Perspective

Hydrogen Economy - An Opportunity for Chemical Engineers?

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Introduction

Fossil fuels have provided a convenient and plentiful energy source, and have been used profitably in all sectors of the global economy. However, continued reliance on fossil resources must take note of, and may even be placed in jeopardy by several factors. First, worldwide oil demand continues to increase, and replacing the produced oil is technically and politically demanding and very capital intensive. Second, known fossil reserves are concentrated in only a few regions of the world. Oil and natural gas reserves, in particular, are in regions geographically separate from those undergoing the most rapid economic growth. Third, the widespread use of oil in the transportation sector contributes to environmental disturbances, such as air pollutants and CO_2.

Various demand-side solutions have been proposed to address the continued, increasing reliance on oil. The perennial solution of improving energy efficiency by way of vehicle fuel economy would curb demand for oil. Major auto manufacturers have entered the hybrid electric vehicle market. Hybrids and fleet-wide fuel economy standards may reduce the growth of oil demand, but fuel substitution in the transportation sector offers another type of solution. One such possibility is the widespread adoption of light-duty electric vehicles (EVs), which could displace substantial oil demand, but which will depend on successful research and development (R&D) on high-energy density battery technology. Also, if the electricity is produced from coal, there is potential for increased CO_2 emissions.

Another possible fuel substitution and end-use combination is the hydrogen (H_2) fuel-cell vehicle (FCV). The major automakers have rolled-out H_2-fueled concept cars coupled to proton exchange membrane (PEM) propulsion systems. As with EVs, there remain substantial cost and technological barriers to the commercial deployment of FCVs.

While there are strong supporters of H_2, it also invokes strong reactions from those who believe that H_2 is unlikely to meet the requirements of an alternate energy source.[1,2] These differences in opinion stem from the fact that like electricity, H_2 is simply an energy carrier. Despite its abundance in nature, H_2 is not available in the free form and must be produced from another energy source. Moreover, H_2 needs to be transported, delivered and stored at the point of end use. All these steps can potentially consume energy. Use of H_2 as an energy carrier is pollution-free and efficient as long as all the steps involved in its production, transportation and use chain are also pollution-free and efficient. Moreover, for H_2 to be a long term alternative, it must be produced from an energy source whose supply is unlimited or sufficiently abundant to last for centuries. The nonbelievers in the H_2 economy conclude that the supply and use chain of H_2 is more inefficient, costly and, furthermore, it is generally more polluting if H_2 were to be produced from a fossil fuel.

This article will focus on the key barriers to assembly of an H_2 infrastructure, and the pros and cons associated with various methods of producing inexpensive H_2. In the long-term, H_2 could be produced in large, central plants and delivered via pipelines to filling stations. In transition to this end-state, a system of distributed production sites, i.e., small production units located at filling stations-could obviate the need for

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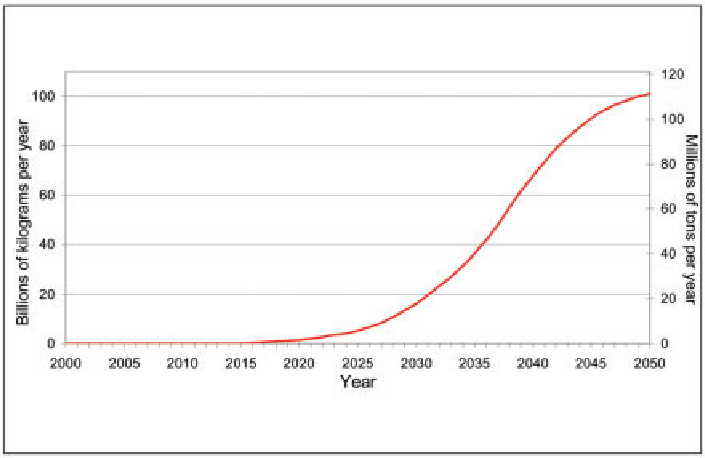

Figure 1. U.S. Hydrogen demand assuming commercialization of the fuel cell vehicles in 2015.

An " optimally plausible" solution based on NRC report.[3]

pipelines, but the production cost and efficiency must be improved significantly.

It will be assumed that the successful widespread deployment of H_2 fuel cell vehicles can be achieved, and, thus, the focus of discussion will be kept on H_2 supply. The discussion will be based on the analysis and assumptions in a 2004 report by the National Research Council.[3] In the report, an economic and engineering analysis of H_2 production and delivery methods was conducted with present technology and future technology — the latter considering *what cost and performance might be possible* if R&D is successful in overcoming the significant barriers in many of the H_2 supply technologies.

To help define the potential role chemical engineering can play in the H_2 economy, this perspective article will address the following issues. What is the true potential of an H_2 economy? Are the expected benefits realistic and can they be achieved? Are the costs and inefficiencies of the various technologies for the H_2 production and use too high? What are the major hurdles in the implementation of H_2 as an energy carrier? What is the realistic time frame to implement an H_2 economy? See in Figure 1, taken from NRC report,[3] shows an "optimally plausible" H_2 penetration curve for fuel cell cars in the United States.

In order to address these questions*, this article will examine hydrogen's potential as a transportation fuel for the light duty vehicles (passenger cars)*. First, the economics and engineering of the H_2 supply chain will be discussed and the thermodynamic underpinning explained. A description follows of the possible benefits of wide-scale implementation of H_2 for light-duty vehicle transportation including the possible CO_2 and security benefits. Next, the various primary resources or feedstocks from which H_2 can be derived are listed, and their pros and cons examined with regard to energy security. The foregoing will provide a framework for the discussion of the major challenges to a successful H_2 energy system and how chemical engineers can turn these challenges into opportunities.

Light duty vehicles are defined as cars and light-trucks having gross vehicle weight under 8,500 pounds.

H_2 Supply chain

The prime fossil fuels for H_2 production are natural gas and coal, although oil could also be used.[4–6] Reforming of natural gas with steam or partial oxidation of natural gas/coal followed by the water gas shift reaction are the pathways for H_2 production.[7] Other major energy sources for H_2 production are nuclear, wind, and solar where electricity would first be generated and then utilized with electrolysis of water to yield H_2. However, when feasible, it can be more efficient to produce H_2 directly without going through electricity. Thus, sulfur-iodine or another suitable cycle can be chosen for thermochemical water splitting using nuclear energy.[8] Attempts are underway to develop processes for H_2 production from the biomass gasification/reforming,[9,10] Similarly research is being done to create photoelectrochemical cells for the direct production of H_2 from water.[11] All of these technologies required additional R&D—some significant—to produce cost and energy competitive H_2 for transportation.

Cost of H_2 Supply Chain. The recent NRC report (2004) estimated the cost of H_2 produced from diverse feedstocks using various infrastructure configurations. In Figure 2, the estimated dispensed H_2 cost for three plant sizes are shown: (1) a 1.2 million kilograms per day (kg/d) central station plant to support about 2 million cars, (2) a 24,000 kg/d midsize plant to support about 40,000 cars, and (3) a 480 kg/d distributed plant to support 800 cars. Three sizes of plants were considered in order to meet the increasing demand for H_2 during the transition period, as the number of H_2 FCVs increase with time. Each bar is divided into segments that show the production, as well as delivery and dispensing costs. For large central station plants, delivery through pipelines was envisioned.[13] For midsize plants, liquid H_2 tankers were used for delivery of H_2 to

In the past, several studies have looked in to the cost, efficiency and environmental impact of the H_2 production, transportation and use. However, most of these studies have only forcused on the spcific aspects of the total supply and use chain. As a result, when conclusions are drawn on the basis ofd more than one study, the assumptions are generally consistant. This makes it difficult to draw a consistant set of conclusions, and is responsible for some of the confusion in the literature. A recent report by Lipman provides a good summary of the depensed H_2 cost for the several feed stocks from several studies.[12]

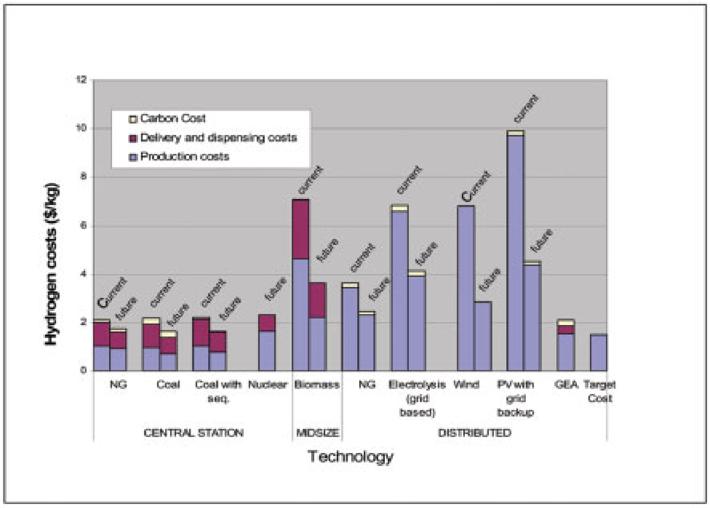

Figure 2. Delivered unit hydrogen costs from various feedstocks. (from the NRC report [3]).

the dispensing/filling stations.[14] Distributed plants were assumed to be located at the dispensing stations and H_2 assumed to be produced on-site. The costs in Figure 2 are shown for the current technology, as well as for the future with potential technological advances. Anticipating a carbon tax, an imputed cost of $50 per ton of carbon emitted was also included. Note that the energy contents of 1kg of H_2 and 1 U.S. gallon of gasoline are approximately the same. In order to compare the cost of one kg of H_2 with gasoline, it is important to note that energy efficiency of a FCV is taken to be better than a gasoline hybrid electric vehicle (GHEV), which in turn is better than a conventional internal combustion engine vehicle (ICEV). The GEA bar in Figure 2 refers to the cost of an equivalent amount of gasoline that is expected to give the same traveled distance for a GHEV as a Kg of H_2 for a FCV. It is worthwhile to point out that the future infrastructure for H_2 is yet to evolve, and this leads to uncertainties in the delivery and dispensing costs in Figure 2. Therefore, it is generally believed that the target price for H_2 to penetrate the market is about $1.50 per kg**.** This target price is shown in Figure 2.

It is possible to conclude from Figure 2 that the costs of the delivered H_2 can be competitive with gasoline, depending on the choice of feedstock, the production method and the progress of R&D. The following can be observed with regard to specific feedstocks and infrastructure strategies:

- *Large Centralized Production.* The cost of H_2 produced from large central plants using fossil fuels or nuclear energy, could approach that of gasoline with future technologies. However, for the large centralized plants, there exits a tremendous amount of uncertainty in the technology and logistics for building the infrastructure to delivery the H_2 to the dispensing station.
- *Midsize and Distributed Production.* The cost of H_2 from both the midsize and distributed size plants is substantially higher than gasoline. This requires major technological breakthrough to defy the conventional wisdom of economy of scale for chemical plants and supply H_2 at a competitive cost. These distributed plants are very important for the first 15 to 20 years of the transition period, as shown in Figure 1.
- *Revewable Energy.* The cost of H_2 from renewable energy sources, such as biomass gasification, wind and photovoltaic (PV) are considerably higher than that of gasoline; these technologies will require R&D breakthroughs to be competitive.
- The high cost of biomass gasification results from low crop yields and gasification efficiency.

For wind and solar, the intermittent nature of these sources adds considerably to the costs. To make better use of the electrolyzer capital investment, the calculations in Figure 2 assumed that grid electricity was used to extend electrolyzer operation around the clock. For the future wind case, the NRC study assumed sufficient technology advancement to increase the wind turbine's capacity factor to 40%, which reduces the cost of electricity to 4 cents per kilowatt hour (kWh). PEM electrolyzer costs are further assumed to decrease to $125 per kilowatt — an eight-fold improvement — in conjunction with possible decreases in the PEM fuel cell costs. Note the PEM electrolyzer and PEM fuel cell are essentially reversible technologies, but with different operating environments. For the future wind case, it is assumed that no back up grid electricity is needed because of advances in both wind and electrolyzer technologies (see NRC report[3]).

In Figure 2, PV is not competitive in either the current or the future cases, even with PV electricity dropping in costs from 20 to10 cents/kWh. For the PV to be competitive this cost would have to drop to 4 cents!

Clearly the renewable energy sources need substantial cost improvements, or different technical approaches including innovation, to fulfill their promise of producing cost/energy efficient H_2.

Well-to-Wheels Energy Efficiency. Energy is consumed in the recovery of a fossil fuel feedstock from its underground reservoir and subsequent transportation to an H_2 plant. Additional energy is needed not only for the conversion of feedstocks to H_2 but also for its transportation, delivery, and dispensing to the on-board storage system of a FCV. Ultimately some energy is lost due to the inefficiencies in the fuel cell system. A similar energy chain exists for gasoline usage. Often such overall system efficiency studies are referred to as well-to-wheels analyses.[15]

Figure 3 shows the well-to-wheels energy use for FCVs using various feedstocks, and for a GHEV and an ICEV. The

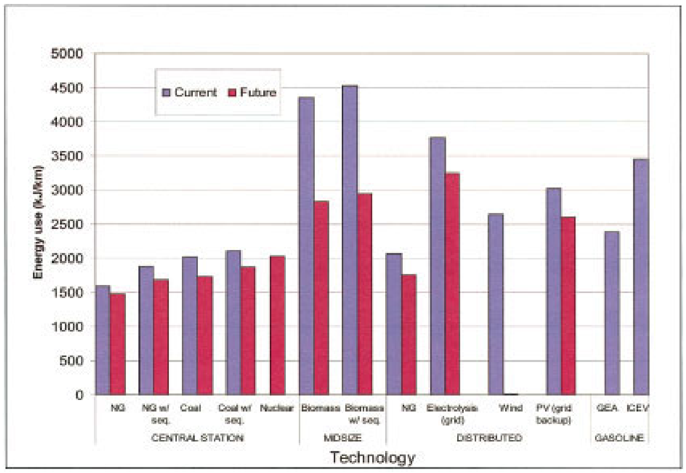

Figure 3. Overall energy used to drive a km using H_2-fuel cell LDVs.
(from the NRC report[3]).

source of the data is again the NRC report, so as to provide compatibility with Figure 2.

The following observations can be made from Figure 3 regarding the efficiency of the various feedstocks and infrastructure strategies:

- *Fossil fuel feedstocks and nuclear energy.* The anticipated well-to-wheels energy use by an H_2 FCV, when a fossil fuel is used as feedstock, is slightly better than that of a GHEV and much better than a conventional ICEV. The same comparison holds true for when nuclear energy is used to produce H_2.
- *Distributed production.* Distributed, electrolytic production of H_2 using grid electricity stands out as well-to-wheels inefficient even with electricity generated at 50% efficiency. This high energy loss results from the multistep process of generating electricity, conversion to H_2, and then back to electricity in the vehicle.
- While distributed natural gas reforming is more well-to-wheels inefficient than large central plants, they are still more efficient than GHEV and ICEVs.
- *Renewable Energy.* All the renewables in Figure 3, except the future technology wind case, consume more energy than the gasoline based GHEV and the ICEV. The majority of the energy used for biomass comes from the biomass itself. Therefore, the major impact of the lower efficiency is in the increase of land use to grow the biomass. (Note that all of the energy usage shown in Figure 3 for the current technology wind case and both the PV cases are due to the use of grid electricity as backup power.)

Storage and Transportation. The costs and efficiencies in Figures 2 and 3 are significantly impacted by the thermodynamic properties of molecular H_2. Compression and storage of H_2 requires 5 to 10% of the energy contained in H_2 on a unit mass basis; the corresponding fraction for its liquefaction can be approximately 30%. As a consequence, the energy required to transport a unit of energy as H_2 from a production plant to the dispensing station is considerably higher than that of gasoline. This is the primary reason for the H_2 delivery and dispensing costs being comparable to the H_2 production costs in the central plant cases (see Figure 2). This is in sharp contrast to gasoline, for which the delivery and dispensing costs are only a minor fraction of the total cost.

Another important property is the low energy density of molecular H_2 which creates significant technical barriers for on-board vehicle storage and vehicle driving range. While on a mass basis, H_2 has high energy content (lower heating value [LHV] of 33.3 kwh/kg); its volumetric energy density is considerably lower. At pressure of 680 atmospheres, LHV of H_2 is about 1.32 kwh/L. The same number for liquid H_2 is 2.35 kwh/L. In contrast to this, the corresponding energy density for gasoline is 8.88 kwh/L. This has several implications. To store the same amount of energy, H_2 needs significantly more volume than gasoline. For example, a light duty vehicle with 40 L of gasoline storage, the (energy-equivalent) storage volume for 680 atm H_2 would be about 160 L, and for liquid H_2 about 90 L. Thus, driving range could be reduced significantly if H_2 physical storage is limited on board. Major R&D efforts are underway to develop material which will adsorb/absorb H_2 in the high density required to give at least a 450 km driving range. A major technical breakthrough to overcome this barrier is required.

Environmental Benefits, Carbon Capture and Storage (Sequestration) and Safety. One of the potential promises of an H_2 economy is to decrease carbon dioxide emissions in the transportation sector. Figure 4, again taken from the NRC report, shows the carbon released for each of several H_2 production feedstocks on a well-to-wheels basis. All calculations are made assuming successful future technologies.

The significant observations are: (1) the use of H_2 has the potential to reduce carbon emissions; (2) the highest carbon release occurs when coal is used to produce H_2, and unexpectedly this number is less than that from gasoline; (3) if H_2 is produced from fossil fuels, co-product CO_2 from the gasification/reforming plants will have to be captured and stored in order to get significant reduction in net carbon releases; (4) capture and storage of carbon from a biomass gasification plant has a potential for an overall net decrease in the environmental CO_2 since carbon is captured and stored during the growth of the biomass, as well as during its conversion to H_2; and (v) renewables, such as wind with no grid backup can provide H_2 with no need to capture and store carbon.

While separation and capture of CO_2 from natural gas and coal plants can be achieved through the use of current and

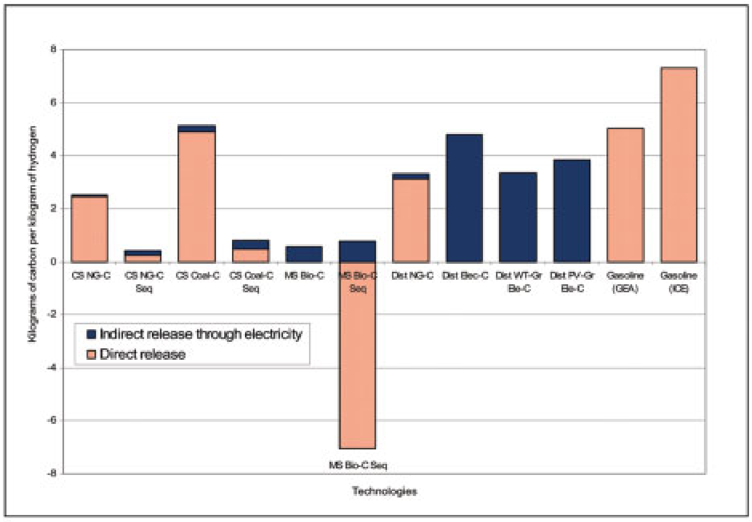

Figure 4. Total carbon released during hydrogen, delivery, dispensing, and end use.

These numbers are for future technologies. (NRC report[3]).

future technologies, the long-term isolation of large quantities of CO_2 requires much more effort.[16-19] Use of depleted oil/gas reservoirs, unmineable coal beds and deep saline aquifers have been suggested. The areas which need attention are CO_2 transport, infrastructure, real reservoir CO_2 capacity, potential CO_2 leakage, contamination and mitigation. This requires study on the integrity of sequestration well seals, monitoring etc. in geological time frame. This is crucial, owing to the potential for CO_2 release, the consequences of which became tragically clear in 1986 when an estimated 80 million cubic meters of natural (i.e., not sequestered) CO_2 erupted from the Lake Nyos Crater in Cameroon, killing 1,800 people.[18] Clearly, massive quantities of CO_2 would be generated during a decades-long period of hydrogen production and use. Thus, a requirement to sequester the CO_2 for centuries would place extreme demands on CO_2 capture and storage systems.

There are many real and perceived safety issues that are barriers to an H_2 Economy. Even though H_2 has been used safely in the hands of experienced chemical plant operators, its use by the unskilled consumer is one of the significant issues. See the NRC report [3] for a detailed discussion of safety.

Resources Availability. Light-duty vehicles consume roughly 40% of petroleum in the U.S., more than half of which is imported. Switching to H_2 fuel on a large scale could reduce oil imports and increase energy security, depending on the H_2 production feedstock, as shown in Figure 3. In fact, except for natural gas, all feedstocks are domestically sourced. While natural gas is produced domestically, it is also imported in increasingly significant quantities and would be subject to the same market instability as is petroleum.

In the H_2 demand scenario posited in the NRC study, by the year 2050, FCVs in the USA would be consuming nearly 100 billion kgs of H_2 per year (see Figure 1). For comparison, the current annual U.S. industrial production of H_2 is about 8 billion kg. Thus, if H_2 economy were to take off, then just for the light-duty vehicle fleet alone, the H_2 production in the Untied States would have to increase by more than an order of magnitude! It is informative to briefly look at the availability of the requisite feedstocks *within the USA* to meet this massive H_2 demand. For a detailed discussion of resource availability see NRC report.[3]

Summary. For H_2 produced from fossil fuels, (1) dispensed H_2 cost could be similar to that of gasoline, (2) transportation and dispensing costs for H_2 are a substantial portion of the overall costs; (3) there is potential for large gain in the overall system efficiency compared to ICEVs, and (4) coal as H_2 source will not increase carbon emission to the atmosphere on a well-to-wheels basis. Therefore, based on these observations, it is not out of the question to consider fossil-fuel-derived H_2 as an energy career. However, there is a limited supply of fossil fuels, and, therefore, the production of H_2 from fossil fuels is not a long term solution. The cost of H_2 from renewable and nuclear energy is currently noncompetitive and it requires major technical breakthroughs to be competitive.

Major Challenges and Opportunities

Chemical engineering is an excellent discipline for the development of technologies for a H_2 Economy. R&D in materials, systems, chemistry, nanoscience, modeling/optimization, biosciences, manufacturing, and process engineering are all required to overcome many of the barriers. Particularly important is the breadth of chemical engineers and their ability to develop interdisciplinary solutions. Some of the major challenges and opportunities for chemical engineers are summarized in Figure 5 and discussed next.

Storage, Transmission and Dispensing

Systems Engineering

Several transition strategies have been proposed.[3,13,14] During the early years, supply from existing production sites to

In 2001, daily supply of motor gasoline in the U.S. was 8.67 million barrels, 93.5 percent of which was used in light duty vehicles.

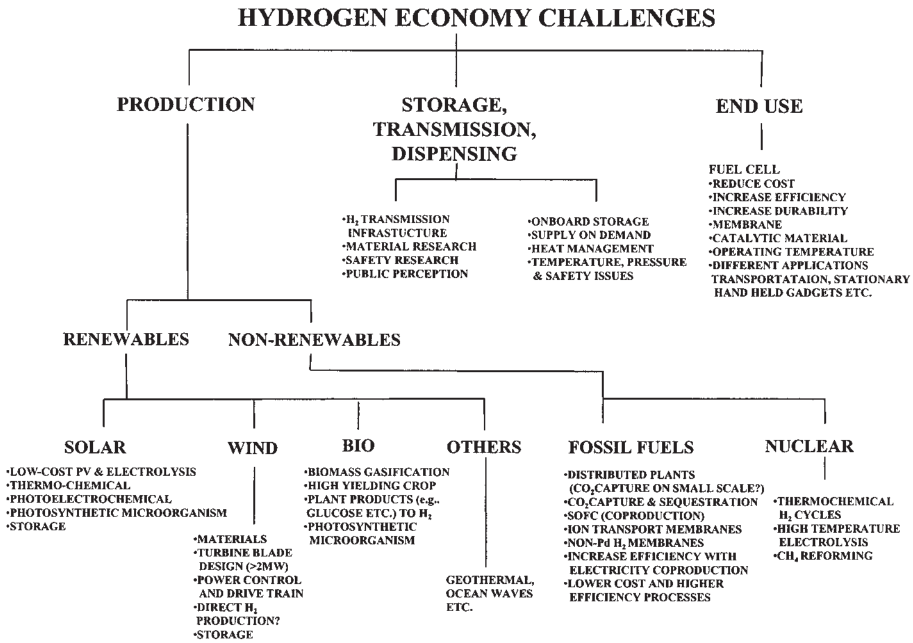

Figure 5. Hydrocarbon economy challenges and opportunities.

filling stations could be accomplished through liquid or compressed H_2 trucks. The demand could also be met through small scale onsite distributed reformers and water electrolyzers - less than 500 kg/day of H_2 capacity. In the long run, commercial scale central plants will produce H_2 that can be delivered through pipelines. Optimization of the overall infrastructure layout and costs as it evolves through several transition stages can benefit from the chemical engineering expertise in systems optimization and process engineering.

H_2 Onboard filling and storage

The onboard H_2 storage technologies developed to date have significant gaps in the energy density consistent with adequate vehicle cruising range (450 km)-a potential show stopper. Furthermore, a storage system is needed that is rapidly refillable, can instantly supply H_2 to the fuel cell on demand, and is perceived to be "as safe as a gasoline tank".[20] If solid or liquid mediums are used for H_2 storage, then heat management associated with H_2 pickup and H_2 release by the medium must be carefully addressed. The temperatures associated with each step are crucial. For example, if a dense medium storage is heated to temperatures higher than the fuel cell operating temperatures to release H_2, then fuel cell waste heat cannot be utilized. This implies that a large fraction of the energy contained in the H_2 will be required as heat energy, making the system quite inefficient. Similarly, if during onboard H_2 fill-up, a large amount of heat is released then it must be properly removed in the short fill-up period. Therefore, there is need for both substantial R&D into new materials for storage, and a well designed process to operate the system. In addition, new sensors and control methods for the onboard H_2 supply system may be required. These are all areas where chemical engineers have expertise.

Production

Distributed H_2 production

One of the production challenges to which chemical engineering expertise could be applied is the design and manufacture of distributed H_2 reformers that will be needed for the transition described in the subsection titled "Cost of H_2 Supply chain". As seen in Figures 2 and 3, the current distributed natural gas reformers produce H_2 with about three times the cost of the central plant, and at lower efficiencies. The challenge is to come up with novel materials and innovative plant designs that will lead to a low cost and efficient reformer that has turndown and on/off capabilities. While it is straightforward to think of small size H_2 plants based on natural gas as a feedstock, can a distributed plant be developed based on other fossil fuels feedstocks, such as coal? An interesting chemical engineering question.

CO_2 Management

For fossil fuels, carbon monoxide (CO) and CO_2 are byproducts and conversion to H_2 is generally limited by the water gas shift reaction. Once again clever reactor and material designs are needed to eliminate this constraint. If co-produced CO_2 is to be sequestered, then better processes will be needed to recover CO_2 at higher pressures.

Nuclear energy

If H_2 were to be produced from nuclear energy, then development of new processes would be required. It has been shown through modeling that electrolysis of water at high temperature (excess of 350°C) can be quite efficient, but it is yet to be used with a nuclear reactor.[21] Similarly, a number of thermochemical cycles for water splitting are in development. However, most of these cycles operate at temperatures in excess of 700°C, and have material corrosion and handling problems. A thermochemical cycle that does not have associated material problems and operates at somewhat lower temperatures could be quite attractive. There are opportunities in the design of processes that will co-produce electricity and H_2.

Biomass

In commonly occurring ecosystems, solar energy is converted into biomass with an overall thermodynamic efficiency of about 0.4%.[22] This low efficiency coupled with land availability will ultimately limit the amount of H_2 that can be produced through this route.. Clearly, there is a need to increase biomass yield per unit of land, and also the gasification efficiency.

Electrolysis

One of the biggest challenges for the carbon free H_2 production methods is competitive cost. Although electricity from wind is now competitive (~6¢/kwh), the high capital cost of electrolyzers-discussed in the section and currently in excess of $1,000/kw-drives up the H_2 cost. There is potential for chemical engineers to bridge technology advances in PEM fuel cells with PEM electrolyzers to significantly impact renewable H_2 costs.

Solar Cells

One way of using solar energy is to first produce electricity and then use an electrolyzer. However, the cost of electricity from the current photovoltaic technology is in the range of 20¢ to 30¢/kWh. There is a great opportunity for the chemical engineers to get involved in the manufacture of solar cells and bring systems approach to the problem. Also with the advent of new methods to form thin films, nanomaterials with tailorable structures and conducting polymers, opportunity exist to apply chemical engineering knowledge to develop new materials for solar cells.

Direct H_2 Production

For solar energy, another, potentially greater opportunity is to produce H_2 directly from water without first going through electricity. Thermochemical and photoelectrochemical processes are in the early phase of development and have a number of material and process related issues that are within the realm of chemical engineering. Recently, fundamental research on H_2 production by photosynthetic organisms has started to receive attention. This is an attractive area for those in bioengineering.

End Use. The cost and performance of the fuel cell itself is another potential showstopper for widespread adaptation of H_2 economy. At present, vehicle fuel cells cost in excess of $1,000/kw and have operating lifetime of less than 1,000 h. In contrast, the conventional internal combustion engines cost in the neighborhood of $35 per kW and easily last operating hours of 5,000 or more.

From a chemical engineer's perspective, the fuel cell design provides a number of opportunities. A new membrane material is needed that operates at a somewhat higher temperature. Currently noble metals such as platinum are used as catalytic materials on the electrode. A cheaper material with a more abundant supply is desirable. The fuel cells operate with moist gaseous streams and have freeze-up problem in cold parts of the world. Clearly a systems design approach is needed to not only eliminate these problems but also decrease the overall cost and increase the lifetime of the system.

Final Thoughts

Energy is one of the grand challenges facing the global community. While the use of H_2 as an energy carrier has been demonstrated, its wide-scale use is laden with potential technical, economic, and societal impasses. Some major obstacles to an H_2 economy are: reduction in fuel cell cost by one order-of-magnitude while enhancing performance attributes; storage and transportation of H_2; and evolution of a suitable infrastructure. The discussion in this article has outlined these and other key technical challenges to which chemical engineers can apply their expertise.

Today the cost of H_2 from renewables such as solar is noncompetitive. Surprisingly, if H_2 were to be produced from fossil fuels, the amount of carbon release to the atmosphere is no more than that from the gasoline driven cars. Therefore, during transition period, H_2 could be produced from fossil fuels. However, this requires the development of cost-effective and efficient distributed fossil fuel based H_2 generators. However, due to limited supply of the fossil fuels, the production of H_2 from fossil fuels is not a long-term solution, and there is a need to reduce cost for H_2 production from a more sustainable source.

If successful, an H_2 economy and associated infrastructure will not be realized for several decades. Because success is not certain, it will be wise to maintain a robust portfolio of energy research and development that includes programs in areas other than H_2. Chemical engineering must play a significant role in developing solutions to these grand energy challenges facing the global community.

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