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PROCESS ANALYSIS WORK FOR THE DOE HYDROGEN PROGRAM - 2000

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Abstract

In 2000, process analysis work conducted at the National Renewable Energy Laboratory for the Department of Energy's Hydrogen Program included cost analyses on both long-term basic research concepts and nearer-term fossil-based technologies. Additionally, a life cycle assessment on wind/electrolysis was performed for comparison of the environmental impacts of hydrogen production with those from steam methane reforming. The goal of this work is to provide direction, focus, and support to the development and introduction of hydrogen through evaluation of the technical, economic, and environmental aspects of hydrogen production and storage technologies. The advantages of performing analyses of this type within a research environment are several-fold. First, the economic competitiveness of a project can be assessed by evaluating the costs of a given process compared to the current technology. These analyses can therefore be useful in determining which projects have the highest potential for near-, mid-, and long-term success. Second, the results of a technoeconomic analysis are useful in directing research toward areas in which improvements will result in the largest cost reductions. Finally, as the economics of a process are evaluated throughout the life of the project, advancement toward the final goal of commercialization can be measured. Life cycle assessment (LCA) is used to identify and evaluate the environmental impacts of emissions and resource depletion associated with a specific process. When such an assessment is performed in conjunction with a technoeconomic feasibility study, the total economic and environmental benefits and drawbacks of a process can be quantified. Material and energy balances are used to quantify the emissions, resource depletion, and energy consumption of all processes required to operate the process of interest, including raw material extraction, transportation, processing, and final disposal of

products and by-products. The results of this inventory are then used to evaluate the environmental impacts of the process so that efforts can be focused on mitigating negative effects.

The studies that were conducted this year are summarized below. The actual milestone report for each study is available from the authors. Analyses were conducted on the following:

- Assessment of wind energy coupled with a reversible fuel cell
- Analysis of the production of hydrogen from Air Products' SER and ITM reactors
- Evaluation of the cost of hydrogen production via photobiological algal systems
- Life cycle assessment of wind/electrolysis, compared to SMR
- Assessment of thermocatalytic hydrogen production from natural gas decomposition
- Summary and map of analysis work funded by the U.S. DOE Hydrogen Program

The analyses conducted by NREL's process analysis task for the Hydrogen Program in 2000 served to refine our understanding of the economic feasibility of many research projects, as well as to quantify the environmental impacts of two methods of hydrogen production. Overall, process analysis at NREL helps the Hydrogen Program to methodically assess the applied research portfolio, in order to focus on those projects that have the potential to significantly contribute to the adoption of clean hydrogen systems. Results from the economic studies help researchers concentrate their efforts on those areas that have the greatest impact on cost, such that novel technologies can be commercialized more quickly. Hand-in-hand with cost analysis, LCA studies help the Program and the hydrogen community quantify the environmental status of various hydrogen technologies. Finally, process analysis helps streamline the transition to the hydrogen economy, balancing environmental requirements and economic constraints.

Assessment of Wind Energy Coupled with a Reversible Fuel Cell

This study examined the economic advantages that could be gained by storing off-peak wind power for sale during peak periods of the day. The report examined a number of different scenarios. In one case, it was assumed that a hydrogen bromide (HBr) fuel cell was used at the wind farm site for storing off-peak power for sale during on-peak periods of the day. In a second scenario, it was assumed that power transmission lines from the wind farm to the metropolitan area where it would be consumed were constrained. Power was therefore transmitted at night and during other off-peak times and stored using the HBr reversible fuel cell system for sale during peak periods of the day. Both of these cases were compared to systems without storage, operating under the same limitations.

There is a major difference between the scenarios mentioned above. With the constrained power transmission lines, no power can be sold directly from the wind turbines to the grid during peak times. In the case with unconstrained power, the system can supply wind power directly to the grid (the most efficient mode of operation) or use stored hydrogen in the HBr system to supply electricity using the HBr fuel cell. Excess power during peak periods could also be stored using the HBr system, but for the highest electricity sales revenue, it was assumed that all the wind power produced during peak periods went directly to the grid.

Although the HBr system was clearly able to increase the electricity selling price, using the HBr storage system for electricity storage results in a 36% loss in power compared to supplying the electricity directly to the grid (i.e., 64% round-trip storage efficiency). In the case of constrained transmission lines, all the off-peak power produced by the wind turbine went through storage and no on-peak power from the turbines could be sold. These factors resulted in a lower volume of electricity sales in all cases and lower overall electricity revenue, despite the higher selling price. The economics of this system naturally looked worse once the capital costs were factored in.

This analysis used Minot, North Dakota, wind turbine performance data for an Atlantic Orient Corporation 15/50 wind turbine and power demand and cost data from the New England Power Pool. These were the data available at the time of the analysis, but another analysis is planned using one of NREL's advanced turbine designs with a more complete wind data set and power data from the Chicago and Denver power markets. The results are not expected to change significantly.

Analysis of the Production of Hydrogen from SER and ITM Reactors

Sorption-Enhanced Reactor

Air Products is developing the sorption-enhanced reactor (SER) to reduce capital costs by operating at a lower temperature and lower pressure, and achieving a higher conversion of methane to hydrogen in the reforming reactor, eliminating the need for subsequent shift reactors. This is accomplished by mixing materials with the reforming catalyst that will adsorb carbon dioxide, shifting the equilibrium in the reactor toward higher hydrogen concentrations.

While the SER process is simpler and has lower capital costs than a conventional steam methane reforming process, the need for purge steam to desorb the carbon dioxide captured by the sorbent results in poor heat integration and additional natural gas consumption. The overall hydrogen yield is therefore lower and results in a hydrogen selling price of $12-$17/GJ (HHV basis). This price may be competitive for customers far from a centralized hydrogen production facility, but would not be directly competitive with large-scale steam methane reforming. Improvements in the economics of the process would depend upon changes in either the reforming catalyst to allow a different purge gas, or changes in the sorbent to allow a higher-pressure purge and improved heat recovery.

The hydrogen selling price for a 2.5 million scfd (246 kg/h) plant was estimated at $16.80/GJ of hydrogen, including a 15% internal rate of return. For a 10 million scfd (984 kg/h) plant, the hydrogen selling price dropped to $12.60/GJ due to economies of scale and proportionally lower labor costs. These prices were based upon the reactor conditions reported by Air Products at the 1999 Hydrogen Program Review. While these selling prices are higher than the $5-$8/GJ estimated price for hydrogen from steam methane reforming, a small-scale SER process might be more economical for onsite generation compared to conventional steam reforming for supplying liquid hydrogen to a remote location, which can cost $20/GJ or more.

Ion Transport Membrane Reactor

Air Products is developing the ion transport membrane (ITM) reactor to reduce the cost of producing hydrogen. The ITM reactor would eliminate the oxygen plant required for conventional partial oxidation hydrogen production, thereby reducing the capital and/or operating costs.

An analysis of the ITM production process resulted in a hydrogen selling price of $21.60/GJ of hydrogen for a 2.5 million scfd (246 kg/h) plant, including a 15% internal rate of return. For a 10 million scfd (984 kg/h) plant, the hydrogen selling price dropped to $18.40/GJ due to economies of scale and proportionally lower labor costs. Some credit was taken for excess electricity produced using an off-gas combustion turbine. While these selling prices are again higher than the $5-$8/GJ estimated price for hydrogen from steam methane reforming, a small-scale ITM process might be economical for onsite generation compared to supplying liquid hydrogen to a remote location from a centralized steam reforming plant. The cost estimates in this study are preliminary because of limited data on the ITM membrane. Information on the cost of the ceramic ITM membrane and its performance characteristics would be needed to make a final comparison with steam methane reforming or other technologies.

These projected hydrogen costs are very dependent upon the cost of the ceramic material used in the ITM reactor. The cost of the ceramic was estimated using information for hydrogen transport membranes, but because the ceramic is a large contributor to the overall plant cost, further information is required from Air Products to better estimate the true capital costs of a full-scale plant. The key to the process is the development of an ion transport membrane capable of efficiently removing oxygen from air to supply a partial oxidation reaction. This membrane would replace the high-cost oxygen generation plant that would normally be required for such a process. If the ITM reactor could be constructed for half the cost, the hydrogen selling price would drop to $15/GJ for the 10 million scfd (984 kg/h) plant size.

Evaluation of the Cost of Hydrogen Production via Photobiological Algal Systems

It was recently discovered that *Chlamydomonas reinhardtii* (green algae), under sulfur-deficient, anaerobic conditions, will spontaneously produce hydrogen gas at measurable rates without any special equipment and without genetic or mutation modification. These results have been verified, but whether photobiological hydrogen production with green algae is economically viable is another, separate question. The purpose of this study was to estimate what the hydrogen production costs might be using the current system, to determine what cost reductions might result from expected improvements, and to identify what design variables have the most importance on the process economics.

The current procedures used in the lab do not resemble what a full scale process might look like, however, the methods used are effective for data collection to model the full-scale system. Using current laboratory conditions, the hydrogen selling price would be estimated at over $5,000/GJ for a system large enough to supply hydrogen to 100 cars per day (300 kg/d). This cost drops to $1,000/GJ with an improved process design, taking into account verified improvements over the current lab procedures. If the current areas of research are successful in meeting their targets, this cost would most likely drop another factor of ten to $100/GJ. Then assuming some breakthroughs in materials and biological function—yet not exceeding what is theoretically possible—the cost could drop another order of magnitude to $10-$20/GJ with a highly simplified production system.

As expected, the analysis results show significant effects from varying the algae concentration, the specific hydrogen yield, the amount of transmitted light and the pond depth. Changing the daily hydrogen production rate showed very high costs at low production rates, but at larger plant sizes, there is very little economy of scale and so there is only a slight increase in profits for facilities larger than 300 kg/d.

The results from varying the algae concentration show that there is an optimum concentration: if the algae concentration is too low, the capital cost for larger tanks and the operating cost for handling more water increase the hydrogen selling price. If the concentration is too high, poor light penetration results, requiring extra production capacity. This optimum concentration is based on economic factors, in addition to light absorbance and kinetic factors.

The specific hydrogen yield had the largest effect on the economics, partly because there are no adverse effects from increasing the yield—the higher the yield, the lower the costs. Likewise an increase in light transmittance due to decreasing the algae antennae size will always result in lower costs. However, if genetically engineered organisms are required to accomplish this, there may be additional regulatory requirements and/or higher design and operating costs associated with maintaining pure strains and preventing contamination.

Another important factor is reducing the recovery time. If any daylight hours are lost to recovery and transition instead of production, this represents a direct loss in production capacity and requires extra pond capacity. Eliminating the recovery step helps reduce the cost a little more, but more importantly allows for a simpler process design.

By varying the pond depth, it was shown that after a certain point, creating a deeper pond results in no added benefit only increased capital costs. This is because the algae are so efficient at absorbing light, the algae more than a few centimeters below the surface see almost no light. Adding more algae capacity below this depth just results in a more costly tank and more material to handle, but because the light intensity is so low, the additional algae are producing very little, if any, extra hydrogen.

Naturally the average hours of sunlight affected the economics. What might be important is whether the hydrogen production rate remains high at low light levels. If this is the case, hydrogen production may still be adequate on rainy or cloudy days.

The cost of the transparent material for constructing the bioreactor is an important consideration. Material costs range over several orders of magnitude going from expensive glass to very thin, cheap sheets of polyethylene plastic. An important consideration includes the hydrogen permeability of the material. For example, the permeability of hydrogen through PVC is several hundred times less than the permeability through polyethylene, but PVC costs almost 100 times more.

Some factors that were shown to be less important were the settled solids density, the wasting rate, the mixing requirements, the pumping requirements, and many of the balance of plant costs. These items may make the difference between prices of $50/GJ and $15/GJ of hydrogen, but other improvements must be made before things like power consumption become a real concern.

The most important conclusions from this study are:

- The current experimental conditions and procedures do not represent what the design criteria would be for a full-scale process.
- No *one* improvement in the cyclic process would result in enough of a cost reduction to make the process economical—work is required on several fronts.
- Successful research and development in multiple areas might result in a hydrogen selling price close to the current program goal of $15/GJ for hydrogen from renewable sources.
- The success of this process will require higher specific hydrogen production rates, increased light transmittance through the algae, shortening of the recovery period and a bioreactor with low material costs that could be designed with a shallow pond depth.

Life Cycle Assessment of Wind/Electrolysis Compared to SMR

Although hydrogen is generally considered to be a clean fuel, it is important to recognize that the steps involved in producing it may have negative impacts on the environment. Examining the resource consumption, energy requirements, and emissions from a life cycle point of view gives a complete picture of the environmental burdens associated with hydrogen production. Life cycle assessment (LCA) is a systematic analytical method that helps identify and evaluate the environmental impacts of a specific process or competing processes. Life cycle assessments were conducted on two hydrogen production systems: steam methane reforming (SMR) and wind/electrolysis. Each LCA was performed in a cradle-to-grave manner. For the SMR system, this included plant construction and decommissioning, natural gas production and distribution, upstream processes required for plant operation such as electricity generation and distribution, the recycling of materials, and the disposal of wastes. Natural gas lost to the atmosphere during production and distribution is also taken into account. Wind/electrolysis is unique in that the resources required, energy consumed, pollutants emitted, and waste generated mostly occur during construction, with almost no emissions resulting from its operation. In contrast, the majority of the environmental stressors in the SMR system are a result of natural gas production and distribution.

In terms of total air emissions, CO_2 is emitted in the greatest quantity, accounting for more than 95 weight percent of the total air emissions for both systems. For the SMR system, the vast majority of the CO_2 (84%) is released at the hydrogen plant. Very few non-CO_2 emissions come from the operation of the SMR plant itself. For wind/electrolysis, 77% of the system's CO_2 is a result of producing concrete and steel for the wind turbines and hydrogen storage. For the wind/electrolysis system, the second highest air emission is particulates. These come primarily from quarrying the sand and limestone needed for concrete production.

The greenhouse gas emissions from these systems are CO_2, CH_4, and N_2O, and can be normalized to describe the systems' total global warming potential (GWP). Normalization factors for CO_2, CH_4, and N_2O are 1, 21, and 310, respectively. The global warming potential (GWP) of the SMR system is 12 times higher than that for the wind/electrolysis system. Table 1 summarizes the total greenhouse gas emissions from each system.

Table 1 - Global Warming Potential

System	GWP	% contribution to GWP		
	g CO_2 eq. per kg H_2	CO_2	CH_4	N_2O
SMR	11,888	89.3	10.6	0.1
Wind/electrolysis	970	97.9	0.6	1.5

The energy balance of these systems can be represented as the net energy ratio, which is the total amount of energy contained in the product hydrogen divided by the total energy consumed by the system that produces the hydrogen. This ratio was calculated to be 0.66 for SMR and 13.2 for wind/electrolysis. Because the SMR system is based on consumption of a non-renewable resource, the amount of energy in the product is less than the amount of energy consumed by the system. In contrast, the wind/electrolysis system delivers more energy than it consumes.

These two studies are the first in a series of assessments to compare the environmental benefits and drawbacks of hydrogen production via different technologies. Future work will involve using these studies to assess integrated systems for the following three hydrogen applications: transportation, remote communities, and residential. These studies can also be compared to hydrogen production via other routes such as biomass and photovoltaics. Additionally, longer-term technologies (e.g., photobiological and photoelectrochemical hydrogen production) can be examined using life cycle assessment to explore opportunities for reducing environmental consequences.

Assessment of Thermocatalytic Hydrogen Production from Natural Gas Decomposition

A technical and economic analysis was performed to examine two process designs for producing hydrogen via thermocatalytic decomposition of natural gas. Research for this process is being conducted by Dr. Nazim Muradov of the Florida Solar Energy Center (FSEC). The first design uses partial oxidation of some of the natural gas and carbon within the reactor to produce heat for the decomposition reaction. The second design uses combustion of natural gas to heat the carbon in a separate vessel. The hot carbon is then recycled back to the reactor. Both methods use pressure swing adsorption (PSA) to purify the product hydrogen, with the PSA off-gas recycled to the reactor to improve hydrogen production efficiency. A pure carbon byproduct, free of sulfur and ash impurities, is assumed to be sold.

Due to the recent volatility in the natural gas market, hydrogen selling price results were presented as a function of natural gas cost. Depending on the size of the plant and natural gas cost, the results of a sensitivity analysis predict the plant gate hydrogen selling price to be $11-$31/GJ for the partial oxidation system, with an expected cost of $19.53/GJ for a 20 million scfd plant and a year 2000 natural gas cost of $3.72/GJ of natural gas. For the three-vessel system, the predicted price range was $7-$21/GJ of hydrogen, with an expected price of $10.71/GJ. These selling prices assume a carbon byproduct selling price of $0.30/kg and a 15% internal rate of return. The following three plant sizes were evaluated: 6, 20, and 60 million scfd (591, 1969 and 5906 kg/h) of hydrogen, with the largest plant size having the lowest hydrogen selling price. Hydrogen storage and transportation contribute an additional $0.10-$13.00/GJ depending on the customer location and delivery method.

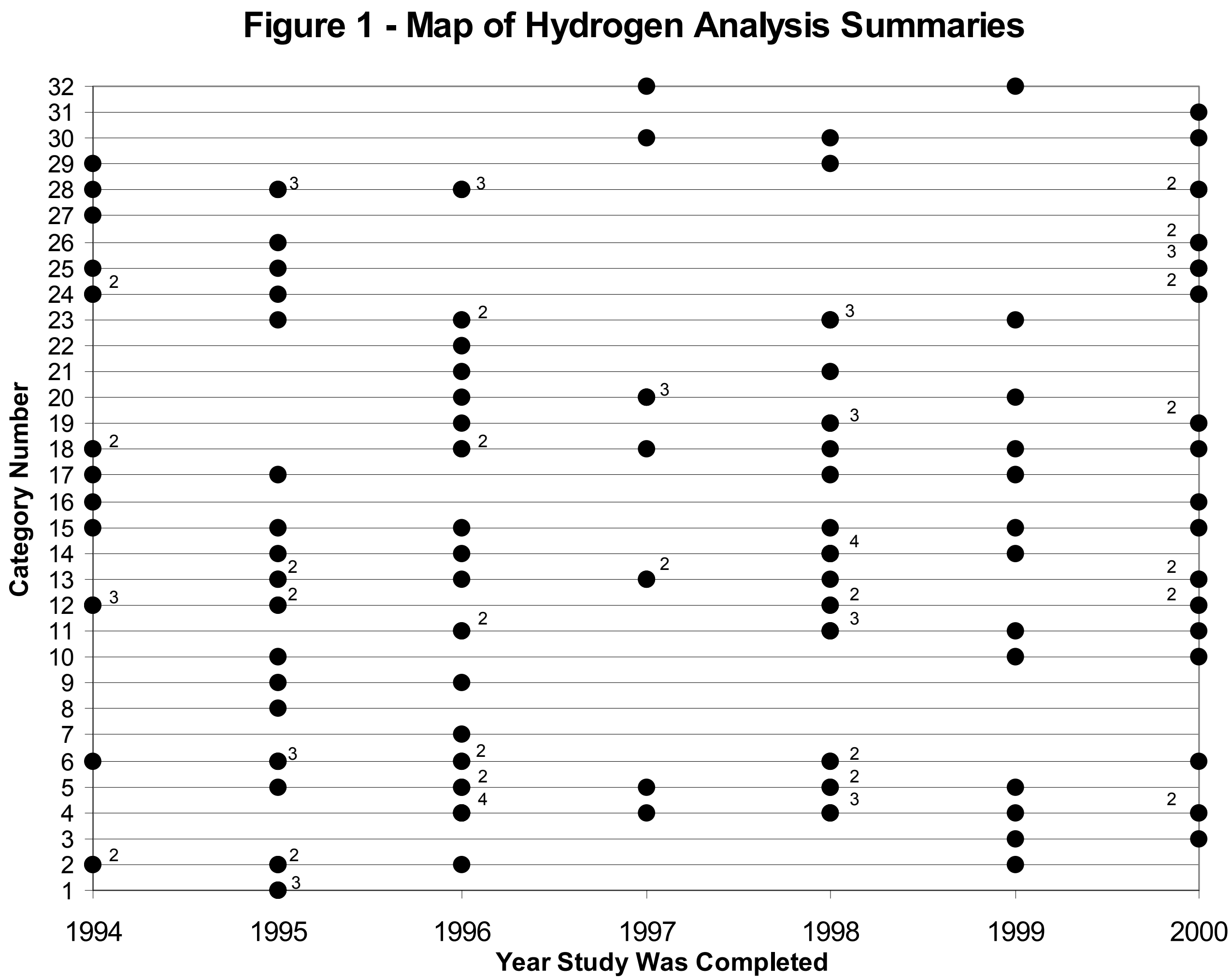
Results from the sensitivity analysis determined the contribution of 25 assumption variables to uncertainty in the hydrogen selling price. Those variables that have the greatest influence on hydrogen selling price are yield of carbon, hydrogen production factor, operating capacity factor, and carbon selling price. In addition to varying carbon selling price with other variables in the Monte Carlo analysis, the carbon price was also varied independently to determine the dependence of hydrogen selling price on carbon selling price alone. If the carbon cannot be sold as a byproduct, the hydrogen selling price increases by $8/GJ from the base case in the partial oxidation system and by $5/GJ in the three-vessel system.

To accurately compare the greenhouse gas emissions from these two processes with those from steam methane reforming (SMR), a life-cycle approach was taken and emissions from the hydrogen production plant, upstream natural gas production, natural gas distribution, and avoided carbon black production were included. Emissions from these sources were reduced by 59% for the partial oxidation system compared to SMR and were reduced 33% for the three-vessel system.

Results of the sensitivity analysis yielded several research recommendations. Current data from Dr. Muradov are based on a single-pass reactor setup. Experimental trials with a carbon recycle to the reactor will give a better understanding of how the carbon's catalytic activity changes over time. Also, the carbon selling price has a large influence on the hydrogen selling price, so in-depth testing of the carbon quality and purity will allow a more accurate determination of the carbon selling price.

Summary and Map of Analysis Work Funded by the U.S. DOE Hydrogen Program

A visual map of hydrogen analysis studies funded by DOE in the past six years was constructed and is shown in Figure 1.



Note: Numbers indicate how many studies were conducted in each category each year. Only one study was conducted if there is no number.

Some preliminary conclusions from this map are:

- Many studies have been done for hydrogen production and hydrogen distribution, however, few studies have been completed concerning newer developing hydrogen technologies and niche markets.
- Many transportation studies have been completed.
- Very few studies are shown in the areas of safety and environmental concerns.

The purpose of this work is to determine areas of focus for future analyses and also to provide a quick reference for finding studies already completed. A total of 76 studies were summarized and sorted into the following categories shown in Table 2.

Table 2: Categories for Analysis Map

H_2 Production
1. Grid electrolysis
2. Natural gas
3. Coal
4. Sunlight
5. Wind
6. Biomass
7. Hydroelectric
8. Geothermal
9. MSW
10. Comparison studies

H_2 Distribution
11. Stationary storage
12. Infrastructure - H_2 transmission
13. Infrastructure - refueling stations

Electricity Generation
14. Renewables
15. Stationary FCs

Market Analysis
16. Transportation
17. Distributed power

Transportation
18. Onboard storage
19. Fuels
20. Fuel cell vehicles
21. Hybrid electric vehicles
22. Internal combustion engine vehicles
23. Comparison studies

Outreach
24. Industry
25. Education

Safety
26. Codes and standards
27. Ventilation systems

Analysis Methodology
28. Project evaluation
29. Modeling

Environmental Concerns
30. CO_2 sequestration
31. Vehicle emissions
32. Life cycle assessment

Outreach

The reports summarized came primarily from the Hydrogen Program Reviews (1994-1999). In addition, articles by subcontractors of the Program were included. Only those efforts supported by the Program were included, while undertakings outside of the Program were not reviewed. The articles reviewed should not be considered exhaustive. Because there is no listing of all projects/publications funded by the Hydrogen Program, it was impossible to ensure that all efforts had been reviewed. However, since all of the Program Reviews were covered, it is likely that the most important efforts have been addressed.

In some cases, the analyses occurred over several years, with progress reports occurring in different Program Review Proceedings and the author list changing. In these cases, only a single entry is noted in the figure. Reports that encompassed more than one analysis area were listed in all applicable analyses areas. The map and categories will be periodically updated as new studies are published and as feedback is received from the authors and Program stakeholders.

Summary

This year's analyses examined several new or developing technologies for hydrogen production. Besides providing an estimated hydrogen selling price for each process, the analyses identified the major contributors to the selling price so efforts can be made to improve the economics. Sensitivity analyses and Monte Carlo help supply insight into the likelihood that certain changes will improve the economics of a process, or whether there are limiting factors that cannot be overcome. Without conducting these periodic assessments of economic potential, a project could be funded for several years without concentrating research efforts in the right areas to achieve the most benefit for the money spent.

Likewise, LCAs provide insight into the environmental aspects of a process. LCAs can be used to study a single process or to compare alternatives. Through a systematic cradle-to-grave investigation, an understanding of the benefits or drawbacks is possible. What may look like a good idea initially, may have far reaching impacts that are not immediately obvious. The next step will be to take the quantitative information on resource depletion, emissions, waste production and energy consumption to evaluate the overall impact of competing technologies on the environment.

Lastly, because it is important to use systems analysis studies to guide the future course of the Hydrogen Program, the mapping and associated database of prior analyses will help identify sources of information already available and show where further work must be done.