II.E Hydrogen Fueling Systems and Infrastructure

II.E.1 Development of a Turnkey Commercial Hydrogen Fueling Station

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Objective

Demonstrate the potential for an economically viable stand-alone, fully integrated hydrogen (H_2) fueling station based upon the reforming of natural gas by striving to:

- Develop a cost-effective solution to the reforming of natural gas to produce a reformate stream;
- Develop an efficient, cost-effective means to purify the hydrogen-rich reformate to pure hydrogen employing pressure swing adsorption (PSA) technology;
- Develop an optimum system to compress, store, meter, and dispense hydrogen into vehicles;
- Efficiently integrate the process steps mentioned above into a safe, user-friendly, cost-effective fueling station;
- Demonstrate the operation of the fueling station at Penn State University;
- Maintain safety as the top priority in the fueling station design and operation; and
- Obtain adequate operational data to provide the basis for future commercial H_2 fueling stations.

Approach

This nine-quarter project is being managed in three phases, with Stage Gate reviews between each phase. These phases overlap in time in order to make efficient use of resources and minimize costs.

- In Phase 1, conceptual design and preliminary cost evaluations for each major sub-system in the fueling station will be completed.
- In Phase 2, sub-system R&D will be performed to test the concepts put forth in Phase 1. Technical viability and fueling station costs will be validated.
- Phase 3 will include fabrication, installation, and testing of the full-scale H_2 generator and dispenser at Penn State University. This H_2 fueling station will be designed to deliver 50 nm^3/hr H_2.

Accomplishments

- Kicked off development work on the novel reforming system.
- Began the process and cost study of the various reforming options available.
- Initiated the H_2 PSA development program at Air Products and Chemicals, Inc. (APCI) and the engineering services study at QuestAir.
- Built a prototype H_2 PSA system to be installed for testing at an Air Products H_2 production facility.
- Started engineering work on the compression and dispensing systems.
- Equipped a laboratory to test H_2 flow meters for use within the dispenser.

Future Directions

In the near term, the development team will conclude the Phase 1 work and hold a Stage Gate review meeting with DOE management. Then, work on all aspects of Phase 2 will commence, followed by Phase 3. The expected schedule for these Phases is outlined in the table below:

Task	Date
Phase 1 Pre-Contract Technical Development	Oct 2001 – March 2002
Cooperative Agreement Award	29 March 2002
Phase 1 Conceptual Design and Economic Evaluation	April 2002 – June 2002
Phase 2 Subsystem Development	July 2002 – March 2003
Phase 3 System Deployment	April 2003 – December 2003
Phase 3 System Deployment – Operation & Testing	January 2004 – June 2004

Introduction

The transition to hydrogen as a fuel source presents several challenges. One of the major hurdles is the cost-effective production of hydrogen in small quantities. In the early demonstration phase, hydrogen can be provided by bulk distribution of liquid or compressed gas from central production plants; however, the next phase to fostering the hydrogen economy will likely require onsite generation to institute a pervasive infrastructure. Providing inexpensive hydrogen at a fleet operator's garage or local fueling station is a key step toward enabling commercialization of direct hydrogen fuel cell vehicles (FCVs). The objective of this project is to develop a comprehensive, turnkey, stand-alone hydrogen fueling station for FCVs with state-of-the-art technology that is cost-competitive with current hydrocarbon fuels. Such a station will promote the advent of the hydrogen fuel economy for buses, fleet vehicles, and ultimately personal vehicles.

Approach

The development efforts are expected to build on preliminary work accomplished by the major partners. Air Products, as the overall project manager, is responsible for the total system integration and final development of the installed equipment. As the system integrator, Air Products will ensure that the system is fully optimized and that all of the individual components are compatible to deliver the lowest cost H_2 fuel. This nine-quarter project is being managed in three phases, with Stage Gate reviews between each phase.

During Phase 1 of the program, subsystem conceptual designs will be formulated and costed. Options will be developed and compared for the reformer system, PSA system, compression, storage, and dispenser. Air Products will work with H2Gen to develop and to evaluate the applicability of a novel convective steam methane reforming (SMR) based reforming system. At the end of Phase 1, we will confirm the preliminary feasibility of cost targets via an initial, pre-developmental definition of scope and execution costs and will identify the partners for further development of components.

In Phase 2, the most promising subsystem designs assessed and selected in Phase 1 will be further developed. Lab testing of certain components will be carried out. Recommendations for the optimal fueling station components will be made. Air Products engineers, working with the selected reforming partner, will optimize the design of the reformer and PSA systems, and build and test components of the systems in laboratories. Air Products will be directly responsible for the design of the dispenser, which will be tested in a shop prior to installation on site. Finally, Air Products will act as the system integrator to pull together the various pieces into a comprehensive turnkey unit and to minimize the total cost of delivered H_2.

During Phase 3, scale-up and detailed engineering design of all equipment will be completed. The engineered system will be analyzed for Design for Manufacture and Assembly (DFMA), and the assembled system will include instrumentation for data collection and provisions for remote monitoring of operation. Fabrication of all equipment and installation at Penn State University will follow. The fueling station will be started up and put into operation, beginning with 6 months of operation and testing. Finally, the cost of H_2 delivered from the installed fueling station will be validated, taking into account the impact of mass-producing components.

Results

As shown in Figure 1, hydrogen can be delivered for use at a refueling station in several ways. It can be piped to the station via a pipeline, delivered in cryogenic liquid form and then vaporized, delivered in compressed gaseous form and stored in on-site tanks, generated on-site via reforming of hydrocarbon feedstocks such as natural gas, or

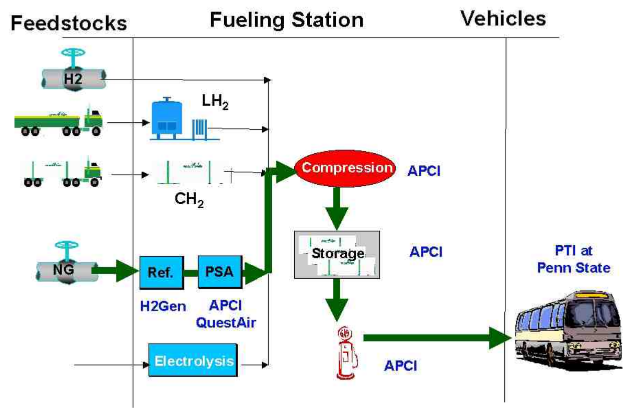

Figure 1. Hydrogen Fueling Station

produced via electrolysis of water with power input. The scope of this program is to develop the route highlighted with the bold arrows in Figure 1 – the reforming of natural gas followed by H2 purification with PSA technology. Subsequently, the high purity H2 will be compressed and stored prior to final dispensing into the H_2 vehicles.

Also highlighted in Figure 1 next to each process unit operation is the development partner responsible to contribute to the development or engineering of that piece of equipment. The development team began work addressing the technical challenges in October 2001. Below is a summary of progress to date:

Regarding aggreements and contracts, the cooperative agreement between DOE and APCI was signed on 29 March 2002. Subsequently, the subcontract with H2Gen was signed for development of the reformer. The subcontract with QuestAir is in review for supply of an improved H_2 PSA purifier design, and the subcontract with Penn State University has been completed for siting of the fueling station.

In the reforming area, H2Gen development work kicked off in October 2001. Catalyst characterization work has begun, and the first prototype reformer is being built. Components have been tested, and the burners have been sized and tested in the lab. In addition, APCI began its engineering study in April 2002 to update the comparison of autothermal reforming (ATR), partial oxidation (POX), and SMR technologies to determine the optimum route to small-scale H_2 production. This kicked off the "Phase 1" portion of the development program.

As part of this Phase 1 study, APCI prepared and sent out a Request For Quotation (RFQ) for the reforming system to several reformer vendors. Included in the RFQ were companies offering SMR, ATR, and catalyst systems.

The development of a H_2 PSA at APCI began in October 2001. Adsorbent development has commenced and step-out approaches to achieving compact PSA designs have been identified. PSA cycle development work is underway to fully utilize the adsorbents' capabilities. Laboratory experiments are underway. Additionally, development of new PSA valves, vessels, and other mechanical components has been initiated; testing plans have been formulated; and laboratories are being equipped for component testing. To hasten the introduction of some of these new concepts, APCI completed detailed design of a prototype H_2 PSA unit to be evaluated at one of APCI's H_2 production facilities. The data collected on this PSA unit will serve to verify several of the significant technical "step-outs" being taken in the new PSA design being developed by the APCI team. Fabrication of this PSA skid was completed in early June, and the system is being installed on site. Finally, in anticipation of an engineering services sub-contract, QuestAir began work to improve their HyQuestor H_2 purifier in October 2001. Their preliminary design and cost summaries are nearing completion.

APCI's compression, storage, and dispensing development work began in October 2001. To date, APCI has completed the preliminary engineering work to determine the optimum configuration and selection of components for the H_2 dispenser. Also, laboratory equipment to test H_2 flow meters for use in the dispenser has been purchased and is being installed.

APCI has completed the initial conceptual process flow diagram (PFD) for the integrated fueling station. This will serve as the basis for engineering discussions related to the Penn State fueling station. To date, process specifications for all major components in the fueling station have been issued. Regarding utilities, APCI has defined a natural gas specification based on North American averages, has defined a potable water specification, and has identified Penn State's specific natural gas and potable water specifications for use as the design basis for the system to be placed there.

Conclusions / Future Directions

Work has begun on this aggressive project to determine the viability of a commercial turnkey H_2 fueling station. Initial conclusions will be communicated at the completion of the Phase 1 tasks and will be included in the Phase 1 report.

II.E.2 Autothermal Cyclic Reforming Based Fueling System

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Objectives

- Design, fabricate, and install a reliable and safe H_2 refueling system, based on autothermal cyclic reforming (ACR), that is capable of producing at least 40 kg/day of H_2 (450 std m^3 per day of H_2), which is sufficient for refueling at least 1 bus or 8 cars per day.
- The current target cost for generation and refueling of hydrogen is $19.2/GJ of hydrogen for a 900 kg/day of H_2 (10,000 std m^3 per day of H_2) system, based on the lower heating value (LHV) of hydrogen. The future target cost is expected to decrease to $17.2/GJ by 2005 and $16.2/GJ by 2010.

Approach

- Phase I (2002): Complete the design of the integrated system and assess the technical and economic feasibility of the design.
- Phase II (2003-4): Perform subsystem development.
- Phase III (2004-5): Demonstrate the fully integrated system.

Accomplishments

- An optimal process configuration was selected, process flow diagrams were developed and efficiencies were calculated.
- In collaboration with another ongoing DOE project, “Fuel Processing Based on ACR for Stationary PEM Fuel Cells” (contract No. DE-FC02-97EE50488), the component design of a fuel processor has been completed and the system is being fabricated. The fabrication is expected to be complete by July 2002.
- A detailed safety assessment including personnel hazard analysis (PHA), hazardous operations (HAZOP) and failure mode and effects analysis (FMEA) has been performed.
- An economic analysis for the hydrogen refueling station is being performed. Based on information from the literature, the cost of each subsystem of the refueling station was expressed as a function of the quantity manufactured and the hydrogen capacity. Preliminary estimates were made for cost of H_2.

Future Directions:

- Complete the system design.
- Complete the economic analysis.
- Develop a plan for Phase II.

Introduction

Autothermal Cyclic Reforming (ACR) is a GE patented technology for converting hydrocarbons to a hydrogen-rich stream. The ACR process operates in a three-step cycle that involves steam reforming the fuel on a nickel catalyst (reforming step), heating the catalyst bed through oxidizing the nickel catalyst to nickel oxide (air regeneration step), and finally reducing the catalyst to its original metal state (fuel regeneration step). The heat required for the endothermic reforming reaction is provided during the exothermic oxidation of nickel to nickel oxide.

Approach

A system design is being developed for the integrated hydrogen refueling system, and the technical and economic feasibility of the design is being assessed. The developmental activities and test work that are needed to both validate the design and identify a viable business model for commercialization, within the capital cost target, will be completed during the remaining part of Phase I (2002).

During Phase II (2003-4), the critical components and subsystems will be developed and tested to achieve the performance goals.

During Phase III (2004-5), the integrated H_2 refueling station will be fabricated, installed and operated. GE will develop the reformer and integrate the full system. Praxair will develop the pressure swing adsorption (PSA) unit, the H_2 compressor, and the H_2 storage tanks. BP will analyze the refueling logistics and safety.

Results

Process Analysis

A preliminary process analysis of the fuel processor, which includes the reformer, shift reactor and PSA unit, has been completed. The major subsystems of the hydrogen refueling station are shown in Figure 1, and they are: 1) autothermal cyclic reformer and PSA unit, 2) hydrogen compressor, 3) hydrogen storage system, and 4) hydrogen dispenser.

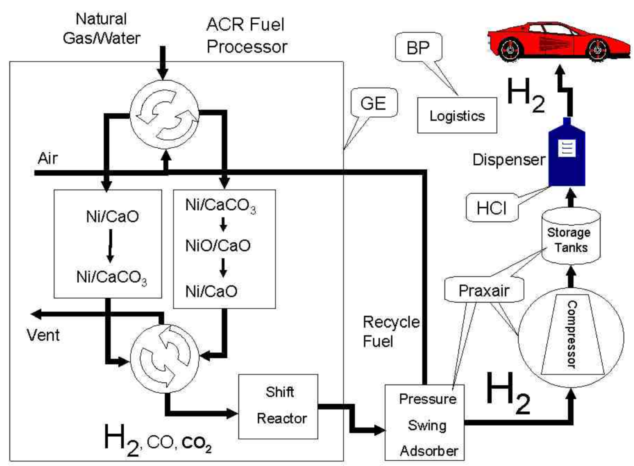

Figure 1. Major Subsystems of a Hydrogen Refueling Station

The efficiency of the fuel processor is defined as the ratio of the lower heating value (LHV) of the hydrogen produced to the LHV of the fuel consumed by the fuel processor. The major factors affecting the efficiency are: 1) the conversion in the reformer and shift reactors, 2) the recovery of hydrogen in the PSA, 3) the recovery of the process heat, and 4) the minimization of heat losses and parasitic requirements in compressors.

Several heat exchanger and compressor configurations were considered, since the thermal integration of the system has a significant impact on the efficiency. An optimal process configuration was selected, and the process flow diagrams were developed. As shown in Table 1, the efficiency of the optimal configuration is 75.2%. Compressor calculations showed that electricity required was

H_2 Recovery in PSA	80%
Electricity Consumed / LHV of fuel	1%
Mol H_2 Produced / Mol Fuel Fed	2.50
Efficiency= LHV of H_2 Produced / LHV Fuel Fed	75.2%

Table 1. Efficiency for the Optimal ACR Fuel Processor Configuration

around 1% of the LHV of the fuel. The operating conditions for the PSA are 7.9 bar (100 psig) and 50°C with 80% hydrogen recovery.

Fabrication of Integrated Fuel Processor

In coordination with another ongoing DOE project, "Fuel Processing Based on ACR for Stationary PEM Fuel Cells" (contract No. DE-FC02-97EE50488), the component design, fabrication and installation of the fuel processor have been completed (see Figure 2). The system can produce 90 kg of H_2 per day (127 kW on a LHV basis). The component design will be modified for hydrogen refueling applications, based on input from Praxair on integration of the PSA.

Figure 2. Prototype ACR Fuel Processor

Safety Analysis and Permitting

A detailed safety assessment including personnel hazard analysis (PHA), hazardous operations (HAZOP) and failure mode and effects analysis (FMEA) has been performed. The assessment will be expanded to ensure that the system is compliant with all applicable building, fire and electrical codes.

Economic Analysis

Based on a literature search, the capital cost for each major subsystem was estimated and then expressed as a function of the quantity manufactured and the hydrogen capacity of the refueling station. Cost models available in the literature for the hydrogen compressor, dispenser and storage subsystems have fairly good agreement. However, there is disagreement among various cost models for reformers. In general, small capacity reformers with optimized thermal integration are expected to cost less than conventional steam methane reformers.

Table 2 shows the information available in the literature[1-4] for capital costs of the reformer (excluding the PSA), hydrogen compressor, storage tanks and dispenser island scaled to a hydrogen capacity of 10,000 std m^3 per day (900 kg of H_2 per day or 1249 kW of H_2 on a LHV basis). Scaling factors were applied to determine the costs of the units as the manufactured quantities increase. The relationships between hydrogen capacity and subsystem capital cost are also shown in Table 2.

The projected preliminary estimate for the cost of a commercial hydrogen generation system based on ACR excluding cost of compression, storage and dispensing is presented in Table 3. The system capacity is 900 kg/day of H_2 (10,000 std m^3 per day of H_2), which can refuel 300 vehicles per day.

The cost of hydrogen was estimated by considering the capital costs, capital recovery factor, the operating expenses of the refueling station, the cost of utilities (fuel and electricity), and the cost of catalysts. The natural gas cost was assumed to be \$5/GJ on a higher heating value (HHV) basis, and the electricity cost was assumed to be 7¢/kWhr. The efficiency of the system (75% on a LHV basis) was used to determine the required amount of natural gas. A capacity factor of 90% for plant utilization was used. The capital recovery factor was determined as 13.1%, assuming 10% interest rate over 15 years. The cost of H_2 generation was estimated to be \$16.0/GJ. This preliminary cost analysis did not consider the cost reduction due to mass production, and did not consider the cost of hydrogen compression, storage and dispensing. These costs are currently being analyzed.

	Capital Cost	10 Stations	100 Stations	1,000 Stations	10,000 Stations
Fuel Processor (not including PSA)	$.88*10^6*(Kg/hr*9.5*10^{-3})^{0.7}$ @10 units	\$424,716			\$115,799
H2 Compressor	1341*(Kg/hr)+20896 @1,000 units	\$141,506		\$70,753	
H2 Storage Tanks	7708.8*(Kg/hr)+228 @10 units	\$286,835		\$200,784	
H2 Dispenser Island	850+1327.56*(Kg/hr) @10,000 units	\$439,043	\$149,484		\$50,208

Table 2. Capital cost for refueling station subsystems as a function of the manufactured quantities. The delivered hydrogen capacity is 67 kg/day.

REFORMER H2 GENERATION CAPACITY		1249	LHV kW
CAPITAL INVESTMENT			
Total Plant Cost (TPC)		\$992,162	
Allowance for Funds During Construction (AFDC)	6.3% of TPC	\$62,506	
Total Plant Investment (TPI)		\$1,054,668	
Royalty Allowance	2.6% of TPI	\$27,421	
Inventory Capital	0.8% of TPI	\$8,437	
Total Capital Requirement (TCR)		\$1,090,527	
LEVELIZED CAPITAL CARRYING CHARGES (ANNUAL BASIS)			
Capital Recovery Factor	13.1% of TCR		\$143,376
OPERATING AND MAINTENANCE COSTS (ANNUAL BASIS)			
Operating Labor	1.0% of TCR	\$10,905	
Maintenance Labor	0.9% of TCR	\$9,815	
Maintenance Material	1.2% of TCR	\$13,086	
Administrative and Support Labor	0.5% of TCR	\$5,453	
Total Operation and Maintenance			\$39,259
SYSTEM EFFICINECY	80% (HHV)		
SYSTEM EFFICIENCY	75% (LHV)		
FUEL & ELECTRICITY COSTS (ANNUAL BASIS)			
Natural Gas Feed	55,150.0 MMBtu/year		
Natural Gas cost per year	\$5.3 per MMBtu HHV		
Natural Gas cost per year	\$5.0 per GJ HHV	\$292,295	
Electricity Required/HHV of Fuel	4.4%		
Electricity Required	711,155.5 kW-hr		
Electricity Unit Cost	7 cents/kW-hr	\$49,781	
Catalysts		\$83,787	
Total Cost of Fuel & Electricity & Catalysts, accounting for capacity factor			\$383,276
NET REVENUE REQUIRED (ANNUAL BASIS)			\$565,911
HYDROGEN GENERATED	GJ/day (LHV)		107.89
CAPACITY FACTOR			90%
COST OF HYDROGEN	\$/GJ (LHV)		\$16.0
COST OF HYDROGEN	\$/kg		\$1.93

Table 3. Estimation of cost of hydrogen generation for a one-of-a-kind 900 kg/day of H_2 system (10,000 std m^3 per day of H_2; excludes cost of compression, storage and dispensing; does not consider mass production)

Conclusions

The thermal integration of the system has a significant impact on the fuel conversion efficiency of the hydrogen production system. An optimal process configuration that generates the process steam with minimum parasitic losses was selected, and the fuel conversion efficiency on an LHV basis was estimated to be 75.2%. Compressor calculations showed that electricity required was around 1% of the LHV of the fuel.

The preliminary analysis indicates that for a 900 kg/day of H_2 (10,000 std m^3 per day of H_2) one-of-a-kind commercial system, the cost of H_2 generation is $1.93/kg ($16.0/GJ) excluding the costs of hydrogen purification, compression, storage and dispensing. Mass production is expected to reduce the cost of hydrogen significantly.

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II.E.3 Development of a Natural Gas to Hydrogen Fuel Station

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Subcontractor: FuelMaker Corporation

Objectives

- Develop cost-competitive technology for high-pressure, hydrogen-based fueling systems.
- Design a fast-fill natural gas-to-hydrogen fueling system with 40-60 kg/day delivery capacity that meets the DOE goal of providing hydrogen at a cost of $2.50/kg or less.

Approach

- Use innovative, compact natural gas steam reforming system and appliance-quality hydrogen compressor technologies.
- Undertake system design and analysis to find pathways for meeting cost and performance targets.
- Conduct development and lab testing to confirm subsystem operation.
- Integrate system and incorporate controls.
- Conduct lab and field testing to validate system performance and reliability.

Accomplishments

- Developed comprehensive model for analyzing hydrogen fueling station costs, including capital, operating, and maintenance cost elements. Included Monte Carlo techniques to account for uncertainty and variability in cost drivers.
- Prepared and presented paper on hydrogen fueling system economics to World Hydrogen Energy Conference.
- Constructed a state-of-the-art high-pressure hydrogen testing environmental chamber. System contains a full-size hydrogen three-bank storage cascade that can be run from –45^{o}C to 85^{o}C.
- Developed a first-principle model for understanding the fast-fill behavior of hydrogen and the effects of temperature rise on cylinder fill performance.

Future Directions

- Complete design phase, including revised estimates of system capital, operating, and maintenance costs.

- Begin work to document the fast-fill behavior of hydrogen over a range of temperatures and starting and ending conditions using cylinders of different construction.
- Begin long-term testing to evaluate and confirm the ability of various advanced materials to provide greater durability under dry gas conditions.

Introduction

A key barrier to expanded fuel cell vehicle use is fueling infrastructure. Along with onboard liquid hydrocarbon fuel reformers, a parallel DOE strategy is development of cost-competitive technology based on high-pressure, hydrogen-based fueling systems and on-board hydrogen storage. This project builds on experience gained with compressed natural gas coupled with targeted research on natural gas-to-hydrogen reformation processes and innovative strategies to meet hydrogen fuel quality requirements (water, carbon dioxide, and carbon monoxide levels). An additional core effort is development of a hydrogen dispenser with an advanced filling algorithm that will permit accurate and complete filling of compressed hydrogen vehicles under a range of conditions.

These advanced subsystems – reforming, fuel cleanup, compression, storage, and dispensing – will be incorporated into an integrated and cost-competitive small natural gas-to-hydrogen fueling station that will support hydrogen fueling infrastructure development and expansion.

The specific goal is a fast-fill natural gas-to-hydrogen fueling system with 40-60 kg/day delivery capacity. DOE goals include providing hydrogen at costs of $2.50/kg or less.

Approach

This project is based on leveraging developments at GTI in the stationary PEM fuel cell and compressed natural gas vehicle market sectors. GTI has been developing high-efficiency steam methane reformers for stationary fuel cells, including design approaches to achieve compact size, reduced cost, and simplified control and operation. Modification of this reformer—as a hydrogen generator with advanced controls—will comprise a core element of this system.

In addition, GTI is building upon its experience with high-pressure natural gas fueling systems and working with key partners to develop hydrogen-capable and compatible versions of our fueling products—including compressors, dispensers, and cascade storage vessels. GTI sees this strategy of product line extension as a near-term pathway for achieving cost reduction and product availability to support early establishment of a hydrogen fueling infrastructure.

In this regard, GTI is working with FuelMaker Corporation to develop a high-pressure hydrogen version of their vehicle refueling appliance (VRA). The FuelMaker VRA is a high-quality appliance-like compression unit that is completely oil free—an important consideration for contaminant sensitive PEM fuel cell stacks.

The project approach includes three phases: 1) Design, 2) Development and Lab Testing, and 3) Field Testing. Through these progressive phases, GTI anticipates having a proven small natural gas-to-hydrogen fueling system that can support the development and expansion of a distributed hydrogen fueling infrastructure.

Results

The project began in February 2002, with a focus on subsystem and system design.

GTI has developed a comprehensive model for hydrogen fueling systems that takes into account all capital, operating, and maintenance cost elements. The model can also be used to assess the effects of factors such as grants and tax incentives. The output, among other dimensions, is the levelized cost for hydrogen.

GTI currently sees capital and energy costs (including the cost of natural gas consumed in the steam reformer and electricity for compression) as the dominant cost factors (see Figure 1). The cost of

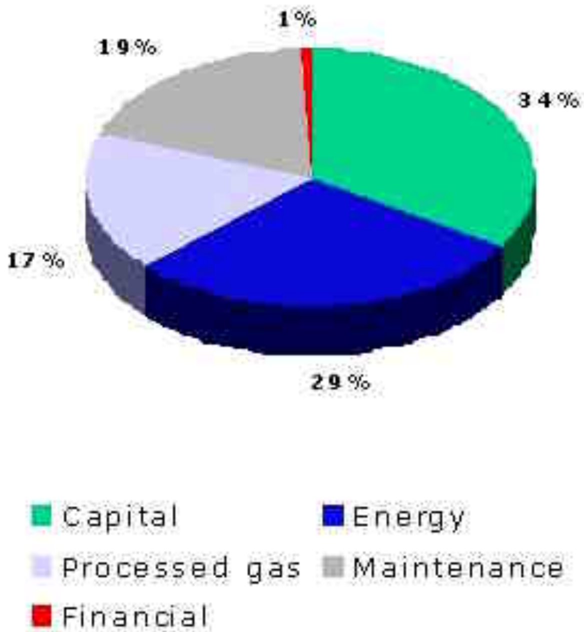

Figure 1. Hydrogen Station Costs

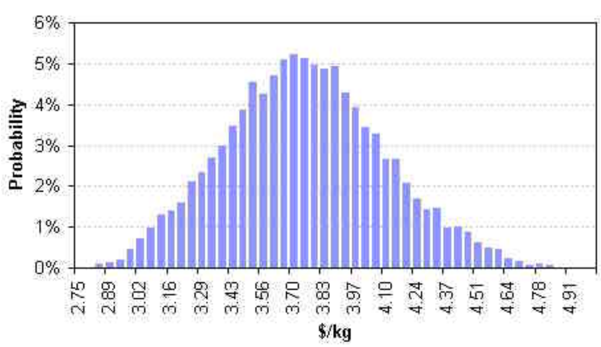

Figure 2. Hydrogen Fuel Station Cost Distribution

"processed gas"—that is, the gas reformed into hydrogen—is less than 20% of the cost of production.

Monte Carlo techniques were used to account for uncertainty and variability in individual cost elements—a facet of the nascent nature of this technology. Figure 2 shows the model results for expected cost. Levelized hydrogen costs are estimated at around $3.70/kg. Further work will be undertaken during the design phase to review these cost factors and revise the model.

GTI is also developing analytical and empirical information on the filling behavior of hydrogen

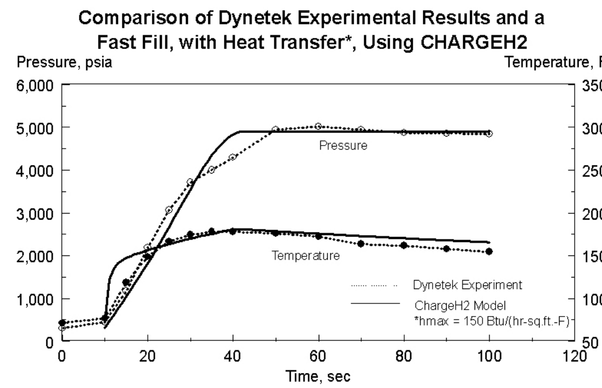

Figure 3. Hydrogen Fast Fill Data and Model

under fast-fill conditions. Work has shown that hydrogen experiences a significant temperature rise under these conditions. GTI has developed a first-principle model called CHARGE H2 that can be used as a predictive tool for this phenomenon. Figure 3 shows early results in comparing this model with empirical data. In this testing, a Dynetek carbon-wrapped, aluminum lined hydrogen cylinder rated at 345 bar (5000 psig) was "fast filled" in a period of less than 60 seconds. This cylinder had an internal water volume of 34 liters. At 345 bar, this implies a total hydrogen storage capacity of about 0.75 kg for this cylinder.

Of note is the nearly 55^{o}C *in situ* gas temperature rise during cylinder filling. While some heat transfer from the gas phase to the cylinder liner occurs, the short duration of the fill process limits the amount of heat that can be dissipated. Longer fill times—for example, 3 to 5 minutes—may somewhat increase the amount of heat transferred. Preliminary indications show the initial cylinder internal heat transfer coefficient may be as high as 6 to 8 times greater than for natural gas.

The temperature rise phenomenon seen in hydrogen as well as natural gas reduces gas density and energy content and ultimately can result in reduced vehicle driving range. GTI will conduct comprehensive testing under a variety of conditions and using cylinders of differing construction to document this behavior and compare the resulting data with its CHARGE H2 model. To counteract this effect, GTI will develop a hydrogen dispenser control algorithm to more accurately fill cylinders and provide underfill compensation that largely offsets this phenomenon.

To conduct this unique hydrogen testing, GTI has constructed a state-of-the-art high-pressure hydrogen environmental chamber. This system contains a full-size hydrogen three-bank storage cascade that can be run from –45^{o}C to 85^{o}C (see Figure 4). The chamber is fully instrumented and connected to a high-speed data acquisition system. Fast-fill hydrogen tests will be run over a wide range of temperature and pressure conditions using cylinders constructed with steel, aluminum, and plastic liners.

Figure 4. GTI Hydrogen Testing Environmental Chamber

Conclusions

Work was begun on this program in February 2002. Preliminary indications are that a natural gas to hydrogen fueling system with reduced cost capabilities is possible. Achieving the stated cost targets of $2.50/kg will be a challenge.

The strategy of leveraging developments in PEM reformers for stationary applications and compressed natural gas vehicle technology appears to be a promising pathway for leveraging technology, experience, and market channels.

References

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II.E.4 Distributed Hydrogen Fueling Systems Analysis: Cost and Performance Comparison of Stationary Hydrogen Fueling Appliances

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Objectives

- Quantify the costs of hydrogen fueling appliances (HFAs) using two natural gas reforming technologies (autothermal reforming versus steam methane reforming) and two gas cleanup technologies (pressure swing adsorption versus metal membrane gas separation) to provide on-site hydrogen for a community of 183 hydrogen fuel cell vehicles (FCVs) (equivalent to 20 refuelings per day or a capacity of 115 kilograms (kg) of hydrogen (H_2) per day (with a 69% capacity factor).
- Estimate the cost of hydrogen using each combination of technologies.
- Estimate the cost reductions from scaling the least expensive technology to a larger unit providing 160 fuel cell vehicle refuelings per day.

Approach

- Design the chemical process, physical implementation, and manufacture and assembly methods for each of the four HFA technology combinations, produced in quantities of 250 units/year.
- Use Design for Manufacture and Assembly (DFMA) cost analysis techniques to estimate the capital costs of each HFA design.
- Apply discounted cash flow analysis to determine a cost per kilogram of hydrogen.
- Use common chemical engineering scale-up factors to scale-up the design producing lowest-cost hydrogen by 8x.

Accomplishments

- Designed complete 115 kg/day capacity HFA systems for low-cost hydrogen from four combinations of reforming-cleanup technologies: steam methane reforming (SMR) with pressure swing adsorption (PSA), autothermal reforming (ATR) with PSA, SMR with metal membrane gas separation, and ATR with metal membrane gas separation.
- Estimated costs of materials, manufacture, and assembly using an adapted DFMA methodology to arrive at capital costs for each HFA design.
- Using discounted cash flow analysis, identified the SMR-PSA system as the technology to provide lowest cost hydrogen ($3.38/kg) for small-scale, small production volume HFAs.
- Estimated up to 45% reduction in cost of hydrogen ($1.87/kg) from scaling HFA size up by 8x.

Future Directions

- Evaluate the cost of renewable hydrogen for transportation applications in the 2030-2050 time frame based on a variety of renewable resources (wind, biomass, geothermal, solar, etc.), transportation, and storage options.
- Determine the most practical and economically feasible plan for the supply of 10 Quads/year of renewable hydrogen for transportation applications in 2030-2050.

Introduction

Over several studies, Directed Technologies, Inc. has analyzed the costs of representative HFAs to supply the early-introduction hydrogen powered FCVs and the cost of hydrogen produced by these HFAs. In previous studies we evaluated the impact of fuel choice on FCV, the cost of other sizes and quantities of HFA's, and the infrastructure maintenance costs of various fuels. In this study we analyzed the costs for an intermediate production rate (250/year) of HFAs sized to support communities of 183 vehicles each (about one-eighth the size of the typical new gasoline station). This small HFA is chosen to allow economical hydrogen production in the early years when there are low numbers of FC's present in any geographical area. While the focus of this report is on the economics of hydrogen production at this small unit size, it is noted that significant hydrogen cost reductions can be achieved by scaling the HFA unit to a larger size.

For the baseline HFA, we compared the costs and efficiencies of two hydrogen-generation technologies (steam methane reforming and autothermal reforming) and two hydrogen purification technologies (pressure swing adsorption and metal membrane gas separation). Each HFA includes components for natural gas desulfurization, reformation, hydrogen purification, compression, storage, and dispensing. The processing options chosen for this comparison emphasize the relative strengths of each process, with the result that there are many other potential variations that involve tradeoffs between capital cost and efficiency.

Approach

Each HFA system required a careful chemical and mechanical engineering analysis to capture the appropriate performance parameters and cost factors. Once moderately detailed mechanical designs and material and energy balances were created for all system components, a complete system Bill of Materials was generated. This Bill of Materials allowed a line-by-line, element-by-element cost assessment to be conducted using a Design of Manufacturing and Assembly (DFMA) costing approach. This methodology is used extensively by industry for product cost estimation and to compare the relative cost of competing manufacturing and assembly approaches. The DFMA methodology is both a rigorous cost estimation technique and a method of product redesign to achieve lowest cost.

Once the capital costs for each design were determined, a discounted cash flow analysis was used to compare reforming options with differing initial investments and operating expenses. The cost of hydrogen was determined by calculating the cost of hydrogen that results in a net-present value of $0 for the HFA over ten years of operation. Solving for the cost of hydrogen at $0 net-present value yields the "wholesale price" at which the reformer operator realizes an after-tax return on investment equal to the cost of capital. The cost of hydrogen calculated in this analysis is somewhere between the wholesale and retail level. We have included the capital cost for storage and dispensing, which would not typically be reflected in the wholesale costs of other fuels, but have excluded retail markup and profit for the HFA operator.

Results

Each HFA system was designed such that the reforming system ([RS], not including hydrogen compressor, storage, and dispenser) could be contained on a skid-mounted pallet (see Figure 1). This pallet has an approximately 8 ft by 13 ft footprint, stands roughly 10 ft tall, and may be enclosed by a canopy and chain-linked fence. The compressor, hydrogen storage tanks, and dispenser would be housed separately.

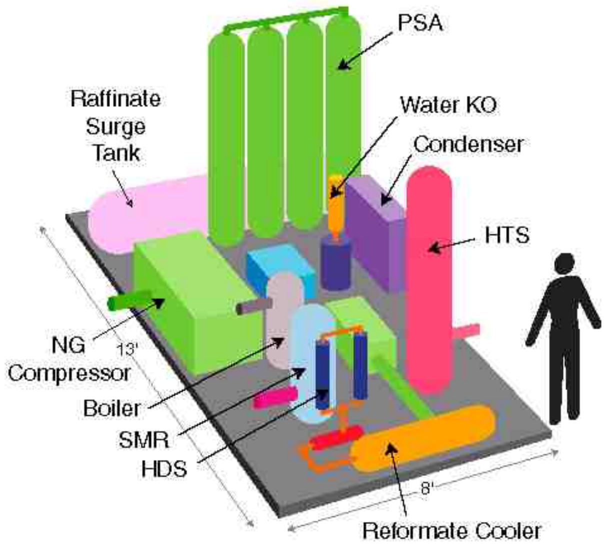

Figure 1. Proposed Layout of 10 atmospheres Steam Methane Reformer System

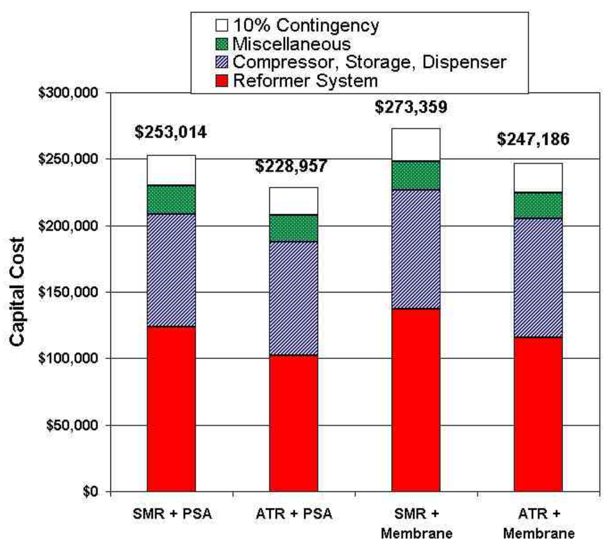

Figure 2. Contribution of Subsystems to Capital Cost for 115 kg/day HFAs. (The "Miscellaneous" category includes on-site installation, freight, taxes & insurance, and initial spares. The "Reformer System" category includes the hydrogen production and gas cleanup subsystems.)

Table 1. Cost of Hydrogen Produced from the 115 kg/day HFA Options

Costs in \$/kg H_2	SMR/ PSA	ATR/ PSA	SMR/ Membrane	ATR/ Membrane
Hydrogen Cost	**\$3.38**	**\$3.59**	**\$3.74**	**\$4.28**
Capital Recovery	1.66	1.50	1.78	1.62
Natual Gas	0.95	1.17	1.01	1.44
Electricity	0.23	0.41	0.37	0.68
O&M	0.33	0.31	0.33	0.33
Taxes & Insurance	0.23	0.20	0.24	0.22
Gasoline Equivalent (\$/gal)	**\$1.55**	**\$1.65**	**\$1.72**	**\$1.96**

HFA is assumed to run an average of 69% of capacity with 98% availability.
Capital Recovery assumes a 10% after-tax return on investment over its 10-year life.
A 38% marginal tax rate (34% federal, 4% state and local) is included in the return on investment calculation.
Natural gas price is based on the 19-year national average commercial rate of \$5.34 per thousand scf.
Electricity price is based on the 19-yar national average commercial rate of 7.5 cent per kW hr.
The cost for water usage is negligible.
O&M inclludes yearly hydrogen desulfurization bed replacement and reformer and shift catalyst replacement after five years. It also includes general maintenance for compressors, valves, etc.
Tax and Insurance costs refer to annual property taxes at 1.5% of capital investment and annual insurance premiums at 1% of capital investment. Highway/road sales taxes are not included.
Gasoline equivalent price is based on an efficiency gain of 2.2 hydrogenc FCVs over current gasoline internal combustion engine vehicles.

While the cost of the RS varies considerably depending on the reformation and cleanup technologies employed, the cost of the hydrogen compressor, storage, and dispenser, as well as unit installation, are independent of RS design. A cost breakdown for each 115 kg/day HFA design and the resulting cost of hydrogen are provided in Figure 2 and Table 1, respectively. Based on this study, we find that the most cost-effective option as determined by the wholesale cost of hydrogen is SMR coupled with PSA hydrogen purification. The initial capital cost to install the preferred SMR-PSA to support 183

Table 2. Cost of Hydrogen from 920 kg/day (8x) SMR/ PSA HFA with Optimistic Assumptions

Costs in \$/kg H_2	16,000 scfh SMR/PSA HFA
Hydrogen Cost	**\$1.87**
Capital Recovery	\$0.77
Natual Gas	\$0.59
Electricity	\$0.15
O&M	\$0.24
Taxes & Insurance	\$0.13
Gasoline Equivalent (\$/gal)	\$0.85

Estimates are based on a scaled-up version of a 2,000 scfh HFA. Scale-up may not retain accuracy of original analysis.
HFA is assumed to run an average of 69% of capacity with 98% availability.
Capital Recovery assumes a 10% after-tax return on investment over a 15-year life.
A 38% marginal tax rate (34% federal, 4% state and local) is included in the return on investment calculation.
Natural gas price is based on the 19-year national average industrial rate of \$3.30 per thousand scf.
Electricity price is based on the 10-yar national average industrial rate of 4.65 cent per kW hr.
The cost for water usage is negligible.
O&M includes yearly hydrogen desulfurization bed replacement and reformer and shift catalyst replacement after five years. It also includes general maintenance for compressors, valves, etc.
Tax and Insurance costs refer to annual property taxes at 1.5% of capital investment and annual insurance premiums at 1% of capital investment. Highway/road sales taxes are not included.
Gasoline equivalent price is based on an efficiency gain of 2.2 hydrogen FCVs over current gasoline internal combustion engine vehicles.

vehicles is \$253,014 per unit. The wholesale cost of hydrogen for this option, including storage and dispensing but excluding sales taxes and retail markup, is \$3.38/kg, or \$1.55 per gallon of gasoline equivalent. Autothermal reforming (ATR) of natural gas is a lower initial-cost option (\$228,957), but the resulting cost of hydrogen is higher (\$3.59/ kg) because the ATR uses more natural gas and electricity than the SMR to produce the same quantity of hydrogen.

Based on the results of the baseline HFA analysis, we estimated the potential hydrogen cost reduction that would result from increasing the size of the HFA from 115 kg/day to 920 kg/day. An HFA of this size would support roughly 1464 vehicles, which is comparable to large modern gasoline stations. A breakdown of the estimated cost of hydrogen for this HFA is given in Table 2. Using scale-up factors common to chemical processes, the capital cost of this 8x HFA was estimated to be \$1.16 million, resulting in a hydrogen cost of \$1.87-\$2.48/ kg (dependent on assumptions about utility discounts, natural gas feedstock cost, and equipment life). Thus, the "small" HFA derived hydrogen cost of \$3.38/kg is appropriate when discussing the early introduction of fuel cell vehicles, and the significantly lower hydrogen cost of \$1.87-\$2.48/kg, produced by a "large" HFA, is appropriate for the future years when the FCV population and population density are much higher.

Conclusions

For HFA's of the baseline capacity (115 kg/day) and production volume (250 units/year), there are two general conclusions that can be taken from this analysis:

- Steam methane reforming is more efficient than autothermal reforming, and the efficiency benefit results in a lower cost of hydrogen over a ten-year system lifetime even with a slightly higher initial capital cost (\$253,014 for SMR vs. \$228,957 forATR). The difference between the SMR and ATR costs of hydrogen shrinks as the cost of the natural gas feedstock decreases, but only with zero-cost natural gas (i.e. free) does the ATR match the SMR. For a given cost of hydrogen the SMR and ATR economic returns are equal by the fourth year of operation, with the SMR advantage increasing every year thereafter.
- PSA is a more economical and reliable option than any other hydrogen cleanup system at this time. Significant reductions in the cost and reliability of membrane purification systems are required to make them competitive with PSA.

The wholesale cost of hydrogen from the SMR-PSA HFA is \$3.38/kg, which is the equivalent of \$1.55/gallon of gasoline for an internal combustion engine vehicle after adjustment for the higher efficiency of the fuel cell engine. (Note that the hydrogen price provided does not include the taxation currently applied to gasoline.) This equivalent gasoline cost is at the upper end of current retail gasoline costs. When there are sufficient FCVs to justify a larger number of higher-volume stations, the cost of hydrogen will decrease by taking advantage of economies of scale in both HFA manufacture and the reforming process.

FY 2002 Publications/Presentations

1. "Cost and Performance Comparison of Stationary Hydrogen Fueling Appliances", submitted to Hydrogen Program Office, Office of Power Technologies, U.S. Dept. of Energy, under Grant No. DE-FG01-99EE35099, April 2002.

2. "Distributed Hydrogen Fueling Systems Analysis-Cost and Performance Comparison of Stationary Hydrogen Fueling Appliances", presentation made by Brian D. James at 2002 DOE Annual Hydrogen Program Review on May 6, 2002.

II.E.5 Technical Analysis: Integrating a Hydrogen Energy Station into a Federal Building

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Objectives

- Evaluate combined fuel cell power/hydrogen production systems (Energy Stations):
  - Analyze energy station systems with 50 kilowatt (kW) proton exchange membrane fuel cells (PEMFCs) that are suitable for installation in Federal buildings
  - Analyze options for system components, including direct hydrogen and reformate fuel cells and various storage, power production, and hydrogen usage configurations
  - Determine cost and energy efficiency for different system configurations
- Assess integration with buildings and potential for cogeneration:
  - Analyze potential for heat recovery from fuel cell/hydrogen production systems
  - Identify potential for cogeneration in Federal building applications
- Identify potential fleets to use hydrogen for vehicle operation
- Establish partnerships for hydrogen fueling and power sales
- Identify barriers to hydrogen use
- Make recommendations for future development
- Identify potential opportunities to develop fuel cell energy stations

Approach

- Analyze system cost and performance
- Assess public/private fleet size and locations
- Evaluate building integration

Accomplishments

- Developed list of possible components that will comprise hydrogen generation and dispensing station
- Developed list of relevant system configurations from possible components, with detailed description and schematics of proposed system configurations
- Selected a baseline system configuration, and initiated a detailed system cost and performance analysis
- Prepared a comprehensive list of potential operating configurations
- Surveyed potential public/private fleets and federal buildings for siting a hydrogen energy station

- Initiated evaluation of building integration and prepared comprehensive list of potential building interfaces

Future Directions

- Continue the analysis and identification of energy station applications in Federal buildings:
  - Explore specific public and private partnerships to support the establishment of a hydrogen energy station in a Federal facility
  - Analyze the cost, emissions, and energy utilization benefits of integrated power and vehicle refueling
  - Identify the key technology, cost, and public perception barriers to hydrogen use
  - Make recommendations for future development

Introduction

The purpose of this project is to analyze the development of a hydrogen infrastructure for transportation applications through the installation of a 50-75 kW stationary fuel cell-based energy station at federal building sites. The various scenarios, costs, designs and impacts of such a station are quantified. It uses a natural gas reformer to provide hydrogen fuel for both the fuel cell stack and a limited number of fuel cell powered vehicles, with the possibility of using cogeneration to support the building heating load.

Approach

The project has three major tasks:

Task 1. Analyze System Cost and Performance

The first task conducted in this project is to evaluate all of the competing technologies that could be utilized for each of the components in the entire fuel cell and vehicle fueling system based on the criteria of cost, performance, and technical feasibility. The goal of this initial, broad-based assessment is to select the most promising (four to five) system designs and technologies on the basis of the above criteria.

Task 2. Assess Public/Private Fleet Size/Locations

Data on the potential for energy stations with fleets is being collected from a representative and diverse composition of stakeholders. We are coordinating with automakers to obtain information about fuel cell vehicle fleet size, location and type projections. Another key source of information for projecting hydrogen vehicle fleet size and location are the Energy Policy Act (EPAct) fleet administrators, who will help us determine their current and projected alternative fuel vehicle (AFV) fleet practices. Finally, other policies, such as the California Zero-Emission Vehicle Mandate and the California Air Resources Board transit fleet regulation, that will either directly or indirectly encourage hydrogen fleets, are being analyzed for their potential impacts.

Task 3. Evaluate Building Integration

Using the results of Task 1 and a limited number of system designs and technologies selected for further analysis, the likely amounts and grades of waste heat that will be produced from the reformer and fuel cell stack(s) will be determined. With this information, cogenerative heat uses and technologies are being researched and evaluated with respect to beneficial utilization in a commercial/government building setting, as well as the cost and technical feasibility of those applications.

Results

Analysis of System Performance (Task 1)

A hydrogen-producing energy station would reform an input fuel to produce hydrogen for fuel cell operation and for dispensing to hydrogen-powered vehicles. The electrical power generated by the fuel cell and/or the residual heat from the system processes may be used to support energy station and nearby building power and heating loads. The fraction of reformer output used for hydrogen

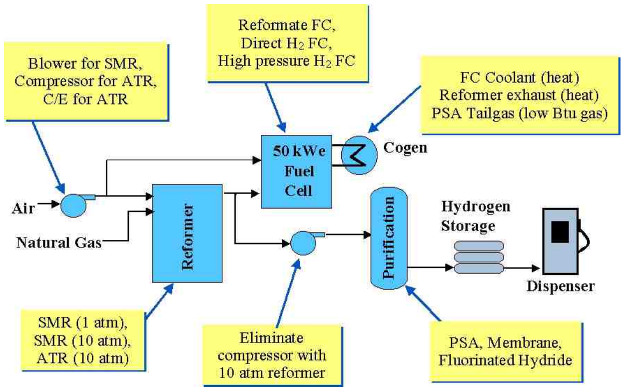

Figure 1. Several Technology Options Exist for System Configuration

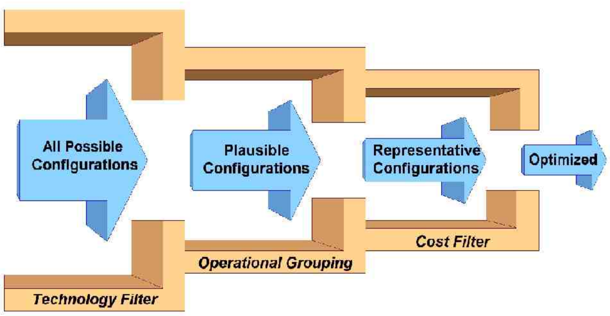

Figure 2. Application of Filters to Determine Optimal Configurations for Analysis

vehicles would be purified and stored for dispensing upon demand. Figure 1 shows the various major components that make up a hydrogen energy station.

In order to determine which system configurations and operational patterns are most viable for an energy station, TIAX developed several criteria for selecting a representative set of technology configurations. TIAX applied these criteria to all possible technology configurations to determine an optimized set, as shown in Figure 2. The remaining cases best illustrate the range of viable energy station configurations and operational profiles. These representative configurations, along with the baseline case, will be used to develop a representative cost and energy output estimate for the energy station (see Figure 3).

The possible operational scenarios for each of the station configurations include peak power

System Attributes	Major Components
Conventional Systems	Air Blower, SMR, PrOx, Reformate Fuel Cell, PSA
Lower-cost Fuel Cell	Air Blower, SMR, PSA, Direct Hydrogen Fuel Cell
Small Scale Purificaiton	Compressor / Expander, ATR, PrOx, Reformate Fuel Cell, Fluorinated Metal Hydride Purification
Simple Cogeneration	Air Compressor, ATR, PSA, Direct Hydrogen Fuel Cell

Figure 3. Representative Energy Station System Component Configurations

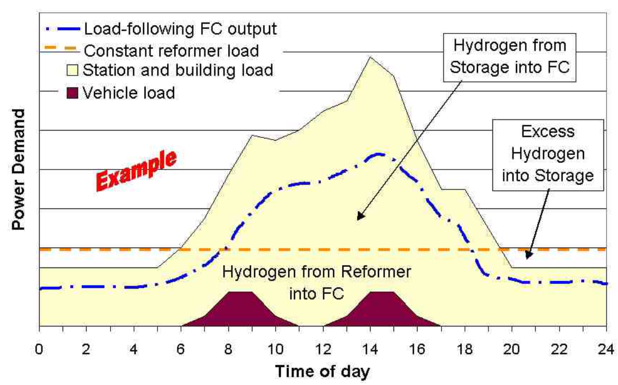

Figure 4. Example Fuel Cell and Reformer System Operation Scenarios

shaving, constant baseload operation, scheduled operation, on demand operation, and/or load following. These options are not necessarily exclusive - in some cases they may be used in combination. Figure 4 shows an example operational mode where the reformer load remains constant,

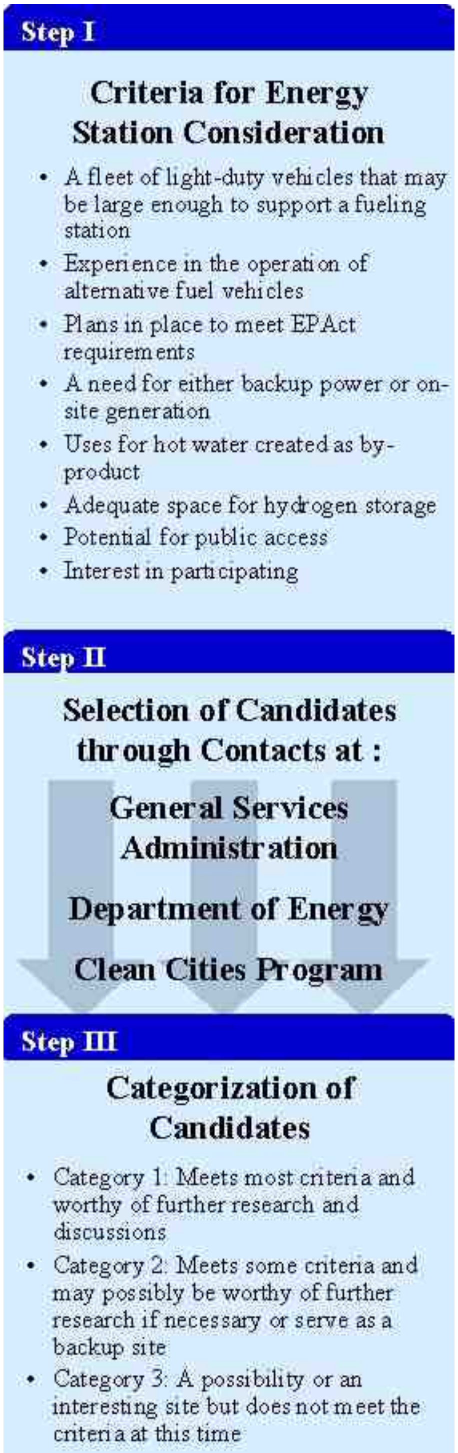

Figure 5. The Process for Choosing Facilities that Would Most Likely Benefit from an Energy Station

while the fuel cell load follows the combined station and building loads.

<u>Assessment of Public and Private Fleet Size and Locations (Task 2)</u>

In its effort to identify candidate federal facilities for the placement of a hydrogen fueling station, TIAX worked with its subcontractor, Bevilacqua-Knight, Inc. (BKI), to create a list of characteristics that the ideal location should possess. These characteristics, shown in Figure 5, formed the criteria by which the facilities would be judged.

For each federal agency contacted, BKI attempted to speak with both the fleet manager and the facility's energy manager. Fleet managers were asked about their existing vehicle fleet, experience with AFVs and plans for future acquisitions. TIAX was particularly interested in facilities that currently operate compressed natural gas (CNG) vehicles since CNG is a gaseous fuel with many properties similar to those of hydrogen. In addition, each agency was asked about how their vehicles were acquired. Lastly, TIAX asked how the facility planned to meet future EPAct requirements.

<u>Evaluation of Building Integration (Task 3)</u>

In order to take advantage of potential cogenerative heat uses and technologies, the likely amounts and grades of waste heat that will be produced from the reformer and fuel cell stack(s) will need to be determined. Using the representative technology configurations above, the opportunities for cogeneration are currently being examined. We are evaluating the potential cogeneration heat requirements in terms of heat load and seasonal variations as well as the hardware requirements required to integrate an energy station into a building.

Conclusions

- TIAX has identified a set of representative technologies and representative operational scenarios that are being analyzed to estimate the size, power output, and cost of a hydrogen energy station.
- Several options have been identified for system configuration and operation, with

each focusing on a different benefit: conventional system components, lower cost, small-scale operation, and design simplicity.

- Several Federal facilities have been identified as potential host sites, meeting most of the energy station host criteria developed as a part of this project. Energy and cost estimates will be presented in the final report of this project.

II.F Crosscutting Hydrogen Production and Delivery Analysis

II.F.1 Hydrogen Technical Analysis

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Objectives

- Identify promising hydrogen (H_2) purification technologies that DOE does not currently fund
- Characterize technical maturity and risks of selected technologies
- Perform detailed performance and cost analysis for the selected purification technologies integrated into a hydrogen fueling station concept and compare to baseline technologies
- Identify key barriers and possible development paths for promising alternative purification technologies

Approach

- Screen purification technologies and select three for detailed analysis
- Evaluate current and projected performance and cost of the selected purification technologies
- Develop system models for each purification technology with various hydrogen fueling station design concepts
- Calculate overall costs and primary energy use based on system model results and capital cost estimates from developers and internal analyses

Accomplishments

- Selected amorphous membranes without noble metals (Zirconium-Nickel [Zr-Ni] alloy), dry fluorinated metal hydrides and the application of this fluorinated metal hydride in a slurry as the three most promising non-DOE funded purification technologies
- Projected future performance and cost parameters for the selected purification technologies based on developers' input and internal analyses
- Calculated overall system efficiencies and hydrogen costs for each purification technology integrated with various reformer types and storage options
- Identified fluorinated metal hydrides as the most attractive option to pursue further, especially in a slurry-based system. Identified need to examine system-level interactions on production / purification technology in hydrogen energy mini-grid

Future Directions

- Evaluate combined fueling and power concepts utilizing central production and storage for both direct-hydrogen vehicle fueling and direct-hydrogen PEMFC power systems

- Evaluate the use of fluorinated metal hydride slurries in a mini-hydrogen grid concept for enhancing co-gen opportunities from combined fueling and power systems
- Determine if combined fueling and power or mini-hydrogen grid concepts provide cost or efficiency savings or other benefits that could encourage hydrogen and PEMFC use

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Introduction

There is increasing interest in the development of small-scale (< 1 million standard cubic feet per day) hydrogen fueling stations to support direct hydrogen fuel cell vehicles when and if these vehicles capture a significant fraction of the U.S. passenger vehicle fleet. Hydrogen for fuel cell vehicle refueling could be generated from conventional or emerging fuels at the fueling station with an on-site system including a reformer, hydrogen purification, storage, and dispensing, along with the necessary safety systems and controls. For this purpose, both higher pressure (around 10 atmospheres [atm]) and lower pressure reformers are being designed. Higher pressure systems would integrate well with the pressure requirements of conventional purification technologies (pressure swing adsorption [PSAs] and membranes). Lower pressure reformers (1-3 atm) would take advantage of designs originally intended for integrated reformer/fuel cell systems for automotive and stationary power applications and could result in lower cost due to synergies with those systems, though they would require the use of expensive and inefficient reformate compressors for integration with conventional purification technologies. It is thus clear that purification technology drives component and system design decisions.

Approach

Three small-scale purification technologies not currently being funded by DOE for on-site hydrogen production at vehicle refueling stations were evaluated. They were analyzed in the context of a larger (690 kilograms [kg] H_2/day) and a smaller (69 kg H_2/day) refueling station and in the context of high and low pressure on-board storage technologies. The analysis included assessments of technical maturity and risks, performance, cost, and a comparison to baseline technologies, as well as the identification of key barriers and an evaluation of possible development paths. We developed detailed flowsheet models for each of the options considered. These were used to estimate the conditions, flowrates, power requirements, and heat duties needed for sizing the necessary equipment. Based on the equipment sizes so calculated, we developed cost estimates from a combination of quotes and existing bottom-up cost models. The three purification technologies selected for analysis are:

<u>Fluorinated Metal Hydrides (Dry)</u>

If properly protected from certain impurities, metal hydrides could purify reformate streams at much lower pressure than conventional technology. Forming a porous fluoride film on the surface of metal hydride particles is a promising way to protect the metal hydride from poisoning by non-hydrogen species that are less likely to penetrate through the fluoride film than hydrogen molecules (particularly carbon monoxide and water). Combining this low pressure purification with hydrogen storage in the same metal hydride has the potential to simplify system integration and improve efficiency and cost for fueling metal hydride vehicles.

<u>Metal Hydride Slurries</u>

Utilizing fluorinated metal hydrides in slurries could improve system integration even further. The metal hydride slurry is pumpable, allowing for its use as a medium for hydrogen purification, storage and transportation simultaneously. Slurry systems also have faster absorption/desorption times than dry metal hydrides, allowing them to be used for purification only with compressed H_2 storage and dispensing. The fast absorption/desorption time also reduces the amount of metal hydride material required for purification, thus minimizing capital cost of the purification process.

<u>Non-Palladium Metal Membranes</u>

Non-palladium metal membranes are a potential low-cost alternative to palladium-based membranes currently in use. Japanese researchers have

Purification Attributes	Units	Small-scale PSA	Zr-based Membranes	Fluorinated MH[1,4]	Fluorinated MH Slurry[1]
Demonstrated Performance					
Inlet pressure	atm	10-20	3[2]	15 (initial)	NA
H_2 Outlet pressure	atm	9-19	~1[2]	1	NA
Operating temperature	°C	0-50	250-350	60, 80	NA
Hydrogen recovery[3]	%	70-90	40-60[2]	85	NA
Assumed Performance					
Inlet pressure	atm	10	10	1.5-10	1.5-10
H_2 Outlet pressure	atm	9	~1	5	5
Operating temperature	°C	40	350	40-110	40-110
Hydrogen recovery[3]	%	70-76	78-86	65-94	64-92

[1] Based on the material and processes investigated in this study. Attributes vary significantly with material.
[2] Current performance with 2 atm (30 psia) pressure difference across the membrane. Hydrogen recovery increases with increasing pressure difference.
[3] Varies depending on inlet pressure and reformate composition (SR versus ATR).
[4] Demonstrated performance based on: Wang, et al 1995.

Figure 1. Demonstrated and Assumed Purification Performance

promising results from amorphous alloy membranes without noble metals (Zr-Ni). Alloys without noble metals may be two orders of magnitude cheaper than palladium-based materials on a weight basis (Hara 2000).

Results

Hydrogen Recovery (Figure 1)

Hydrogen recovery was estimated for each purification technology and inlet condition. Demonstrated performance and our assumptions for inlet and outlet pressures, operating temperature, and hydrogen recovery are shown in Figure 1. Hydrogen recovery for the PSA case was based on vendor quotes for typical autothermal reformer (ATR) and steam reformer (SR) impurity concentrations. Zr-based membrane recovery was estimated based on current and estimated membrane performance characteristics, hydrogen pressure gradient across the membrane, and assumed permeability decrease due to carbon monoxide presence in the feed stream. Fluorinated metal hydride recovery was estimated based on the operating conditions and metal hydride cycling hydrogen capacity.

Efficiency (Figures 2 and 3)

- Steam reformer based systems result in lower primary energy use than autothermal reformer systems largely because steam reformers can utilize the non-recovered hydrogen from the purification step.
- For high-pressure dispensing options (compressed H_2 vehicles), PSA purification with a high-pressure steam reformer results in the lowest primary energy use, provided highly efficient waste heat integration is possible.
- PSA and membrane purification for use with low pressure reformers tend to have higher power-based primary energy use due to the need for compression prior to purification.
- Fluorinated metal hydride (Fl MH) purification options achieve very high hydrogen recovery rates compared with a PSA; but dehydriding energy requires an auxiliary burner for use with steam reformers, raising energy consumption.
- Autothermal reformers have enough waste heat to significantly reduce or eliminate an auxiliary burner for use with Fl MH systems, provided a significant fraction of the waste

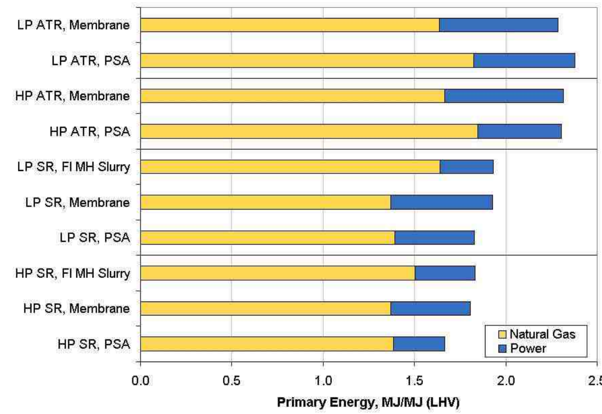

Figure 2. Primary Energy Use for Compressed H_2 Vehicle Fueling Stations

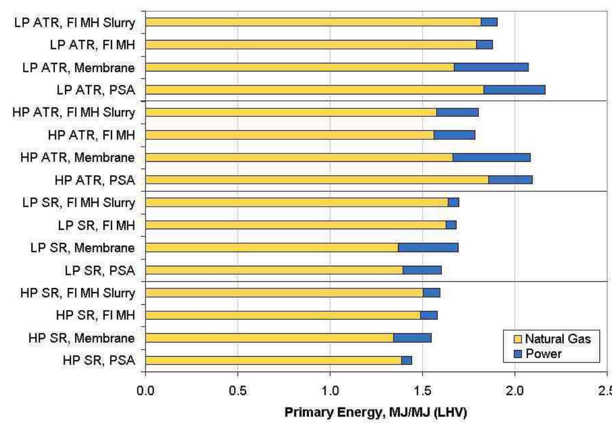

Figure 3. Primary Energy Use for MH Vehicle Fueling Stations

heat can be stored and used as needed during fueling.

With Fl MH purification, hydrogen recovery does not strongly depend on reformate quality, and hence is the preferred option with ATRs and purification of syngas streams from renewable sources (e.g. biomass gasification or pyrolysis).

Hydrogen Cost (Figures 4 and 5)

Notes on figures: purification category includes reformate compressor costs for low-pressure reformers with PSA and membrane purification. Cost categories include energy, maintenance, and capital recovery costs. "Other" costs include labor, rent, utilities, profit, and capital recovery for site preparation and central controls and safety.

- Under our cost assumptions, low-pressure (high production volume) reformers are cheaper than high-pressure (low production volume) reformers, but result in about the same overall cost for hydrogen due to higher purification costs.
- Although membrane cost may ultimately be low for non-palladium membrane purification, compression costs off-set the benefits this provides compared with PSA purification, except for use with low-pressure ATRs.
- Unlike PSAs and membranes, Fl MH systems are projected to have very similar purification cost regardless of reformate composition, making them particularly suitable for ATR and renewable-based hydrogen production.
- Fl MH purification scales down in size better than the other purification options, making it a more attractive technology for small fueling stations, though low-capacity stations still cost at least 50% more than large-capacity stations (not shown in figures).
- Liquid hydrogen delivery is projected to have the lowest cost of the central hydrogen production options, and the lowest cost of all compressed H_2 options provided transportation distances are short (delivery distance is assumed to be 50 miles).

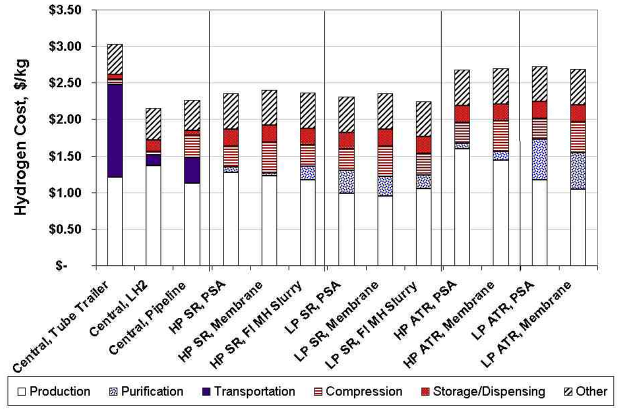

Figure 4. Hydrogen Cost for Compressed H_2 Vehicle Fueling - 690 kg H_2/day Capacity

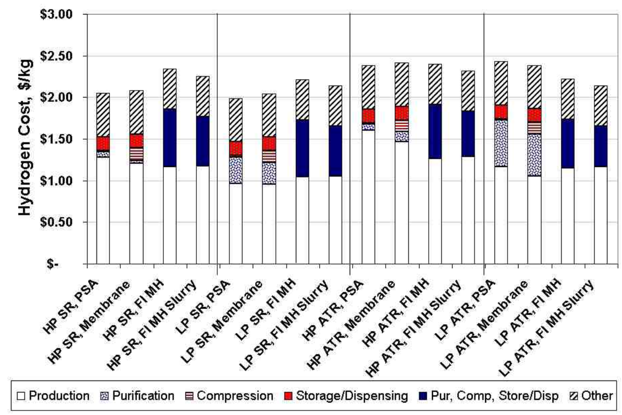

Figure 5. Hydrogen Cost for MH Vehicle Fueling - 690 kg H_2/day Capacity

However, central options could not be used ubiquitously, because costs will increase significantly with transportation distance.

Conclusions

Our analysis indicates that the use of fluorinated metal hydrides in slurry form could reduce overall hydrogen cost, especially if the slurry is used for purification only. In addition, if high-pressure storage is of concern due to safety or regulatory issues, Fl MH purification and storage could provide significant benefits. Slurries could also provide benefits in terms of hydrogen transmission to decentralized fuel cell power systems in a mini-hydrogen grid. It is not likely that significant energy savings can be expected over a well-integrated PSA combination, though improvements over the state-of-the-art systems are possible. Some technology development will be required to optimize the slurry system, and significant development will be required to develop a stable and effective fluorinated metal hydride that can be produced cost-effectively.

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II.F.2 Hydrogen Infrastructure Studies

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Objectives

- Address energy efficiency, cost competitiveness and environmental impact of integrated hydrogen systems through participation in three integrated system teams as called for by the International Energy Agency's (IEA) Hydrogen Agreement Annex 13: "Design and Optimization of Integrated Systems."

Approach

- Provide independent modeling and assessment of integrated hydrogen systems, with an emphasis on spreadsheet models
- Maintain consistency among the three teams with respect to assumptions of cost and performance
  - Lead the Transportation Applications analysis, focusing on hydrogen refueling infrastructure - particularly the production sources, distribution, and storage of hydrogen. The effort addresses several general areas:
  - Cost of hydrogen fuel dispensed to the vehicle
  - Sensitivity of that cost to numerous assumptions, including future hydrogen production and delivery options
  - Emissions (tailpipe and station), compared with alternative vehicle types
  - The impact of codes and standards on hydrogen storage footprints
- Attend Expert Team meetings and Task Definition Workshops
- Interact with the U.S. Operating Agent (Cathy Gregóire Padró), as needed

Accomplishments

- The transportation infrastructure analysis has been completed, including the following sensitivity studies:
  - Station utilization
  - Station size
  - Projected component costs for on-site hydrogen generation
  - Costs of natural gas and electricity (including renewables)
  - Upstream infrastructure costs (new central reformers and pipelines)
  - Transport distances
- The fuel economy and emissions analysis evaluated the following for alternative vehicle and fuel types:
  - Fuel economy

- Cost of a 300-mile fill-up
- Tailpipe emissions, gallon/mile
- Major local / station emissions (kilogram [kg]/year)
- Minor local / station air pollutants (kg/year)

- The final report on this analysis has been submitted and is part of an overall IEA package including all three project reports and a cost model
- A topical analysis and report of relevant (and changing) fire codes and the impact on station footprints were also completed

Future Directions

- Annex 13 was concluded at the end of June 2002. New tasks for a new Annex were proposed through two Task Development Workshops and are currently being developed for approval by the IEA Executive Committee. A new Annex or study task could address the following issues:
  - Validation of models using data from case studies
  - Use of models to assist in the design and optimization of demonstrations / projects
  - An analysis of legacy projects that lead from demonstration to commercial practice
  - An assessment of the impact of portable hydrogen system development (i.e., small devices) on larger system needs
  - Additional analysis of the impact of codes and standards on system design and cost
  - Comparison of different countries' demands, supplies, experiences and policies

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Introduction

The U.S. Department of Energy participates in various activities of the International Energy Agency (IEA) through an Implementing Agreement and its Annexes. Hydrogen Agreement Annex 13, "Design and Optimization of Integrated Systems," calls for the U.S. to participate in three integrated system teams. The three teams and their projects are:

- Remote Power Systems
- Home/Residential Systems
- Transportation Applications
- Longitude 122 West serves as U.S. Team leader for Annex 13 activities

The goal of the analysis has been to provide independent modeling and assessment, especially of capital and operating costs, for the integrated systems. The current emphasis is on spreadsheet modeling, to make comparisons between system configurations and technologies easier. Other factors being considered are efficiency, environmental impact, and the role of codes and standards. The present task addresses infrastructure to support transportation applications.

Approach

The analysis of capital costs, operating costs, and footprints, fuel economy and emissions has been conducted using Excel spreadsheet modeling. Data sources included vendor data sheets and website information, vendor quotes and communications, case study experience, published literature (including Environmental Protection Agency data), theses, and engineering estimates. Major assumptions for the analysis include:

- Station serves 100 vehicles per day
- Each hydrogen fueling event delivers 4 kg of hydrogen
- Station operates 24 hours/day, 365 days per year
- Liquid hydrogen is delivered weekly; round trip delivery distance is 1,000 miles; storage is oversized by 30%

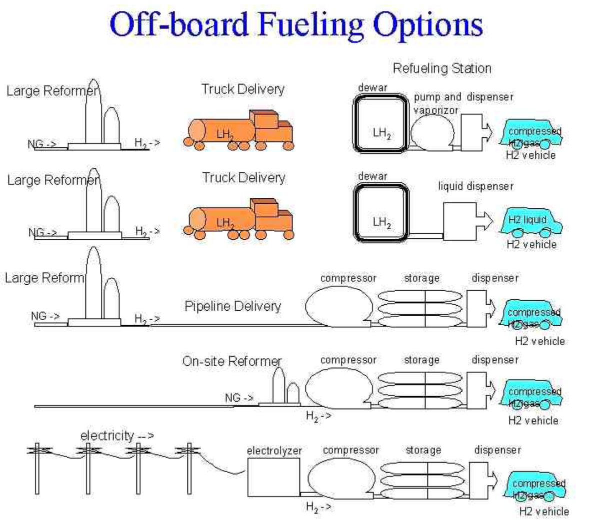

Figure 1. Refueling Station Alternatives Studied in this Work

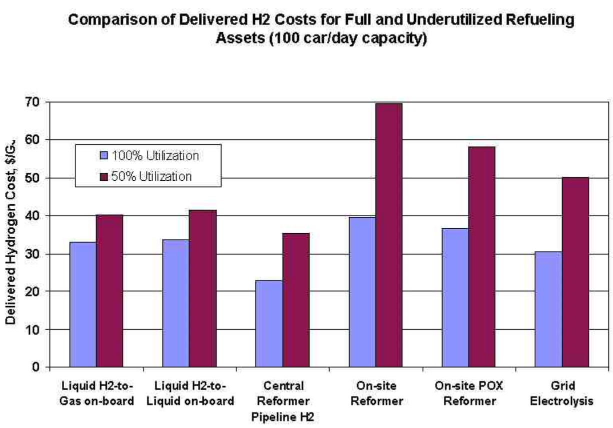

Figure 2. Cost of Dispensed Hydrogen ($/GJ) for Base Case and Station Utilized at 100% and 50% (100 Cars/Day Capacity)

- Gaseous hydrogen is delivered by pipeline or generated on-site; storage is sized for one day's service plus 40%
- On-site generators are sized / rated to fill storage in 18 to 24 hours, depending on electricity rates

The 6 scenarios differ by whether the hydrogen is produced off-site and transported by truck or pipeline, or whether the hydrogen is produced on-site by steam methane reformer (SMR), partial oxidation POx) reforming, or grid electrolysis. The scenarios are depicted in Figure 1.

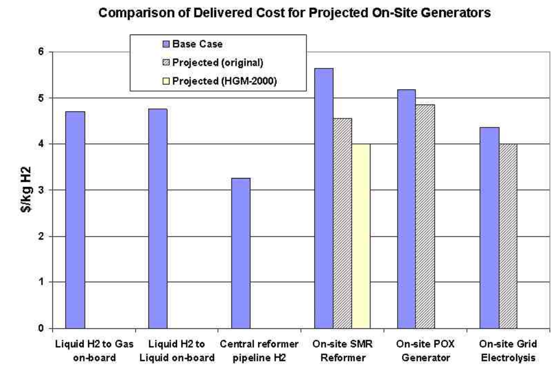

Figure 3. Sensitivity of Cost Results to Projected Costs of On-Site Generation Technologies

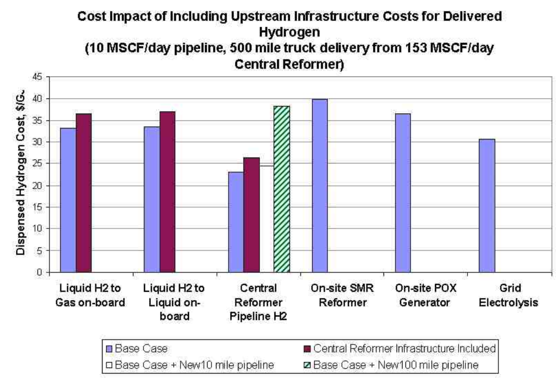

Figure 4. Sensitivity of Cost Results to the Inclusion of Upstream Infrastructure Costs

Results

Key results are the cost of dispensed hydrogen for the 6 cases. These are compared for a number of important parametric variations. The sensitivity to station utilization factor is shown in Figure 2, for both the base case of 100% utilization and under-utilization at 50%. The results are also sensitive to the projected cost of on-site production equipment, as shown in Figure 3. [1,2]

Another key result is that the construction of upstream production and delivery infrastructure (central SMR and pipelines) is not ruled out by including the amortization of these costs in the dispensed hydrogen cost, as shown in Figure 4.

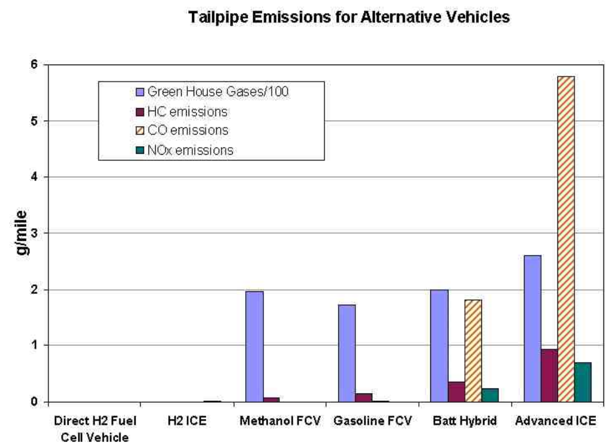

Figure 5. Tailpipe Emissions for Alternative Vehicles and Fuels

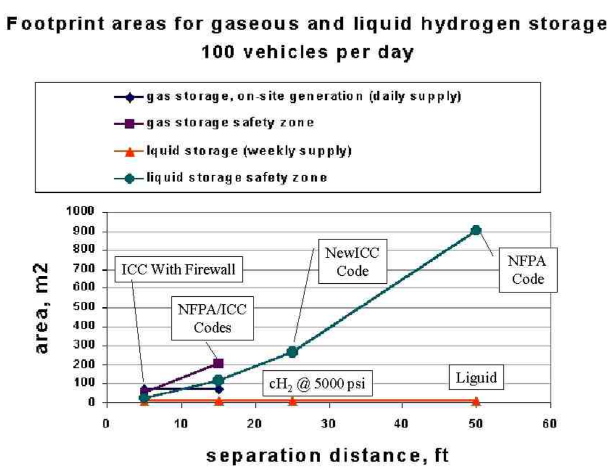

Figure 6. Footprints of Station Alternatives Showing Impact of Varying Fire Codes for Hydrogen Storage

Major and minor emissions from the tailpipe of alternative vehicles and the different refueling station options were calculated. The results show the pipeline and on-site electrolyzer to be the cleanest local approaches. Tailpipe emissions for alternative vehicles and fuels are shown in Figure 5.

Footprints are strongly dependent on the interpretation and implementation of fire codes and standards for local hydrogen storage [3]. As shown in Figure 6, a conservative safety stand-off zone requires a significantly larger footprint than a more practical standard.

Conclusions

Hydrogen refueling infrastructure can be provided for passenger vehicles by several alternative means, including bulk delivery of hydrogen to a station via truck or pipeline, or on-site generation using electrolysis or reforming techniques. The price of the various alternatives can be comparable, depending on the transport distance and production capacity.

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2. Susan M. Schoenung, "A Comparison of Hydrogen Vehicle and Refueling Infrastructure Alternatives: An Analysis Developed for the International Energy Agency," proceedings 14th World Hydrogen Energy Conference, Montreal, Canada, June 2002

3. Technical staff seminar at South Coast Air Quality Management District, October 2002