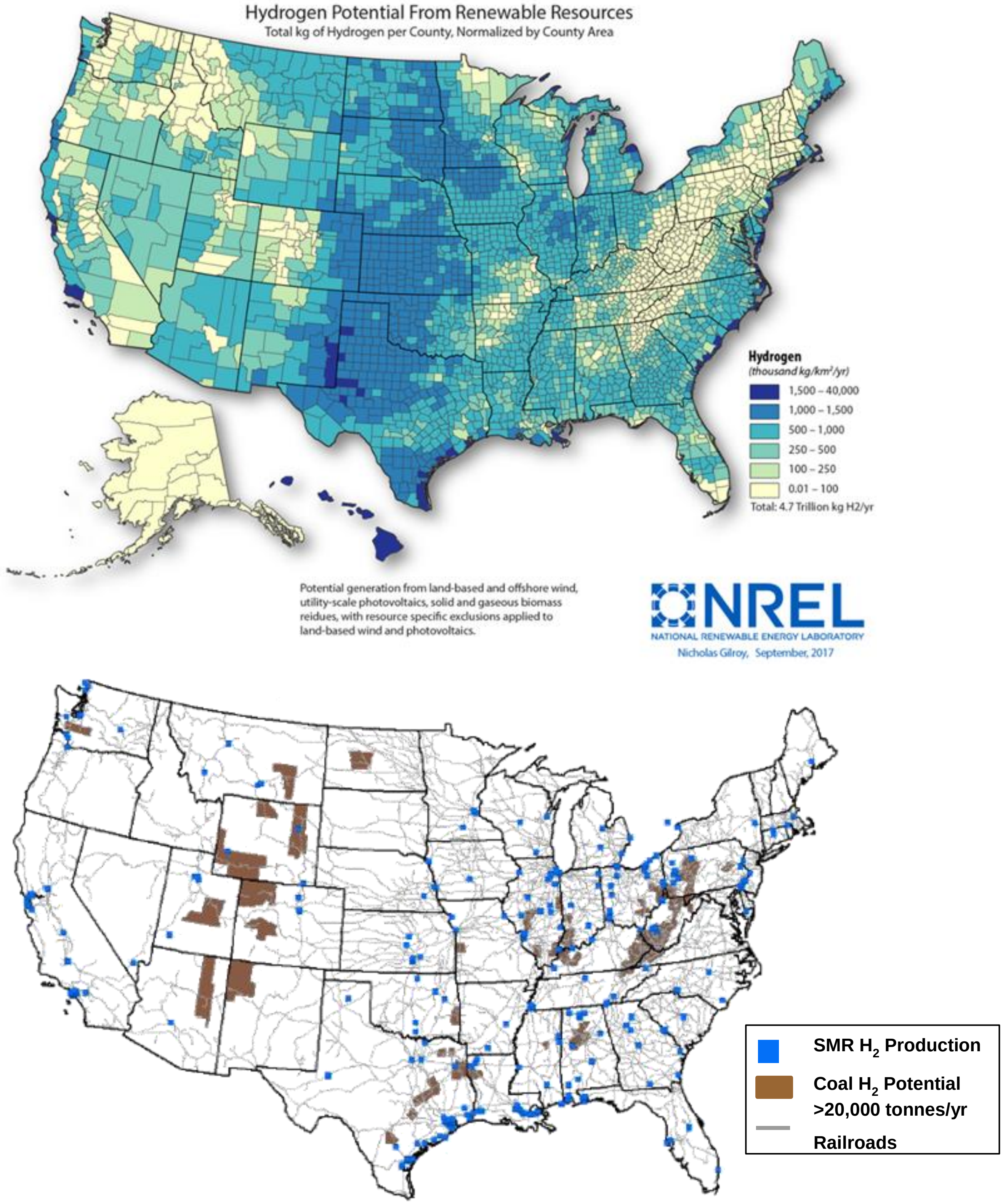
[7] NREL Technical Report, Resource Assessment for Hydrogen Production, a 2017 update (draft).



Hydrogen Potential From Renewable Resources

Total kg of Hydrogen per County, Normalized by County Area

Potential generation from land-based and offshore wind, utility-scale photovoltaics, solid and gaseous biomass reidues, with resource specific exclusions applied to land-based wind and photovoltaics.

NREL NATIONAL RENEWABLE ENERGY LABORATORY

Nicholas Gilroy, September, 2017

Figure 1 Combined hydrogen production potential from biomass, wind and solar (top) and current hydrogen production from natural gas using steam-methane reforming (SMR) and potential hydrogen production from coal (bottom).

DOE R&D Leadership

The DOE Fuel Cells Technologies Office (FCTO) within the Office of Energy Efficiency and Renewable Energy (EERE) focuses primarily on early-stage R&D to ultimately enable the widespread commercialization of a portfolio of hydrogen and fuel cell technologies by industry, across sectors and applications. One way the FCTO can accelerate its mission is through participation in the U.S. DRIVE Partnership, a voluntary, non-binding, and nonlegal government-industry partnership focused on advanced automotive and related energy infrastructure technology R&D. The Partnership provides peers in the technical community an opportunity to discuss pre-competitive, technology-specific R&D needs and challenges, set targets to guide the development of affordable and competitive technologies, identify possible solutions, and evaluate progress toward jointly-developed technical goals,

The FCTO has historically been organized into distinct sub-programs that address the specific research and supporting activities needed to overcome the barriers to hydrogen and fuel cell commercialization, including

- hydrogen production and delivery;
- hydrogen storage;
- fuel cells;
- technology validation;
- market transformation;
- safety, codes and standards;
- education; and
- systems analysis and integration.

Within the FCTO, the Hydrogen Production sub-program works on the development of hydrogen production technologies, integrating foundational and early-stage applied research. To adequately address the diverse range of technologies and feedstocks associated with hydrogen production, the office is closely coordinated with activities within the DOE Offices of EERE, Nuclear Energy (NE), Fossil Energy (FE), and Science (SC). It also interacts with the Advanced Research Projects Agency-Energy (ARPA-E), and agencies outside of DOE, such as the National Science Foundation (NSF). The U.S. Department of Transportation (DOT) participates in activities involving codes and standards development, infrastructure safety, and hydrogen vehicle safety. In addition, the Hydrogen Production sub-program participates and co-Chairs the HPTT, one of 13 U.S. DRIVE technical teams that work to accelerate the development of pre-competitive technologies to enable a full range of efficient and clean advanced light-duty vehicles, as well as related energy infrastructure.

Tied to the related energy infrastructure within the U.S. DRIVE's scope is a new DOE initiative, H2@Scale, a concept that explores the potential for wide-scale hydrogen production and utilization in the United States to enable resiliency of the power generation and transmission sectors, while also aligning diverse multibillion dollar domestic industries, domestic competitiveness, and job creation. As H2@Scale gains momentum and early stage R&D projects begin to receive funding through the FCTO, there will be an opportunity for the U.S DRIVE HPTT and other Tech Teams to offer input and guidance on the energy infrastructure as it pertains to hydrogen production via project reviews and related workshops.

HYDROGEN PRODUCTION

Production Scales and Locales

Hydrogen can be produced in small-, medium-, and larger-scale facilities. HPTT envisions that, for purposes of producing hydrogen for transportation, small-scale (distributed) facilities would produce from 100 to 1,500 kilograms of hydrogen per day with the production site at the fueling stations. Medium-scale (also known as semi-central or city-gate) facilities would produce 1,500 to 50,000 kilograms per day on the outskirts of cities. The largest (central) facilities would produce more than 50,000 kilograms of hydrogen per day. Co-production facilities, which would combine the production of hydrogen, fuel, heat, and electric power, are also being explored in the H2@Scale initiative. Utilization of hydrogen from the central plants for vehicle refueling is currently limited by the lack of hydrogen delivery and distribution infrastructure.

DOE Cost Goal

DOE has established a cost goal of < $4.00 per gge delivered, dispensed and untaxed for hydrogen fuel. An apportioned value of <$2.00 per gge of hydrogen has been allocated for production costs.[8, 9] DOE determined the methodology and other assumptions used to establish the cost goal with input from multiple stakeholders, including the Partnership's Hydrogen Production and Fuel Pathway Integration Technical Teams and others.[10] Currently, hydrogen can be produced from steam methane reforming (SMR), using commercially available technology, at a projected high-volume production cost of <$2.00 per gge (in 2007$) over a wide range of natural gas prices.[11] Other pathways of interest need further R&D to reach the cost target as illustrated in Figure 2, which are discussed in subsequent sections.

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[8] DOE Hydrogen and Fuel Cells Program Record #12001 (Washington, DC: U.S. Department of Energy, 2012), http://www.hydrogen.energy.gov/pdfs/12001_h2_pd_cost_apportionment.pdf.

[9] The hydrogen threshold cost is a DOE threshold cost and not a Partnership goal or target.

[10] DOE Program Record (Offices of Fuel Cell Technologies) #11007 (Washington, DC: U.S. Department of Energy, 2011), http://hydrogen.energy.gov/pdfs/11007_h2_threshold_costs.pdf.

[11] DOE Hydrogen and Fuel Cells Program Record #12024 (Washington, DC: U.S. Department of Energy, 2012), http://www.hydrogen.energy.gov/pdfs/12024_h2_production_cost_natural_gas.pdf .

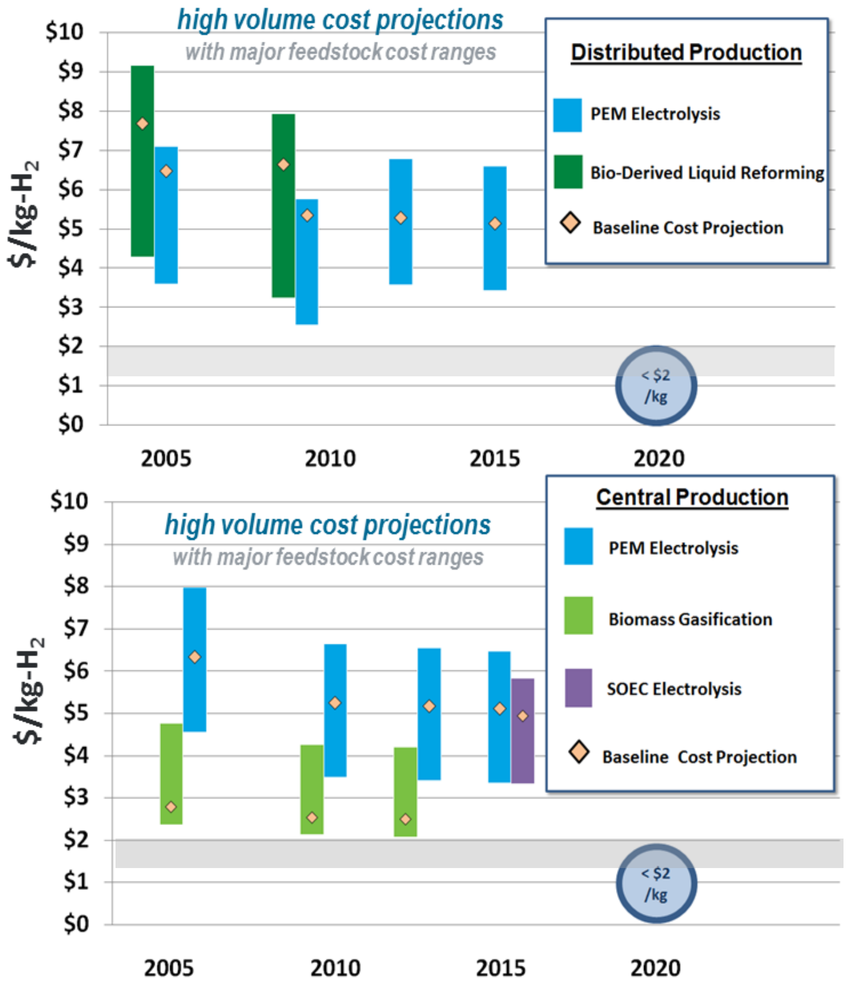

Figure 2 Current range of hydrogen production costs (un-dispensed and untaxed, reported in $/kg H_2 (where 1 kg H_2 roughly equals 1 gge) including feedstock and capital cost variability for high volume production[12]. The grey shaded area represents the cost of hydrogen when produced by SMR for natural gas prices ranging from $2-7.50 MMbtu. Costs shown in 2007$.

Types of Resources: Three Major Categories of Technology Pathways

A major benefit of hydrogen is that it can be produced from diverse, domestic resources. As previously mentioned, most hydrogen is produced from fossil fuels, predominantly from natural gas. Electricity is also used to produce hydrogen via water electrolysis, but at relatively modest scales due to higher current costs compared with natural gas reforming. In the longer term, solar energy and biomass can be used directly to generate hydrogen. For the purpose of this Roadmap, and to align with the portfolio organization within the FCTO Hydrogen Production sub-program, the production technology pathways of interest have been grouped into three major categories: fossil resources, biomass resources and direct water splitting. Within each category there are multiple technology pathways, each with their own R&D challenges, priorities and timeline for widespread adoption. The main production opportunities are illustrated in Figure 3. Within each resource class, the relative timescale to widespread adoption is

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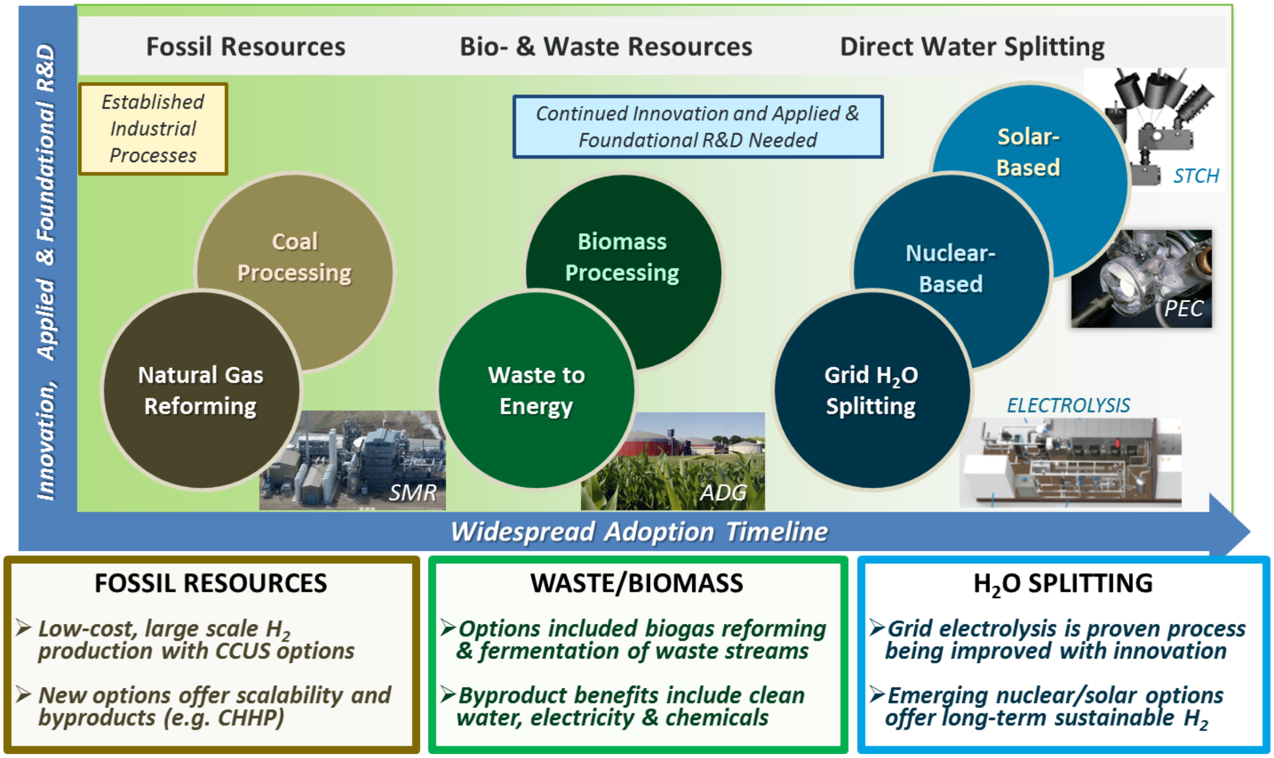
[12] Fuel Cell Technologies Office Program Record #14005, 2014
https://www.hydrogen.energy.gov/pdfs/14005_hydrogen_production_status_2006-2013.pdf

depicted by the relative ordering along the timeline axis. For example, natural gas reforming is already a commercialized, widely adopted process whereas coal processing technology is developed but not widely adopted; and, while grid electrolysis at large scale is underway, solar based hydrogen production at scale is in the very early research and development stage.



FOSSIL RESOURCES

- *Low-cost, large scale H_2 production with CCUS options*
- *New options offer scalability and byproducts (e.g. CHHP)*

WASTE/BIOMASS

- *Options included biogas reforming & fermentation of waste streams*
- *Byproduct benefits include clean water, electricity & chemicals*

H_2O SPLITTING

- *Grid electrolysis is proven process being improved with innovation*
- *Emerging nuclear/solar options offer long-term sustainable H_2*

Figure 3 Diverse domestic resources allow for a broad portfolio of near- to longer-term H_2 production technology options that are being developed and optimized through comprehensive R&D[13]. Technologies include fossil-based resources using natural gas reforming and coal processing with and without carbon capture, utilization and storage (CCUS) options, waste/biomass technologies, water splitting technologies such as solar thermochemical (STCH), photoelectrochemical (PEC) and electrolysis. Combined heat, hydrogen and power (CHHP) options are also considered.

Fossil Resources.

Fossil fuels such as natural gas or coal are the source of most of the hydrogen produced in the world and the hydrogen production processes based on these resources are advanced and mature. Today, almost all the hydrogen produced in the United States is made by SMR in large central plants fed by the existing natural gas infrastructure. This is an important pathway for near-term production that will need to be supplemented with other sustainable production pathways as the demand for renewable or low-carbon hydrogen increases. Combining SMR and coal gasification processes with carbon capture, utilization and storage (CCUS), is a promising option for low-carbon hydrogen production.

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[13] K. Randolph. "HydroGEN: Accelerating Advanced Water Splitting Materials Discovery & Development," 231st Electrochemical Society Meeting, New Orleans, LA. May 28 – June 1, 2017.

Biomass Resources.

Biomass is an abundant sustainable resource that can be produced domestically and converted to hydrogen and other byproducts through a number of methods. In addition to using biomass directly via biomass gasification or co-fed in coal gasification, bio-derived liquid reforming or fermentation, there are opportunities to produce hydrogen from waste streams (e.g., municipal solid waste or agricultural crop residues) containing biomass which offer the additional benefit of waste clean-up.

Direct Water Splitting.

Direct water splitting processes involve the use of electricity, high temperature heat, or light energy (photons) to generate hydrogen and oxygen from water. Electrolysis can be driven by electricity from the traditional fossil-fuel based grid or a variety of diverse domestic and sustainable resources including solar and wind. Thermally driven water splitting processes can utilize heat from concentrated solar power or waste heat from advanced nuclear reactors. Photons can be absorbed via semiconductors and the energy trapped can be used to drive the chemical reaction to split water. Direct or advanced water splitting (AWS) technologies for hydrogen production include advanced high- and low-temperature electrolysis, solar thermochemical (STCH) water splitting, and photoelectrochemical (PEC) water splitting.

KEY CHALLENGES

There are numerous technical barriers to high-volume production of hydrogen using next-generation technologies. Those that are common to multiple production pathways are described here.

Hydrogen Quality

Hydrogen purity is a major issue for hydrogen destined for use in FCEVs. Platinum-Group-Metal (PGM) catalysts used in most FCEVs can be easily poisoned by impurities in the hydrogen, ultimately rendering them ineffective. Therefore, hydrogen production technologies must either produce high-purity hydrogen directly or incorporate additional purification processes downstream.

Scale

Many of the potential technology pathways face serious scale up challenge to meaningfully impact the existing hydrogen supply market.

Control and Safety

All hydrogen production technologies will be required to meet strict safety requirements. The permitting process relies on proven technology reliability and safety. Production units for placement at refueling stations, in particular, must be designed to operate with minimal manual assistance. This capability will use back-up and fail-safe modes, remote monitoring, and intermittent maintenance schedules.

Codes, Standards, and Regulations

Inspection, testing, certification, and permitting necessary to transfer new hydrogen production technologies into commercialization may require amending existing and creating new regulations, codes, and standards. This process will require extensive outreach to familiarize regulatory agencies with the technologies.

Regulations, codes, and standards have been in place for many years to address the public safety issues associated with large-scale centralized hydrogen production through natural gas reforming and may be leveraged for emerging technologies. However, these technologies will have unique safety concerns and distributed production at hydrogen fueling stations represents a new application and product design.

Issues relating to on-site feedstock storage, gas emissions, and waste (solid/liquid) storage and disposal will also need to be addressed. Some areas not effectively covered by current regulations, codes, and standards include operations and maintenance plans; certification testing; permitting; and waste storage and disposal.

Further information on the codes, standards and regulations associated with hydrogen can be found in the Codes and Standards Tech Team Roadmap.

Codes, Standards, and Regulations

The establishment and adoption of codes and standards is performed on a national level through code and standard development organizations and federal agencies. On the state level, state legislatures and various agencies determine which codes and standards will be adopted. Local Authorities Having Jurisdiction, of which there are approximately 144,000 in the United States, can further increase the regulatory requirements through adoption of more stringent codes and standards than those adopted into state regulatory law. In addition, for permit approvals, local communities can provide input on whether a new technology should be installed and operated in or around their neighborhoods.

Community Acceptance Barriers

New technologies require accompanying outreach efforts to encourage public acceptance. FCEVs and hydrogen fueling stations will be no different. Community barriers that are shared by all production pathways include regulations, codes and standards, and education to assure wide public acceptance of hydrogen fuel.

Capital and Operating Costs

To offer a competitive energy alternative, hydrogen must be economically attractive to American consumers. Capital costs for many hydrogen production technologies today are too high for cost competitiveness. These costs are expected to drop as developers apply the principles of design for manufacturing, identify better materials, and move into larger-scale manufacturing. Operating costs will similarly decline as equipment developers identify improved materials, consolidate processing steps, and enhance equipment performance and integration.

Critical Technology Needs

Collectively, the critical R&D activities for each technology pathway described in this roadmap make up the Hydrogen Production sub-program. The technologies are in different stages of development, and each offers unique opportunities, benefits, and challenges. Economics favor certain technologies over others in the near term, but as the technologies mature and market drivers shift, a broad range of technologies is expected to become economically viable, taking advantage of the range of energy and feedstock resources available in each region.

1.0 Pathways Utilizing Fossil Resources

Fossil fuels can be reformed to release hydrogen from the constituent hydrocarbon molecules through three main reforming technologies: steam reforming, partial oxidation, and autothermal reforming.[14]

Steam reforming is typically the preferred process for hydrogen production in industry. In steam reforming processes, the hydrocarbon is reacted with steam at high temperature over a catalyst to produce syngas (H_2 + CO), which is then further reacted with steam in a Water-Gas-Shift reactor to convert CO into additional hydrogen ($CO+H_2O \rightarrow CO_2+H_2$). Following this, pure H_2 is separated usually using a Pressure Swing Adsorption (PSA) technology.

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[14] J. D. Holladay, K. Hu, D. L. King, and Y. Wang, “An Overview of Hydrogen Production Technologies,” *Catalyst Today* 139 (2009): 244–260.

Partial oxidation (POX) converts hydrocarbons to syngas by partially reacting (combusting) the hydrocarbon with oxygen in an exothermic reaction. The major advantage of POX is that it does not require a catalyst, and therefore the POX reactor is not susceptible to catalyst poisoning that is encountered in catalytic reformers (e.g., steam and autothermal reforming). The challenges for POX include high reaction temperatures which require more expensive reactor construction materials, some soot formation, and a low H_2/CO ratio (1:1 to 2:1) which means less hydrogen is produced per molecule of hydrocarbon fuel compared to steam and autothermal reforming. As with the steam reforming process, a WGS reaction is required to increase the hydrogen content.

Autothermal reforming (ATR) combines steam reforming with partial oxidation. POX provides the heat for the endothermic steam reforming process, in theory, resulting in a thermally neutral process. Since the heat for the steam reforming is provided by the exothermic POX reaction, an external heat source for the reactor is not required. However, POX and ATR both require expensive and complex oxygen separation unit. Since a large amount of carbon monoxide (CO) is produced, a WGS reactor is required to maximize the hydrogen production. While ATR produces a higher amount of hydrogen per hydrocarbon molecule than POX, it is still less than what steam reforming would produce.

All three reforming technologies release carbon as carbon dioxide. Combining this processes with carbon capture, utilization, and storage (CCUS) can reduce the CO_2 emissions.

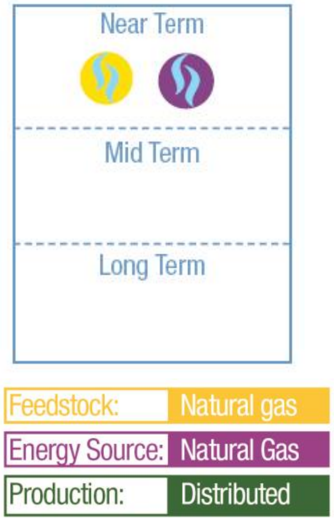
1.1 Natural Gas Reforming

95% of the hydrogen produced in the United States today is made by steam methane reforming (SMR) of natural gas (NG) in large central plants. This is an important pathway for near-term hydrogen production.

Status

Abundant supply of inexpensive NG makes hydrogen produced in central facilities through existing SMR process cost-competitive with gasoline on an energy basis. The main barrier is the high cost of hydrogen transportation from the central plant to the station owing to the lack of the distribution infrastructure.

Distributed Natural Gas Reforming



Small-scale modular distributed natural gas reforming (DNGR) units have been developed which can be configured to achieve the desired scale of distributed production of hydrogen from NG. DNGR offers a potentially economical and technically viable near-term approach to supply hydrogen to vehicles, offering early availability which is key to promoting acceptance of FCEVs and hydrogen fuels and creating the market demand.

As illustrated in Figure 4, projections based on high-volume production of DNGR systems indicate the potential for a \$1.50/gge or less when the price of natural gas is below \$4/MMBtu (million British thermal units).[15] Because of this, DOE is no longer supporting research in conventional natural gas reforming

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[15] Sara Dillich, Todd Ramsden, and Marc Melaina, "Hydrogen Production Cost Using Low-Cost Natural Gas," *DOE Hydrogen and Fuel Cells Program Record* (Washington, DC: U.S. Department of Energy, 2012), http://www.hydrogen.energy.gov/pdfs/12024_h2_production_cost_natural_gas.pdf.

processes, although innovative approaches leveraging flex-fuels and byproduct benefits remain under investigation. It is anticipated that industry will continue to make incremental improvements to the standard SMR technologies as part of base business operations.

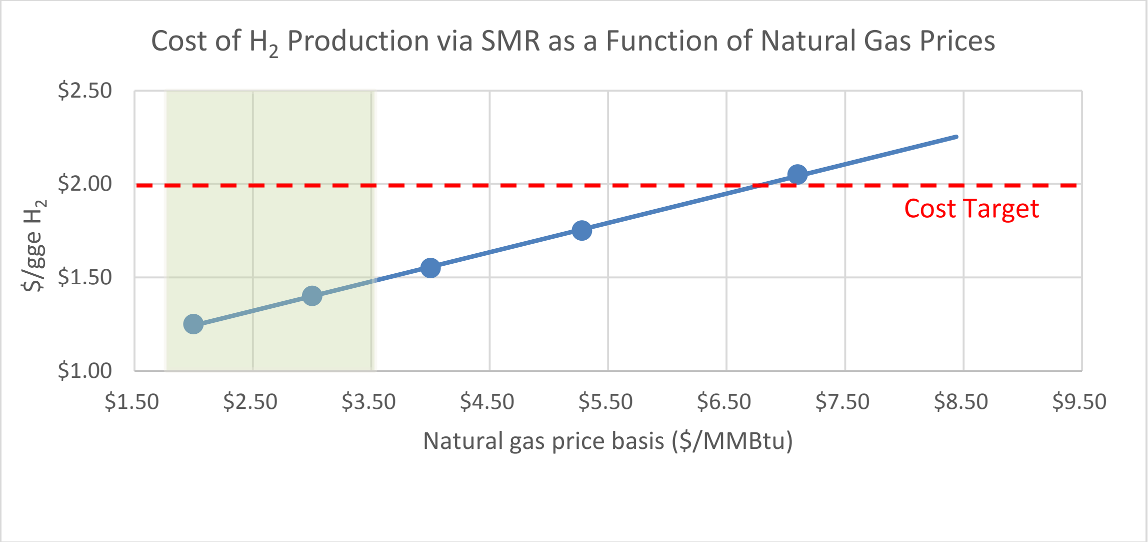

Figure 4 H_2 production cost ($/gge untaxed) at varying natural gas prices for current DNGR technology (assuming 1,500 gge/day plant size and economy of scale in plants deployment). Cost target for hydrogen (<$2.00/gge) can be met with a price of NG < $7.00 /MMBTU. The shaded area represents the range of natural gas spot prices for 2016.[16]

Gaps and Technical Barriers

Driving DOE’s research activities are specific barriers identified in the Fuel Cell Technologies Office Multi-Year Research, Development and Demonstration Plan (MYRD&D),[17] as well as others identified by the U.S. DRIVE Partnership’s HPTT. The DOE updates the MYRD&D periodically and the USDRIVE Roadmap will also be updated to be consistent with MYRD&D as required.

Reduce Reformer Footprint

The DNGR plant footprint is a critical barrier. Refueling stations providing an average of 1,500 gge per day of hydrogen will tend to occupy a relatively large footprint owing to the size and amount of process equipment involved. Reformer and BOP size need to be reduced through process intensification and overall system flowsheet optimization to enable wider adoption of distributed generation technologies.

Reduce Reformer Capital Costs

Equipment capital cost is a significant factor in hydrogen production costs using DNGR technologies. Efforts associated with process intensification, combining process steps such as separations, simplifying equipment lists, etc., are needed to lower capital costs. Design for Manufacture and Assembly (DFMA) will be a key component of cost reduction efforts. In the near term, the focus should be on developing reformer designs that incorporate commonly available materials and use common tooling and standard sizing for procured components. For

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[16] EIA Henry Hub NG pricing data: https://www.eia.gov/dnav/ng/hist/rngwhhdM.htm

[17] Office of Energy Efficiency and Renewable Energy, *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan* (Washington, DC: U.S. Department of Energy, June 2015), Section 3.1, https://energy.gov/sites/prod/files/2015/06/f23/fcto_myrdd_production.pdf.

widespread deployment, on-site reformers will be manufactured in large quantities (hundreds of systems per year), and the goals will shift towards incorporating optimal high-volume production methods such as use of common, interchangeable components, automated joining processes, and low-cost stamping and extrusion methods. BOP components also constitute a significant part of the capital cost. Improved low-cost pumps, blowers, sensors, control actuators and monitoring equipment need to be developed.

Optimize System to Manage Variable Demand. Demand for hydrogen refueling will vary significantly over the course of a day. This demand variability may be handled through a combination of on-site hydrogen storage and load-responsive capability of the reformer. The extent to which each of these two strategies is used to handle demand variability will have a significant impact on capital costs and the station footprint. Sizing the reformer to handle peak demand will increase capital costs for the reformer, whereas increasing storage will increase the system footprint to accommodate storage tanks. Optimizing this balance also requires considering the relative impacts on maintenance costs and safety.

Improve Catalysts. Large-scale SMR typically use a low-activity nickel-based catalyst. Although inexpensive, the nickel-based catalysts are prone to coking, require complicated start up and shut down protocols and owing to their low activity, the reactors must be relatively large.[18] Most DNGR applications tend to use a precious metal-based catalyst.[19] Some precious metal catalysts have a higher activity and are less prone to coking; however, their cost is higher. Lower-cost catalysts are needed that can provide high yields to help increase the energy efficiency of distributed production.

Improve Feedstock Pre-Treatment. Typically, reforming catalysts require odorant-free natural gas and de-ionized water. Feedstock pretreatment systems that achieve these conditions can represent a significant share of the capital, operating, and maintenance costs. Several approaches can reduce the costs associated with these systems and will need to be further explored.

Reduce Operating and Maintenance Costs

Costs for O&M also have a significant impact on the overall cost for producing hydrogen. Improvements in process design that increase energy efficiency and/or allow for greater variability and higher levels of contaminants in feedstocks will reduce O&M costs. Leaks of NG or hydrogen must be eliminated to ensure safety, and minimize loss of process efficiency. Heat loss and heat rejection must also be minimized through well-designed insulation and heat integration.

O&M costs will also be reduced by reducing on-site labor through the use of automated process control and remote monitoring, automatic fault detection, improving process controls for cycle optimization, and development of better and less expensive sensors and better turn-down capability.

Increased Equipment Reliability. The reliability of BOP equipment with moving parts (such as pumps, compressors, and blowers) is often a limiting factor in overall system reliability. Increasing the reliability of these components along with minimizing equipment complexity is critical for improving system reliability.

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[18] J. D. Holladay, K. Hu, D. L. King, and Y. Wang, "An Overview of Hydrogen Production Technologies," *Catalyst Today* 139 (2009): 244–260.

[19] U.S. Department of Energy, *2011 NREL/DOE Hydrogen and Fuel Cell Manufacturing R&D Workshop Report* (Washington, DC: U.S. Department of Energy, 2011), https://www1.eere.energy.gov/hydrogenandfuelcells/pdfs/mfg2011_wkshp_report.pdf

Strategy to Overcome Barriers and Achieve Technical Targets

Analysis of central and distributed SMR technology status indicates that federal R&D partnerships have addressed the major technical and cost challenges to the extent that private industry should be able to tackle the remaining technical and cost barriers and complete the commercial development of this production technology without additional DOE resources. The barriers discussed above remain for industry to resolve in commercialization and mostly apply to DNGR.

1.2 Coal Gasification

Status

Gasification of coal or other carbonaceous (carbon-based) raw materials is a mature technology for production of synthesis gas (syngas) and hydrogen that has been practiced for nearly two centuries.[20] Gasification generally occurs in large scale, high temperature/pressure vessels where oxygen (or air) and steam are directly contacted with the coal or other solid feed material causing a series of chemical reactions to occur that convert the feed into syngas composed primarily of the colorless, odorless, highly flammable carbon monoxide (CO) and hydrogen (H_2) and ash/slag mineral residues. To produce pure H_2, CO in the syngas can be further converted (or shifted) to more H_2 and carbon dioxide (CO_2) by adding steam and reacting over a catalyst in a water-gas-shift reactor and then pure hydrogen gas separated, generally through a pressure swing adsorption (PSA) process. CO_2 can be efficiently captured from syngas, preventing emission to the atmosphere and enabling its utilization or underground storage.

Gaps and Technical Barriers

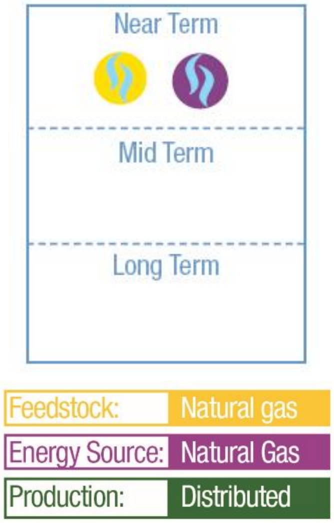
Many of the barriers to widespread adoption of the coal gasification technology are similar to the barriers for SMR technology listed in the above section. Additional factors limiting broader deployment of coal gasification technology for production of hydrogen are its lower efficiency and higher capital cost relative to SMR (about 60% efficiency for coal gasification vs 70-80% for SMR and x1.4-2.5 times higher cost[21,22]). Furthermore, because of large amounts of solids participating in the process (both the solid feed and the ash removal) coal gasification is not particularly amendable to scaling down and generally practiced only for large-scale centralized hydrogen production plants.

Continuous operations are very important to the economics of a gasification plant. With current, state-of-the-art technology, many integrated gasification combined cycle (IGCC) designs incorporate a spare gasifier in order to achieve acceptable overall plant availability, which entails a higher capital cost.

Strategy to Overcome Barriers and Achieve Technical Targets

R&D is being conducted to increase the availability of the gasifier and decrease the cost of operation and maintenance to substantially optimize gasifier operations. Examples include advanced materials development for

Coal Gasification



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[20] https://www.netl.doe.gov/File%20Library/Research/Coal/energy%20systems/gasification/gasifipedia/index.html
[21] Capital and Operating Cost of Hydrogen Production from Coal Gasification (Apr 2003), Final Report by Parsons for NETL
[22] https://www.netl.doe.gov/research/Coal/energy-systems/gasification/gasifipedia/technologies-hydrogen

refractory and the development of a reliable, practical and cost-effective means of monitoring real-time temperature in the gasifier through advances in sensors and instrumentation.

In addition to development of technologies such as advanced refractories and sensors, current research efforts also include development of gasifiers for low-rank coal, creating models to better understand the kinetics and particulate behavior of fuel inside a gasifier, and developing practical solutions to mitigate the plugging and fouling of syngas coolers.

1.3 Other fossil based options

Hydrogen production through SMR or coal gasification with Carbon Capture

SMR and coal gasification extract hydrogen from carbonaceous fuel, while releasing CO_2. Efficiency for both technologies have been improved over time to the point where CO_2 emissions are close to the theoretical minimum. Further reduction of CO_2 can be achieved by integration of these processes with CCUS technologies.

One CCUS option is to remove CO_2 from the high-pressure syngas stream which is present immediately after the carbonaceous fuel conversion in the first stage of the process before separation of H_2. This is analogous to the pre-combustion CO_2 removal in a coal power plant with CCUS. The advantage of this capture strategy is that the syngas stream has high pressure and CO_2 is present at high-concentration, requiring lower cost equipment but limiting CO_2 capture to only about 50-60% of the total produced in the overall process.[23] Another CCUS option is to remove CO_2 from the low-concentration, low-pressure post-combustion stream at the exhaust of the overall process (analogous to post-combustion capture in power plants). As much as 90% of the overall CO_2 can be removed in the post-combustion capture but this requires higher capital cost equipment. Recent techno-economic analysis of six different cases of CCUS integration with a large scale SMR plant suggests that the levelized cost of H_2 increases by 18-45% from the base case without CCUS depending on the carbon capture option, cost of fuel, etc. [23] Also the cost of CCUS installation with a coal gasification plant is about 40% higher than for and SMR plant. [24]

Two large scale demonstration projects integrating carbon capture with hydrogen SMR plants have been implemented in recent years in North America. One project is the Air Product's SMR plant at Valero refinery at Port Arthur, TX. [25] The other is Quest SMR at Shell's Scotford Upgrader in Alberta, Canada.[26] Each project is utilizing the pre-combustion integration strategy and is capturing about 1 million metric tonnes of carbon dioxide per year. Currently utilization of captured CO_2 is mainly directed to enhanced oil recovery (EOR) or to sequestration in geological formations. Both applications are limited to large projects on the order of millions tonnes per year and only can be applied to large scale industrial SMR and gasification plants.

Methane pyrolysis, the non-oxidative thermal decomposition of methane to hydrogen and solid carbon, is an alternative to SMR that facilitates carbon capture.[27] Thermal and plasma-based processes for methane pyrolysis are currently more expensive than SMR, but continued R&D is expected to result in cost reductions. An added benefit is that the produced carbon (e.g., carbon black, carbon fibers, etc.) could potentially be sold as a co-product to help offset the hydrogen production costs.

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[23] Techno-Economic Evaluation of SMR Based Standalone (Merchant) Hydrogen Plant with CCS. IEAGHG Technical Report 2017-02. February 2017.

[24] Assessment of Hydrogen Production with CO2 Capture Volume 1: Baseline State-of-the-Art Plants, August 30, 2010; DOE/NETL-2010/1434

[25] https://www.netl.doe.gov/research/coal/major-demonstrations/industrial-carbon-capture-and-storage/iccs-air

[26] https://www.globalccsinstitute.com/projects/quest

[27] R. Dagle, V. Dagle, M Bearden, J. Holladay, T. Krause, S. Ahmed, "Research and Development Opportunities for Development of Natural Gas Conversion Technologies for Co-Production of Hydrogen and Value-Added Solid Carbon Products", Technical Report by the Argonne National Laboratory and the Pacific Northwest National Laboratory (2017).

Distributed hydrogen production through methanol reforming

Methanol (MeOH) reforming is another option for distributed hydrogen production. The market price for methanol is much higher than for NG (varying in the $1.7-3.4 /gge range for MeOH vs. $0.4-0.8 /gge for NG over the last 5 years) making NG a preferred fuel for central hydrogen production. However, MeOH has some advantages for distributed hydrogen production. It can be converted at low temperatures (< 300°C for MeOH conversion vs. ~ 900°C for NG reforming), over low-cost Cu based catalysts and with high selectivity to H_2 and CO_2 over CO, eliminating the need for a water-gas-shift reaction. This significantly reduces complexity and capital cost of the MeOH reforming system and at small production scales can compensate for the higher cost of the feedstock. Furthermore, MeOH is liquid at most ambient conditions, so there is no special infrastructure required. With an existing commercial MeOH distribution infrastructure already throughout the United States, distributed hydrogen production through MeOH reforming where small capacity MeOH reforming plants are located directly at the refueling stations may be an attractive option for the initial development of the hydrogen refueling infrastructure.

Currently, most commercially distributed MeOH is produced from NG; however, it can also be produced from renewable sources such as biomass and even from renewable hydrogen and captured CO_2. As more renewable MeOH enters the global mix, the developing infrastructure may gradually transition from fossil sources to renewable sources for hydrogen production. Most barriers to widespread application of distributed MeOH reforming technology are the same as for DNGR. Distributed MeOH reforming would need to compete with DNGR on price and availability.

MeOH toxicity may create an additional barrier to widespread utilization. While MeOH is often cited as a hazardous material, in fact it is less toxic than many common liquid fuels and household chemicals. In a 1991study the DOE concluded that gasoline is considered to be more hazardous to human health and the environment than pure methanol.[28] Methanol is readily miscible with water, so leaks or spills may be diluted to below the hazardous concentrations.

As with DNGR, MeOH reforming technology is sufficiently advanced so that private industry should be able to tackle the remaining technical and cost barriers and complete the commercial development of this production technology without additional DOE resources.

2.0 Pathways Utilizing Biomass Resources

Another major resource that the United States can tap for energy is biomass, with the potential for over a billion dry tons of biomass available annually.[29] In general, the two types of biomass feedstocks available for use in hydrogen production are (1) primary biomass such as energy crops like poplar, willow, and switchgrass and (2) biogas produced from anaerobic digestion of organic residues from sources such as landfill, animal waste, and municipal solid waste.[30] Primary biomass can be gasified using well established technology similar to the coal gasification process previously described. It can also be processed into bio-derived liquids for subsequent reforming. Biogas, with additional cleanup requirements, can be reformed to produce hydrogen using the SMR process previously discussed. Waste streams can be used to produce hydrogen through biological-based processes such as fermentation and microbial electrolysis.

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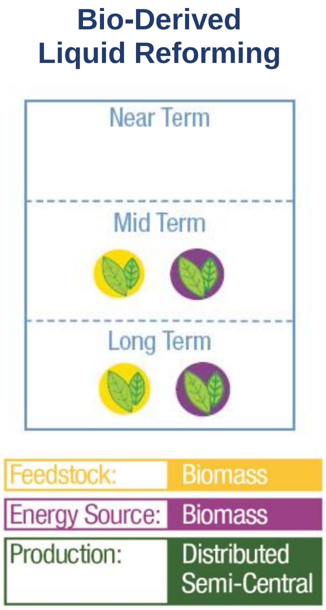
[28] United States Department of Energy, October (1991). Assessment of Costs and Benefits of Flexible and Alternative Fuel Use in the US Transportation Sector. Technical Report No. 7: Environmental, Health, and Safety Concerns

[29] U.S. Department of Energy. 2016. *2016 Billion-Ton Report: Advancing Domestic Resources for a Thriving Bioeconomy, Volume 1: Economic Availability of Feedstocks*. M.H. Langholtz, B.J. Stokes, and L.M. Eaton (Leads)., ORNL/TM-2016/160. Oak Ridge National Laboratory, Oak Ridge, TN. 448p. doi: 10.2172/1271651. https://energy.gov/eere/bioenergy/2016-billion-ton-report.

[30] National Research Council and National Academy Of Engineering, *The Hydrogen Economy: Opportunities, Costs, Barriers, and R&D Needs* (Washington, DC: National Academies Press, 2004), http://www.nap.edu/openbook.php?isbn=0309091632.

2.1 Reforming of Bio-Derived Liquids

Status



Hydrogen can be produced by distributed or semi-central facilities that employ gas-phase or aqueous-phase reforming of bio-liquids such as sugars, cellulose slurries, ethanol, or bio-oils, which can be extracted from primary biomass feedstocks. Bio-liquid reforming is similar to NG reforming but is usually challenged by limited catalyst activity and durability.

In addition to the three reforming technologies described in the Pathways Utilizing Fossil Resources section 1.0 above, which all can be applied to reforming biomaterial feedstocks, aqueous phase reforming (APR) can also be used to convert biomass or bio-derived liquid directly to hydrogen. For aqueous phase reforming, water soluble organics are decomposed at high pressure (~2 Mpa and relatively low temperatures, <300°C) to hydrogen. The high pressure keeps the components in the liquid phase and the relatively low temperatures favor CO_2 formation over CO, thus maximizing the hydrogen yield without the need of a water gas shift (WGS) reactor. As APR is still in developmental stages, researchers and developers are trying to address some of the issues related to catalysts and process development.

Based on the latest detailed cost analysis published[31], the cost of hydrogen from bio-derived liquid reforming using a representaitve feedstock is $6.60/gge. Based on the cost breakdown illustrated in Figure 5, the main driver is the feedstock cost. The DOE has recently invested in R&D for bio-derived liquid reforming with some promising results that indicate innovative, process intensification approaches in addition to projected reductions in bio-oil costs[32] that there is a pathway to meet the DOE cost target of $2/gge[33].

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[31] DOE Hydrogen and Fuel Cells Program Record #14005. October 7, 2014. https://www.hydrogen.energy.gov/pdfs/14005_hydrogen_production_status_2006-2013.pdf

[32] M. Ringer, V. Putsche and J. Scahill, "Large-scale Pyrolysis oil production: A Technology Assessment and Economic Analysis," Technical Report NREL/TP-510-3779, National Renewable Energy Laboratory, US Department of Energy, November 2006. http://www.nrel.gov/docs/fy07osti/37779.pdf

[33] W. Liu, S. Li, E. Cutsforth, K. Rapppe, R. Zheng, Y. Wang, B. Xu, C. Bertole, "Monolithic Piston-type Reactor for Hydrogen Production through Rapid Swing of Reforming/Combustion Reactions," 2016 FCTO Annual Merit Review, June 8, 2016. https://www.hydrogen.energy.gov/pdfs/review16/pd111_liu_2016_o.pdf

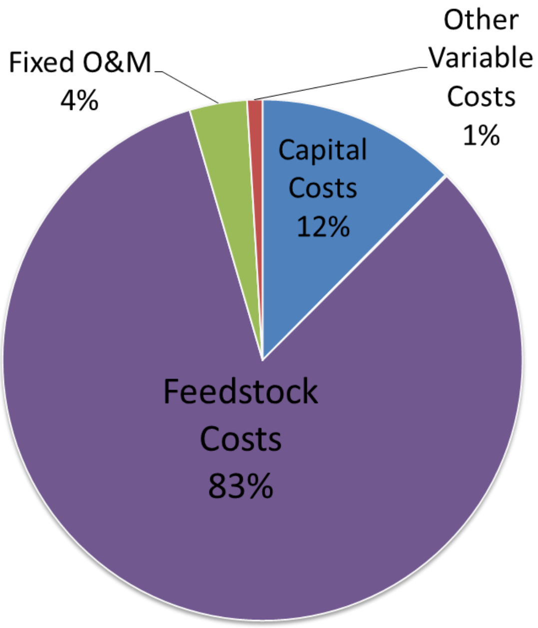

Figure 5 Cost breakdown for bio-derived liquid. Feedstock cost is the most significant cost driver.

Gaps and Technical Barriers

Specific barriers to implementing hydrogen production from the biomass resources, such as bio-derived liquid reforming, have been identified by the MYRD&D [34] and by the U.S. DRIVE Partnership's HPTT. These barriers are generally similar to that for hydrogen production from the fossil resources.

Reformer Capital Costs

Currently, the capital cost of small-scale distributed reformers for bio-derived liquid feedstock is too high to achieve target hydrogen production costs. High capital costs are caused by high catalyst costs, low conversion efficiencies, and multiple complicated unit operations. Additionally, installation costs can be significant, while components have reliability, durability and life span challenges. The most developed reformers operate at high temperatures (>700°C), requiring more expensive construction materials. Lower-temperature reactors are under development but have issues with coking. Either lower-cost materials for high-temperature operation are needed, or the lower-temperature reactors need to be improved. Finally, the high purity of hydrogen required for fuel cells puts upward pressure on capital costs by requiring expensive metal membranes or multiple pressure swing adsorption units. Considerable additional R&D is still needed.

Reformer Manufacturing

Distributed reformer units are currently considered niche. The capital cost contribution is higher for smaller hydrogen production facilities designed for distributed applications. This limited manufacturing approach results in expensive system components with poor life span and

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[34] Office of Energy Efficiency and Renewable Energy, *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan* (Washington, DC: U.S. Department of Energy, June 2015), Section 3.1, https://energy.gov/sites/prod/files/2015/06/f23/fcto_myrdd_production.pdf.

durability, as well as increased BOP component cost. Finally, current systems are too large and too expensive, in part because of the need for site-specific fabrication of subsystems.

Station Footprint

The specific location of a distributed or semi-central liquids reforming station determines the constraints on the station footprint. Refueling stations providing an average 1,500 gge per day of hydrogen will tend to occupy a relatively large footprint because of the size and amount of process equipment involved. Reformer and BOP size reduction may be needed to decrease this footprint and enable wider adoption of distributed generation technologies.

Feedstock Issues

Feedstock costs, including transportation costs, are typically the single largest factor determining economic viability of hydrogen from bio-derived liquids.[35] Feedstock availability may be limited — owing to competition for biomass or lack of crops in some areas, for example — and the lower-cost feedstock may change throughout the year. Without significant reductions in feedstock cost, hydrogen from bio-derived liquids would not be economically viable.

Operations and Maintenance

All system components (e.g., contaminant removal, reforming, controls, utilities, sensors, compression, storage, dispensing, and safety) must be considered in O&M cost projections, which currently are too high. Hydrogen quality monitoring is also a potential barrier, as described in the Introduction. Although similar to DNGR, reforming of bio-derived liquids is more complex and will require a more complicated overall system. For distributed production, however, the O&M issues related to scheduled maintenance and demand management are nearly identical to those for DNGR systems (see Section 1.1).

Catalysts. The reformer and WGS unit operations require large amounts of catalysts and considerable maintenance. Commercial catalysts are designed for continuous use, whereas in distributed production, the reactors are turned on and off almost daily, causing thermal cycling that may degrade catalyst performance. Therefore, long-life, inexpensive, durable catalysts are needed. Gas-phase reforming of liquids is very similar to natural gas reforming and has many of the same barriers. The main differences are that vaporization must occur, the catalysts may need to be adjusted, and the steam-to-carbon ratio typically needs to be higher to avoid catalyst deactivation caused by coking and charring. APR has been primarily proposed for reforming of biomass or the aqueous phase of the pyrolysis oil. However, the aqueous phase of pyrolysis oil often contains significant amounts of carboxylic acid, such as acetic acid, which are very difficult to decompose to desired products, making catalyst development a primary need for APR.

Durability. For current systems, necessary repairs are frequent, and repair cost can be significant. Down time may adversely affect co-located businesses (e.g., convenience store, car washes).

Control and Safety

Control and safety barriers associated with reforming include poor performance of start-up and shut-down processes, insufficient turn-down capability, general feedstock issues, a lack of rapid on-off cycling, and feedstock storage tank refilling difficulties. Many of the control systems issues for renewable liquids reforming are the same as those for NG reforming. Reforming control and safety costs are high owing to complex system configurations and too many regulation-mandated sensors. The permitting process critically relies on the proven reliability and

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[35] J. D. Holladay, K. Hu, D. L. King, and Y. Wang, "An Overview of Hydrogen Production Technologies," *Catalyst Today* 139 (2009): 244–260.

safety of these units in the forecourt environment, and these criteria will be key qualification targets.

Strategy to Overcome Barriers and Achieve Technical Targets

Table 1 lists the critical R&D needs to reduce the cost of bio-derived liquid reforming. Process integration and catalyst durability are key areas where additional R&D can significantly improve hydrogen yield and meet cost targets.

Table 1 Bio-derived Liquid Reforming Hydrogen Production — Critical Technology Needs.

Barrier	Strategy
Capital Costs	➔ Integrating separate processes in to a single unit, such as combining a two-step water-gas shift and PSA separation into a single step water-gas shift with integrated separations, can significantly reduce capital cost of the reformer.[36] ➔ Incorporate alternative gas clean-up approaches
O&M Costs	➔ Improve heat integration ➔ Improved catalyst durability by mitigating coking and charring
Feedstock	➔ Use feedstock-flexible processes
Yield	➔ Design processes that produce higher hydrogen yields ➔ Improve selectivity through catalyst research

2.2 Biogas Reforming

Status

Biogas can be produced by anaerobic digestion of organic matter, such as municipal solid waste, discards from food processing, animal manure, sewage, stillage and glycerin from biofuels production, as well as energy crops and agricultural residues. In the anaerobic digestion process the organic matter is broken down in an oxygen-free environment producing significant amounts of methane. The U.S. total methane potential in raw biogas is estimated at about 16 million tonnes per year, with the net availability calculated at about 6.2 million tonnes (Table 2). For comparison, the U.S. NG consumption in 2016 was about 600 million tonnes[37].

Landfills represent the largest potential source of methane and hydrogen from both a total perspective as well as current net availability. Waste water treatment plants (WWTPs) can also be a significant source of methane for hydrogen production. The total potential from industrial, institutional and commercial (IIC) sources is slightly less than from the other biogas sources, yet it still represents a significant source of methane and hydrogen. Animal manure is a more dispersed resource found in rural areas. However, it can be a significant source of biogas if some of the economic issues of collection and aggregation can be overcome. It can provide a source of

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[36] Bio-derived Liquids to Hydrogen Distributed Reforming Working Group Background Paper, September 2016. https://energy.gov/sites/prod/files/2014/03/f10/biliwg_nov06_background_paper.pdf

[37] U.S. Energy Information Administration. "U.S. Natural Gas Monthly: Table 2 - Natural Gas Consumption in the United States, 2009-2014." 2014. Available from: www.eia.gov/oil_gas/natural_gas/data_publications/natural_gas_monthly/ngm.html

hydrogen for bridging transportation corridors between major metropolitan areas and bringing economic opportunities for rural areas.

Table 2 U.S. Methane and Hydrogen Potentials by Source [38]

Source	**Methane Potential (thousand tonnes/yr)**		**Hydrogen Potential (thousand tonnes/yr)**	
	Total	Available	Total	Available
WWTPs	2,339	1,927	618	509
Landfills	10,586	2,455	2,795	648
Animal manure	1,905	1,842	503	486
IIC organic waste	1,158	N/A	306	N/A
Total	*15,988*	*6,224*	*4,221*	*1,643*

The geographic distribution of the biogas sources shown in Figure 6 suggests that the largest biogas resources are located in close proximity to population centers, as would be expected as the majority of it is the result of human activity. This is also where the demand for hydrogen in industrial and vehicle refueling applications is expected to be highest. The estimates suggest that biogas and hydrogen from biogas produced from local, sustainable resources can supply upwards of 5% of the current U.S. vehicle fleet if that portion were replaced by FCEVs and, therefore, can aid with early FCEV rollout[38]. In addition reducing waste through the use of anaerobic digestion and utilization of produced biogas can help decrease greenhouse gas emissions and other environmental pollution to the air and water.

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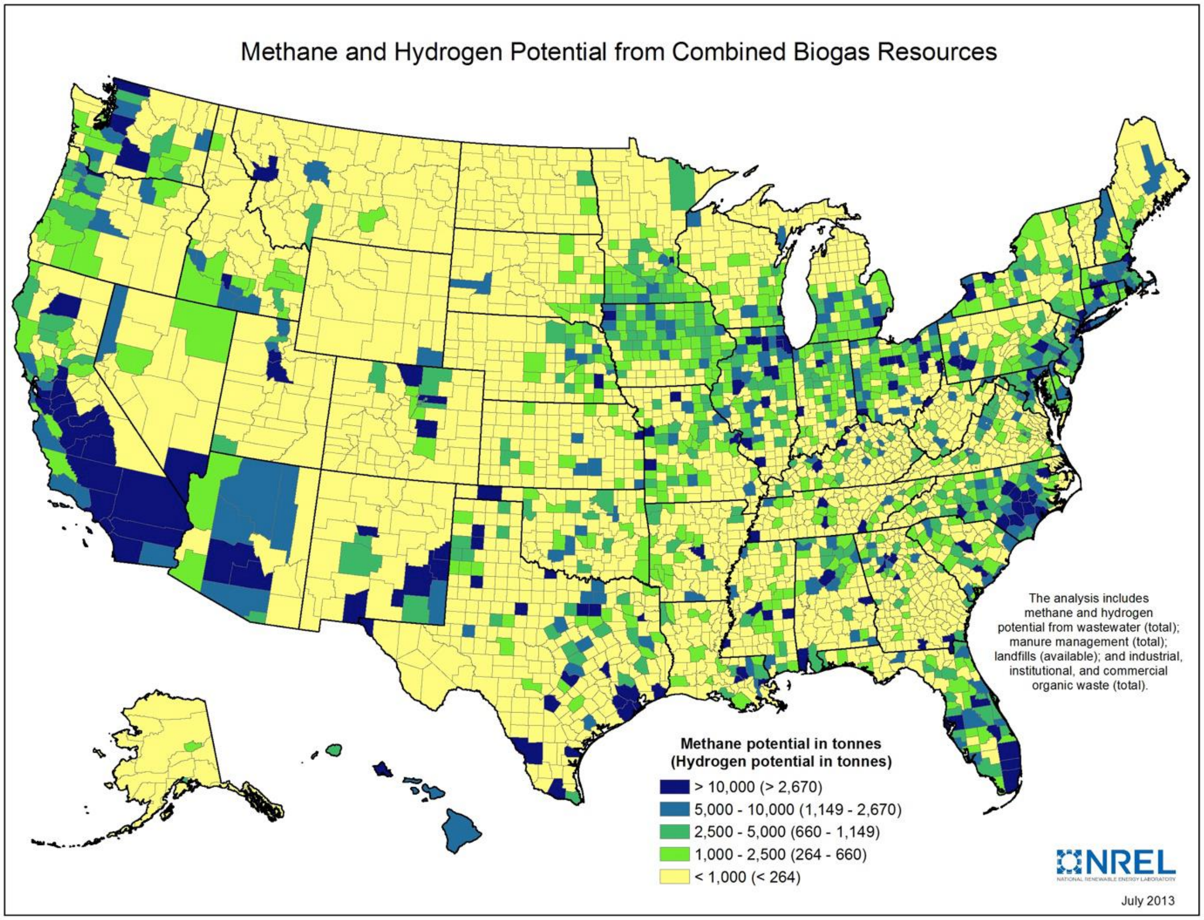
[38] G. Saur and A. Milbrandt, Renewable Hydrogen Potential from Biogas in the United States. NREL report, 2014



The analysis includes methane and hydrogen potential from wastewater (total); manure management (total); landfills (available); and industrial, institutional, and commercial organic waste (total).

July 2013

Figure 6 Methane and hydrogen potential from combined biogas sources in the United States by county.

As methane is the main component of biogas, it can be converted to hydrogen through the same processes as NG, as described in the fossil resources section. Though, unlike NG, which consist mainly of methane and have relatively few impurities, biogas contains methane at only 50%–70% level with 30%–50% CO_2 and large amounts of nitrogen and other particulates and contaminants which complicate processing. Sulfur, siloxanes, and halogens are the most damaging impurities which need to be removed to sub-ppm levels, which adds to the cost of clean-up as well as fuel quality monitoring. Therefore, additional clean up steps are required in biogas processing before it can be converted into hydrogen. Various chemical and biological purification processes are available on the biogas market. The efficiency of separating biomethane from biogas has been estimated to be 87% [39,40,41]. Once the biogas has been upgraded to natural-gas-quality biomethane, it can be used as a substitute for natural gas in an SMR process to produce hydrogen.

Gaps and Technical Barriers

Most technical barriers to converting biogas to hydrogen are similar to those for conversion of natural gas using SMR based systems. In addition, the need to pre-condition and clean up biogas before reforming constitute additional set of challenges to widespread application of hydrogen production from biogas. Estimates showed the clean-up of biogas costs ~2 cents per kWh of electricity, and ~30% of the O&M costs in an anaerobic digester gas fueled FC power plant [42].

Strategy to Overcome Barriers and Achieve Technical Targets

R&D needed to address the challenges of biogas clean up include:

- Developing affordable analytical equipment and methods suitable for rapid onsite analysis to overcome uncertainties and variations in the impurity levels and the lack of affordable sensors for the impurities at low detection limits
- Developing high capacity sorbents that are unaffected by moisture and hydrocarbons
- Developing accelerated test protocols for evaluating effective clean-up systems
- Developing ways to convert fuel impurities or spent sorbents into useful byproducts – this would convert a disposal problem to a revenue source and improve economics
- Manufacturing scalable, environmentally friendly, portable, low cost clean-up systems to drive down capital costs.

2.2 Biomass/Waste Conversion to Energy

Pathways for fermentative hydrogen production include traditional dark fermentation and microbial-aided electrolysis. In dark fermentation, bacteria decompose biomass into hydrogen and by-products without the need for sunlight.[43] Microbial-aided electrolysis combines the energy from microbial decomposition of organic matter with an additional small electric current to produce hydrogen;[44] the term microbial electrolysis cell (MEC) will be used in this document to encompass all the related system designs.

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[39] California Air Resources Board. “Detailed California-Modified GREET Pathway for Compressed Natural Gas (CNG) from Landfill Gas, Version 2.1.” California Environmental Protection Agency, 2009.

[40] California Air Resources Board. “Detailed California-Modified GREET Pathway for Compressed Natural Gas (CNG) from Dairy Digester Biogas, Version 1.0.” California Environmental Protection Agency, 2009.

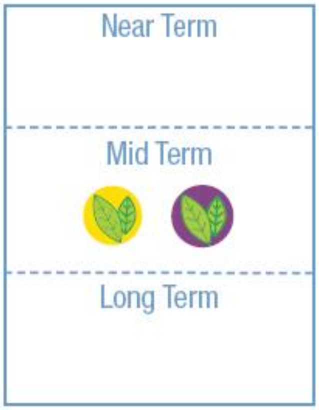
[41] Williams, R. B. et al. “Estimates of Hydrogen Production Potential and Costs from California Landfill Gas.” May 7–11, 2007, Berlin, Germany. 15th European Biomass Conference & Exhibition.

[42] Gas Clean-Up for Fuel Cell Applications Workshop report, 2014. https://energy.gov/sites/prod/files/2016/04/f30/fcto_gas_cleanup_workshop_report.pdf

[43] W. S. Kontur, D. R. Noguera, and T. J. Donohue, “Maximizing reductant flow into microbial H_2 production,” *Curr Opin Biotechnol.* 23, no. 3 (June 2012): 382–9, doi: 10.1016/j.copbio.2011.10.003; P. C. Hallenbeck, M. Abo-Hashesh, and D. Ghosh, “Strategies for improving biological hydrogen production,” *Bioresour Technol.* 110 (April 2012): 1–9, doi: 10.1016/j.biortech.2012.01.103.

[44] B. E. Logan, *Microbial Fuel Cells* (New York: John Wiley & Sons, 2008).

Fermentative Hydrogen Production



Feedstock:	Water Biomass
Energy Source:	Solar Biomass
Production:	Distributed Semi-Central Central

Fermentation uses microorganisms that break down biomass to produce hydrogen as a metabolic product or through microbe-aided electrolysis. This is a mid- to long-term technology that will most likely be suitable for distributed, semi-central, and central hydrogen production facilities, depending on the feedstock used.

Status

Hydrogen fermentation and MECs are in an early phase of development, requiring both fundamental and applied R&D. Perhaps the nearest-term opportunity for these technologies are systems that produce a usable fuel by using industrial, municipal or agricultural wastes as a feedstock. Pilot systems using these feedstocks currently exist for both fermentation and MECs, but hydrogen yields and rates are low.[45] These systems may be made feasible due to their distributed hydrogen production potential and by offsetting other costs, even if hydrogen production yields and rates are low. For example, systems that utilize a waste stream could become economical, in part, by replacing costly wastewater treatment processes while producing a valuable fuel.[46]

Dark Fermentation

Dark fermentation uses anaerobic bacteria on carbohydrate-rich substrates grown, as the name indicates, without the need for light. As the microbes break down the biomass substrate, a number of pathways can result in hydrogen production.[47] Many different metabolic steps are needed to either reduce or oxidize these electron carriers, depending on the initial feedstock and other conditions. Some by-products of this metabolism, such as organic acids, may be broken down further by microbes for energy but would not produce the necessary reduced ferredoxin or NADH to produce additional hydrogen.

For large-scale fermentative processes to be efficient, the biomass feedstock needs to be bioavailable, available in large quantities with consistent supply and quality, inexpensive, and possess high carbohydrate content[48]. Pure, simple sugars (such as glucose and lactose) are easily biodegradable but are more expensive and must be refined from biomass sources, so microorganisms are now being developed that can use other, less costly feedstocks, including wastes.[49] Hydrogen production rates and yields vary widely for different feedstocks, but as an example, fermentation of cellulose yielded 3.2 moles H_2/mole

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[45] R. D. Cusick et al., "Performance of a pilot-scale continuous flow microbial electrolysis cell fed winery wastewater," Appl Microbiol Biotechnol 89, no. 6 (March 2011): 2053–63, doi: 10.1007/s00253-011-3130-9; T. M. Vatsala, Raj S. Mohan, and A. Manimaran, "A pilot-scale study of biohydrogen production from distillery effluent using defined bacterial co-culture," International Journal of Hydrogen Energy 33, no. 20 (October 2008): 5404–5415, http://www.sciencedirect.com/science/article/pii/S0360319908008367.

[46] M. L. Chonga et al., "Biohydrogen production from biomass and industrial wastes by dark fermentation," International Journal of Hydrogen Energy 34, no. 8 (May 2009): 3277–3287.

[47] W. S. Kontur, D. R. Noguera, and T. J. Donohue, "Maximizing reductant flow into microbial H2 production," Curr Opin Biotechnol. 23, no. 3 (June 2012): 382–9, doi: 10.1016/j.copbio.2011.10.003; P. C. Hallenbeck, M. Abo-Hashesh, and D. Ghosh, "Strategies for improving biological hydrogen production," Bioresour Technol. 110 (April 2012): 1–9, doi: 10.1016/j.biortech.2012.01.103.

[48] DOE Hydrogen and Fuel Cells Program Record #16016, February 27, 2017. https://www.hydrogen.energy.gov/pdfs/16016_h2_production_cost_fermentation.pdf

[49] M. L. Chonga et al., "Biohydrogen production from biomass and industrial wastes by dark fermentation," International Journal of Hydrogen Energy 34, no. 8 (May 2009): 3277–3287; N. Ren et al., "Biohydrogen production from molasses by anaerobic fermentation with a pilot-scale bioreactor system," International Journal of Hydrogen Energy 31, no. 15 (December 2006): 2147–2157, http://www.sciencedirect.com/science/article/pii/S0360319906000814.

equivalent of glucose.[50] Using known metabolic pathways, a maximum of 4 moles H_2/mole of glucose can be produced. Industrial-scale fermentation for other products is well-developed, so although fermentation to produce hydrogen would have unique requirements, many of the necessary components have been developed and are available at large scales.

An analysis was conducted by Strategic Analysis, Inc. using the Hydrogen Analysis version 3.101 (H2A Production v3.101) model and its associated assumptions[51],[52] for a centralized production facility with a production capacity of 50,000 kg H_2/day.[53] The analysis utilizes a system design based on lab-demonstrated hydrogen production procedures and using capital costs derived from a 2013 NREL report[54] on the production of hydrocarbons from lignocellulosic compounds. The projected "current case" results in prohibitively high production costs of >$50/gge, but more importantly identifies real R&D opportunities to advance the current state-of-the-art and bring costs down significantly. The projected "future case" is based on technological advancements deemed feasible by 2025, including increasing the feedstock loading from ~13 (current case) to 175 g/L, consistent with the DOE Bioenergy Technologies Office target for biomass hydrolysis. This advancement, combined with other improvements, results in a projected cost of $5.65/gge for a 50,000 kg/day hydrogen production facility when a byproduct credit is considered.

HPTT 2016 Accomplishment

Pathway to Economic H_2 from Biomass Fermentation Case Study Developed

In 2016, the HPTT highlighted work supported by DOE through Strategic Analysis Inc. that provided a detailed cost analyses identifying a potential pathway for fermentative H_2 production to reach < $4/gge. Achieving this cost will require significant research success

Table 3 Sensitivity analysis results for the projected Future case (with byproduct credit). Results of H_2 production cost for parameters varied are reported in 2007$ below the adjusted parameter[55].

Case Study	Optimistic Value (2007$/gge H_2)	Baseline Value (2007$/gge H_2)	Conservative Value (2007$/gge H_2)
Current Case (2015)	$59.76	$67.71	$75.67
Current Case (2015) with byproduct credit	$40.88	$51.02	$61.16
Future Case (2025)	$7.68	$8.56	$9.43
Future Casei[56](2025) with byproduct credit	$3.40	$5.65	$7.91

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[50] Office of Energy Efficiency and Renewable Energy, *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan* (Washington, DC: U.S. Department of Energy, June 2015), Section 3.1, https://energy.gov/sites/prod/files/2015/06/f23/fcto_myrdd_production.pdf.

[51] H2A is a discounted cash-flow model providing transparent reporting of process design assumptions and a consistent cost analysis methodology for hydrogen production at central and forecourt facilities. H2A addresses cost scenarios where sufficiently high annual and cumulative volumes have been reached so that economies of scale for capital and unit costs have been achieved. See also at: http://www.hydrogen.energy.gov/h2a_production.html.

[52] DOE Hydrogen and Fuel Cells Program Record #16016, February 27, 2017. https://www.hydrogen.energy.gov/pdfs/16016_h2_production_cost_fermentation.pdf

[53] H2A Production v3.1 Dark Fermentation Cases are at http://www.hydrogen.energy.gov/h2a_prod_studies.html. See Table 2 for a summary of case input parameters.

[54] Davis, R. et al. Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbons : Dilute-Acid and Enzymatic Deconstruction of Biomass to Sugars and Biological Conversion of Sugars to Hydrocarbons Process Design and Economics for the Conversion. (2013). doi:10.2172/1107470

[55] DOE Hydrogen and Fuel Cells Program Record #16016, February 27, 2017. Fermentation Record https://www.hydrogen.energy.gov/pdfs/16016_h2_production_cost_fermentation.pdf

[56] Uses 6.86¢/kWh effective electricity price (levelized over 40 yr. life) as electricity byproduct selling price.

Microbial Electrolysis Cells

MECs are a variation of microbial fuel cells. In microbial fuel cells, a microbial culture decomposes organic matter, excreting protons and transferring electrons to the anode; the electrons travel to the cathode and combine with oxygen and the protons to produce water, along with a low voltage.[57] In an MEC, a small voltage is added, resulting in the recombination at the cathode to produce hydrogen gas instead of water (Figure 7). With the bacteria breaking down the organic matter to electrons and protons and generating power, less external electric power is required as compared to standard water electrolysis. MECs can use feedstocks that would not support fermentative hydrogen production. Although CO_2 is produced at the anode through the metabolic processing, reactor designs can be made to ensure that the gas collected at the cathode is nearly pure hydrogen.

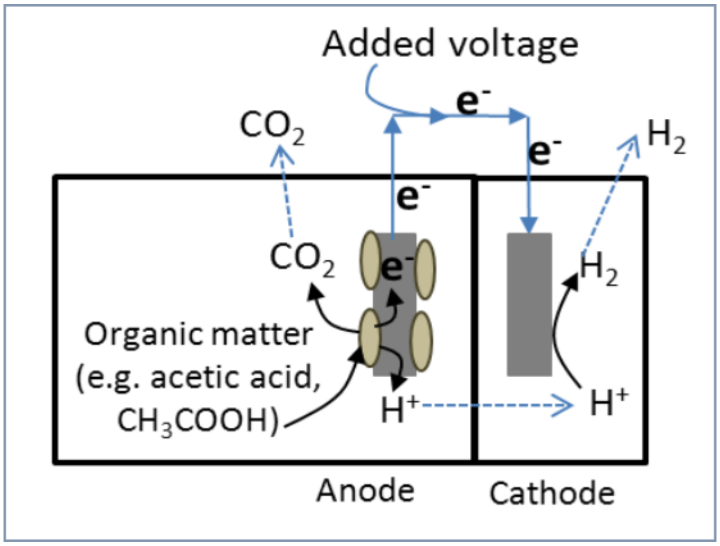

Figure 7 Microbial Electrolysis Cell.

For both fermentative and MEC hydrogen production, current microbial strains do not yet meet the production rates needed to meet the production cost goal of <$2/gge. There are ongoing efforts to improve the current strains and conditions, as well as to identify organisms with improved characteristics. In recent years, the number of microorganisms identified for potential use in these technologies has increased substantially.[58] Only a small fraction of naturally occurring microorganisms have been discovered and functionally characterized.[59] Research is ongoing to discover strains with the necessary characteristics and optimal growth conditions (e.g., pH, temperature, feedstock loading) for high hydrogen production rates and yields are being investigated.[60] Known organisms are being modified to improve their characteristics[61] and several recent review articles provide in-depth descriptions of the reaction pathways and types of enzymes being used in studies of biological hydrogen production.[62]

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[57] B. E. Logan, Microbial Fuel Cells (New York: John Wiley & Sons, 2008).

[58] G. Davila-Vazquez et al., "Fermentative biohydrogen production: trends and perspectives," Reviews in Environmental Science and Bio/Technology 7, no. 1 (January 2008): 27–45; S. Rittmann and C. Herwig, "A comprehensive and quantitative review of dark fermentative biohydrogen production," Microb Cell Fact. 11 (August 27, 2012): 115, doi: 10.1186/1475-2859-11-115.

[59] Vigdis Torsvik, Lise Øvreås, and Tron Frede Thingstad, "Prokaryotic Diversity — Magnitude, Dynamics, and Controlling Factors," Science 296, no. 5570 (May 10, 2002): 1064–1066.

[60] G. Davila-Vazquez et al., "Fermentative biohydrogen production: trends and perspectives," Reviews in Environmental Science and Bio/Technology 7, no. 1 (January 2008): 27–45; S. Rittmann and C. Herwig, "A comprehensive and quantitative review of dark fermentative biohydrogen production," Microb Cell Fact. 11 (August 27, 2012): 115, doi: 10.1186/1475-2859-11-115.

[61] P. C. Maness, "Fermentation and Electrohydrogenic Approaches to Hydrogen Production" (2012 Annual Merit Review Presentation, May 16, 2012), http://www.hydrogen.energy.gov/pdfs/review12/pd038_maness_2012_o.pdf.

[62] W. S. Kontur, D. R. Noguera, and T. J. Donohue, "Maximizing reductant flow into microbial H2 production," Curr Opin Biotechnol. 23, no. 3 (June 2012): 382–9, doi: 10.1016/j.copbio.2011.10.003; P. C. Hallenbeck, M. Abo-Hashesh, and D. Ghosh, "Strategies for improving biological hydrogen production," Bioresour Technol. 110 (April 2012): 1–9, doi: 10.1016/j.biortech.2012.01.103; G. Davila-Vazquez et al., "Fermentative biohydrogen production: trends and perspectives," Reviews in *Environmental Science and Bio/Technology* 7, no. 1 (January 2008): 27–45; M. D. Redwood, M. Paterson-Beedle, and L. E. Macaskie, "Integrating dark and light biohydrogen production strategies: towards the hydrogen economy," *Reviews in Environmental Science and Bio/Technology* 8, no. 2 (2009): 149–185.

Combined Systems

Integration of different technologies may make it possible to create an economically and technically viable system without overcoming all of the individual technology barriers. Combining an MEC reactor with a dark fermentation reactor has been shown to increase overall hydrogen yield (at the laboratory scale), resulting in production of hydrogen from the biomass feedstock at levels approaching the stoichiometric maximum for the combined system, increasing the total hydrogen production capability vs. stand-alone, single-technology systems.

Both fermentation and MEC systems have the potential, alone or in combination, to be integrated with waste treatment systems in which a bioavailable waste product (food waste, sewage, etc.) could act as the feedstock.[63] As mentioned earlier, such a system could reduce the net costs of hydrogen production by replacing costly wastewater treatments with a system that could both treat waste and produce a useable by-product. In this case, production could occur on a distributed or semi-central scale with the reactor systems installed at the site of waste production. Different waste products would have different challenges with respect to feedstock utilization and may have lower stoichiometric hydrogen yields, but the economic and sustainability considerations may allow this production pathway to reach commercial viability earlier than other biological production pathways.

Gaps and Technical Barriers

DOE's research activities are being driven by specific barriers identified in the MYRD&D[64], as well as others identified by the U.S. DRIVE Partnership's HPTT. Barriers facing cost-effective fermentative and MEC hydrogen are described on the following pages. In addition to these, the lack of identified species and consortia, condition characterization and tool development are common barriers to biomass/waste energy conversions.

Dark Fermentation

Hydrogen Production Yields and Rates

Hydrogen yield and production rates are both too low. Methods to increase yield and production must be developed. Trade-offs between yield and rate must be identified and considered. The ultimate goal of this technology pathway is to generate 10 moles H_2/mole glucose, or the equivalent yield for other carbohydrates. Limiting factors include metabolic by-product accumulation, including waste acids and solvents, and competing metabolic pathways. In addition, selectivity to hydrogen over other products such as ethanol needs to be improved.

Waste By-products

Waste by-products (e.g., butyric acid and ethanol) may compete with hydrogen production in fermentation and/or inhibit further hydrogen production. Metabolic pathways that reduce the production of waste acids, or methods to utilize these waste acids, must be identified or developed.

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[63] B. E. Logan, Microbial Fuel Cells (New York: John Wiley & Sons, 2008); M. L. Chonga et al., "Biohydrogen production from biomass and industrial wastes by dark fermentation," International Journal of Hydrogen Energy 34, no. 8 (May 2009): 3277–3287; N. Ren et al., "Biohydrogen production from molasses by anaerobic fermentation with a pilot-scale bioreactor system," International Journal of Hydrogen Energy 31, no. 15 (December 2006): 2147–2157, http://www.sciencedirect.com/science/article/pii/S0360319906000814.

[64] Office of Energy Efficiency and Renewable Energy, *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan* (Washington, DC: U.S. Department of Energy, June 2015), Section 3.1, https://energy.gov/sites/prod/files/2015/06/f23/fcto_myrdd_production.pdf

Feedstock Issues

Feedstock is a major cost driver for hydrogen production using this technology. Refined sugars such as glucose may result in a higher molar yield but are expensive. Currently available cellulolytic microbes and other organisms do best with relatively pure feedstocks and still have insufficient yields. This lack of flexibility drives up feedstock costs. For raw biomass, seasonal availability must also be considered. Pathways and microbes for using lower-cost feeds must be identified.

Reactor Systems

Reactor systems will need to be developed to remove and separate the hydrogen gas from the reactor headspace. Materials that are hydrogen-compatible may need to be incorporated into current industrial-scale reactor system designs. Prevention of methanogen (microorganisms that produce methane by consuming the hydrogen and CO_2 released by the dark fermentation process) contamination is also required.

MECs

Biological System Performance

Evaluation of different microbial communities that enable improved hydrogen production need to be evaluated, and conditions that best balance production rates and total yields with reactor performance must be identified.

Material Development

This technology uses materials similar to polymer electrolyte membranes (PEM) electrolyzers in conjunction with microbes for the anode. Novel durable cathodes and non-precious metal catalysts are needed for the cathode to enhance hydrogen evolution. Lower-cost materials and/or multifunctional materials are being identified and evaluated for long-term performance and need to be tested for larger-scale systems. Electrode materials range from carbon cloths and papers to graphite rods, plates, brushes and granules.[65] Materials with improved durability, greater strength, and lower costs are needed for practical scale units. In addition, electrodes with high surface areas are required for high reaction rates.

Reactor Design

MEC reactors for practical applications will be scaled up from the current laboratory-scale devices in use.[65] The scaled-up reactors will need to offer performance similar to or surpassing that of the current lab-scale reactors while minimizing BOP, maintenance, and cost. The lab-scale reactors have shown high molar yields (2-3.2 moles H_2/mole hexose, which is 50-80% of the theoretical molar yield), but the rate at which the hydrogen is produced needs to be increased substantially. Methods to monitor and control the microbes and conditions must also be considered.

Feedstock Issues

This technology has been shown to operate on acetic acid and several other volatile acids (commonly produced as fermentation end products), glucose, and cellulose, and other sources of organic matter (e.g., municipal and industrial wastewater). Systems that can reach high yields and production rates using low-cost, abundant feedstocks are needed to improve the economics of hydrogen production. In theory, acetic acid and other organic compounds could be obtained from the waste product of the dark fermentative hydrogen production, solving the feedstock problem for microbial electrolysis and the waste problem for the fermentative process.

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[65] B. E. Logan, Microbial Fuel Cells (New York: John Wiley & Sons, 2008); M. L. Chonga et al., "Biohydrogen production from biomass and industrial wastes by dark fermentation," International Journal of Hydrogen Energy 34, no. 8 (May 2009): 3277–3287; N. Ren et al., "Biohydrogen production from molasses by anaerobic fermentation with a pilot-scale bioreactor system," International Journal of Hydrogen Energy 31, no. 15 (December 2006): 2147–2157, http://www.sciencedirect.com/science/article/pii/S0360319906000814.

Strategy to Overcome Barriers and Achieve Technical Targets

Table 4 lists critical technology needs for biological hydrogen production. Discussion of these efforts follows the exhibit. Note that a single R&D activity may address more than one barrier, and multiple R&D activities may be needed to address a single barrier.

Table 4 Fermentative and MEC Hydrogen Production — Critical Technology Needs.

Barrier	Strategies
Microorganism Functionality	➔ Identify and characterize microorganisms and consortium with hydrogen production activity ➔ Identify conditions that optimize hydrogen production ➔ Develop or engineer strains and consortia with improved feedstock utilization, hydrogen production rates and yields, and reduced by-products ➔ Integrate the optimal functionality of the microorganisms into single organism or consortium
Feedstock Costs	➔ Identify low-cost feedstocks available in large supplies that can be efficiently converted to hydrogen (for example, through R&D funded by the DOE Bioenergy Technologies Office or through utilization of waste streams as feedstocks) ➔ Develop microbial strains or consortia that can flexibly and efficiently utilize low-cost feedstocks
Materials Needs	➔ Identify or develop low-cost, durable, high-efficiency MEC materials
Capital Costs	➔ Identify or develop robust, low-cost microorganisms and consortia ➔ Reduce materials and component costs ➔ Reduce manufacturing and installation costs
Fermentation/MEC Integration	➔ In theory, acetic acid and other organic compounds could be obtained from the waste product of the dark fermentative hydrogen production, solving the feedstock problem for microbial electrolysis and the waste problem for the fermentative process.

Addressing all of the barriers to meet commercialization cost targets for fermentative and MEC hydrogen production will require simultaneous R&D efforts in several areas, along with efforts to develop policy, standards, and delivery infrastructure technology. Although these efforts are taking place concurrently, the impact of each effort on the entire hydrogen production system must be kept in mind and integrated into systems optimization efforts.

In the near term, developing microorganisms and conditions with increased hydrogen productions rates and yields is a high priority, especially using economical feedstocks at higher loadings. For MECs, low-cost, durable, high-efficiency materials are a priority, as are system designs that allow scaled-up reactors with production rates and yields similar to bench-scale systems. In the longer term, large-scale system designs must be developed that consider reductions in O&M and capital costs.

2.3 Other biological based options

Photobiological hydrogen production uses microorganisms to convert solar energy into hydrogen. Photolytic production uses microorganisms, such as green microalgae or cyanobacteria, and sunlight to split water through direct or indirect photolysis routes. In photofermentative hydrogen production, sunlight is the driver for photosynthetic bacteria to break down organic compounds (either generated by the microbes themselves or supplied to them), releasing hydrogen. By using sunlight and water (added organic compounds are also an option), photobiological hydrogen production offers a potential for clean, sustainable hydrogen production. These biological hydrogen production methods are in the early-stage of research and present 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. Due to the early-stage of the research in this area, the HPTT has recommended that research in this area would be appropriate for Basic Energy Sciences.

Another biological pathway showing potential for increased hydrogen yield is in vitro synthetic enzymatic biosystems to convert sugar to hydrogen. Current research has theorized it possible to approach the theoretical hydrogen yield.[66]

3.0 Pathways Utilizing Direct Water Splitting

Direct water splitting pathways encompass both near and long-term pathways, including both low- and high-temperature water electrolysis as well as emerging solar to hydrogen pathways based on direct photoelectrochemical (PEC) and solar thermochemical (STCH) water splitting.

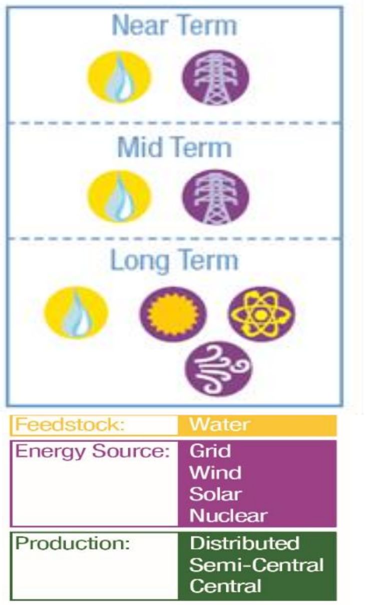
The near-term pathway for hydrogen production through water electrolysis calls for using the existing infrastructure for water and electricity. Emission impacts of this technology will be greatly reduced when the electricity to power electrolysis is supplied by near-zero emissions sources such as wind, solar, or nuclear energy. Water electrolysis is being pursued for distributed, semi-central, and central production. DOE's current R&D priorities focus on materials development, and integration with renewable electricity sources.

A long term goal for large-scale, centralized hydrogen production is solar water splitting via PEC and/or STCH production pathways. These pathways use solar energy directly, providing for enhanced energy security independent of the grid; and offering the potential for meeting DOE cost targets (if the considerable R&D challenges can be addressed).

3.1 Water Electrolysis

Electrolysis is a promising option for hydrogen production that uses electricity to split water. Electrolyzers (the unit in which the electrolysis reactions take place) can range in size from small, appliance-size equipment that is well-suited for small-scale distributed hydrogen production to large-scale, central production facilities that can be tied directly to the grid or to renewable or other non-greenhouse-gas-emitting forms of electricity production.

Water Electrolysis



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[66] https://www.hydrogen.energy.gov/pdfs/review17/pd127_zhang_2017_o.pdf

There are several types of electrolyzers. In a polymer electrolyte membrane (PEM) electrolyzer water reacts at the anode to form oxygen and positively charged hydrogen ions (protons). The electrons then flow through an external circuit and the hydrogen ions selectively move across the PEM to the cathode where the hydrogen ions combine with electrons from the external circuit to form hydrogen gas. This process is illustrated in Figure 8.

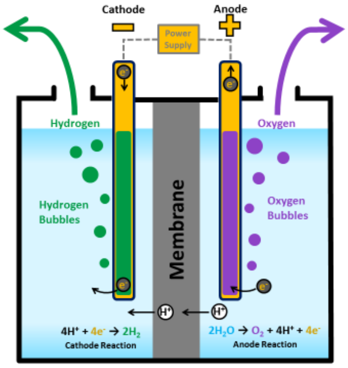

Figure 8 Schematic of a polymer electrolyte membrane (PEM) electrolyzer.

Alkaline electrolyzers operate via transport of hydroxide ions (OH-) through the electrolyte from the cathode to the anode with hydrogen being generated on the cathode side. Electrolyzers using a liquid alkaline solution of sodium or potassium hydroxide as the electrolyte have been commercially available for many years. Newer approaches using solid alkaline exchange membranes as the electrolyte are showing promise on the laboratory scale.

Solid oxide electrolyzers use a solid ceramic material as the electrolyte that selectively conducts negatively charged oxygen ions at elevated temperatures, but with lower electricity requirements (i.e. higher electrical efficiency). Water at the cathode combines with electrons from the external circuit to form hydrogen gas and negatively charged oxygen ions which then pass through the solid ceramic membrane and react at the anode to form oxygen gas and generate electrons for the external circuit.

The different electrolyzer types typically operate over different temperature ranges. Solid oxide electrolyzers must operate at temperatures high enough for the solid oxide membranes to function properly (typically 700°–800°C), compared to PEM electrolyzers, which operate at 70°–90°C, and commercial alkaline electrolyzers, which operate at 100°–150°C. The solid oxide electrolyzers can effectively use heat available at these elevated temperatures (from various sources, including nuclear energy) to decrease the amount of electrical energy needed to produce hydrogen from water, but the elevated temperatures also pose additional materials challenges.

Status

Distributed commercial hydrogen production via water electrolysis is considered a near- to mid-term technology and is being deployed on site at distributed/ forecourt hydrogen refueling stations, where it could stimulate market acceptance. In the longer term, centralized production has the potential to expand substantially the commercial supply of hydrogen by water electrolysis. Larger semi-central and central production via wind and nuclear heat and power is being investigated by both DOE's EERE and NE Offices.

Distributed hydrogen production via electrolysis has near- to mid-term potential because many existing forecourt stations may be able to incorporate an electrolysis unit, albeit with potentially higher electricity costs compared to central production. There are hydrogen fueling stations today that use electrolysis to generate hydrogen onsite[67]. Low-temperature, modular electrolysis units have the potential to be reasonably small (~100 kg/day) and able to use the existing water and electricity infrastructures. The compact, modular nature of the technology enables hydrogen production to grow as demand increases simply by adding electrolysis units. This modularity decreases initial installation costs, while electrolysis at larger, central facilities can take advantage of economies of scale. Water can be obtained and treated in

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[67] CaFCP members ITM Power, Hydrogenics, and H2Logic develop stations that use onsite electrolysis., https://cafcp.org/blog/resources-californias-hydrogen-stations-webinar-august-31, accessed 8/31/2017

high volumes at low cost. Large electrolysis modules can be built, and cascaded modules can then be brought on line as needed.

Electrolytic hydrogen production may be particularly useful for load-leveling of the electricity generated from wind turbines, reducing fluctuations in capacity or augmenting capacity during periods of peak electricity demand. Therefore, it may be feasible to negotiate favorable electricity rates by operating the electrolyzers during off-peak periods. Electrolyzers potentially have a secondary use for grid stabilization (e.g., by mitigating frequency disturbances), helping the overall economics. As a further example, in Europe, electrolysis is being pursued as a means of grid stabilization through hydrogen storage. In one approach, excess wind energy, which would otherwise not be utilized, drives electrolysis and the hydrogen produced is then injected into the natural gas grid as a means of storage and renewable gas production.[68,69] These concepts of intermittent electrolyzer operation during periods of low electricity cost with multiple value streams for the hydrogen generated form the basis for DOE's H2@Scale initiative which could ultimately provide a route for low cost hydrogen for FCEVs.

Further, there are possible advantages to high-temperature electrolysis operation using available process heat from sources such as concentrated solar power or next-generation nuclear reactors. DOE-NE has examined the option of using heat from nuclear power plants to provide thermal energy for high-temperature electrolysis. High-temperature electrolyzers require about two-thirds of the electrical energy needed by low-temperature electrolyzers to produce the same amount of hydrogen; the additional energy is provided by heat added to the system.[70]

Recent technoeconomic analyses have been performed and published by Strategic Analysis, Inc. including current cases (based on lab-proven technology) and future cases (based on expected technology advancements) for PEM central and forecourt and SOEC central hydrogen production technologies[71,72]. In both cases, there is the potential to bring costs down through R&D, but the significant cost driver is the cost of electricity as illustrated in the cost breakdowns in Figure 9.

Table 5 Current case and future case baseline costs of central SOEC and PEM and forecourt PEM.

	Current Case Study Baseline ($/gge H_2)	**Future Case Study Baseline** ($/gge H_2)
Central SOEC	$4.95	$3.83
Central PEM	$5.12	$4.20
Forecourt PEM	$5.14	$4.23

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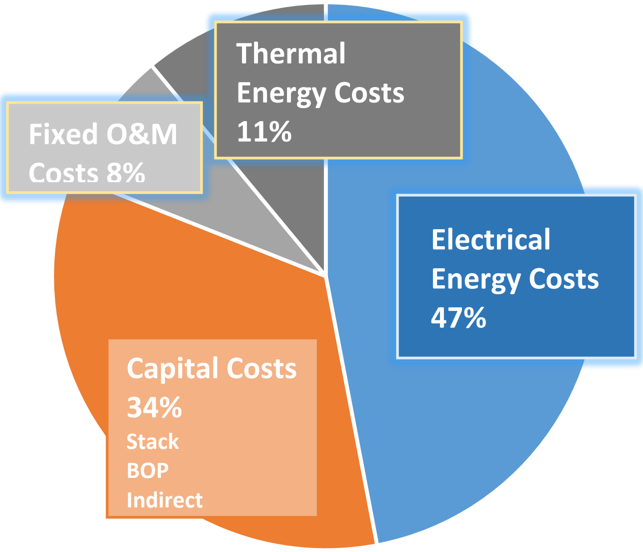
[68] M. Peters, "Renewable Electrolysis Integrated Systems Development and Testing," https://www.hydrogen.energy.gov/pdfs/progress16/ii_b_1_peters_2016.pdf

[69] FCH Joint Undertaking, "Study On Early Business Cases For H2 in Energy Storage and More Broadly Power to H2 Applications" (2017): http://www.fch.europa.eu/sites/default/files/P2H_Full_Study_FCHJU.pdf

[70] J. D. Holladay, K. Hu, D. L. King, and Y. Wang, "An Overview of Hydrogen Production Technologies," Catalysis Today 139 (2009): 244–260.

[71] https://www.hydrogen.energy.gov/pdfs/16014_h2_production_cost_solid_oxide_electrolysis.pdf

[72] https://www.hydrogen.energy.gov/pdfs/14004_h2_production_cost_pem_electrolysis.pdf



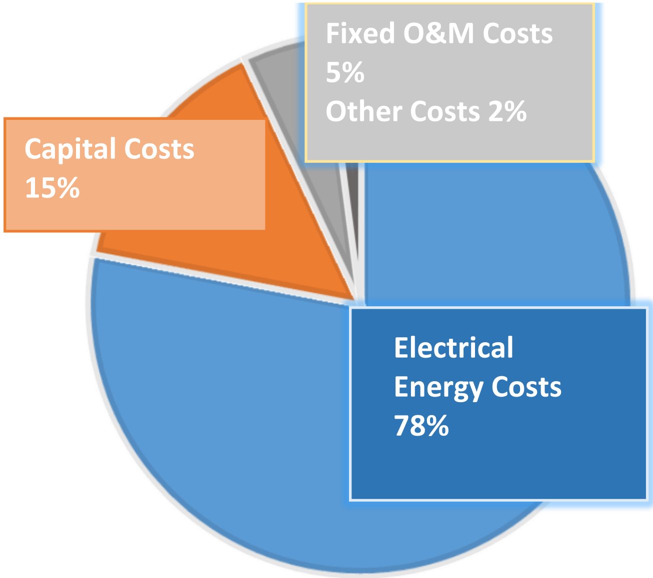


Figure 9 Cost breakdown for SOEC (top) and PEM (bottom). In both cases, the electricity feedstock cost is the largest cost driver.

Gaps and Technical Barriers

DOE's research activities are being driven by specific barriers identified in the MYRD&D[73], as well as others identified by the U.S. DRIVE Partnership's HPTT. Barriers facing cost-effective hydrogen using electrolysis are described on the following pages.

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[73] Office of Energy Efficiency and Renewable Energy, *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan* (Washington, DC: U.S. Department of Energy, June 2015), Section 3.1, https://energy.gov/sites/prod/files/2015/06/f23/fcto_myrdd_production.pdf

System Efficiency and Electricity Cost

For electrolyzers across all applications, electricity is the most significant portion of the hydrogen production cost. Major inefficiencies exist in current electrolysis stacks, drying subsystems, and power electronics.

Current low-temperature electrolysis stack- and system-level efficiencies are up to 74% and 67%, respectively (based on the lower heating value [LHV] of hydrogen and all systems and auxiliaries except compression). Based on analysis to achieve the DOE cost targets, the system efficiency needs to increase to 75% (LHV) with electricity costs decreasing to <$0.04/kWh.[74] The primary losses associated with the electrolyzer stack are currently in the oxygen-generating electrode. Improved catalysts and membranes may enable some efficiency improvements. In addition, operating at high temperatures, made possible with use of solid oxide electrolyzer technology, will increase the stack electrical efficiency with it approaching theoretical maximum for LHV. These higher-temperature systems will need greater durability, requiring development of corrosion-resistant materials and improved seals.

Producing the hydrogen at higher pressures within the electrolyzer stack may decrease the need for compressors and make it feasible to eliminate the compressors completely in some applications. Most commonly, water electrolysis is carried out at lower pressures (100-300 psig), but current laboratory testing shows it can be performed at pressures as high as 10,000 psig. Losses in stack efficiency and throughput limitations resulting from high-pressure operation may be compensated by reductions in compression costs. Optimization of high-pressure electrolyzer operation and subsequent compression is needed to determine the proper balance.

Once the hydrogen is produced, residual water needs to be removed prior to compression. Depending on the method used to dry the gas, 10% or more of the generated hydrogen may be lost, or a significant amount of electricity may be consumed. Improved processes must be identified and deployed to decrease these losses.

Power electronics that convert alternating current (AC) power to direct current (DC) power suitable for electrolysis operation can be the source of significant power losses. Power supplies are often quoted at 90% to 95% efficiency, but in the field, testing has shown otherwise. At higher temperatures and non-optimal varying operating currents, the measured efficiency can be closer to 75% to 80%, representing significant loss. Further work is needed to develop optimized power electronic systems optimized for integration with electrolyzer systems.

Renewable and Nuclear Electricity Generation Integration

Better integration of electrolysis systems with renewable energy is needed. The variability of renewable energy is a concern when powering water electrolysis. Electrolyzers have shown sub-second response time to changing power profiles so they should be able to operate effectively with intermittent power, though there remains some concern of the impact of this intermittent operation on the long-term durability of the electrolyzer cell components, especially for next generation, low PGM loaded electrodes. Integration with nuclear generation presents barriers associated with system component designs as well as with certifications, codes, and standards.

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[74] Office of Energy Efficiency and Renewable Energy, *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan* (Washington, DC: U.S. Department of Energy, June 2015), Section 3.1, https://energy.gov/sites/prod/files/2015/06/f23/fcto_myrdd_production.pdf.

Capital Costs

Capital costs for current electrolyzer technologies are a barrier to attaining the targeted hydrogen production cost. High capital costs are caused by expensive materials, relatively small systems, relatively low efficiencies, customized power electronics and other BOP components, and labor-intensive fabrication.

The high costs of noble metals and the lack of durability drive up electrode and membrane costs. Current production rates are below targeted levels, and systems are incapable of efficiently operating at the high current densities that would allow decreased stack size. Cell and stack architecture are often too complex and do not have a long enough life span. Generally, production volume is insufficient to meet projected future demand. Custom-built power electronics and other BOP components also contribute to increased capital costs. Higher-temperature systems also need low-cost thermal management (e.g., vaporizers, recuperators).

Manufacturing

Electrolysis units are currently produced in low volume. Mass production is capital-intensive, and manufacturers must therefore have assurance that the product demand will be high enough to enable adequate return on investment. The industry expects that manufacturing techniques can progress sequentially from hand processes to low-volume, semi-automated, automated, and finally high-volume automated processes, similar to automotive manufacturing. A step change in cost is anticipated for each change in manufacturing technique. Currently, low-volume manufacturers have little leverage to obtain lower costs or preferred materials from suppliers. For example, solid oxide electrolyzers require stainless steel manifolds and interconnects. The optimal thickness of the steel is not a standard size, and to get the desired thickness would require a steel run of approximately 70,000 pounds. At low-volume production, manufacturers would be forced to pay extra for the steel or use plates that are of less than optimal thickness.

Site-specific fabrication drives up manufacturing costs of crucial system and BOP components, often resulting in systems that are larger than necessary. In order to increase the hydrogen production capacity, stacks and cells will need to be scaled-up in a high volume manufacturing process while maintaining performance and other required characteristic is challenging

Operations and Maintenance

O&M costs for distributed hydrogen production from water electrolysis remain high. For distributed production, some of the O&M issues related to durability, scheduled maintenance, and demand management are nearly identical to those for DNGR systems (see Section 1.2). Central hydrogen production entails O&M costs, and even though the specific needs and constraints may vary from the distributed case, the themes are similar. All system components must be considered in O&M, including power conditioning/management, feed pre-conditioning (e.g., water purification), controls, utilities, QA/QC (e.g., sensors), compression, storage, dispensing, and safety.

Efficiency. The major cost during operation is electricity, so the efficiency of the electrolysis system (stack, BOP, power conditioning/management, etc.) is crucial. However, there are trade-offs between efficiency and capital cost. The stacks could be operated at extremely high efficiencies, but to achieve the desired production rates, larger stacks (increased capital cost) would be required. Techno economic analysis can be used to help determine the projected optimal balance between efficiency and capital costs.

Durability. Commercial PEM electrolyzers can run for tens of thousands of hours; however, there are some potential durability concerns with the more advanced cell components which are still at the lab scale. High-temperature stacks require improved materials that are inexpensive, efficient, and highly resistant to corrosion. In addition, high-temperature seals must be able to operate at moderate pressures and withstand thermal cycling.

Transients and Duty Cycles. For central wind and distributed production cases, water electrolysis units will not be operated at constant levels because of variations in power (wind) or fluctuating demand (distributed). Water electrolysis systems face challenges in achieving efficient operation over a wide range of conditions and there is a potential impact on durability as well.

Control and Safety

Control and safety barriers associated with water electrolysis include the efficiency of start-up and shut-down processes, turn-down capability, and the capability for rapid on-off cycling. Control and safety system costs remain high owing to complex system designs and necessary high-cost sensors. For distributed production, the permitting process relies on the proven reliability and safety of these units. These units must be designed to operate in an environment requiring no manual assistance, which will necessitate back-up/fail-safe modes, remote monitoring, and sparse maintenance schedules. Centralized production will require development of new control and safety procedures. This is particularly true for central generation using nuclear power.

Strategy to Overcome Barriers and Achieve Technical Targets

Table 6 lists critical technology needs for water electrolysis hydrogen production. Discussion of these efforts follows. Note that a single R&D activity may address more than one barrier or multiple R&D activities may be needed to address a single barrier.

Table 6 Water Electrolysis — Critical Technology Needs.

Barrier	Strategies
Capital Costs	➔ Materials with improved corrosion resistance and conductivity, and lower costs ➔ Low PGM and PGM-free catalysts with improved durability and activity ➔ Optimized membrane electrode assemblies ➔ Novel, integrated system architecture, including efficient thermal integration ➔ Lower cost balance of plant components ➔ System optimization to manage variable demands ➔ DFMA/high-volume equipment manufacturing
Operations and Maintenance Costs	➔ Automated process control ➔ Improved reliability ➔ Improved system efficiency ➔ More efficient H_2 quality control/hydrogen drying ➔ Efficient water conditioning ➔ Increase capital utilization ➔ Strategies for operation only at times of low electricity costs

Meeting the foregoing challenges and achieving the cost targets for commercially-competitive hydrogen production from water electrolysis will require diverse R&D efforts as well as the development of policies and standards. Many nuclear facilities currently have hydrogen safety protocols that may be adapted for production. In addition, standardizing certifications, codes, and standards will minimize control and safety concerns. Technology improvements must be developed in the context of a stringent regulatory environment, limited physical space, and resource limitations.

The cost of producing hydrogen from water electrolysis is largely determined by the electricity cost and, to a lesser extent, capital equipment costs. Thus, improved system efficiency and reduction of capital cost are the primary technology needs.

3.2 Photoelectrochemical Hydrogen Production

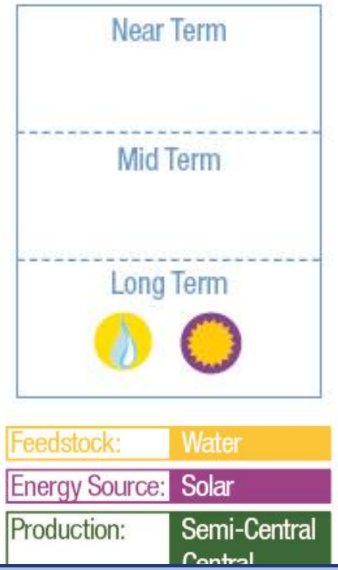
The PEC water splitting process uses semiconductor materials to convert solar energy directly into chemical energy in the form of hydrogen. The semiconductor materials used in the PEC process are similar to those used in photovoltaic solar electricity generation, but for PEC applications the semiconductor is immersed in a water-based electrolyte, where sunlight energizes the water-splitting process.

PEC is attractive among solar to hydrogen (STH) conversion technologies because efficient STH conversion can potentially be achieved at low operating temperatures using cost-effective thin-film and/or particle-based materials. It is an early-stage development technology that will be suitable for semi-central and central hydrogen production.

PEC reactors can be constructed in panel form (similar to photovoltaic panels) as electrode systems, or as slurry-based particle systems, with each approach having its own advantages and challenges. To date, panel systems have been the most widely studied because of their similarities with established photovoltaic panel technologies.

Since the 1972 publication of Fujishima and Honda's seminal paper describing the PEC water-splitting process on a titanium dioxide photoelectrode,[75] significant technical advances in photoelectrode R&D have resulted in numerous functional bench-scale systems. To date, PEC photoelectrode panel reactors composed of crystalline III-V semiconductors have demonstrated STH efficiencies as high as 16.2%[76] while multi-junction thin-film PEC cells have yielded efficiencies up to ~8% [77,78] at the bench-top laboratory scale. Primary technology development hurdles include durability, efficiency, and cost.

Photoelectrochemical Production



HPTT 2016 Accomplishment

New World Record Achieved for Direct Solar-to-Hydrogen Conversion

In 2016, the HPTT highlighted work supported by DOE through NREL, who recently made significant progress on the quest to high efficiency PEC systems by developing a cell which is over 16% efficient based on a novel III-V semiconductor tandem structure – achieving a new world record for immersed photoelectrodes

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[75] A. Fujishima and K. Honda, "Photolysis-decomposition of water at the surface of an irradiated semiconductor," Nature 238 (1972): 37–38.

[76] J. L. Young, M.A. Steiner, H.Döscher, R. M. France, J. A. Turner, and T. G. Deutsch, "Direct solar-to-hydrogen conversion via inverted metamorphic multi-junction semiconductor architectures", Nature Energy 2, (2017).17028

[77] S. Y. Reece, J. A. Hamel, K. Sung, T. D. Jarvi, A. J. Esswein, J. J. H. Pijpers, and D. G. Nocera, "Wireless solar water splitting using silicon-based semiconductors and earth-abundant catalysts," Science 334 (2011): 645–648.

[78] R. E. Rocheleau, E. L. Miller, and A. Misra, "High-efficiency photoelectrochemical hydrogen production using multijunction amorphous silicon photoelectrodes," Energy & Fuels 12 (1998): 3–10.

In panel reactors (illustrated in Figure 10a), the PEC water-splitting process begins with the absorption of a solar photon by the semiconductor device to form an excited electron-hole pair. The electron and hole are separated by an internal electric field, established by the semiconductor–electrolyte interface or by solid-state junctions buried within the semiconductor. The separated electron and hole are then collected at different surfaces, where they drive the hydrogen- and oxygen-evolving reactions, respectively. PEC systems can incorporate a single photon-absorbing semiconductor, or multiple absorbers in a higher-efficiency tandem device.[79]

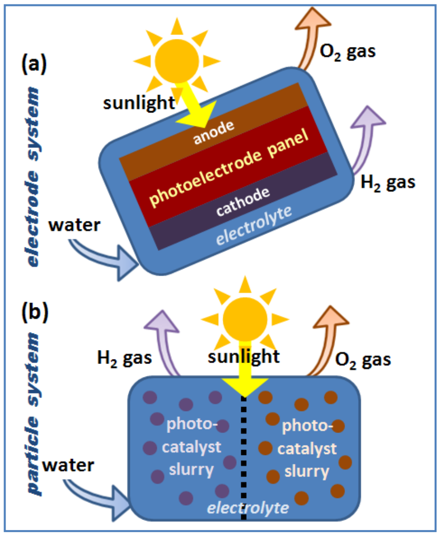

Figure 10 PEC Solar Water-splitting Reactors–(a) photo-electrode and (b) photocatalyst-

PEC hydrogen production may also be accomplished through the illumination of light-absorbing, semiconductor photocatalyst particles dispersed in water. Hydrogen and oxygen are evolved from separated H_2 and O_2 photocatalyst particles, as shown in Figure 10b. The overall water-splitting reaction is coupled by an intermediate ionic species "X" in solution (such as Fe^{3+}), which is reduced by the O_2 photocatalyst (e.g., to Fe^{2+}) and re-oxidized by the H_2 photocatalyst in a continuous closed-loop process.

The merits of the various reactor configurations for PEC systems must be evaluated in the context of broader technoeconomic analyses to determine the best paths forward for meeting the DOE production cost goal (<$2/gge). PEC devices have been fabricated with relatively high STH efficiencies ranging from 4% to over 16%.[80] Photocatalyst systems, however, offer the potential for lower overall cost of hydrogen due to elimination of panel and panel-mount infrastructure. Early technoeconomic models of PEC reactor systems based on the H2A tool[81] indicate long-term potential for cost-effective hydrogen production through both approaches. Current R&D priorities are focused on materials discovery and development, along with reactor design and engineering. As described below, these activities are directed to improve device performance (specifically, efficiency and durability) and decrease cost.

Through current R&D efforts, efficient, durable and cost-effective PEC materials systems and devices are being developed with the assistance of state-of-the-art methods in materials theory, synthesis and characterization, and with development of standardized methods for testing and reporting on PEC materials experimental work.[82]

Gaps and Technical Barriers

Driving DOE's research activities are specific barriers identified in the MYRD&D[83], as well as

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[79] E.L. Miller, A. DeAngelis, and S. Mallory, "Multijunction Approaches to Photoelectrochemical Water Splliting," in Photoelectrochemical Hydrogen Production, eds. R. van de Krol and M. Grätzel (New York: Springer, 2012) 205–276.

[80] https://www.hydrogen.energy.gov/pdfs/progress16/ii_0_miller_2016.pdf

[81] B. D. James, G. N. Baum, J. Perez, and K. N. Baum, *Technoeconomic Analysis of Photoelectrochemical (PEC) Hydrogen Production*, DOE Contract No. GS-10F-009J, produced by Directed Technologies Inc., Arlington, VA (Washington, DC: U.S. Department of Energy, 2009).

[82] Z. Chen, T. F. Jaramillo, T. G. Deutsch, A. Kleiman-Shwarsctein, A. J. Forman, N. Gaillard, R. Garland, K. Takanabe, C. Heske, M. Sunkara, E. W. McFarland, K. Domen, E. L. Miller, J. A. Turner, and H. N. Dinh, "Accelerating materials development forphotoelectrochemical hydrogen production: Standards for methods, definitions, and reporting protocols," *Journal of Materials Research* 25 (2010): 3–16.

[83] Office of Energy Efficiency and Renewable Energy, *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan* (Washington, DC: U.S. Department of Energy, June 2015), Section 3.1, https://energy.gov/sites/prod/files/2015/06/f23/fcto_myrdd_production.pdf

others identified by the U.S. DRIVE Partnership's HPTT described below.

Conversion Efficiency

PEC semiconductor efficiency is limited by light absorption, charge separation and charge transport in the bulk, and by energetics and charge transfer at the solid–liquid interface. Further development is needed for materials systems, such as tandem configurations, with appropriate bandgap for light absorption (e.g., <2.2 eV), with band-edges aligned energetically for hydrogen and oxygen evolution, with low-loss charge separation and transport in the solid state, and with interfaces kinetically favorable for the photoelectrochemical water-splitting half reactions. Technoeconomic analysis has indicated that meeting DOE cost targets will require durable PEC semiconductor material systems that provide a STH efficiency of >25% (photo-electrode configuration) or >10% (photo-particle configurations)[84] (as a point of reference, PEC efficiencies in excess of 30% STH are possible under ideal circumstances.[85]) Standardized theoretical, synthesis, and characterization methods in materials discovery and screening are important tools in the basic understanding of the bulk and interface loss mechanisms that limit efficiency.

Materials/Interface Durability

PEC semiconductor/electrolyte junctions are prone to both dark- and light-induced degradation due to corrosion reactions that compete with water-splitting half-reactions at the interfaces. Durable materials with the appropriate characteristics for high-efficiency PEC hydrogen production are still under development. For example, the high-efficiency materials currently available are prone to corrosion, while the most durable materials studied to date have demonstrated substantially lower STH conversion efficiency. Discovery of stable and efficient materials would be an ideal solution to this barrier, but such a finding represents a significant challenge. Promising alternative approaches focus on modification of surfaces through coatings or dispersions that stabilize the interface (energetically or kinetically) and protect the bulk. The use of PEC theory, synthesis, and characterization methods can facilitate a better understanding of corrosion mechanisms for development of mitigation schemes to enhance durability.

Materials Cost

Cost of the PEC semiconductor material system has a direct impact on capital costs and, thus, the cost of hydrogen. High-efficiency crystalline III-V materials systems are being developed to meet efficiency and durability requirements, but the cost of these materials could be prohibitive to large-scale deployment. Solar concentrator schemes to reduce the semiconductor footprint and new synthesis technologies are possible approaches for overcoming the cost barriers to utilizing crystalline semiconductors in PEC reactors. Lower-efficiency materials systems based on lower-cost thin-film or particle semiconductors are also being developed. Improved efficiencies are needed in these material systems.

Auxiliary Materials

In addition to the semiconductor absorber materials, auxiliary materials for integrated PEC devices include surface treatments, interface/linking materials (including soluble, transparent redox mediators for the particle-based systems) and separators that insure safe gas separation. Techniques are needed to synthesize these integrated device configurations while maintaining each component material's integrity,

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[84] Office of Energy Efficiency and Renewable Energy, *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan* (Washington, DC: U.S. Department of Energy, June 2015), Section 3.1, Office of Energy Efficiency and Renewable Energy, *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan* (Washington, DC: U.S. Department of Energy, June 2015), Section 3.1, https://energy.gov/sites/prod/files/2015/06/f23/fcto_myrdd_production.pdf.

[85] H. Döscher, J.F. Geisz, T.G. Deutsch, J.A. Turner, "Sunlight Absorption in Water– Efficiency and Design Implications for Photoelectrochemical Devices", Energy & Environmental Science 7 (9), (2014): 2951-2956

and appropriate manufacturing techniques based on these synthesis routes will be needed to scale device configurations to commercial scales.

Integrated Devices

Achieving ultimate targets in PEC solar hydrogen production requires efficient and stable integrated devices combining the best available PEC semiconductors, surface treatments and auxiliary interface and separator materials. These can be planar-integrated devices for photo-electrode reactor configurations or functionalized particle devices for photocatalyst reactor configurations. Integrated device designs that combine functionalized materials optimized for light absorption, charge transport and interfacial catalysis could simultaneously address issues of durability and efficiency. Even with the best available semiconductor absorber materials with properties consistent with efficient PEC solar water splitting, integration into optimized high-efficiency devices requires specific applied and engineering R&D efforts.

System-Level Considerations

Determination of the most cost-effective reactor configurations will require rigorous technoeconomic analysis, taking into account materials performance and cost parameters in addition to O&M costs. Technoeconomic models to compare the cost-effectiveness of different PEC reactor approaches need to take into account the system-level costs and the performance and cost parameters of the PEC materials systems under development. Reactors and systems must be designed to account for such elements as diurnal operation, water purity, ion transport (e.g., cell resistance), and gas handling (including drying and compression); and these systems must be evaluated based on costs of commodity materials of construction and system components. In addition, the overall cost sensitivity of hydrogen must be estimated as a function of these various engineering parameters.

Strategy to Overcome Barriers and Achieve Technical Targets

Table 7 lists the critical technology development needs for PEC hydrogen production. R&D activities within these categories address the critical technology barriers to the ultimate commercialization of PEC solar hydrogen generation.

Table 7 Photoelectrochemical — Critical Technology Needs.

Barrier	Strategies
Materials and Device Challenges	➔ Development of light-absorbing semiconductor materials systems compatible with high STH efficiency devices (>25% for photo-electrode configurations and >10% for photo-particle systems, typically requiring material system bandgap less than 2.0 eV for absorbing a high percentage of the solar irradiance) ➔ Develop Redox mediators for photo-particle PEC that are stable and transparent to visible light ➔ Improved catalytic/protective surface coatings compatible with operating conditions of high-efficiency STH devices ➔ Improved methods of fabrication that yield photo-electrode/ photocatalyst materials at target costs and target STH efficiencies
Supporting Scientific and Engineering Methodologies	➔ Advanced theoretical models of PEC semiconductor bulk and interface properties ➔ Advanced theoretical models of particle PEC that provide estimates of system efficiency as a function of particle size, bandgap, and rate of back reactions (i.e., with the redox mediator) ➔ Comprehensive portfolio of standard and advanced characterization tools for evaluating PEC materials and interfaces ➔ Wide portfolio of state-of-the-art techniques for synthesis of PEC materials and devices ➔ Theory-guided screening tools for discovery and development of novel PEC materials systems

	➔ Experimental combinatorial synthesis/rapid screening tools for discovery and development of novel PEC materials systems ➔ Standardized protocols for evaluation and reporting of PEC materials and device physical and operational parameters
System-Level Technoeconomic Analysis	➔ Perform detailed technoeconomic models of photo-electrode-based PEC reactor systems, including sensitivity analysis of prime contributing factors to hydrogen production cost ➔ Perform detailed technoeconomic models of photo-particle-based PEC reactor systems, including sensitivity analysis of prime contributing factors to hydrogen production cost ➔ Prioritization of fundamental and applied R&D needs for addressing the critical factors for reducing hydrogen production costs to meet DOE cost threshold targets

Addressing all of the barriers to commercialization cost targets for PEC hydrogen production will require simultaneous R&D efforts in several areas, along with efforts to develop policy, standards, and delivery infrastructure technology. Although these efforts are taking place concurrently, the impact of each effort on the entire hydrogen production system must be kept in mind and integrated into systems optimization efforts.

Current R&D priorities in PEC solar hydrogen production include fundamental, applied and engineering efforts to discover, develop and optimize materials systems and device configurations capable of achieving DOE targets. To achieve the overall DOE hydrogen production cost target, a number of trade-offs can be made among the efficiency, durability, and cost parameters of the materials and devices. System-level technoeconomic analysis remains an important activity for developing long-term technical and cost targets for both photo-electrode and photocatalyst reactor systems. Efforts to develop detailed reactor designs, however, are not expected to become a priority until appropriate materials systems and devices have been established.

Current PEC materials research is progressing simultaneously on three fronts. The first is the study of highly efficient light absorbers, typically with limited lifetimes and relatively high cost (e.g., Group III-V crystalline semiconductor materials), to establish performance benchmarks and to quantify PEC hydrogen generation versus corrosion mechanisms. The second is the study of stable thin-film materials systems, typically with lower visible light absorption efficiency and relatively lower cost (e.g., metal- and mixed-metal oxide thin films, silicon alloy thin films, and chalcopyrites and other emerging efficient thin-film absorbers) to mitigate optical and electronic losses for improving efficiency toward benchmark values. The third is 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. Current R&D efforts are using state-of-the-art methods in materials theory, synthesis and characterization to develop efficient, durable and cost-effective materials systems. These research efforts are supported by the development of standardized methods for testing and reporting on PEC materials experimental work.[86] Further advanced work will be needed on integration schemes into high-performance photo-electrode or photocatalyst devices and reactors. Commercially viable large-scale deployment will require identifying and developing cost-effective methods of engineering and manufacturing the best available PEC materials, devices and systems.

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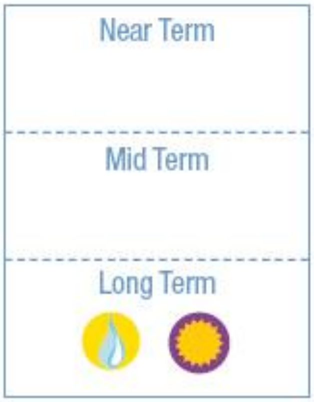
[86] Z. Chen, T. F., E. L. Miller, and H. N. Dinh, “Photoelectrochemical Water Splitting: Standards, Experimental Methods, and Protocols”, SpringerBriefs in Energy (2013) .

3.3 Solar Thermochemical Hydrogen Production

STCH



Feedstock:	Water
Energy Source:	Solar
Production:	Semi-Central Central

Thermochemical water splitting uses high temperatures—from concentrated solar power or from the waste heat of nuclear power reactions—and chemical reactions to produce hydrogen and oxygen from water. The chemicals used in the process are reused within each cycle, creating a closed loop that consumes only water and produces hydrogen and oxygen. This is a long-term technology pathway and calls for producing hydrogen in semi-central and central facilities. Numerous solar thermochemical water-splitting cycles have been investigated for hydrogen production, each with different sets of operating conditions, engineering challenges, and hydrogen production opportunities. In fact, more than 300 water-splitting cycles are described in the literature.[87] STCH offers a potential technology for clean, sustainable, high volume hydrogen production with current R&D priorities focused on materials development for both the reactive material as well as the reactor material and design.

Broadly, the STCH processes can be divided into “direct” cycles, which use only the concentrated solar thermal energy, and “hybrid” cycles, which additionally incorporate an electricity-driven electrolysis step as part of the water-splitting cycle. Typically, the direct thermal cycles offer lower complexity but require higher operating temperatures. With the energy added to the electrolysis step in hybrid cycles (typically less energy-consumptive than direct water-splitting electrolysis), these cycles can operate at relatively lower temperatures, offering practical advantages for reactor design and durability. Disadvantages of the hybrid systems include added complexity and extra requirement for electric input (which perhaps could be generated on site using waste heat from the STCH reactor). Examples of direct thermal and hybrid STCH cycles are, respectively, the simple two-step cerium oxide thermal cycle and the hybrid copper chloride cycles, as shown in Figure 11.

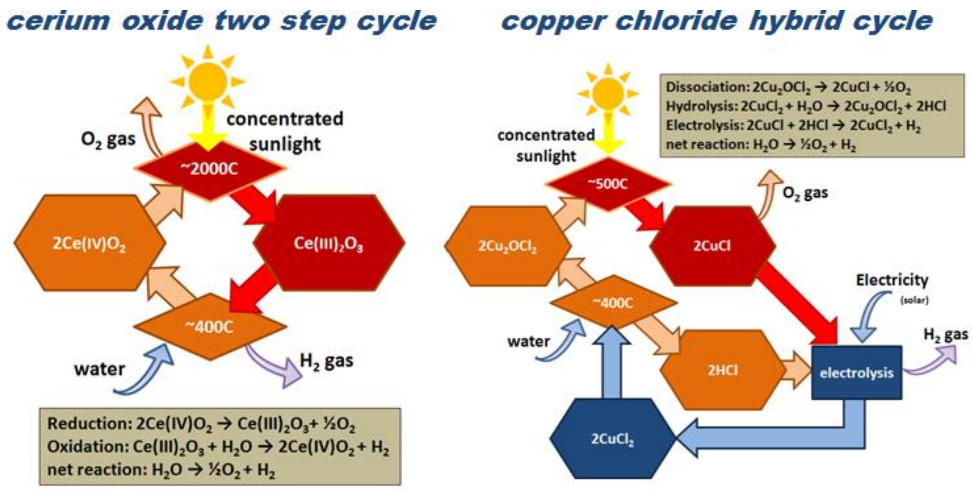


Figure 11 Examples of Solar Thermochemical Cycles for Hydrogen Production.

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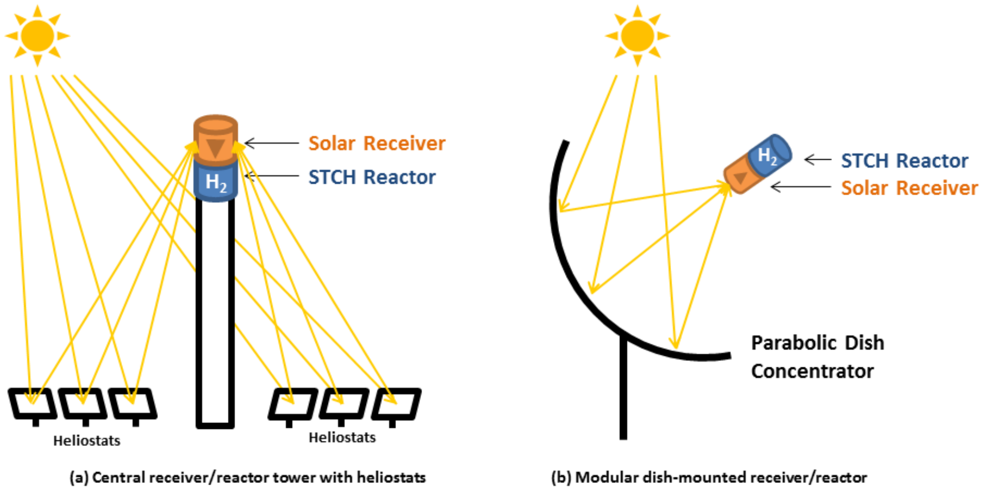
[87] R. Perret, *Solar Thermochemical Hydrogen Production Research (STCH)*, SAND2011-3622 (Albuquerque, NM: Sandia National Laboratories, 2011), https://www1.eere.energy.gov/hydrogenandfuelcells/pdfs/solar_thermo_h2.pdf.

The high temperatures necessary to split water via the "direct" STCH processes require the use of concentrated solar power. One approach is the deployment of a central STCH reactor in a solar receiver tower surrounded by heliostat fields (fields of sun-tracking mirrors) of a suitable size. Another approach is the use of multiple smaller-scale STCH reactor modules, each coupled to a tracking dish concentrator. Both approaches are illustrated in Figure 12. Each approach has unique advantages and disadvantages; however, both can incur significant capital expense because of the solar resource's diffuse nature, requiring large areas and infrastructure for efficient collection and concentration.



(a) Central receiver/reactor tower with heliostats

(b) Modular dish-mounted receiver/reactor

Figure 12 Two mirror based approaches for focusing sunlight on a thermochemical reactor to produce temperatures up to 2000°C are illustrated: (a) a field of heliostat mirrors concentrates sunlight onto a central reactor tower; and (b) dish mirrors focus sunlight.

Independent of the solar concentration approach, STCH cycles face obstacles that include high-temperature operations, highly corrosive chemicals, difficult separations of chemicals during sequential cycle steps, multiple reaction steps necessary to close the cycle, or side reactions with stable products that poison the process upon recycling. Many of these barriers can be overcome, but generally at the expense of energy efficiency, consumption of feedstocks other than water (e.g., electricity in the hybrid cycles), and possibly extremely high temperatures to drive reactions to completion. All of these measures add cost to the product, inhibit acceptable production rates, or prevent the realization of plant designs with acceptable lifetimes.

With solar radiation as the driving energy source, overcoming these barriers is made even more difficult, primarily because of the source's transient nature and relatively low power density. The low power density characteristic of solar power requires large collector areas and efficient concentrators to drive energy-intensive processes such as water splitting. Additionally, reactors must endure daily cycling from low to high temperatures resulting from the sun's day/night cycles, as well as weather effects. One option is decreasing reactor cycling by storing the thermal energy in salts or other materials to enable continuous production. A combination of thermal storage and/or backup power might be needed to ensure continuous operation.

STCH reactor systems have the potential to achieve high theoretical STH efficiencies.[88, 89] Based on boundary level technoeconmic analyses, STH efficiencies >25% would be needed in order to ultimately reach the hydrogen cost goal. However, bench-scale demonstrations of full-cycle STCH solar hydrogen production to date have been limited to <5% STH owing to materials, receiver and reactor losses.[90]

Making STCH technically viable will require long-term, fundamental and applied research efforts. The technology is not expected to meet DOE's cost targets in the next 10 years; however, the potential opportunity to harvest such tremendously clean energy makes this risk acceptable at this time.

Gaps and Technical Barriers

DOE's research activities are being driven by specific barriers identified in the MYRD&D[91], as well as others identified by the U.S. DRIVE Partnership's HPTT.

Thermochemical Cycle Selection

The literature has over 300 thermochemical cycle candidates, and new cycles continue to emerge. The most promising cycles need to be identified for further development. The complete set of criteria for selection, described in recent publications,[92] include thermal efficiency, operation temperature (lower temperatures are desired), minimal numbers of steps, and low raw materials costs, among others. In order achieve the DOE MYR&D targets, the projected thermal-to-chemical efficiency will need to exceed 35%, and the complete solar-to-hydrogen efficiency will need to exceed 25%.

Materials Development

The solar thermochemical cycles require high reaction temperatures, sometimes in excess of 1500°C for the high-temperature reaction step. Many of the materials for the reactants, reactor, seals, catalysts, and supports do not possess adequate thermal, physical, or chemical stability at these temperatures and rapid temperature transients. Thermal compatibility in reactor components, seals, etc., can also be problematic considering the wide temperature swings entailed by STCH. Reactant materials need to be developed not only with sufficient thermal and chemical stability but also with optimized heat exchange and surface kinetics for efficient thermal-to-chemical conversion efficiency.

Materials must endure extreme heat and corrosive and reactive environments, posing major challenges for development of durable, inexpensive materials for reactants, reactor, receiver, and any included thermal/chemical storage. Moreover, these materials would have to be easy to manufacture and capable of enduring extreme thermal shock. Some of the chemical cycles may require catalysts and/or supports, which will also need to endure aggressive environments. The materials will need to endure daily cycles and severe thermal temperature cycling. Ceramics that can endure high temperatures have issues with the cycling and with seals. Metals, such as Hastelloy steel, have better cycle life and fewer seal issues but have a lower usable temperature.

Hybrid STCH cycles also require materials R&D for major components of the electrolysis step. These materials include membranes, catalysts and support structures. Important materials parameters require

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[88] A. Steinfeld, "Solar thermochemical production of hydrogen—a review," Solar Energy 2005, 78:603–615

[89] N. Siegel, J. Miller, I. Ermanoski, R. Diver, E. Stechel, "Factors affecting the efficiency of solar driven metal oxide thermochemical cycles," Ind Eng Chem Res 2013, 52:3276–3286

[90] W. Chueh, C. Falter, M. Abbott, D. Scipio, P. Furler, S. Haile, and A. Steinfeld, "High-Flux Solar-Driven Thermochemical Dissociation of CO_2 and H_2O Using Nonstoichiometric Ceria," Science 330 (2010): 1797–1801.

[91] Office of Energy Efficiency and Renewable Energy, Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan (Washington, DC: U.S. Department of Energy, June 2015), Section 3.1, https://energy.gov/sites/prod/files/2015/06/f23/fcto_myrdd_production.pdf

[92] R. Perret, *Solar Thermochemical Hydrogen Production Research (STCH)*, SAND2011-3622 (Albuquerque, NM: Sandia National Laboratories, 2011), https://energy.gov/sites/prod/files/2014/03/f9/solar_thermo_h2.pdf

optimization to achieve low-voltage–high-efficiency operations as well as long operational lifetimes with minimum contamination and/or cross-over degradation and materials durability.

Chemical Reactor Development

At the hydrogen production scales of interest, STCH chemical plants are expected to be capital-intensive. STCH chemical reactor designs need to be efficient and inexpensive and entail minimal BOP to meet the DOE cost targets.

High-temperature operation necessitates extreme thermal management to achieve high efficiencies. Thermal losses result from inefficient process flow and a lack of integration among unit operations. Heat recuperation is vital to attaining the conversion efficiencies required to meet hydrogen production cost goals.

Other barriers to reactor development and capital costs include cycle phase separation and purification, including the extraction of sufficiently pure hydrogen product. Ideally, the product stream will be composed of only hydrogen and water. However, there may be small amounts of other contaminants similar to those in hydrogen produced via water electrolysis. In hybrid cycles, efficiency of the electrolysis step needs to be optimized in terms of low voltage, high efficiency, long lifetime and efficient reactant/product management to reduce overall system losses.

Solar Receiver Development

STCH reactors can be broadly classified as directly heated by the sun or indirectly heated (e.g., a thermal transfer medium absorbs the thermal energy and transfers the energy to the reactor). The solar receiver is the focal point of the solar concentrator (e.g., heliostat field or dish concentrators) and directs the thermal power to the reactor and/or thermal storage. Efficient heat transfer at the interface with the heliostat remains a barrier as the cycles move toward commercialization.

The interface with the chemical reactor is an important consideration in selecting a solar receiver. For directly heated reactors (e.g., rotating disk, fluid wall, and centrifugal), the receiver and reactor are integrated, enabling solar flux to heat the reactor. Ideally, the solar thermal input rate would match the heat of reaction at constant temperature. However, the chemistry and dynamics of each system establish the equilibrium temperature required.

The solid particle and volumetric receivers are heated indirectly by the sun. For these reactors, the heat is absorbed by solid particles (e.g., sand) or molten salts, which then heat the reactors. Heat addition is, therefore, not isothermal. In addition, the amount of energy transferred to the thermochemical reaction from the intermediate heat transfer media depends on the range of temperature absorbed by the chemical reaction. The non-isothermal nature of these receivers may be suitable for cycles with steps requiring different temperatures. In addition to interfacing with the receiver, the reactor must also interface with thermal storage, if used.

Solar Intermittency

Cost-effective solar-driven hydrogen production may require cycles that incorporate either thermal/chemical storage or some form of backup power to enable time-shifted hydrogen production to compensate for intermittent solar energy input; however, the appropriate materials or processes have yet to be identified or developed. Storage or backup power can enable continuous plant operations, which will extend the operational lifetime of the STCH reactor. However, this will add cost to the receiver–reactor interface. In addition, insulated storage sites and increased BOP components would be required, adding to the capital and O&M costs. Any storage or backup power approaches will need to be thermally efficient, inexpensive, and chemically compatible with the STCH process.

Solar Concentrator Technologies

The solar concentrator (e.g., the heliostat field or dish concentrators) is a key unit in the development of STCH production. Currently, the units are too expensive, and development is needed to reduce their cost. High costs are in part due to a lack of standardization in their designs, as well as inefficient manufacturing and poor durability. Leveraging R&D efforts (for example, the DOE SunShot Initiative)[93] is expected to be critical in developing more cost-effective solar concentrator technologies (for solar electricity, solar fuels, and solar hydrogen).

Operations Costs

All system components must be considered in O&M costs, including feed pre-conditioning, solar concentrators, solar receivers, reactor, hydrogen purification, controls, utilities, QA/QC (e.g., sensors), compression, storage, and safety. Control/safety system costs may remain high because of system complexity and/or substantial sensor count to assure reliability. These units must operate in an environment of minimal manual assistance, which will require attributes such as back-up fail-safe mode, remote monitoring, and sparse maintenance schedules. Solar power availability and fluctuations will strongly influence the design, performance, and economic viability of this technology.

Land and Capital Costs

As with all solar hydrogen technologies, large-scale STCH hydrogen production will require large areas for collecting sufficient sunlight, with the associated levels of land and capital costs. Maximizing conversion efficiency to reduce the solar collectors' overall footprint remains critical to cost reduction. Reducing capital costs in the receiver–reactor components and in all BOP components is also necessary.

Strategy to Overcome Barriers and Achieve Technical Targets

Table 8 lists critical technology needs for STCH. R&D activities within these categories address the critical technology barriers associated with the ultimate commercialization and successful development of the STCH production pathway.

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[93] https://energy.gov/eere/sunshot/sunshot-initiative

Table 8 Solar Thermochemical Hydrogen — Critical Technology Needs in Promising Cycles.

Reactant Materials Challenges	➔ Engineer known chemical cycle materials to optimize heat transfer, kinetics and durability; and to minimize cost ➔ Discover and develop new materials/materials classes, guided by theory and experimentation, with the potential for high efficiency, long cycle lifetime and low cost ➔ Validate cycle efficiency and cycle life associated with all cycle reactant materials/phases
Innovative Thermochemical Reactor Designs	➔ Develop receiver materials and designs to minimize re-radiation losses and optimize lifetime ➔ Develop receiver /reactor interface materials and designs for maximum thermal coupling, minimum loss and long lifetime ➔ Develop thermal management and heat recuperation in receiver/reactor designs ➔ Develop system to manage cycle reactants and products, including phase separations and purification ➔ Develop system to manage variable demand and solar power, including thermal/chemical storage and required interfaces
Improved Electrolysis (Hybrid Cycles)	➔ Improved membrane materials with optimal conductivity, minimal chemical cross-over, and high durability ➔ Improved end plate and catalyst materials ➔ Optimize electrolyzer for low voltage, high efficiency and long lifetime
Need for Practical Storage	➔ Develop thermal storage materials/strategies ➔ Develop chemical storage materials/strategies
High Solar Concentrator Costs	➔ Reduce heliostat system cost (leveraging CSP R&D) ➔ Reduce dish concentrator systems (levering CSP R&D)
BOP and O&M Costs	➔ All system components must be considered in reducing BOP and O&M costs, including feed pre-conditioning, solar concentrators, solar receivers, reactor, hydrogen purification, controls, utilities, QA/QC (e.g., sensors), compression, storage, and safety
Technoeconomic Analysis	➔ Develop detailed technoeconomic models of prospective STCH reactors based on promising cycles implemented in promising reactor systems (including concentrator/receiver/reactor capital and O&M projected costs) to guide R&D efforts toward meeting H_2 cost threshold goals

Addressing all of the barriers to commercialization cost targets for STCH production will require simultaneous R&D efforts in several areas, along with efforts to develop policy, standards, and delivery infrastructure technology. Although these efforts are taking place concurrently, the impact of each effort on the entire hydrogen production system must be kept in mind and integrated into systems optimization efforts.

Identifying and developing the most promising cycle chemistries is the highest near-term research priority. Exploring cycle materials that provide operational durability and improved thermodynamics and kinetics is essential. Design and demonstration of efficient reactors and receivers suitable for the chemistries identified will also be important for achieving technical targets. To facilitate R&D of STCH reactant and reactor materials and systems, standardized testing and reporting protocols and metrics are being developed in conjunction with the broader solar fuels research community. Other important activities — e.g., minimizing losses through effective thermal management and reducing solar-concentrator capital costs — are expected to leverage the R&D efforts of solar fuels initiatives and the DOE Solar Energy Technologies Office.

O&M costs will also have a significant impact on the overall cost of STCH hydrogen production and will need to be minimized through process and engineering advances. Ultimately, additional efforts will be needed to develop and implement DFMA that will facilitate mass production of equipment and development of lower-cost, easier-to-manufacture, and more durable materials.

3.4 Direct Water Splitting: Path Forward

Direct water splitting hydrogen production pathways hold great promise for sustainable, large-scale production of hydrogen from diverse and domestic resources, but the costs of all these pathways need to be significantly reduced, and as such have become a priority area for DOE supported R&D. As discussed above, there are significant barriers that need to be addressed for these direct water splitting pathways, but common and most critical to all are the needs for materials discovery and development that will address durability and efficiency issues associated with each pathways. These materials challenges are highlighted again here.

1. **Advanced Electrolytic (AE) Hydrogen Production:**

- *Low-and high-temperature electrolysis (including alternative chemistries)*
  Materials challenges include, but are not limited to: membrane and electrolyte conductivity, corrosion, materials stability/durability under aqueous and high temperature conditions, balance of stack components such as seals, overpotential losses and current density constraints for the oxygen evolution reaction and hydrogen evolution reaction (HER) catalysts, contamination, integration of components including interfacial consideration, porous transport layer and bipolar plate issues, catalyst and electrode synthesis scale-up, and lowering components costs at high volume production.

2. **Solar Thermochemical Hydrogen (STCH) Production:**

- *Two-step metal oxide thermochemical cycle*
  Materials challenges include (but are not limited to): discovery and development of water-splitting active oxides with high oxygen storage capacity at lower reduction temperature, optimize HER thermodynamics and kinetics, and develop oxides resistant to extreme thermal and chemical stresses induced by cycling with efficient heat transfer at sufficiently low cost.
- *Hybrid and other multi-step cycles*
  Materials challenges include (but are not limited to): development of efficient electrolytic technologies in hybrid cycles that incorporate next-generation membranes that are resistant to corrosive electrolytes and demonstrate high conductivity at high temperatures. These materials include membranes, catalysts and support structures. Important materials parameters require optimization to achieve low-voltage/high-efficiency operations as well as long operational lifetimes with minimum contamination and/or cross-over degradation.

3. **Photoelectrochemical (PEC) Hydrogen Production:**

- *Integrated assemblies based on photovoltaic-grade semiconductor material systems for photoelectrodes*
  Material challenges include (but are not limited to): bandgap tuning, stability and durability of functional materials and interfaces, reduction in required overpotential through surface catalysis, development of stable and low-loss protective coatings and schemes, reduction in defects during thin film synthesis, and scale up of integrated systems including interface mechanical and chemical stability.

- *New semiconductor material systems and novel approaches (including particle systems)* Material challenges include (but are not limited to): development and validation of new material systems with simultaneously optimized bandgap, electronic and ionic transport properties, catalytic surfaces and stability; and innovative reactor designs.

In an effort to more effectively address these critical barriers and accelerate the advancement of water splitting materials systems for sustainable hydrogen production, DOE has established the HydroGEN[94] Consortium as part of its Energy Materials Network. HydroGEN is focused early-stage applied R&D to enable viable commercial-scale hydrogen production through advanced electrolytic, photoelectrochemical, and thermochemical water-splitting processes. Its foundational approach is to closely integrate state-of-the-art theory and experimentation at all stages of materials discovery and development, taking advantage of the unique capabilities and expertise available through the U.S. National Laboratory System. The HydroGEN Consortium includes the National Renewable Energy Laboratory, Sandia National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Idaho National Laboratory and Savanah River National Laboratory. Implementation of the HydroGEN consortium is expected to enhance the current approach to DOE funded R&D by streamlining stakeholder access to the vast resources at the National Laboratories relevant to water splitting technologies, thereby offering stronger collaborative opportunities among industry, academia and the labs.

To date, more than 80 unique research capabilities have been established within the HydroGEN Consortium, and detailed white papers on each can be found at the HydroGEN website using the site's extensive search engine. Moving forward, new projects with industry, academia, and non-consortium national laboratories collaborators will leverage the capabilities and expertise within HydroGEN to address the key technology-specific and cross-cutting material challenges using advanced methodologies such as combinatorial synthesis and high-throughput characterization, guided by computational studies and fundamental materials science knowledge. The overall end goal is to support the research needs identified though the HPTT, H2@Scale, and other stakeholder engagement, for enabling development of direct water splitting technologies capable of industrial-scale hydrogen production at a cost <$2/gge.

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[94] HydroGEN Consortium on Advanced Water Splitting Materials website: https://www.h2awsm.org/