September 1995 • NREL/CP-430-20036

Proceedings of the 1995 U.S. DOE Hydrogen Program Review

Volume I

April 18-21, 1995
Coral Gables, Florida

Sponsored by the
Advanced Utility Concepts Division
Office of Energy Management
U.S. Department of Energy

NREL

National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, Colorado 80401-3393
A national laboratory of the U.S. Department of Energy
Managed by Midwest Research Institute
for the U.S. Department of Energy
Under Contract No. DE-AC36-83CH10093

NREL/CP-430-20036 • UC Category: 1360 • DE95009296

Proceedings of the 1995 U.S. DOE Hydrogen Program Review

Volume I

April 18-21, 1995
Coral Gables, Florida

Sponsored by the
Advanced Utility Concepts Division
Office of Energy Management
U.S. Department of Energy

National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, Colorado 80401-3393
A national laboratory of the U.S. Department of Energy
Managed by Midwest Research Institute
for the U.S. Department of Energy
Under Contract No. DE-AC36-83CH10093

Under Task No. HY511010

September 1995

MASTER

ds

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

TABLE OF CONTENTS

Volume I

Systems Analysis

Utilization

Volume II

Storage

Production

HYDROGEN ENERGY SYSTEMS STUDIES

Joan M. Ogden, Margaret Steinbugler, E. Dennis,
Siván Kartha, Laura Iwan, Andrew Jones
Center for Energy and Environmental Studies
Princeton University
Princeton, NJ 08544

Abstract

For several years, researchers at Princeton University's Center for Energy and Environmental Studies have carried out technical and economic assessments of hydrogen energy systems. Initially, we focussed on the long term potential of renewable hydrogen. More recently we have explored how a transition to renewable hydrogen might begin. The goal of our current work is to identify promising strategies leading from near term hydrogen markets and technologies toward eventual large scale use of renewable hydrogen as an energy carrier. Our approach has been to assess the entire hydrogen energy system from production through end-use considering technical performance, economics, infrastructure and environmental issues. This work is part of the systems analysis activity of the DOE Hydrogen Program.

In this paper we first summarize the results of three tasks which were completed during the past year under NREL Contract No. XR-11265-2: in Task 1, we carried out assessments of near term options for supplying hydrogen transportation fuel from natural gas; in Task 2, we assessed the feasibility of using the existing natural gas system with hydrogen and hydrogen blends; and in Task 3, we carried out a study of PEM fuel cells for residential cogeneration applications, a market which might have less stringent cost requirements than transportation. We then give preliminary results for two other tasks which are ongoing under DOE Contract No. DE-FG04-94AL85803: In Task 1 we are assessing the technical options for low cost small scale production of hydrogen from natural gas, considering a) steam reforming, b) partial oxidation and c) autothermal reforming, and in Task 2 we are assessing potential markets for hydrogen in Southern California.

Introduction

Since 1986, researchers at Princeton University's Center for Energy and Environmental Studies have carried out technical and economic assessments of hydrogen energy systems. Initially, we focussed on the potential of renewable hydrogen (Ogden and Williams 1989, Ogden and Nitsch 1993, Ogden 1993, Larson and Katofsky 1992, Katofsky 1993). Our results suggest that renewable hydrogen used in energy efficient end-use devices (e.g. fuel cells) could become competitive, beginning in the early part of the next century.

More recently we have explored how a transition to renewable hydrogen might begin (Ogden, Dennis and Strohbehn 1994, Ogden, Dennis, Steinbugler and Strohbehn 1995). The goal of our current work is to identify promising strategies leading from near term hydrogen markets and technologies toward eventual large scale use of renewable hydrogen as an energy carrier. Our approach has been to assess the entire hydrogen energy system from production through end-use from several perspectives (fuel producer, consumer, society) considering technical performance, economics, infrastructure and environmental and resource issues. This work is part of the systems analysis activity of the DOE Hydrogen Program.

A key challenge to developing hydrogen energy is the current lack of distribution infrastructure. Thus, we focussed on making hydrogen initially from readily available energy carriers (natural gas and electricity). Two potentially large markets were examined: zero emission hydrogen vehicles and distributed stationary power cogeneration using fuel cells. In this paper we summarize the results of three tasks which were completed during the past year (under NREL Contract No. XR-11265-2) and give preliminary results for two other tasks which are ongoing (under DOE Contract No. DE-FG04-94AL85803).

Assessment Of Near Term Options For Supplying Hydrogen Transportation Fuel From Natural Gas

Hydrogen vehicles are among the leading contenders in the emerging market for zero emission vehicles (ZEVs). One of the main roadblocks to the widespread use of hydrogen as a transportation fuel is the lack of infrastructure. Unlike systems in place for electricity, natural gas or gasoline, there is at present no widespread transmission and distribution system for hydrogen.

The US hydrogen distribution infrastructure today consists of a few hundred miles of industrial hydrogen pipeline plus fleets of trucks delivering liquid hydrogen or compressed hydrogen gas. Although about 1 EJ (1 EJ =1 Exajoule =10^{18} Joules) of hydrogen is consumed per year in the US, most of this is produced and used onsite for ammonia synthesis, oil refining and other chemical processes. Merchant hydrogen (hydrogen which is distributed by truck or pipeline) amounts to only about 5% of the total (0.05 EJ/yr) (Kerr 1993).

This compares to potential hydrogen transportation fuel demand in the LA Basin alone of 0.015 EJ/yr by 2010 (assuming that 10% of the cars were hydrogen fuel cell vehicles), and 0.1 EJ/yr by 2030, (if

50% of the cars were hydrogen FCVs) (see ongoing Task 2 below). If all US light duty vehicles were hydrogen fuel cell vehicles, projected hydrogen demand would be about 5 EJ/yr at projected 2030 driving levels. Clearly, we would need to either greatly expand the existing hydrogen delivery system or make hydrogen near the point of use from widely available energy carriers (natural gas or electricity), if hydrogen is to become a major transportation fuel.

In this Task, we examined how a refueling infrastructure for hydrogen vehicles might evolve over the next few decades (Ogden, Dennis, Steinbugler and Strohbehn 1995).

For this study, we chose high pressure gaseous hydrogen as the onboard storage method. [Although gaseous hydrogen storage systems have a lower energy density than those for liquid hydrogen, the simplicity, speed of refueling, and similarity to compressed natural gas (CNG) vehicle technology are attractive features. Moreover, with high efficiency vehicles such as fuel cell or hybrid IC/electric vehicles (Smith 1993), a reasonable travelling range (say 400 km) could be achieved even wth compressed gas cylinders (DeLuchi 1992, Ogden and DeLuchi 1993, Kuhn 1994)]. It is further assumed that commercially available or near commercial equipment is used for refueling stations, pipelines, etc., and that the hydrogen produced must be of sufficient purity for PEM fuel cells (less than 1 ppm CO or purity of 99.999%). The daily demand for a hydrogen refueling station is estimated to be in the range 0.1-2.0 million scf H_2/day (Ogden et. al 1995).

Although there are many possibilities for producing and delivering compressed gas hydrogen to vehicles, we consider the following near term possibilities:

* hydrogen produced from natural gas in a large, centralized steam reforming plant, and truck delivered as a liquid to refueling stations,

* hydrogen produced in a large, centralized steam reforming plant, and delivered via small scale hydrogen gas pipeline to refueling stations,

* hydrogen produced at the refueling station via small scale steam reforming of natural gas,

* hydrogen produced via small scale electrolysis at the refueling station.

To compare these alternatives, we addressed the following questions:

* How would a hydrogen refueling station be designed for various options?

* What are the refueling station capital cost and delivered cost of hydrogen transportation fuel for various supply options and levels of demand?

* What are the emissions benefits for each case?

* What are the synergisms between these near term options and phasing in longer term supplies such as renewable hydrogen?

Alternatives for Supplying Compressed Gas Hydrogen Transportation Fuel

Production Of Hydrogen Via Large Scale, Centralized Steam Reforming Of Natural Gas W/ Liquid Hydrogen Truck Delivery

A gaseous hydrogen refueling station based on truck delivery of liquid hydrogen is sketched in Figure 1. Filling station equipment includes a dewar for liquid hydrogen storage, a liquid hydrogen pump, a vaporizer, and a gaseous hydrogen dispensing system. Liquid hydrogen is delivered daily to refill the dewar. The liquid is then pressurized to the desired pressure using a liquid hydrogen pump (pressures of up to 6000 psia are commercially available), and evaporated to produce pressurized gas as needed. The delivered hydrogen cost is shown as a function of station capacity. The cost of liquid hydrogen is the largest part of the delivered cost of about $20/GJ ($2.7/gallon gasoline equivalent). The station capital cost is a relatively small fraction of the total cost.

Truck delivery of liquid hydrogen would have the advantage of being widely used in industry at present. Also liquid hydrogen could be delivered over long distance via truck to regions where natural gas pipeline service is not available (Moore 1994). This argues that the first hydrogen refueling stations might be based on truck delivery of liquid hydrogen. However, the delivered hydrogen cost would be relatively high. Also liquifying hydrogen incurs substantial energy penalties at the production plant, which make it less attractive from the point of view of fuel cycle efficiency (e.g. efficiency of converting natural gas into hydrogen into energy at the wheels of the vehicle).

Production Of Hydrogen Via Large Scale, Centralized Steam Reforming Of Natural Gas W/ Gaseous Pipeline Delivery

Another possibility is producing hydrogen in a large, centralized steam reforming plant and distributing it via gas pipelines, similar to natural gas. Large scale production of hydrogen would allow lower production costs. To take full advantage of economies of scale, production capacities of 25-100 million scf/day would be required, enough hydrogen to fuel about 50,000 to 200,000 cars per day (or a fleet of 500,000 to 2 million cars). Thus, centralized production facilities for fuel production might not be built until a fairly large, geographically concentrated demand for hydrogen has developed. In the near term, small dedicated pipelines might be built to serve customers near an existing large hydrogen plant. This is done in a few cases today. The economics and feasibilty would depend strongly on the site.

Each refueling station along the pipeline would consist of a hydrogen compressor, compressed gas storage cylinders, and a hydrogen dispensing system (Figure 2), analogous to compressed natural gas vehicle stations today. The delivered cost of hydrogen transportation fuel is seen to be in the range $25/GJ (for a refueling station serving 80 cars/day) to $12/GJ for a station serving 1600 cars/day. At refueling station capacities of 300 cars/day or more, the dominant cost is pipeline hydrogen at the station (assumed to be $8/GJ in this example). This cost depends on the hydrogen production cost in a centralized plant, and the pipeline distribution cost.

Production Of Hydrogen At The Refueling Station Via Small Scale Steam Reforming Of Natural Gas

Hydrogen can be produced from natural gas at the refueling station via small scale steam reforming of natural gas (Ogden et.al 1995, Dennis 1994). The hydrogen is then compressed, stored and dispensed to vehicles as needed (Figure 3). The capital cost of the refueling station and delivered hydrogen cost are strongly dependent on the capital cost of the reformer, which in turn has strong economies of scale in the size range needed for refueling stations (see Figure 16). Large refueling stations (800 cars or more per day) would have a lower delivered hydrogen cost, because of reformer scale economies and because labor costs are a less significant factor. There appears to be the potential to reduce the reformer capital cost, which could significantly reduce the hydrogen cost.

The delivered cost of hydrogen varied from about $12/GJ (for large refueling stations serving 1600 vehicles/day) to about $20/GJ for a station serving 300 vehicles/day to about $40/GJ for a small station serving 80 cars/day. To achieve a low delivered fuel cost with onsite reforming with existing technology, it would be desirable to have large station size and low natural gas costs. Development of compact, standardized reformers could lead to significant cost reductions. Optimization and mass production of other station components (compressors and storage cylinders) could also reduce costs.

Production Of Hydrogen At The Refueling Station Via Electrolysis Using Off-Peak Power

Hydrogen could also be produced electrolytically from off-peak power (Figure 4), compressed and stored for later use. The delivered cost of hydrogen is shown, assuming that off-peak power costing 2 cents/kWh is available 12 hours/day. The delivered cost of hydrogen is seen to be about $16-25/GJ depending on the refueling station capacity. The capital cost of small scale electrolyzers is assumed to have fairly steep scale economies at sizes less than about 1 MW. If PEM electrolyzers are commercialized, these costs might be considerably reduced (Thomas 1995).

Economic Comparisons

Comparison Of Hydrogen Supply Options

In Figures 5 and 6, we compare the station capital cost and delivered hydrogen cost over a range of refueling station sizes for each alternative. We see that no one hydrogen supply option is a clear winner for all cases. The lowest delivered hydrogen cost depends on the type of demand, and on energy prices. Technical improvements (for example, in small scale reformer technology) could change the relative cost of various hydrogen supply options. The advantages and disadvantages of each hydrogen supply option are summarized in Table 1.

Comparison Of Hydrogen And Other Transportation Fuels

In Figure 7 we compare the delivered cost of hydrogen to other transportation fuels gasoline, compressed natural gas, methanol (from natural gas, biomass and coal), and electricity (Ogden, Larson and Delucchi 1994). We see that hydrogen from natural gas would be the least costly source of hydrogen, but would cost more than gasoline. Figure 8 shows the fuel cost per kilometer travelled for gasoline and CNG cars using internal combustion engines (ICEVs), for fuel cell cars run on hydrogen and methanol (FCVs) and for battery powered electric cars (BPEVs). Because fuel cell vehicles would have an efficiency of 2-3 times that of comparable internal combustion engine vehicles, the fuel cost per km would be considerably less with a FCV using hydrogen from natural gas than with a gasoline ICEV.

The lifecycle cost of transportation, including all the expenses of owning and operating a vehicle (vehicle cost, fuel, misc. O&M) is shown for alternative fueled automobiles in Figure 9 (Ogden, Larson, Delucchi 1994), based on projections for mass-produced fuel cell vehicles. We see that hydrogen fuel cell vehicles would have a lifecycle cost comparable to that of gasoline internal combustion engine vehicles. Hydrogen from near term sources would be an economically acceptable transportation fuel, if fuel cell vehicles are commercialized on a large enough scale to bring fuel cell manufacturing costs down.

Emissions

There would be substantial emissions benefits to introducing hydrogen transportation fuel, made initially from natural gas. With fuel cell vehicles tailpipe emissions are essentially zero. The fuel cycle emissions of greenhouse gases (including fuel production, transmission, delivery and use) are shown in Figure 10 for ICEVs and FCVs using various fuels. With fuel cell vehicles using hydrogen from natural gas, greenhouse gases emissions per km would be only 31% of those from gasoline ICEVs (DeLuchi 1992).

Resources for Hydrogen Production from Natural Gas and Renewables

Worldwide natural gas resources have been estimated at 10,700 EJ, with about 1500 EJ in the United States. If 50% of US light duty vehicles were converted to hydrogen by 2025 and assuming that fuel cell vehicles were used, about 3 EJ/yr of hydrogen (or 4 EJ/yr of natural gas) would be needed. Adding this to the projected 2025 US natural gas use of 15 EJ/yr, we see that natural gas supplies could contribute to hydrogen production for several decades.

The potential for renewable hydrogen production is vast and inexhaustible. Solar resources alone could meet all US transportation energy demands using 0.2% of the US land area. Wind and biomass hydrogen could also be significant in the US and many other parts of the world (Ogden and Nitsch 1993).

Strategies For Developing Refueling Infrastructure For Hydrogen Vehicles

An important question is how to produce and deliver an increasing amount of hydrogen to ZEVs.

Figure 11 shows how the existing merchant hydrogen system might expand, with liquid hydrogen truck delivery to the first few hydrogen refueling stations, followed by development of a small pipeline system with lower delivered hydrogen costs. We show an example of a pipeline serving 80,000 fuel cell cars (the number of ZEV cars projected for the South Coast Air Basin in about 2001). The delivered cost of hydrogen transportation fuel is about $13/GJ, a cost of energy equivalent to about $1.7/gallon gasoline.

Alternatively, it might be possible to "piggyback" on the existing natural gas system (Figure 12), adding onsite reformers as needed. As demand increased, a hydrogen pipeline system might be developed along gas utility rights of way. These systems also gave a delivered hydrogen cost of about $12-14/GJ. Once a pipeline system was in place, hydrogen from renewable sources (biomass, MSW, wind, solar) might be phased in as natural gas became more expensive.

It has been proposed that the existing natural gas pipeline system might be adapted for use with hydrogen, saving a large capital investment. Although it would be technically feasible to convert local natural gas distribution lines to hydrogen, a large demand for hydrogen for ZEVs might arise before other natural gas users on the system would be ready to convert to hydrogen. A rapidly growing ZEV market could lead to development of a pure hydrogen local pipeline distribution system in parallel to the existing natural gas utility system. Because of the wealth of local resources for hydrogen production (natural gas, biomass, wind solar) available in the United States, it may never be necessary to build long distance hydrogen transmission pipelines, even in the long term.

Another option is making hydrogen via electrolysis using utility electricity (derived increasingly from renewable sources) or stand alone PV electrolysis systems (Figure 13). The cost of hydrogen via electrolysis is estimated to be somewhat more expensive than hydrogen produced from natural gas or biomass. However, the lifecycle cost of transportation would still be acceptable with fuel cell vehicles.

Initially, for the first fleet tests, refueling stations based on truck delivery of liquid hydrogen or onsite reforming or electrolysis might be used. Dispersed production (onsite reforming or electrolysis) would allow expansion in relatively small increments and provide fuel where needed. However, the delivered hydrogen cost would be somewhat higher than might be achieved with large scale centralized production. Once the fleet of hydrogen vehicles reached several tens of thousands (e.g. several million scf/day), the lowest cost near term option might be to build a small dedicated hydrogen pipeline from an existing nearby refinery or large scale hydrogen production plant with excess hydrogen capacity to several refueling stations. Once a large enough hydrogen vehicle population was established, new hydrogen capacity might be built and a distribution network might be developed. In the long term, the cost of natural gas is likely to increase and hydrogen derived from renewables (biomass, MSW, solar or wind) could be introduced.

Conclusions and Recommendations for Future Work

- Using near term, commercially available technologies, compressed hydrogen gas could be delivered to vehicles at a cost of $12-40/GJ.
- The best hydrogen supply option depends on the type of demand and energy prices.
- With hydrogen fuel cell vehicles, the fuel cost/km would be less than for gasoline vehicles, and the projected lifecycle cost of transportation would be comparable.
- There would be substantial emissions benefits to introducing hydrogen transportation fuel made initially from natural gas.
- Onsite production has the advantage of adding capacity in small increments, where needed.
- Steam reformers have strong scale economies at the size range needed for onsite reforming. Large station size (800 cars/day or more) would be prefered. Because commercially available reformer technology has not yet been optimized for this type of application, it may be possible to reduce reformer capital costs considerably.
- Once a large demand developed (at least 10 million scf/day or a fleet of 80,000 ZEVs), small scale pipeline delivery gave the lowest delivered cost (improvements in small scale reformer technology could change this.)
- US natural gas resources are large enough that hydrogen could be made from this source for several decades, providing a bridge to renewables.
- In the longer term, hydrogen from biomass, wind and solar could be an economically acceptable, environmentally desirable alternative transportation fuel.

We recommend further research, development and demonstrations in the following areas:

- R&D on small scale technologies for converting natural gas to hydrogen
- Assess small scale electrolysis technology as an option
- Site specific study of development of hydrogen refueling infrastructure

Assessment Of The Feasibility Of Using The Existing Natural Gas System With Hydrogen And Hydrogen Blends

Building a new transmission and distribution system for hydrogen would be a costly undertaking. If part or all of the existing natural gas infrastructure could be used with hydrogen it might save a large investment.

In this Task, we examined how existing natural gas long distance, transmission and local distribution and end-use systems might have to be changed to allow the use of pure hydrogen and hydrogen blends. [Note: we use the term "transmission system" refers to long distance, large diameter pipelines operated at typical pressures of up to 1000 psia. "Distribution system" refers to a gas utility type local distribution system, operated at pressures of 15-500 psia. "End-use systems" are gas using equipment (space and water heating systems, gas engines, boilers, etc.) See Johnson et.al. (Johnson et.al. 1977) for an excellent discussion of the natural gas system.]

Use of hydrogen and hydrogen blends in the existing natural gas system raises a host of technical issues. In particular we are interested in how an increased percentage of hydrogen might impact:

* materials used in pipes, seals, etc.

* compatibility of existing natural gas pipeline and distribution system equipment, including compressors, meters, etc.

* the energy flow and leak rate from the system

* safety

Equally important are systems issues. The development of a transmission and distribution system for hydrogen or hydrogen blends will depend on how demand for these fuels grows. Here we look at the following questions:

* What are projected demands for hydrogen and hydrogen blends over the next several decades?

* What are the alternatives for delivering these amounts of hydrogen and hydrogen blends to users? Is adapting the existing natural gas system the best option in terms of cost, environmental benefits and feasibility to bring low polluting fuels (hydrogen and hydrogen blends) to users?

* What are the potential environmental benefits of using hydrogen and hydrogen blends?

* Is hydrogen blending attractive in terms of cost, environmental benefits, and feasibility? What level of blending is feasible? Is blending an evolutionary strategy toward use of pure

hydrogen? Could the fraction of hydrogen in natural gas be increased continuously from 0 to 100%?

* What are some plausible scenarios illustrating how the natural gas transmission and distribution system might adapt to the demand for hydrogen and hydrogen blends?

Many studies have been done on the use of hydrogen and hydrogen blends in the existing natural gas system. Our approach is to revisit the technical possibilities, with a new set of environmental and systems questions in mind.

Our results are summarized below:

* It has been demonstrated in the chemical industries that it would be possible to construct and safely operate end-use devices, local distribution systems and long distance, high pressure pipelines designed for hydrogen.

* The cost of long distance, high pressure transmission pipelines designed for hydrogen might be 50% higher than those designed for natural gas (Leeth 1977, Christodoulou 1984, Pottier et.al 1988, Kelley and Hagler 1980, Ogden and Williams 1989).

* The absolute cost of building a new distribution system for hydrogen would be large suggesting that the possibility of using the existing natural gas system should be examined. However, the contribution of pipeline distribution to the total delivered cost of hydrogen is still relatively small, perhaps 10-20% of the total delivered cost (Leeth 1977, Christodoulou 1984, Ogden and Williams 1989).

* Existing natural gas end-use systems could be used with blends of up to 15-20% hydrogen by volume; above this level significant changes might be needed (USERDA 1977, Kelley and Hagler 1980, Blazek 1993, Jasionowski 1993, Bunger et. al. 1994).

* It appears that hydrogen blends and pure hydrogen could be used in existing natural gas local distribution systems with relatively minor changes (Blazek et.al. 1992, Johnson et.al 1977, Jasionowski and Huang 1980, Jasionowski, Johnson and Pangborn 1979, Pangborn, Scott and Sharer 1977).

* Although it would be technically feasible to do so, it is unlikely that natural gas local distribution lines will be converted to pure hydrogen unless most of the end-users on the system have converted. To meet projected demands for hydrogen vehicles, it is likely that more distribution capacity will be needed, and a pure hydrogen distribution system will probably grow in parallel with the existing natural gas system, along existing rights of way.

* Because of the higher pressures and materials used (lower strength steels), hydrogen embrittlement could be a serious issue for existing long distance, high pressure natural gas

pipelines carrying pure hydrogen or hydrogen blends (Holbrook et.al. 1982, Holbrook et.al. 1986, Cialone et.al 1984).

- However, since the US has a wealth of local resources (natural gas, solar, wind, biomass) for hydrogen production (Ogden 1993), it may not be necessary to transmit hydrogen long distances even in the long term. Instead hydrogen might be made from the best local resources. Once a very large demand has developed and a local distribution system was in place, it might make sense to run a long distance pipeline to a low cost, but distant source of hydrogen. This is analogous to what happened when natural gas replaced manufactured gas.

- It has been suggested that existing gas utility local distribution systems might accomodate users of both natural gas and hydrogen, if hydrogen is blended with natural gas at 15-20% by volume (USERDA 1977). This would not require natural gas users to change their end-use devices and hydrogen could be "skimmed" out by users requiring pure hydrogen. Onsite separation of low percentages (15-20%) of hydrogen from methane blends would be economically unattractive, because of the high cost of small scale gas separation technologies. It would be much less expensive to obtain hydrogen via onsite reforming, truck delivery or pipeline delivery. The decision whether to blend hydrogen into a utility gas supply must rest on the potential environmental benefits of blends.

- A number of applications have been identified (hythane vehicles, hydrogen enhanced combustion) where the addition of hydrogen to natural gas could reduce emissions of CO and/or NOx (Folsom and Mehta 1993, Hansel et.al. 1993, Lynch 1992, Bunger 1994, Moskinskis 1994). The efficacy of hydrogen blending for emissions reduction should be examined for a particular gas utility.

Assessment Of PEM Fuel Cells For Residential Cogeneration

Improvements in proton exchange membrane (PEM) fuel cell technology have focussed attention on these devices as possible power plants for zero emission vehicles. Automotive internal combustion engine power plants typically cost $25-50/kW, while installed costs for cogeneration systems are typically about $1000/kW. This suggests that before PEM fuel cells become competitive for vehicle applications, they will become competitive for distributed power applications. Distributed power generation is a promising entry market for fuel cells, because they are clean, quiet and easily sited.

In this study, we consider use of a PEM fuel cell stack for residential cogeneration of electricity and domestic hot water. The fuel cell is owned and operated by the utility, but located in a house. The utility dispatches the fuel cell to meet peak and intermediate loads; the waste heat from the fuel cell heats the customer's domestic hot water, which is stored in a tank to meet customer demand (Figure 14). The cost to the utility of producing distributed electricity is estimated with and without credits for distributed generation, emissions reductions and fuel diversity. This is compared to the lowest cost central station option for meeting peak demand, a combined cycle gas turbine.

We make the following assumptions:

- The utility dispatches the fuel cell whenever the load exceeds 50% of peak capacity. Synthetic hourly load data from a summer peaking electric utility with high winter peaks (Zaininger et.al. 1977) were used to find the number of hours per year that the fuel cell operates.
- The fuel cell stack is sized to provide all the domestic hot water (DHW) needs of a typical family. The hourly hot water demands varied by day of the week, but were assumed to have no seasonal variation (Perlman and Mills 1985).
- Hydrogen is available from a neighborhood-scale steam reformer, through a low pressure, local distribution system at a cost of $8-12/GJ.
- The fuel cell stack operates on pure hydrogen and air at near atmospheric pressure, based on data from Los Alamos (Wilson and Gottesfeld 1992). The fuel cell operating curve is shown in Figure 15. Hydrogen utilization in the fuel cell stack is 90%. 75% of the waste heat from the fuel cell can be recovered as domestic hot water.
- Estimates of the value of distributed power were based on an EPRI study (Rastler 1992).
- The customer pays the utility the same amount required to fuel a 60% efficient natural gas fired water heater (e.g. the customer has the same heating bill as before).

Our method for sizing the system was as follows:

- The thermal energy needed for each hour of the week for DHW was calculated
- The fuel cell stack is sized so that the total thermal energy provided in the winter is enough to meet DHW demands for each hour of the week. (Winter is chosen for sizing the fuel cell because the peak electric demand is intermediate between summer and srping/fall.)
- The fuel cell operating point is chosen to keep the fuel cell size relatively small, and the capital cost lower.
- The operating point of the fuel cell is varied each season to meet the thermal demand needed for spring/fall and summer seasons.
- Hot water storage is sized to meet the demand for DHW over an entire week. (The hot water produced each hour of the week is estimated, and the level of the storage tank is computed by subtracting the hot water demanded that hour. The maximum of this running total over a week gives the required storage tank volume.

The cost of electricity generation to the utility is found considering the capital and operating expenses of the fuel cell system and the value of distributed generation. The fuel cell alternative is compared to the best available central station peaking technology, the combined cycle gas turbine.

The capital cost of the fuel cell system includes the fuel cell stack, a utility interactive inverter and the cost of hot water storage above what the homeowner would need with a conventional system. The utility's operating costs include hydrogen to run the fuel cell. It is also assumed that the customer pays the utility an amount equal to what it would have paid for natural gas to run a conventional 60% efficient gas-fired water heater. Table 2 shows the estimated cost of generation for fuel cell capital costs of $1000, $1500 and $2000/kW, hydrogen costs of $8,$10, and $12/GJ, and residential natural gas prices of $5, 5.5 and 6/GJ. This assumed that the system lifetime was 15 years. This is then compared to the cost of electricity generation with a combined cycle gas turbine, assuming that gas prices for utility generation are about $2.8/GJ lower than residential prices.

We see that, if no credits are given for distributed generation, fuel diversity or low emissions, the fuel cell system is unable to compete with the low cost electricity from the combined cycle gas turbine.

However, the value of distributed power can be quite substantial. This is shown in Table 3, where the various benefits have been quantified for three electric utilities (Rastler 1992). When these benefits are figured in, the relative economics of peak power generation can sometimes favor fuel cell systems. This is shown in Table 4 where the cost of power generation including distributed benefits is estimated. When the value of distributed generation includes credits for fuel diversity and low emissions, we found that PEM fuel cell cogeneration was competitive with gas turbines for nearly all combinations of fuel cell capital cost, lifetime, hydrogen cost, and natural gas price considered.

Conclusions

Even at projected market entry costs of $2000/kW, for PEM fuel cell systems may be cost effective for cogenerating domestic hot water and electricity in locations where distributed benefits have a high value. For more modest estimates of distributed benefits, fuel cell cogenerated power may be attractive as fuel cell system costs are reduced, lifetimes extended, and where low cost hydrogen is available.

Recommendations for Future Work

It would be interesting to look at the feasibility of PEM cogeneration systems in commercial buildings.

Assessment Of Small Scale Reformer Technologies

Small scale production hydrogen from natural gas is likely to be an important technology in the early stages of a hydrogen economy. Unless pipeline hydrogen is available, onsite reforming of natural gas could be the best option for applications such as distributed power generation with fuel cells or hydrogen vehicle refueling stations.

In this task, we are assessing the technical options for low cost, small scale production of hydrogen from natural gas considering: 1) catalytic steam reforming, 2) partial oxidation and 3) thermocatalytic (or autothermal) reforming.

We are investigating the following questions:

* What are the performance, cost and emissions of small scale steam reformer technology now on the market? How does this compare to partial oxidation and autothermal systems?

* How do the performance and cost of reformer technologies depend on scale? What critical technologies limit cost and performance of small scale hydrogen production systems? What are the prospects for potential cost reductions and performance improvements as these technologies advance?

* How would reductions in the reformer capital cost impact the delivered cost of hydrogen transportation fuel?

Approach

* First, we contacted manufacturers to gather preliminary cost and performance data on commercially available small scale reformer technologies and those now under development. Table 5 summarizes performance and cost data for small scale reformer systems.

* To gain insight on reformer design, we are developing computer models of 1) equilibrium steam reformer reactions, 2) conversion of methane in a single reformer tube, and 3) a hydrogen plant based on steam reforming, incuding upstream and downstream processing and heat recovery.

* We are continuing discussions with manufacturers and researchers to better understand design and cost issues for small scale reformers.

Survery of Existing Technologies for Small scale Production of Hydrogen from Natural Gas

Catalytic Steam Methane Reforming

Catalytic steam reforming natural gas is a well known, commercially available process for hydrogen production. The steam reforming reaction

$$CH_4 + H_2O \rightarrow CO + 3\,H_2 \qquad \Delta h = +206.16\ \text{kJ/mol}\ CH_4 \quad (1)$$

is endothermic and is favored at temperatures > 800°C, and pressures of 5-15 atmospheres. External heat needed to drive the reaction is often provided by the combustion of 10-20% of the incoming natural gas feedstock (or from fuel cell anode exhaust). Heat transfer to the reactants is accomplished indirectly through a heat exchanger. Generally, the methane feed plus steam (to prevent coking) are introduced into high alloy nickel chromium tubes containing nickel based catalysts. Because the heat flux (and, thus, the reaction kinetics) are limited by the need for indirect heating, heat exchangers in steam reformers have relatively large surface areas, and can be quite bulky. (Typical tube lengths for commercially available reformers are 12 meters.) The design of low cost, compact steam reformers is largely a problem of designing the heat exchange system.

After reforming, the resulting syngas is sent to one or more shift reactors, where the hydrogen output is increased via the water-gas shift reaction:

$$CO + H_2O \rightarrow CO_2 + H_2 \qquad \Delta h = -\,41.15\ \text{kJ/mol CO} \quad (2)$$

This reaction is favored at temperatures of less than about 600°C, and can take place as low as 200°C, with sufficiently active catalysts.

Hydrogen is then purified. Options include preferential oxidation to reduce the CO content, pressure swing adsorption or membranes. For PEM fuel cell quality hydrogen, pressure swing absorption (PSA) systems or palladium membranes are used to produce hydrogen at 99.999% purity.

Data on commercially available steam methane reforming plants were gathered from several vendors (Howe-Baker, Hydrochem, Haldor-Topsoe). In discussons with vendors, we found that the minimum commercially available size is about 100,000 scf H_2/day. Below this size, plant capital costs decrease very little, and other sources of hydrogen (such as truck delivery or electrolysis) are usually less expensive (King 1993). Most steam reforming units built to date have larger capacities than the 0.1-2.0 million scf/day needed for refueling stations or fuel cell cogeneration applications. Typical applications are for refineries or ammonia production, where 25-100 million scf/day might be needed. However, a number of smaller reformers have been built for chemical processing needs.

Manufacturers' installed capital cost data for steam reforming plants in the range 0.1 to 2.0 million scf H_2/day are shown in Figure 16 (costs include the reformer, shift reactor, PSA system, and NOx control). Commercially available small scale steam reformers are costly, ranging from about \$1,500,000 for a plant producing 100,000 scf H_2/day to \$3,000,000 for a plant producing 1 million scf/day. There are strong scale economies in this size range, with installed capital costs varying as

$$\text{Installed cost} = \$3 \times 10^6 \times (\text{plant capacity in million scf/day})^{0.3}.$$

One of the main capital cost drivers for commercially available steam reformers is the reformer tubes. Because of the high temperatures and pressures and long lifetime required for chemical plant applications, tube materials are expensive.

The energy efficiency (= hydrogen energy out/methane in) of small scale reformers is quite high, typically about 80-85%.

To achieve long equipment lifetime, good performance and low emissions, manufacturers indicated that the reformer should be run continuously, preferably at constant output. The reformer start-up time is 4 to 6 hours, and the response time to changes in load is relatively slow, so that following a rapidly varying hydrogen demand would be difficult. Small scale reformers are designed for automated operation, with occasional monitoring.

The only significant pollutants emitted from a steam reforming system would be nitrogen oxides (NOx). NOx can be controlled through a low NOx burner design or with selective catalytic reduction (SCR) to levels that meet stringent California air quality standards.

Operating conditions and costs for a hydrogen plant producing 0.366 million scf/day (enough to fuel about 300 fuel cell cars/day) is shown in Table 6.

In addition to commercially available units, small scale natural gas reformers are being developed for fuel cell applications. (For example, a reformer coupled to a fuel cell with a 200 kW electrical output would require about 500 kW of hydrogen or 120,000 scf/day.) Projections for near term technology estimate about \$500/$kW_{electric}$ as the reformer's contribution to the cost (Barbir 1994, Prater 1994, Wheeler 1995). For a 200 kW fuel cell, this corresponds to a capital cost of about \$100,000 for a reformer producing 120,000 scf/day of hydrogen. Fuel cell reformer systems are not yet commercialized as stand alone units, but are part of an integrated packaged cogeneration system. Steam methane reformers coupled to fuel cells may not be directly comparable to commercially available stand-alone hydrogen plants for several reasons : 1) they are heat integrated with the fuel cell system, 2) some fuel cell reformers are designed to produce hydrogen for phosphoric acid fuel cells which require much lower purity hydrogen than that needed chemical plant applications, 3) cost and compactness are more important issues for fuel cells.

Reformer manufacturers contacted stressed that commercially available small scale steam reforming systems had not yet been optimized for cost or compactness. The much lower costs projected for reformers coupled to fuel cells suggest that it may be possible togreatly reduce costs.

Partial Oxidation

Small scale partial oxidation systems have just become commercially available, but are still undergoing intensive R&D (Moard 1995, Loftus 1994). In partial oxidation reforming, methane is oxidized to produce carbon monoxide and hydrogen according to

$$CH_4 + 1/2\,O_2 \; \text{->} \; CO + 2\,H_2\,, \qquad \Delta h^\circ = -36 \text{ MJ/kmol } CH_4$$

The reaction is exothermic and direct heat exchange can be used. No catalyst is required because of the high temperature. However, the hydrogen yield per mole of methane input (and the system efficiency) can be significantly enhanced by use of catalysts (Loftus). The reactor is more compact than a steam reformer, where heat must be added indirectly via a heat exchanger. The efficiency of the partial oxidation unit is relatively high (70-80%). However, partial oxidation systems are typically less energy efficient than steam reforming because of the higher temperatures involved (and the problem of heat recovery). A hydrogen plant based on partial oxidation would include a shift reactor and hydrogen purification equipment. Partial oxidation systems have a fast response time, making them attractive for following rapidly varying loads. Partial oxidation systems can handle a variety of fuels.

Partial oxidation systems are under development by Arthur D. Little (Loftus 1994) and by Hydrogen Burner Technology (Moard 1995). Because they are more compact, and do not require heat exchangers, it is likely that partial oxidation systems could be lower cost than steam reformers.

Autothermal Reforming

In autothermal reformers, some fuel undergoes partial oxidation, which supplies heat to drive a catalytic steam reforming reaction. The autothermal reformer requires no external heat source and no indirect heat exchangers. This system has a higher efficiency than partial oxidation, and is only slightly more bulky. Autothermal reforming systems are not commercially available at present, but are now being developed by Rolls Royce, (Shoesmith 1992) International Fuel Cells, and Chiyoda. Because they are more compact and less costly, this approach may eventually offer lower cost than steam reforming.

Potential for Low Cost Small Scale Steam Reforming

In catalytic steam reforming, the heat must be transfered indirectly through a tube. The design of low cost steam reformers is basically a problem in heat-exchanger design. Several low cost designs have been proposed for steam reformers, where the heat flow path is made more compact. (As an example, Figure 17 shows a compact, cylindrically symmetric design by Haldor Topsoe as compared to a conventional steam reformer used in chemical plant operations, with long tubes, externally heated).

Comparing the cost of commercially available steam reformers to the cost of reformers in fuel cell cogeneration packages suggests that there may be considerable opportunity to reduce the cost. For example, a commercially available steam reforming plant producing 120,000 scf/day might cost about $1.5 million, while a reformer in a fuel cell producing this much hydrogen might cost only about $100,000. As a first approach to assessing the potential for low cost reformers, we tried to understand why fuel cell reformers were projected to be so much less expensive that commercially available steam reformers.

In discussions with reformer manufacturers and fuel cell developers a number of possible reasons were mentioned to explain why fuel cell reformers are lower in cost.

* Commercially available reformers are generally designed for chemical plant applications, providing hydrogen at a particular purity, pressure and temperature. The reformer is designed to provide as much hydrogen as possible from each tube. Pressures are higher, a longer tube lifetime is required and more costly materials must be used.

* Commercially available reformers are custom designed for each application, so that engineering costs are considerable. Costs for fuel cell reformers assume mass production of a standardized design.

* Fuel cell reformers are designed for an application, where low cost and compactness are at a premium. The operating pressure and temperature may be lower, and a lower tube lifetime than 20 years may be tolerable. Also for some types of fuel cells (phosphoric acid) the required hydrogen purity may be lower.

We are pursuing this question further in continuing discussions with reformer companies and through simulations of steam reformers.

Reformer Simulations

To better understand the design of steam reformers, we have written several computer simulation programs (Jones 1995).

* First, a program was written to model the equilibrium products in a reformer as a function of temperature and pressure. This was checked with results from the ASPEN program for simulation of chemical processes and gave good agreement.

* Then a 1-D model of a single reformer tube was developed based on models by Hyman (Hyman 1968). The results of this simulation were checked with experimental curves given in Rostrup-Nielsen (Rostrup-Nielsen 1984), and good agreement was found. The program allows us to estimate how the fraction of methane, hydrogen, CO, CO_2 and H_2O vary along the length of the reformer tube with operating temperature, pressure, catalytst activity and flow rate.

* Finally, we are working on a model of a full hydrogen plant based on steam reforming, including feed purification, reforming, shift reactor, hydrogen clean-up and heat integration.

We are using these programs to gain insight into proposed designs for low cost, compact steam reformers.

Implications of Low Cost Reformers for Hydrogen Transportation Fuel Cost

For refueling stations based on steam reforming, the capital cost of the reformer is a major contributor to the delivered cost of hydrogen transportation fuel. From Figure 3 we can see how the delivered cost of hydrogen would vary, if the reformer capital cost were reduced. We see that is the cost could be reduced by a factor of two from present commercial technology, the cost of hydrogen would decrease by $11- 5/GJ (or $1.4-0.7/gallon gasoline equivalent), for refueling stations with a capacity in the range 0.1-1.0 million scf H_2/day.

Future Work

As we continue this task we will try to understand the main cost drivers in steam reformer plants, considering the cost of: tube materials catalyst materials, engineering design, manufacturing costs, installation, clean-up of feedstock, and purification of hydrogen.

Similarly, we will investigate partial oxidation systems and autothermal reformer systems.

Assessment Of Potential Markets For Hydrogen In Southern California

We are conducting a case study of how hydrogen markets might develop in Southern California over the next five years. It is likely that fleets of hydrogen vehicles will be introduced in California in the early part of the next century, in response to the zero emissions vehicle (ZEV) mandate. Other possible uses of hydrogen energy in this time frame include co-firing and fuel cells. In this task we are estimating the size of these potential hydrogen markets. We are also estimating the hydrogen supply projected for the next 5-10 years. This work is being carried out in collaboration with Southern California Gas Company, South Coast Air Quality Management District, and industrial hydrogen suppliers.

Thus far we have concentrated on understanding the potential markets for ZEVs in Southern California. Table 7 shows the mandated implementation levels for ZEVs in California. In Table 8, the projected number of light duty vehicles are shown. Assuming that the mandated levels are realized and that these cars remain on the road for 10 years, the number of ZEV cars sold each year and the cumulative number of ZEV cars can be projected for each year. Figures 18 and 19 illustrate how ZEV populations and hydrogen demand might grow in the Los Angeles basin, if mandated levels of ZEVs are introduced in California. We see that by 2003, over 200,000 ZEV cars will be on the road in the LA Basin, and by 2010 about 800,000 (assuming that 10% of the new vehicles sold between 2003 and 2010 must be ZEVs). If half the ZEVs in the LA Basin were hydrogen fuels cell cars, this would require about 55 milllion scf/day of hydrogen, enough to support a large centralized steam reforming plant.

Proposed Future Work

Assess the role of hydrogen as a fuel for fuel cell vehicles

Fuel cell vehicles have the potential to be zero emission vehicles with a reasonably long range and a fast refueling time. All fuel cells proposed for vehicles in the near to mid-term require hydrogen as a fuel. However, a number of alternatives have been suggested for supplying hydrogen onboard fuel cell vehicles, including: 1) storing pure hydrogen onboard, 2) reforming methanol onboard the vehicle, 3) converting hydrocarbon fuels (similar to gasoline or Diesel) to hydrogen via partial oxidation onboard the vehicle.

We would compare hydrogen and other fuels for fuel cell vehicles considering 1) the relative difficulty of developing a refueling infrastructure, 2) onboard fuel storage requirements, 3) fuel cost, 4) vehicle complexity, 5) vehicle performance, 6) vehicle cost, 7) resources for fuel production, 8) vehicle emissions, and 9) fuel cycle emissions.

Assess the value of hydrogen as a pollution reducing additive to natural gas

In the 1970's hydrogen blending was proposed as a way of extending natural gas supplies. Renewed discussion of hydrogen/methane blends has arisen over the last few years as a way of reducing emissions. In general, the higher the proportion of hydrogen in the blend, the larger the potential emissions benefits (assuming end-use equipment designed for the blend). With pure hydrogen, zero or near zero emissions would be possible. In this task we would examine the efficacy of using hydrogen/natural blends when the object is to reduce air pollution.

Case study of developing a hydrogen vehicle refueling infrastructure in Southern California

Building on our work assessing the economics of supplying hydrogen from natural gas, we would apply our insights on hydrogen infrastrucure development to the case of Southern California. This work would build on our ongoing analysis of hydrogen markets in Southern California.

Assessment of PEM cogeneration systems for commercial buildings

Proton exchange membrane (PEM) fuel cells offer the potential of low cost in mass production. Distributed power generation and cogeneration could be markets which would become economically competitive before transportation markets. In our previous year's work, we assessed the possibility of using PEM fuel cells for residential cogeneration. It was found that PEM fuel cells sited in houses and run on hydrogen could become competitive as utility owned peak power devices, if credits for distributed generation, fuel diversity and environmental benefits were counted. Here we would continue expand this study to look at PEM fuel cell cogeneration in commercial buildings.

Strategies for introducing hydrogen from Biomass and MSW

Gasification of biomass and municipal solid waste (MSW) could be the lowest cost renewable sources of hydrogen. In this task, we would examine systems issues involved in a transition from natural gas derived hydrogen to hydrogen from MSW or biomass, sometime in the early part of the next century.

Technology Transfer and Interactions With Other Groups

Because we have focussed on near term issues for hydrogen energy, interactions with industry are an important component of our work. In our studies of the past two years we have developed contacts at gas utilities (Southern California Gas Company), reformer manufacturers (Howe-Baker Engineering, Hydrochem, Haldor Topsoe, Hydrogen Burner Technology, A,D, Little), industrial gas suppliers (Praxair, Air Products, British Oxygen Company), manufacturers of hydrogen compressors and storage systems (RIX compressors, Christy Park Industries), and fuel cell manufacturers (Energy Partners, H-Power, Ballard Power Systems, International Fuel Cells). We have received useful comments and advice from researchers at the Institute of Gas Technology and the National Hydrogen

Association. For our study of Southern California hydrogen markets, data were obtained from the South Coast Air Quality Management District. We have had discussions with researchers at oil companies (Exxon, Mobil) and automotive companies (Chrysler, Mazda, Daimler-Benz) involved with fuel cell vehicles. We have given an invited presentation at a meeting of the Clinton Administration's Partnership for a New Generation for Vehicles (PNGV) program, which is seriously considering fuel cell vehicles as one of the only viable contenders for tripling automotive efficiency. We have also contacted researchers at national laboratories (ORNL, LLNL, Sandia, LANL) and academia (UC Davis, Texas A&M).

Acknowledgments

The authors would like to thank Carol Bailey (Southern California Gas Company), Frano Barbir (Energy Partners), Chris Blazek (Institute of Gas Technology), Chris Boroni-Bird (Chrysler), Jeff Chen (Princeton University), David Crain (So.Cal.Gas), Mark Delucchi (UC Davis), R. Dowling (Christy Park Industries), Gary Fenner (Praxair), Ranji George (SCAQMD), Pat Grimes (consultant), Walt Jasionowski (IGT), Ryan Katofsky (A.D. Little), Art Kaufmann (H-Power), Michael Kerr (Praxair), David King (Howe-Baker Engineers), Ira Kuhn (Directed Technologies, Inc.), Paul Kydd (British Oxygen Company), Eric Larson (Princeton University), Al Mezzina (consultant), Robert Miller (Air Products and Chemicals), David Moard (Hydrogen Burner Technology, Inc.), Robert Moore (Air Products and Chemicals), David Nahmias (National Hydrogen Association), Venkat Raman (Air Products and Chemicals), B.D.Savidge (RIX Industries), Robert Schock (LLNL), Suman Singh (ORNL), J. Ray Smith (LLNL), Sandy Thomas (Directed Technologies, Inc.), Niels Udergaard (Haldor Topsoe), David Watkins (Ballard Power Systems), John Werth (H-Power), Douglas Wheeler (International Fuel Cells) and Robert Williams (Princeton University) for useful conversations and comments.

References

Barbir, F., Energy Partners, private communications 1994.

Blazek, C.F., R. Biederman, S. Foh, and W. Jasionowski, "Underground Storage and Transmission of Hydrogen," Proceedings of the Third Annual US Hydrogen Meeting, March 18-20, 1992, Washington, DC.

Blazek, C., Institute of Gas Technology, private communications, 1993.

Bunger, U., W. Zittel, T. Schmalschlager, "Hydrogen in the Public Gas Grid-A Feasaibility Study about its Applicability and Limitations for the Admixture within a Demonstration Project for the City of Munich," presented at the 10th World Hydrogen Energy Conference, Cocoa Beach, FL, June 20-24, 1994.

Christodoulou, D., "Technology and Economics of the Transmission of Gaseous Fuels via Pipeline," Thesis, Master of Science, Department of Mechnical and Aerospace Engineering, Princeton University, April 1984.

Cialone,H.P., P.M. Scott, J.H. Holbrook, K. Sieradzki, and N. Bandyopadhyay, "Hydrogen Effects on Conventional Pipeline Steels," in Hydrogen Energy Progress V, Pergamon Press pp. 1855-1868.

DeLuchi, M.A., "Hydrogen Vehicles: An Evaluation of Fuel Storage, Performance, Safety and Cost," International Journal of Hydrogen Energy, v. 14, pp. 81-130, 1989.

DeLuchi, M.A., "Hydrogen Fuel Cell Vehicles," Institute of Transportation Studies Technical Report, UCD-ITS-RR-92-14, University of California, Davis, September 1992.

Dennis, E.B. "The Design and Feasibility of a Hydrogen Refueling Station Supplied by On-site Reforming of Natural Gas," Senior Thesis, Department of Chemical Engineering, Princeton University, May 2, 1994.

Folsom, B.D. and B. Mehta, "Hydrogen Enhanced Combustion for Utility Applications," Proceedings of the Fourth Annual US Hydrogen Meeting, National Hydrogen Association, Washington, DC, March 25-26, 1993, EPRI Report No. TR-103183, Research project 1086-22, p. 8-35.

George, R., South Coast Air Quality Management District, Diamond Bar, CA, private communications, 1994.

Hansel, J., D. Kielan, F. Lynch, R. Ragazzi, V. Raman, B. Willson, "Hythane-Status Report," Proceedings of the Fourth Annual US Hydrogen Meeting, National Hydrogen Association, Washington, DC, March 25-26, 1993, EPRI Report No. TR-103183, Research project 1086-22, p.7-13.

Holbrook, J.H., H.J. Cialone, M.E. Mayfield, and P.M. Scott, "The effect of hydrogen on low-cycle-fatigue life and subcritical crack growth in pipeline steels," Battelle Columbus Laboratories, 505 King Avenue, Columbus, OH 43201, BNL--35589, DE85 006685, 1982, 102 pp.

Holbrook, J.H., E.W. Collings, H.J. Cialone, and E.J. Drauglis, "Hydrogen degradation of pipeline steels," prepared for Energy Applications and Analysis Division, Department of Applied Science, Under Subcontract No. 550722-S, Brookhaven National Laboratory, Associated Universities, Inc., Upton, NY 11973, Under Contract No. DE-AC02-76CH00016 with the U.S. Dept. of Energy; Report numbers BNL--52049, DE87 005585; 165pp.,March 1986

Hyman, M.H., "Simulate Methane Reformer Reactions," Hydrocarbon Processing, July 1968, pp. 131-137.

Jasionowski, W., Institute of Gas Technology, Private communications, 1993.

Jasionowski, W., D. Johnson, and J. Pangborn, "Suitability of Gas Distribution Equipment in Hydrogen Service," IGT Report, paper presented at the 14th Intersociety Energy Conversion Engineering Conference, Boston, MA August 5-10, 1979.

Jasionowski, W. and H. Huang, "Gas Distribution Equipment in Hydrogen Service," IGT Report, paper presented at the 15th Intersociety Energy Conversion Engineering Conference, Seattle, WA, August 18-22, 1980.

Jewett, R.P., R.J. Walter, W.T. Chandler, and R.P. Frohmberg. "Hydrogen environment embrittlement of metals," NASA CR-2163, Prepared by Rocketdyne, Division of North American Rockwell, Canoga park, CA 91304, March 1973, pp. 235.

Johnson, D.G., W.J. Jasionowski, D.L. Albright, J.B. Pangborn, N.R. Baker, "Study of the Behavior of Gas Distribution Equipment in Hydrogen Service," Final Report to the U.S. Department of Energy, Contract No. EY-76-C-02-2907, April 1979.

Jones, A.T., "Simulation of Small Scale Steam Methane Reformers," Senior Thesis, Department of Chemical Engineering, Princeton University, May, 1995.

Katofsky, R.E., ÒProduction of Fluid Fuels from Biomass,Ó Princeton University, Center for Energy and Environmental Studies Report No. 279, June 1993.

Kelley, J.H. and R. Hagler, "Storage, Transmission and Distribution of Hydrogen," International Journal of Hydrogen Energy, v. 5, pp. 35-54, 1980.

Kerr, M., "North American Merchant Hydrogen Infrastructure," Proceedings of the Fourth Annual US Hydrogen Meeting, National Hydrogen Association, Washington, DC, March 25-26, 1993, EPRI Report No. TR-103183, Research project 1086-22, p.8-61.

King, D., Howe-Baker Engineers, private communications, 1993.

Kuhn, I., Directed Technologies, Inc., private communications 1994.

Kumar, R. and S. Ahmed, "Multi-Fuel Reformer R&D," Proceedings of the Annual Automotive Technology Development Contractors' Coordination Meeting 1991, Dearborn, MI, Oct 28-30, 1991, p.229.

Kydd, P., British Oxygen Company, private communications 1993, 1994.

Larson, E.D., and R.E. Katofsky, ÒProduction of Methanol and Hydrogen from Biomass,Ó Princeton University, Center for Energy and Environmental Studies Report No. 271 July 1992.

Leeth, G.G., in K.E. Cox and K.D. Williamson, eds., Hydrogen: Its Technology and Implications, volume II: Transmission and Storage, CRC Press, Cleveland, OH, 1979.

Loftus, P., J. Thijssen, J. Bentley, J. Bowman, "Development of a Multi-Fuel Partial Oxidation Reformer for Transportation Applications," A.D. Little, Inc., Cambridge, MA, presented at the 1994 Fuel Cell Seminar, San Diego, CA, Nov.28-Dec.1 1994.

Lynch, F., "Near Term Pathways Toward Hydrogen Energy," Proceedings of the Third Annual US Hydrogen Meeting, National Hydrogen Association, Washington, DC, March 18-20, 1992.

Moard, D., Hydrogen Burner Technology, Inc., private communications, 1995.

Moore, R., Air Products and Chemicals, Inc., private communications, 1994.

Moskinskis, G., "The Role of Utilities and Hydrogen," Proceedings of the Fifth Annual US Hydrogen Meeting, National Hydrogen Association, Washington, DC, March 23-24, 1994, p. 4-15

Ogden, J.M. and R.H. Williams, Solar Hydrogen : Moving Beyond Fossil Fuels, World Resources Institute, Washington DC, October 1989.

Ogden, J.M. and J. Nitsch, ÒSolar Hydrogen,Ó Chapter 22 in T. Johansson, H. Kelly, A.K.N. Reddy and R.H. Williams, Renewable Energy: Fuels and Electricity from Renewable Sources, Island Press, Washington, DC, 1993.

Ogden,J.M., Renewable Hydrogen Energy Systems Studies, final report for NREL Contract No. XR-2-11265-1, June 24, 1993.

Ogden, J.M. and M.A. DeLuchi, ÒSolar Hydrogen Transportation Fuels,Ó Chapter 8, in D. Greene and D. Santini, eds., Proceedings of the Conference on Transportation and Global Climate Change, American Council for an Energy Efficient Economy, Washington, DC, 1993.

Ogden, J.M., J.W. Strohbehn and E. Dennis, ÒHydrogen Energy Systems Studies,Ó Proceedings of the USDOE Hydrogen Program Review Meeting, April 19, 1994.

Ogden, J.M., E. Dennis and J.W. Strohbehn, ÒA Technical and Economic Assessment of the Role of Natural Gas in a Transition to Hydrogen Transportatio Fuel,Ó presented at the 10th World Hydrogen Energy Conference, Cocoa Beach, FL, June 21-24, 1994.

Ogden, J.M., E.D. Larson and M.A. Delucchi, ÒAn Assessment of Renewable Transportation Fuels and Technologies,Ó report to the US Congress Office of Technology Assessment, May 27, 1994.

Ogden, J.M., E. Dennis, M. Steinbugler, and J. Strohbehn, "Hydrogen Energy Systems Studies," Final Report to NREL for Contract No. XR-11265-2, January 18, 1995.

Pangborn, J., M. Scott and J. Sharer, "Technical Prospects for Commercial and Residential Distribution and Utilization of Hydrogen," International Journal of Hydrogen Energy, v. 2, pp. 431-445, 1977.

Perlman, M. and B.E. Mills, "Development of Residential Domestic Hot Water Use Patterns, ASHRAE Transactions 1985, Part 2A, Volume 91, pp. 657-679, ASHRAE, Atlanta, GA, 1985.

Pottier, J., E. Blondin, and A.Garat, "Large Scale Transmission and Storage of Hydrogen," in T.N. Veziroglu and A.N. Protosenko, eds., Hydrogen Energy Progress VII, Proceedings of the World Hydrogen Energy Conference, Moscow, USSR, 25-29 September 1988.

Prater, K., Ballard Power Systems, private communications, 1994.

Rastler, D., "Modular Power Systems: Distributed Generation," EPRI Journal, vol. 17, April/May 1992, pp. 28-30.

Rostrup-Nielsen, J.R., "Catalytic Steam Reforming," Springer-Verlag, New York, 1984.

Shoesmith, J.P., R.D. Collins, M.J. Oakley and D.K. Stevenson, "Status of solid polymer fuel cell development," Journal of Power Sources, v. 49, 1994, pp. 129-142.

Smith, J.R., "The Hydrogen Hybrid Option," 1993 Car Conference, Riverside, California.

Thomas, S., Directed Technologies, private communications, 1995.

US Energy Research and Development Administration Ad Hoc Committee, "An Evaluation of the Use of Hydrogen as a Supplement to Natural Gas," USERDA Chemical and Thermal Storage Systems Branch, Report No. TID-27747, June 1977.

Wagner, E.S. and G.F Froment, "Steam Reforming Analyzed," Hydrocarbon Processing, July 1992, pp. 69-77.

Wilson, M.S. and S. Gottesfeld, "High Performance Catalyzed Membranes of Ultra-Low Pt Loadings for Polymer Electrolyte Fuel Cells," Journal of the Electrochemical Society, vol. 139, No. 2, February 1992, pp. L28-L30.

Zaininger, H.W., A.J. Wood, H.K. Clark, T.F. Laskowski and J.D. Burns, "Synthetic Electric Utility Systems for Evaluating Advanced Technologies," EPRI-EM-285, Electric Power Research Institute, February 1977.

Tables

TABLE 1. COMPARISON OF VARIOUS METHODS OF MAKING HYDROGEN TRANSPORTATION FUEL FROM NATURAL GAS

METHOD	ADVANTAGES	DISADVANTAGES
Onsite steam reforming of natural gas at refueling station	1) Add capacity as needed 2) Hydrogen delivery infrastructure not neccessary 3) Commercially available technology with large cost reduction potential 4) Low delivered hydrogen cost at station sizes of > 1 million scf H2/day	1) High capital cost for refueling station 2) Relatively complex equipment at refueling station 3) High delivered hydrogen cost at station sizes of less than about 0.4 million scf H2/day 4) Requires natural gas feedstock
Centralized steam reforming, with liquefaction and truck delivery of liquid hydrogen to refueling station	1) Current industrial practice 2) Liquid hydrogen could be delivered even where natural gas is not available 3) Low capital cost for refueling station	1) High delivered cost of fuel at station except at small station sizes (less than 0.4 million scf/day) 2) High energy penalty for liquefaction reduces fuel cycle energy efficiency
Centralized steam reforming, with gaseous pipeline delivery of hydrogen to refueling station	1) Lowest delivered cost of fuel 2) Other centrally produced sources of hydrogen (from renewables) could replace natural gas when needed.	1) Requires large demand (tens of millions of scf H2/day) 2) Possible issues with obtaining rights of way, permits, etc.

TABLE 2. COST OF GENERATING ELECTRICITY ($/KWH) FUEL CELL COGENERATION COMPARED TO GAS TURBINE WITH NO CREDITS FOR DISTRIBUTED GENERATION

		Fuel cell electricity cost								
NG Price	w/NG Turb.	H2 cost =$8/GJ			H2 Cost=$10/GJ			H2 Cost=$12/GJ		
		Fuel cell cost ($/kW)			Fuel cell cost ($/kW)			Fuel cell cost ($/kW)		
$/GJ		1000	1500	2000	1000	1500	2000	1000	1500	2000
5.0	0.035	0.086	0.096	0.106	0.108	0.118	0.128	0.130	0.140	0.150
5.5	0.040	0.082	0.092	0.102	0.104	0.114	0.124	0.126	0.136	0.146
6.0	0.044	0.079	0.088	0.098	0.101	0.110	0.120	0.123	0.132	0.142

TABLE 3. THE VALUE OF DISTRIBUTED POWER ($/KWH)

Benefit	Los Angeles Dept. Of Water And Power	Central And South West Corporation	Oglethorp Power
Spinning Reserve	0.0011	0.0018	0.0020
Peak Operation	0.0006	0.0007	0.0014
Reserve Margin	Not quantified	0.0009-0.0017	0.0017-0.0034
T&D Deferral	0.0011-0.0071	0.0017-0.013	0.0015-0.0048
Energy Loss Savings	0.0019-0.016	0.0041-0.0171	0.0036
Improved Reliability	0-0.0013	0.0027-0.013	0
Low Emissions	0.0082-0.021	0.0002-0.058	0.0001-0.038
Fuel Diversity	0-0.0084	0.0008-0.020	0
(1)	0.0030-0.0184	0.0095-0.0336	0.0073-0.0090
(2)	0.0111-0.0478	0.0177-0.116	0.0074-0.0470

Value of distributed benefits in row (1) includes spinning reserve, reserve margin, energy loss savings, and improved reliability. Row (2) also includes value oflow emissions and fuel diversity.

TABLE 4. COST OF GENERATING ELECTRICITY ($/KWH) WITH CREDITS FOR DISTRIBUTED GENERATION, LOW EMISSIONS AND FUEL DIVERSITY

		Fuel cell electricity cost								
NG Price	w/NG Turb.	H2 cost =$8/GJ			H2 Cost=$10/GJ			H2 Cost=$12/GJ		
		Fuel cell cost ($/kW)			Fuel cell cost ($/kW)			Fuel cell cost ($/kW)		
$/GJ		1000	1500	2000	1000	1500	2000	1000	1500	2000
5.0	0.035	-0.026	-0.016	-0.006	-0.004	0.006	0.016	0.018	0.028	0.038
5.5	0.040	-0.029	-0.020	-0.010	-0.007	0.002	0.012	0.015	0.024	0.034
6.0	0.044	-0.033	-0.023	-0.013	-0.011	-0.001	0.009	0.011	0.021	0.031

TABLE 5. PERFORMANCE AND COST CHARACTERISTICS OF SMALL-SCALE METHANE REFORMERS

Company	Capacity H2 out (scf/day)	Feed Pressure	Feed Purification	Reformer Temp	Shift reactor	Hydrogen Purification	Efficiency	Dynamic response	Physical Size and Cost
CATALYTIC STEAM REFORMERS									
Halder-Topsoe	67,000-3.3 million	Supply pressure	Zinc-oxide	1525°F	high and low temp.	99.999% w/PSA	80%	Cold start in 3 hours, 25-100% load in 30 seconds	$500/kW, 30' high, 8' diameter
Howe-Baker Engineers	1-5 million	300 psig	Zinc-oxide	1550-1600°F	High temp (675-800°F)	99.999% w/PSA	80%	Cold start in several hours	$3 million for 1 million scf/day
Hydro-chem	120,000-5 million	275 psig	Zinc-oxide		High temp	99.99% pure w/PSA		Cold start in 2-4 hours, 100% to 30% load in 1 hr	40' high, 40x80' area, $1 million for 120,000 scf/day
KTI									
Glitsch	300,000			Steam Reformer					$1-1.3 million
International Fuel Cells/ONSI	48,000-140,000	Supply pressure		Steam Reforming Fuel Processor Unit in Fuel Cell Cogeneration Package	High temp.	Less than 75% pure H2, product contains H2, CO, CO2	84%	Cold start in less than 3 hours, idle to 100% load in 1 second	10' high, 4' diameter, $300/kWe for refomerBeing developed as part of a phosphoric acid fuel cell cogen package
Ballard Power Systems	6000 120,000	Supply pressure				99.99% pure (for use with PEM fuel cell)	80% eff.		Being devel. as part of a fuel cell package est. $500/kWe
Chiyoda (JAPAN)				Stea, Reformer used with 100-200 kW Phosphoric Acid Fuel Cells					
PARTIAL OXIDATION SYSTEMS									
Arthur D. Little	12,500		Zinc oxide	1600-1800°C (catalytic POX)	high and low temp.	Pref. oxidation	80% eff	Fast	R&D only, not commercial yet
Hydrogen Burner Technology	12,000 96,000			2500°F (POX)	High and low temp	Palladium membrane 99.999% pure	75-80%	Fast	less than $200,000 for 96,000 scf/day unit with production of a few systems
AUTOTHERMAL REFORMERS									
Rolls-Royce/ Johnson-Mathey	7-25 kW H_2 (1700-6200 scf H_2/day)	ambient pressure		Exeprimental Autothermal Reformer Unit			>90%	Fast	60 liters
International Fuel Cells/ONSI	1.5-20 kW			Autothermal Reformer under development				Fast	

TABLE 6. OPERATING CONDITIONS AND COSTS FOR A SMALL SCALE HYDROGEN PLANT WITH STEAM REFORMING OF NATURAL GAS

Operating Temperature	845-870 ^{o}C
Operating pressure	10 atmospheres
Hydrogen production capacity	0.366 million scf/day
Hydrogen purification	Pressure Swing Adsoprtion (PSA)
Outlet pressure from PSA	200 psig
Hydrogen purity	99.999%
Installed capital cost	$2.22 million
Natural gas consumption	0.400 MBTU/1000 scf H_2
Energy conversion efficiency	86% (HHV)
Electricity consumption	0.6 kWh/1000 scf H_2 = 220 kwh/day
Cooling water	200 gallons/1000 scf H_2 =73,200 gallons/day
Boiler water consumption	40 lb./1000 scf H_2 =760 gallons/day
Catalysts	$0.65/1000 scf H_2 =$8683/yr
Misc. O&M	3.5% x capital cost =$77,000/yr
Equipment lifetime	20 years
Land area	80 ft x 30 ft
Height	40 ft
Labor requirements	Automated with occasional monitoring
Emissions (NOx) control	Selective catalytic reduction

Source: D. King, Howe-Baker Engineering, private communications, 1993

TABLE 7. DATA AND PROJECTIONS FOR VEHICLE POPULATION AND ENERGY USE IN THE SOUTHERN CALIFORNIA SOUTH COAST AIR BASIN

YEAR	# PASSENGER CARS	ENERGY USE PASSENGER CARS (EJ/YR)	AVERAGE MILES/YR PASSENGER CARS	TOTAL # VEHICLES	ENERGY USE ALL VEHICLES (EJ/YR)
1990	7,073,945	0.420	10,614	9,402,672	0.744
2000	8,317,394	0.430	11,486	11,102,001	0.799
2010	9,439,696	0.458	11,788	12,636,470	0.871

SOURCE: R. George, South Coast Air Quality Management District, 1994.

TABLE 8. MANDATED IMPLEMENTATION RATES FOR LOW POLLUTING PASSENGER CARS IN THE SOUTH COAST AIR BASIN

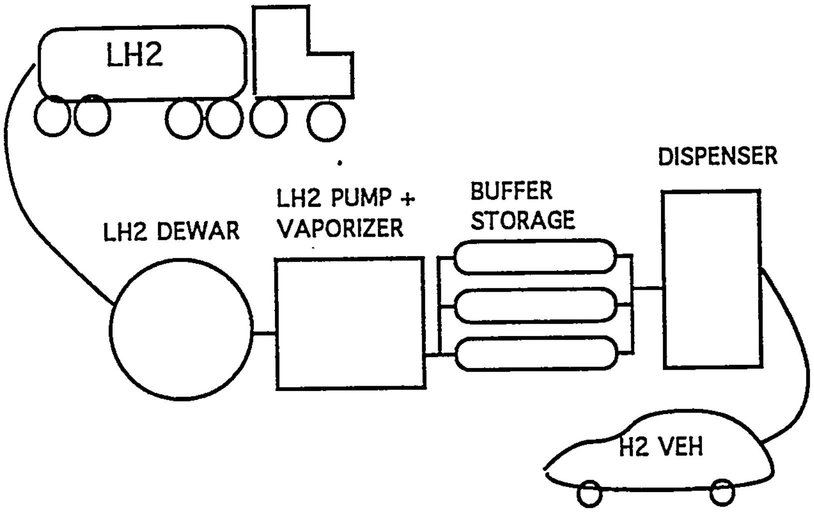
MODEL YEAR	NOx =0.39 g/mi	NOx = 0.25 g/mi	TLEV	LEV	ULEV	ZEV
1994	10%	80%	10%			
1995		85%	15%			
1996		80%	20%			
1997		73%		25%	2%	
1998		48%		48%	2%	2%
1999		23%		73%	2%	2%
2000				96%	2%	2%
2001				90%	5%	5%
2002				85%	10%	5%
2003				75%	15%	10%

SOURCE: A.Lloyd, South Coast Air Quality Management District, 1991.

Figures

Figure 19. Hydrogen demand required to fuel ZEVs in the South Coast Air Basin, if all ZEVs are hydrogen fuel cell cars.

FIG. 1. REFUELING STATION WITH LH2 DELIVERY



DELIVERED COST OF COMPRESSED GAS H2 TRANSPORTATION FUEL VS. STATION CAPACITY : TRUCK DELIVERED LIQUID H2

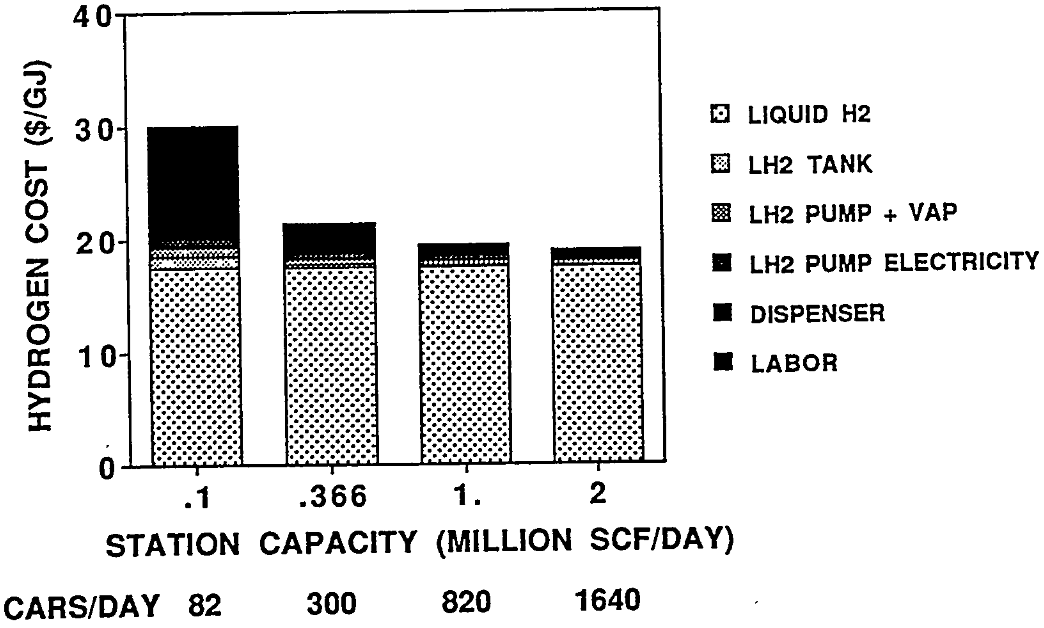
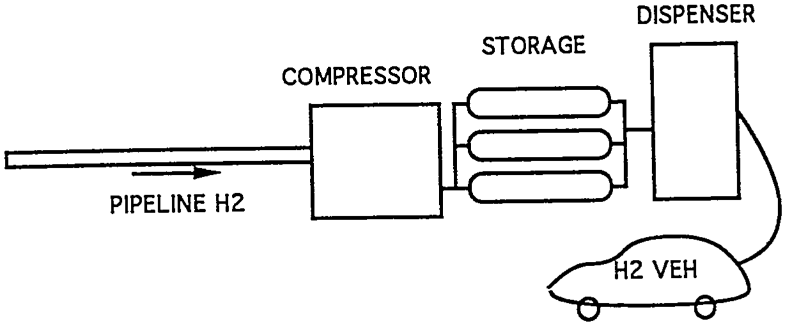


FIG. 2. REFUELING STATION WITH PIPELINE HYDROGEN



DELIVERED COST OF HYDROGEN TRANSPORTATION FUEL VS. STATION SIZE : PIPELINE HYDROGEN

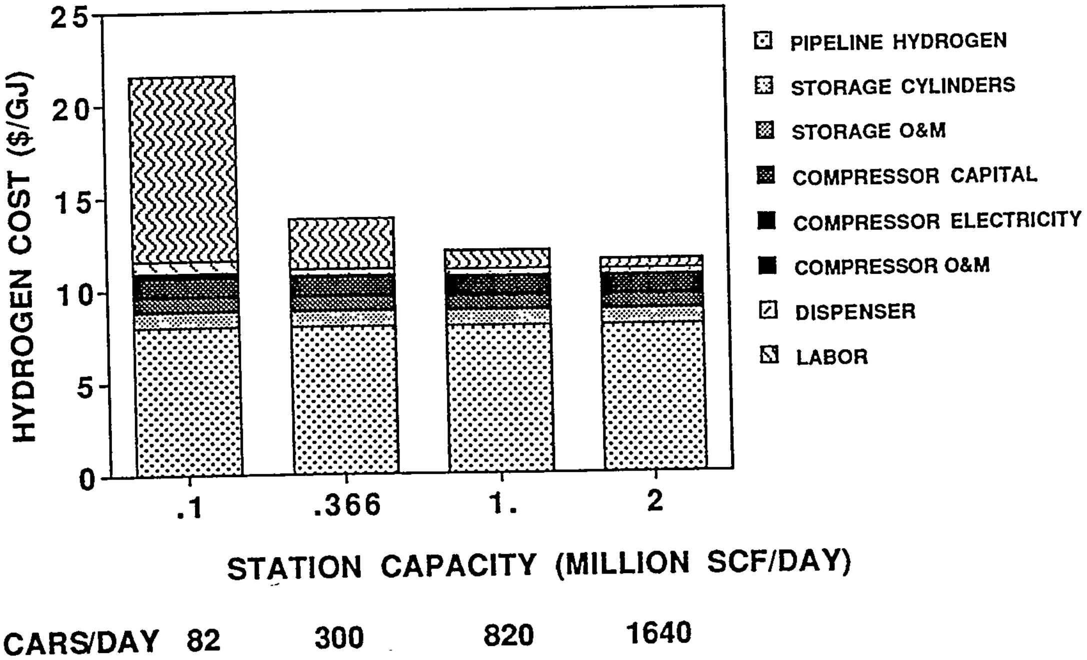
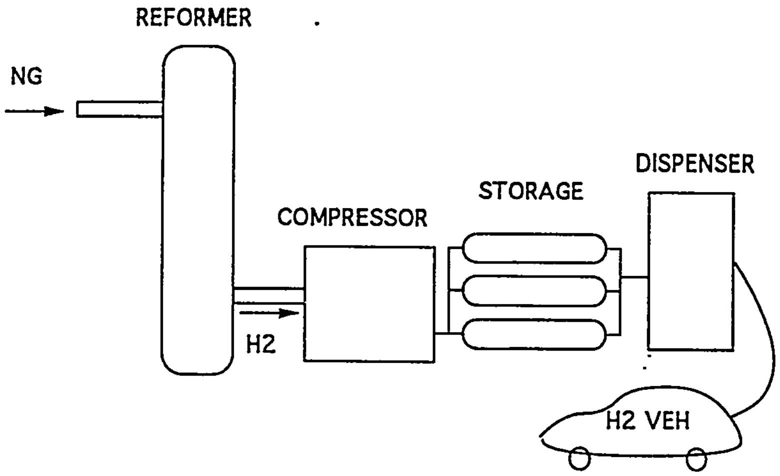


FIGURE 3. REFUELING STATION WITH ONSITE REFORMING



DELIVERED COST OF HYDROGEN TRANSPORTATION FUEL VS. STATION CAPACITY : ONSITE REFORMING OF NG

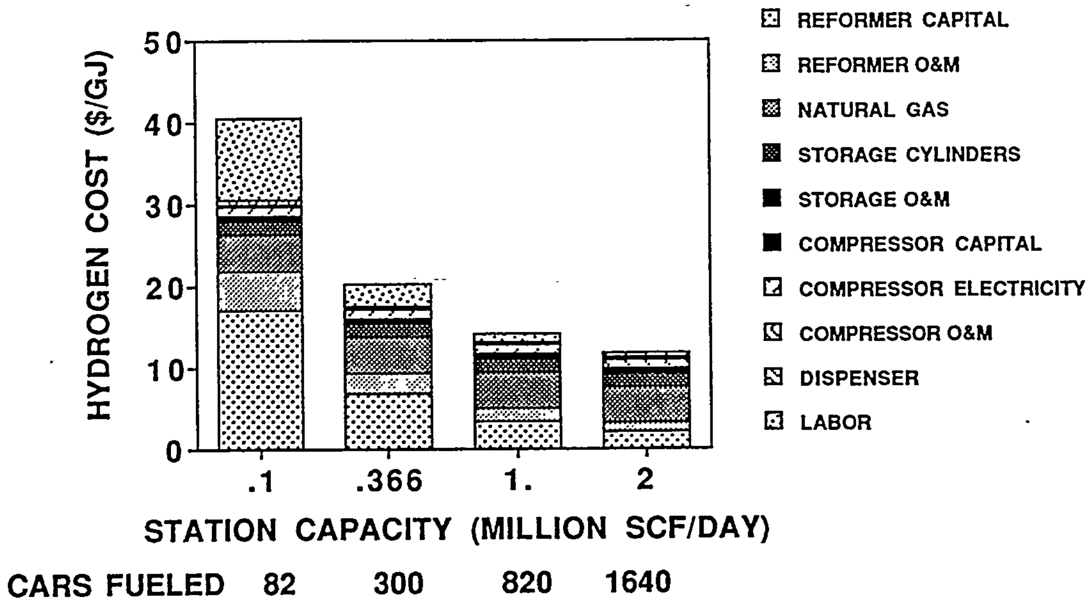
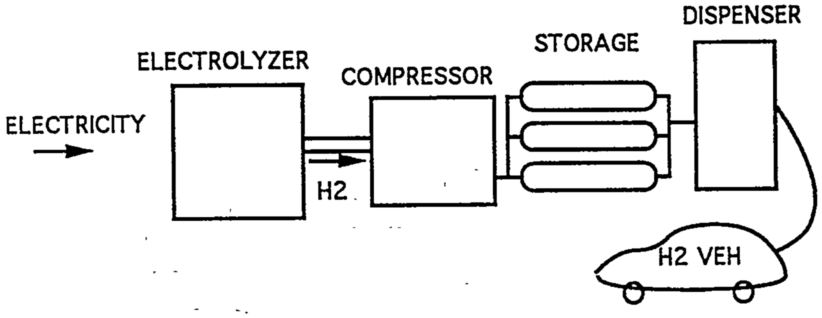
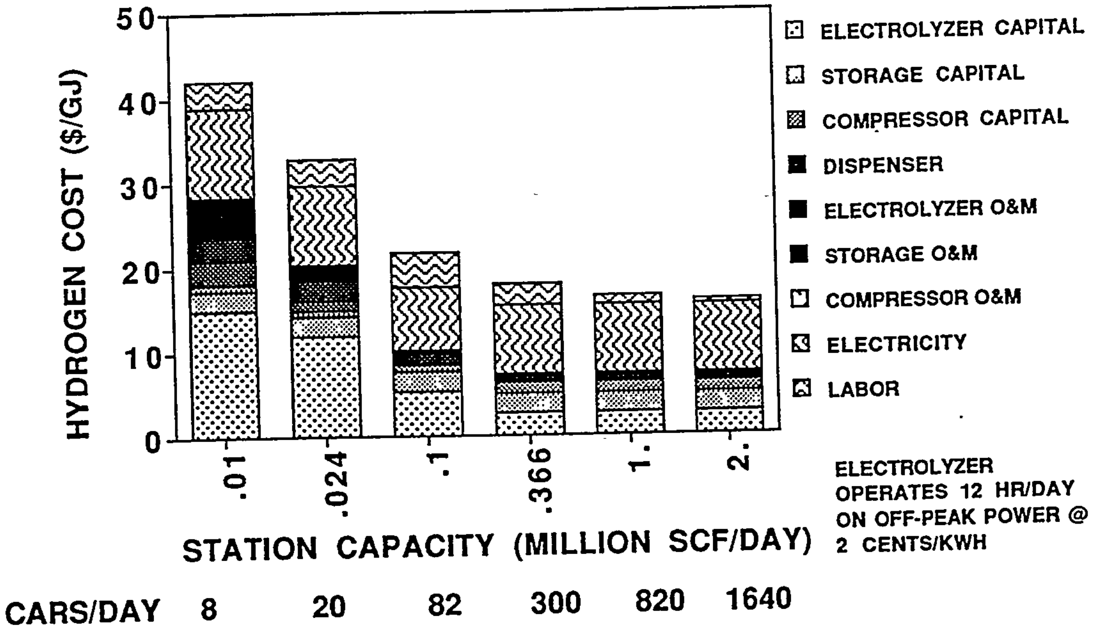


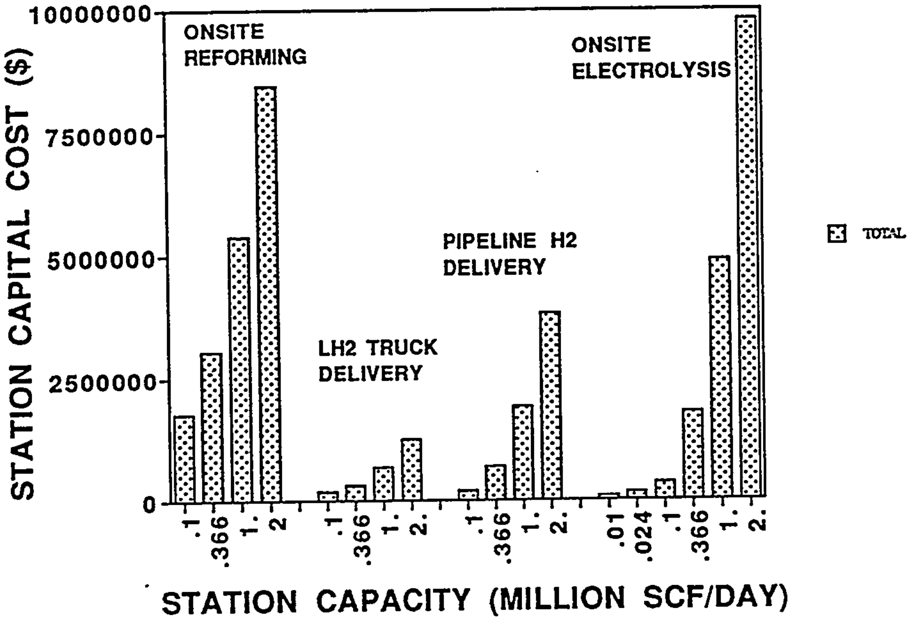
FIG. 4. REFUELING STATION WITH ONSITE ELECTROLYSIS




DELIVERED COST OF HYDROGEN TRANSPORTATION FUEL VS. STATION CAPACITY: ONSITE ELECTROLYSIS

ELECTROLYZER OPERATES 12 HR/DAY ON OFF-PEAK POWER @ 2 CENTS/KWH

FIGURE 5. REFUELING STATION CAPITAL COST



DELIVERED COST OF HYDROGEN TRANSPORTATION FUEL

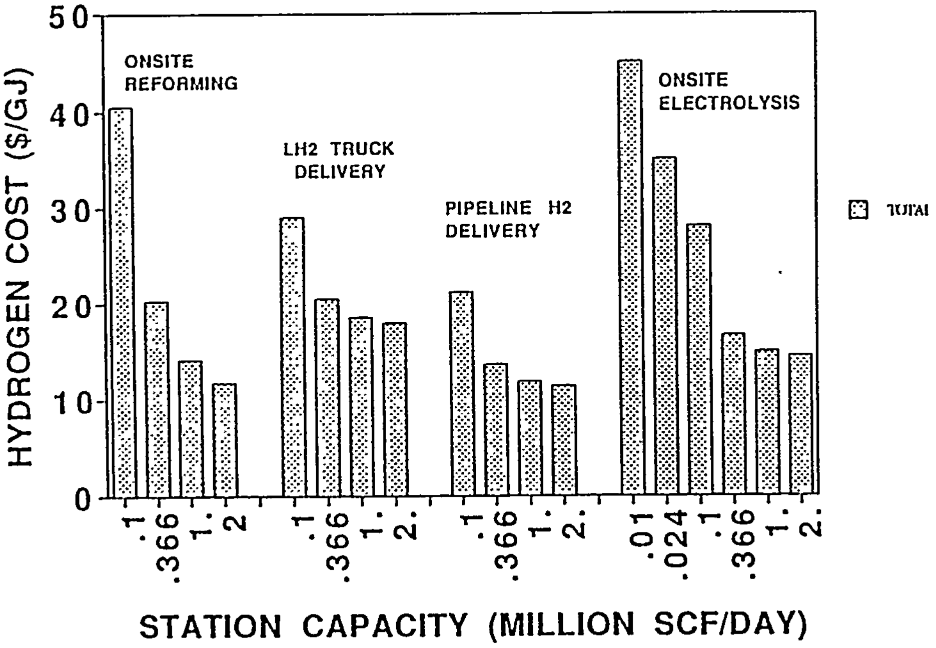


Figure 7. Delivered Cost of Alternative Transportation Fuels ($/Ga Gasoline Equiv.)

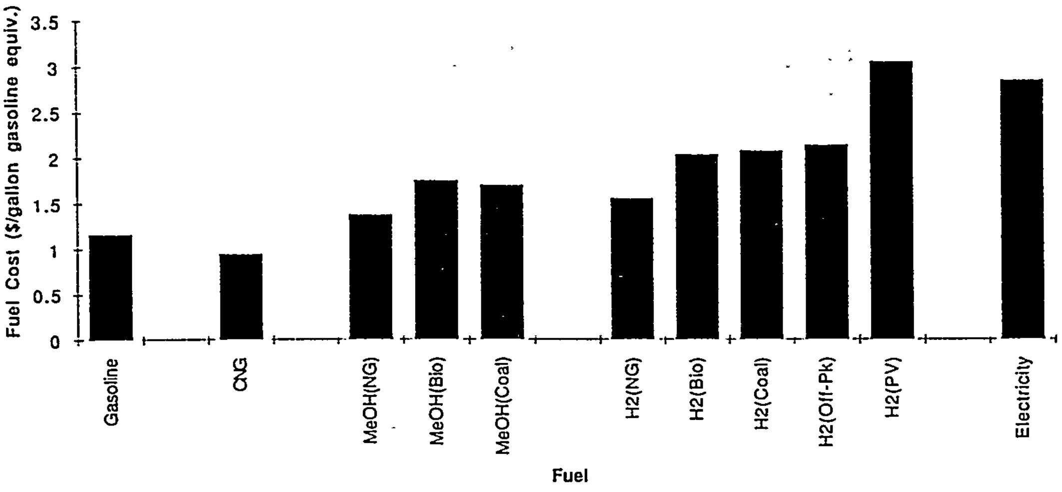


FIGURE 8. FUEL COST (CENTS/KM)

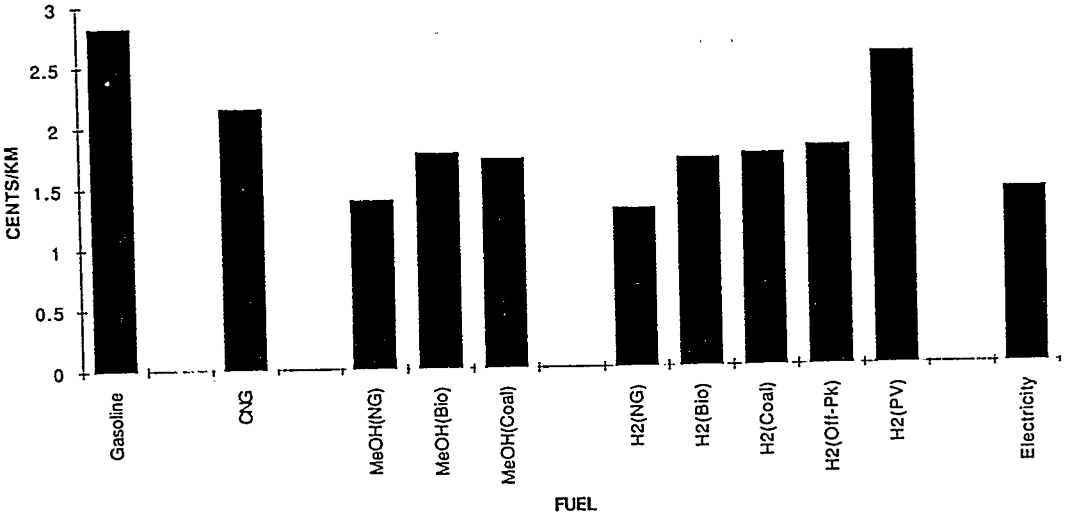


FIGURE 9. LIFECYCLE TRANSPORTATION COST

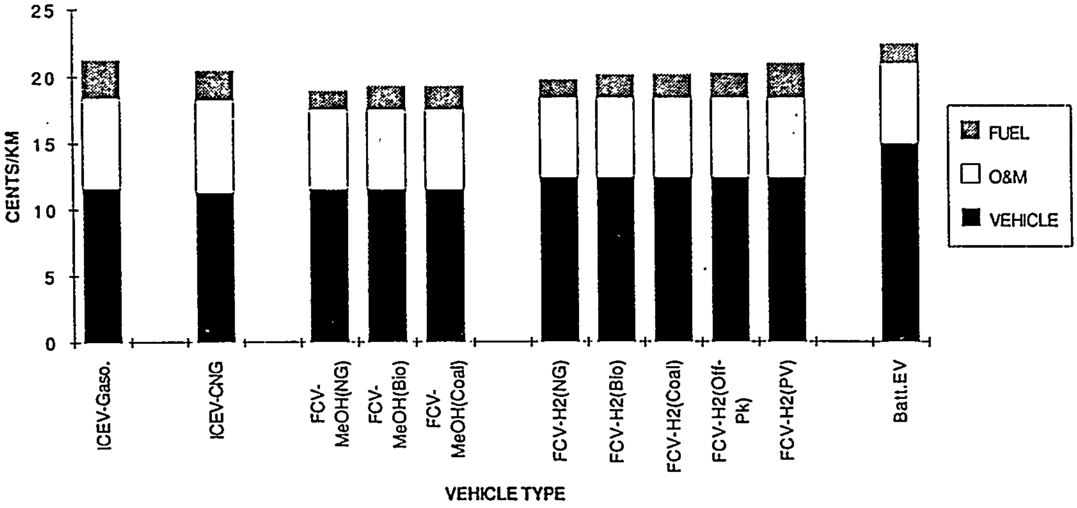


Figure 10. Fuel cycle CO_2 equivalent greenhouse gas emissions relative to emissions from internal combustion engine vehicles using reformulated gasoline.

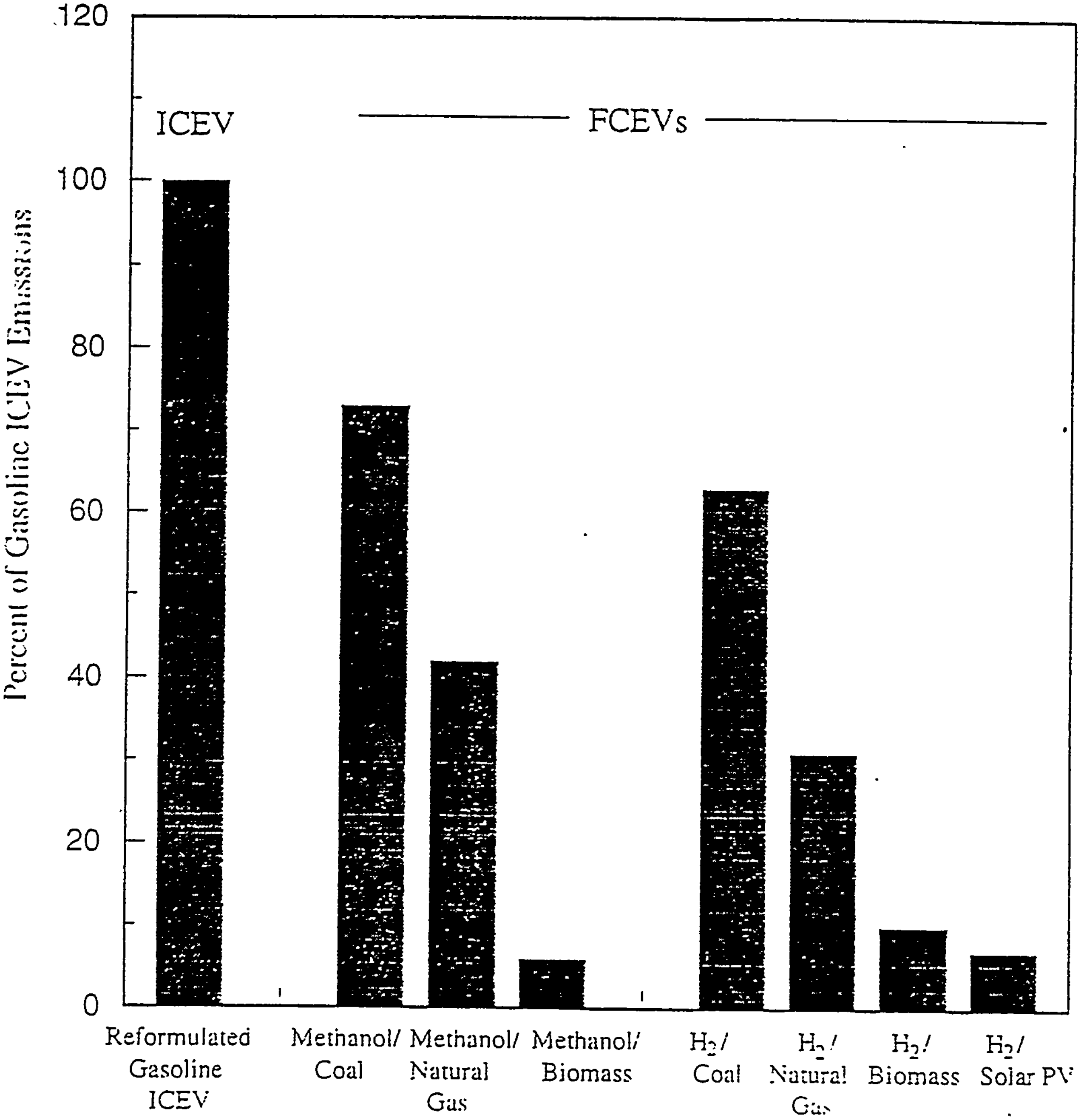
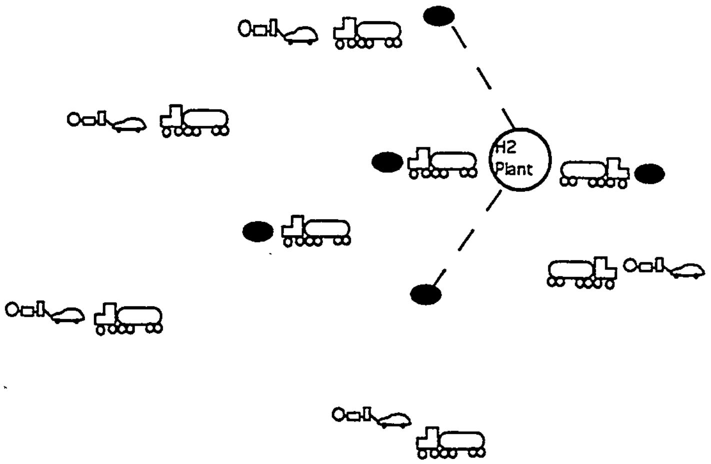


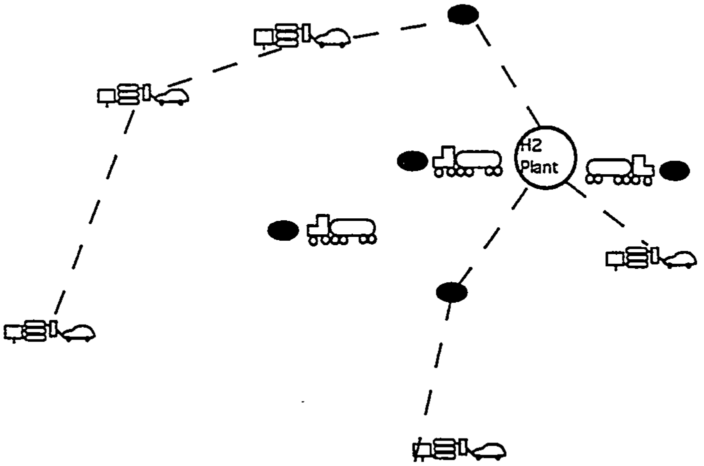
Figure 11. Scenarios for expanding the merchant hydrogen system to provide hydrogen transportation fuel

EXPAND MERCHANT H2 SYSTEM



LH2 Truck delivery
Capital cost for 1 million scf/day
refueling station: $680,000
Delivered Cost H2 Transp. Fuel $19/GJ

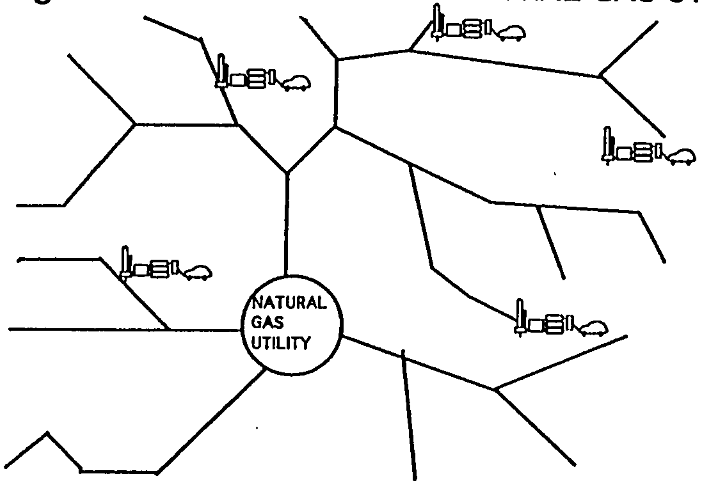
EXPAND MERCHANT H2 SYSTEM



80,000 fuel cell cars requiring
10 million scf/day,
10 refueling stations

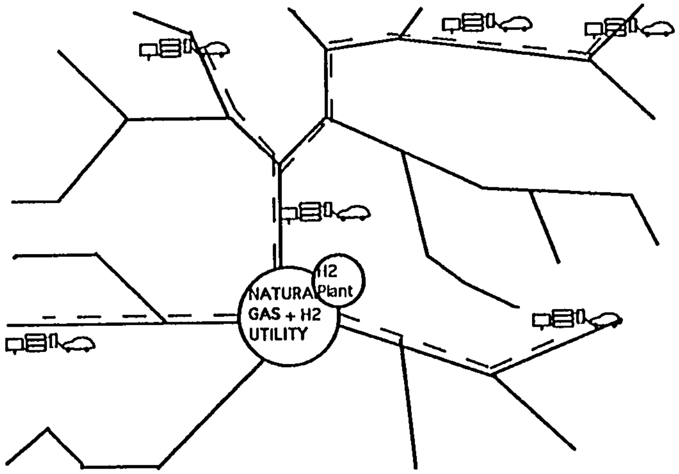
60 km pipeline w/compressed
gas refueling stations:
Capital cost = $43 million
Delivered H2 cost = $13/GJ

Figure 12. PIGGYBACK ON NATURAL GAS SYSTEM



Onsite Reforming
Capital Cost $5.4 million for 1 million scf/day station serving 800 fuel cell cars/day
Delivered H2 Cost: $14/GJ

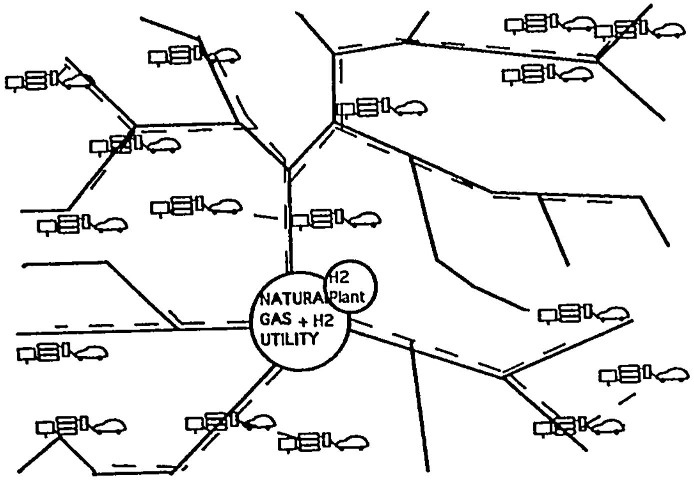
PIGGYBACK ON NATURAL GAS SYSTEM



80,000 fuel cell cars requiring
10 million scf/day,
10 refueling stations

60 km, 10 million scf/day utility H2 pipeline along NG rights-of-way:
Capital cost $43 million
Delivered hydrogen cost $13/GJ

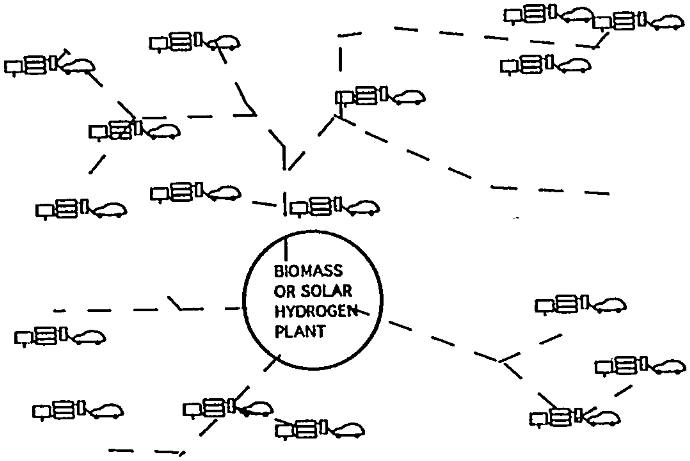
PIGGYBACK ON NATURAL GAS SYSTEM



800,000 fuel cell cars requiring
100 million scf/day,
100 refueling stations

600 km utility H2 pipeline along NG rights-of-way:
Capital cost $455 million
Delivered hydrogen cost $12/GJ

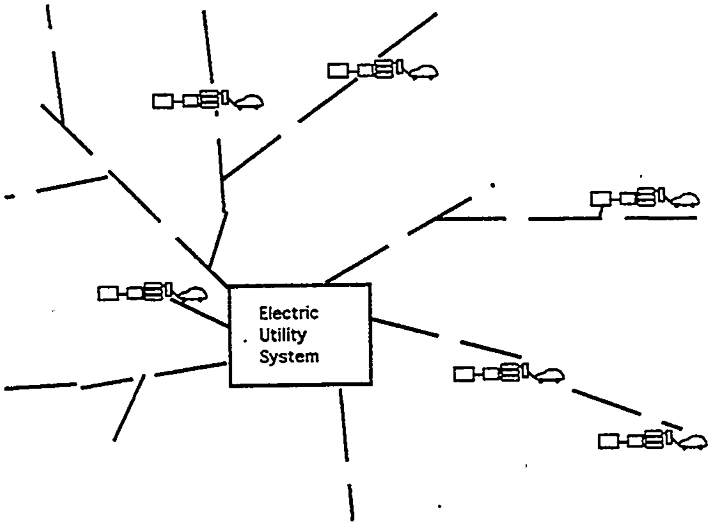
TRANSITION TO RENEWABLE H2



Utility Biomass or Solar Hydrogen Plant
Delivered H2 cost: $15-25/GJ

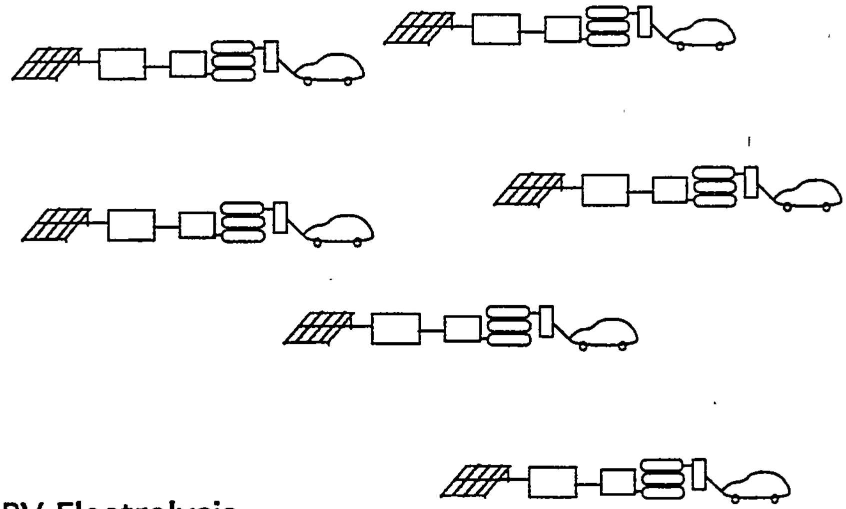
Figure 13. Scenarios for electrolytic hydrogen production

PIGGYBACK ON THE ELECTRICITY DISTRIBUTION SYSTEM



Onsite electrolysis, off-peak power @ 2 cents/kWh:
Capital cost for 1 million scf/day station $6.2 million
Delivered H2 cost: $17/GJ

STAND ALONE PV HYDROGEN



PV Electrolysis,
Capital Cost for 1 million scf/day refueling station: $18-28 million
Delivered H2 Cost $18-25/GJ

Figure 14. A utility owned PEM fuel cell system for cogeneration of electricity and domestic hot water

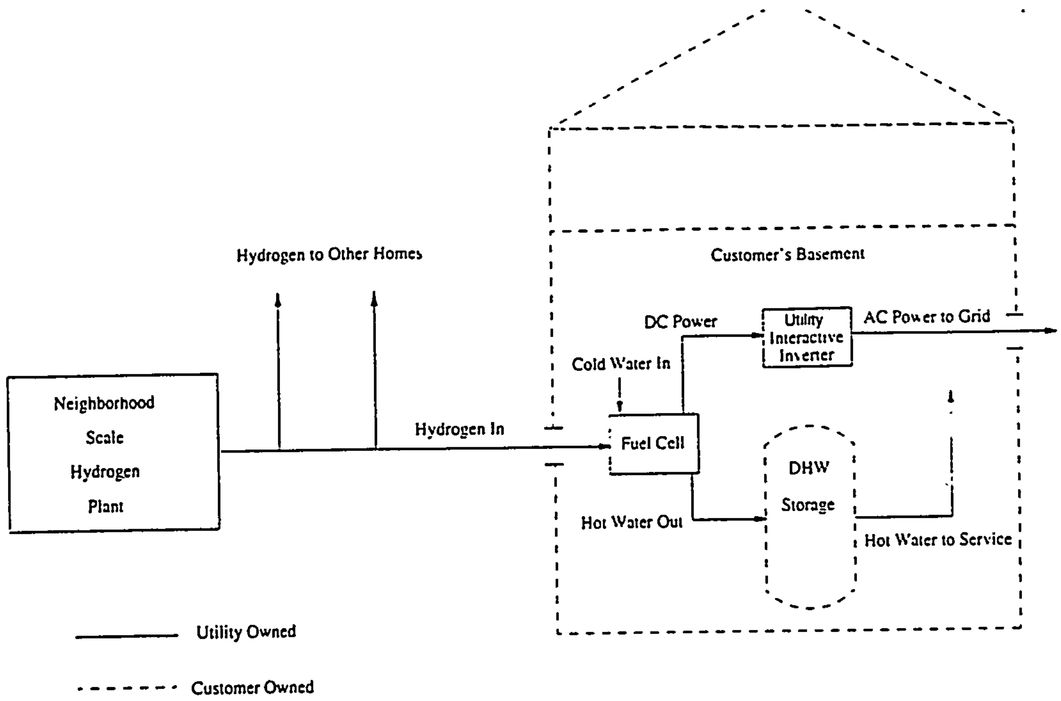


Figure 15. Assumed fuel cell performance curve.

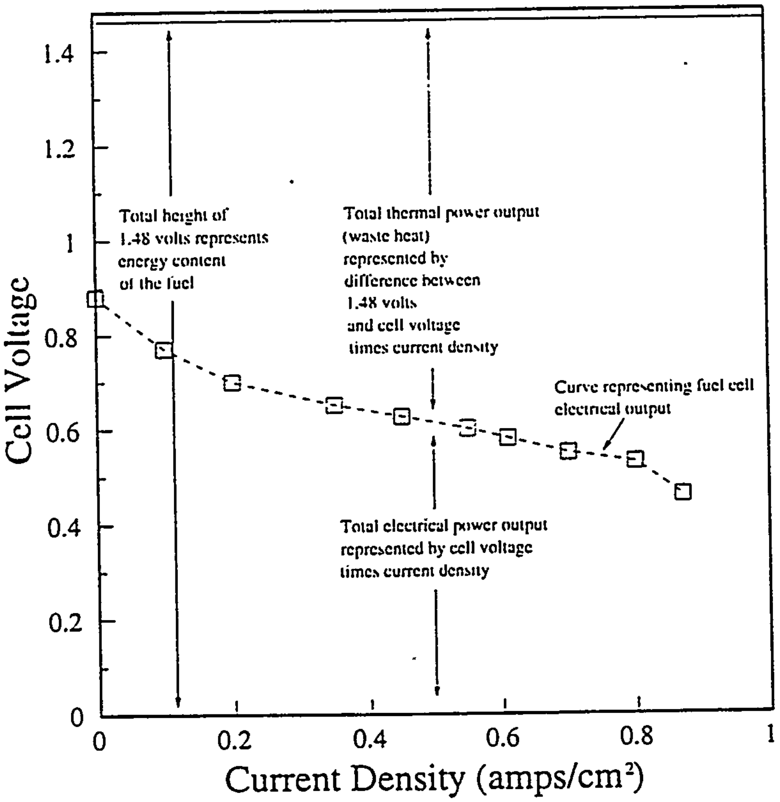


FIG. 16. INSTALLED CAPITAL COST OF SMALL SCALE STEAM METHANE REFORMING H2 PLANT W/PSA

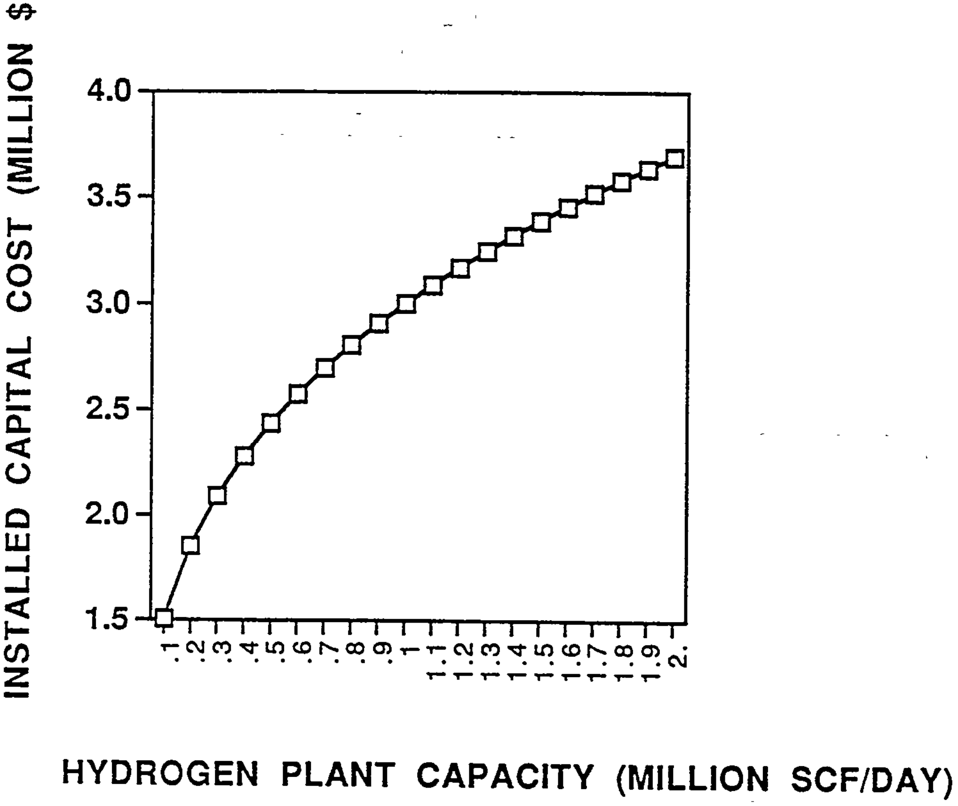


Figure 17. A conventional large scale steam methane reformer with long tubes A compact small scale steam reformer design

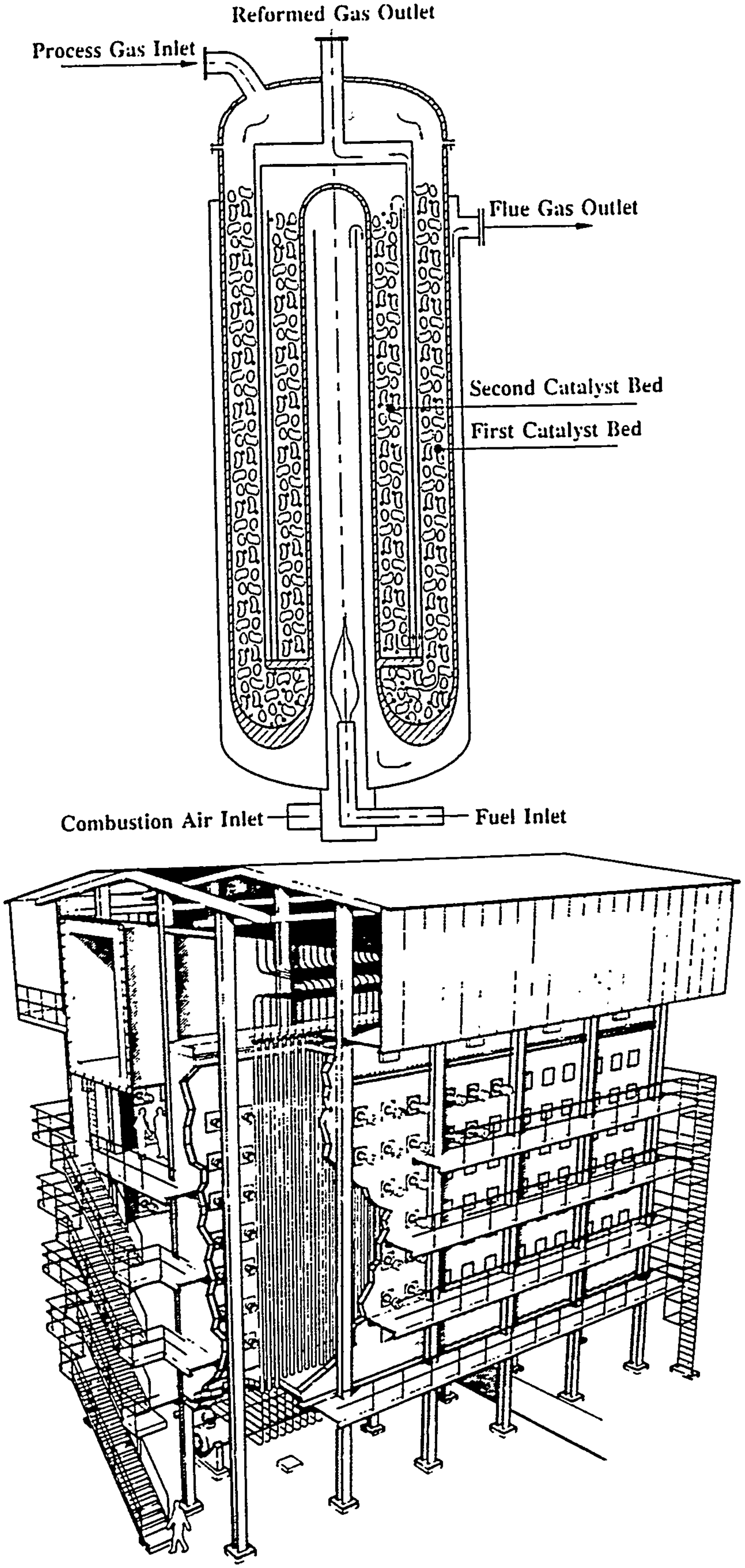


FIG. 18. PROJECTIONS FOR ZERO EMISSION VEHICLES IN THE SOUTH COAST AIR BASIN

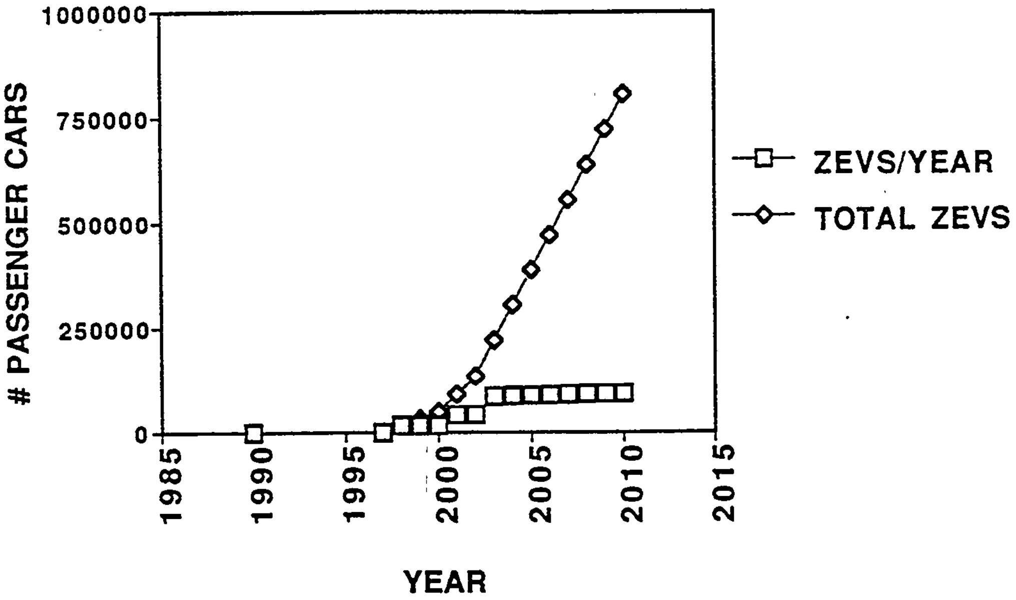
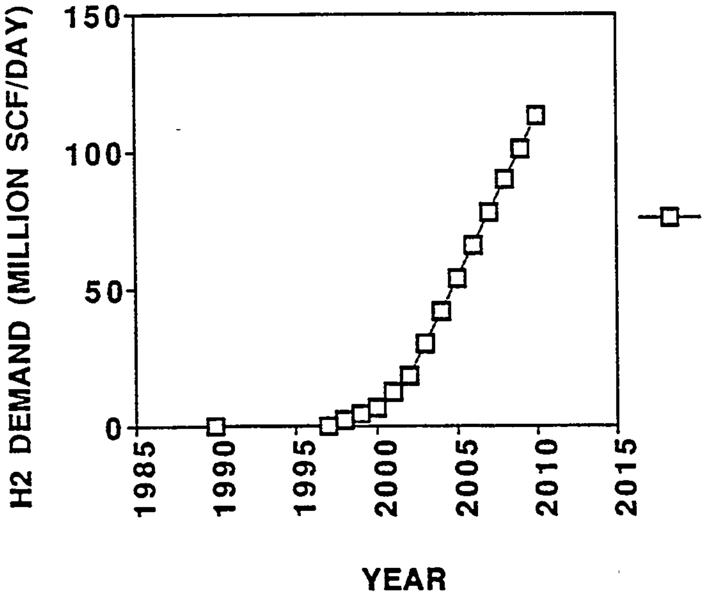


FIG. 19. HYDROGEN DEMAND TO FUEL ALL ZEV CARS IN SOUTH COAST AIR BASIN



ANALYSIS OF NEAR-TERM PRODUCTION AND MARKET OPPORTUNITIES FOR HYDROGEN AND RELATED ACTIVITIES

Robert Mauro and Susan Leach
National Hydrogen Association
Washington, DC 20036
202-223-5547 Fax: 202-223-5537

Introduction

This paper summarizes current and planned activities in the areas of hydrogen production and use, near-term venture opportunities, and codes and standards. The rationale for these efforts is to assess industry interest and engage in activities that move hydrogen technologies down the path to commercialization. Some of the work presented in this document is a condensed, preliminary version of reports being prepared under the DOE/NREL contract. In addition, the NHA work funded by Westinghouse Savannah River Corporation (WSRC) to explore the opportunities and industry interest in a Hydrogen Research Center is briefly described. Finally, the planned support of and industry input to the Hydrogen Technical Advisory Panel (HTAP) on hydrogen demonstration projects is discussed.

Near-term Hydrogen Production and Utilization

An assessment of the current sources and uses of hydrogen and the capability of the existing hydrogen infrastructure was made. Producers of merchant hydrogen were surveyed, potential sources of inexpensive hydrogen from industrial process by-products were identified and evaluated, and the economic feasibility of transporting by-product and excess hydrogen from the southeastern region to Southern California via pipeline was investigated. In this work, the objective was to answer three basic questions:

1. How much hydrogen is being produced in the U.S. for the merchant hydrogen market?
2. Is there excess hydrogen production in the Gulf States due to their industrial mix?
3. Is it economically feasible to build a hydrogen pipeline from the southeastern region to Southern California?

Survey of Hydrogen Sources & Uses

Hydrogen is one of a number of industrial gases produced by major gas producers. Nearly 2.5 trillion cubic feet of hydrogen was produced in the U.S. in 1993. Of that, 96% is for captive uses; only 4% is for merchant use. The largest captive uses are ammonia production, refineries, and methanol production, constituting over 90% of total hydrogen use in the United States. Of the 4% of the market represented by merchant hydrogen, over 80% of the sales are onsite or transported by pipeline. The remaining merchant sales are transported in bulk or cylinder by tractor-trailer, barge, or rail. Nearly all hydrogen is consumed in gaseous form. The gaseous hydrogen business is focused on producing an industrial gas to be used as a feedstock or to provide a controlled atmosphere for an industrial unit process. The liquid hydrogen production business is dominated by NASA, and is focused on producing a fuel. NASA consumes approximately 14 million pounds of liquid hydrogen annually, depending on their test programs and the number of launches per year.

To obtain information from producers on the sources and uses of merchant hydrogen, a literature search was conducted, and a questionnaire was developed and distributed. The questionnaire represented NHA's first attempt to obtain current information on hydrogen production and use from members. It contained five sections: gaseous hydrogen production, liquid hydrogen production, steam reforming plant costs (not discussed here), hydrogen pipelines when applicable, and gaseous and liquid hydrogen production in the southeastern region and Southern California. The data requested included the number and location by region of hydrogen production facilities, production capacity by region, feedstocks used, primary sources of by-product hydrogen and quantity purchased for resale, quantity shipped by region, customer type by region, and nominal delivered price.

The questionnaire was sent to Air Products & Chemical, Inc., BOC Gases, Air Liquide America Corp., and Praxair, Inc. in June 1994. Responses were received in October 1994. No proprietary information was provided, and results are aggregated so that individual company responses are not given.

Gaseous Hydrogen Survey

There are forty plants owned by the major producers of gaseous hydrogen in the U.S. These plants have a production capacity of about 114,250 million cubic feet of hydrogen annually. Gaseous hydrogen production capability is expected to increase in the West South Central region[1] by over

---

[1] See Appendix for a list of states per region.

64,000 million cubic feet of hydrogen, and 72,000 million cubic feet in the Pacific region. The production numbers, which include by-product hydrogen production, are presented by region in Table 1. The feedstocks for the hydrogen produced in the plants included natural gas; chemical off-gases from ethylene, styrene, petroleum, methanol, olefins, oxo-alcohol production; chlor-alkali production, and vaporized liquid hydrogen. Three of the four major hydrogen producers in North America steam reformed natural gas to produce hydrogen. Large steam reforming facilities using inexpensive natural gas tend to set the minimum cost for hydrogen in the United States.

Table 1. Gaseous Hydrogen Plant Capacity by Region

Region	Number of Plants	Production Capacity (MMSCF/yr)
New England	1	19
Middle Atlantic	5	3,117
East North Central	8	3,725
West North Central	1	400
East South Central	1	12
West South Central	16	101,750
South Atlantic	3	1,730
Mountain	0	0
Pacific	5	1,500

By-product purchases of hydrogen are typically for resale on a regional basis. The quantities purchased in 1993 are presented in Table 2. The sources of by-product hydrogen include the chlor-alkali industry, ethylene production, and other sources such as petroleum, petrochemicals, and oxo-alcohol production.

Table 2: Hydrogen By-Product Sales by Region for 1993

Region	By-Product Hydrogen Sales (MMSCF/yr)
New England	0
Middle Atlantic	6
East North Central	18
West North Central	0
East South Central	15
West South Central	29,003
South Atlantic	257
Mountain	0
Pacific	0

Most sales of merchant hydrogen are made to refineries and the chemical industry. Other major users of merchant hydrogen are in the edible fats and oils, agriculture, electronics, aerospace, and steel industries, and industries requiring hydrogen as a controlled atmosphere in manufacturing. Increases or decreases in hydrogen use by industry are shown in Table 3.

Table 3: Industry Trends in Hydrogen Sales

Industry	Increase or Decrease in Hydrogen Use
Refining	Increase
Food	Same or Decrease
Agriculture	Increase
Electronics	Increase
Aerospace	Decrease
Chemicals	Increase --one response indicated a decrease
Steel	Same
Other	Increase

Liquid Hydrogen Survey

The ten production plants producing liquid hydrogen serving the U.S. market have a combined production capacity of over 146,000 tons of liquid hydrogen per year. An additional 5,250 tons per year of liquid hydrogen production is scheduled to come on line in Canada. The regional distribution and current production levels of liquid hydrogen are shown in Table 4.

Table 4: Liquid Hydrogen Plant Capacity by Region

Region	# of Plants	Production Capacity (000 tons per year)
New England	0	0
Middle Atlantic	1	40
East North Central	0	0
West North Central	0	0
East South Central	1	26
West South Central	2	25
South Atlantic	1	11
Mountain	0	0
Pacific	2	24
Canada	3	20

The chemical feedstocks used for liquid hydrogen production include natural gas and off gases produced by ethylene, sodium chlorate, and chlor-alkali production. One Canadian plant produces hydrogen electrolytically. The total quantity of liquid hydrogen shipped between regions is about 39,000 tons per year. At least 27% of the liquid hydrogen produced was shipped from on region to another, suggesting that the market for liquid hydrogen is national in scope. In fact, over half of the liquid hydrogen produced in Canada was shipped to the United States. Much of the Canadian liquid hydrogen is produced from purchased gaseous by-product hydrogen as an off-gas from ethylene and other processes. Additional information on by-product sources of purchased hydrogen were not provided except that by-product hydrogen from chlor-alkali plants is used in some liquid hydrogen production in the United States. The range of prices for delivery of liquid hydrogen over the fence ranged from \$5/MSCF to \$15/MSCF. This is equivalent to from \$.96/lb to \$2.88/lb for liquid hydrogen excluding transport.

Conclusion

The conclusions reached as a result of the survey are:

- Hydrogen use is growing.
- The greatest hydrogen production is in the West South Central region.
- Major hydrogen production facilities are being built in Texas and California. This may be due to a perceived increased demand for hydrogen in energy sector for reformulated gasoline. It appears that hydrogen facilities are being built to respond to market needs.
- Liquid hydrogen is shipped throughout the United States and Canada. The information provided on gaseous hydrogen is insufficient to determine whether or not gaseous hydrogen is distributed nationally or in regional markets.

Gaseous hydrogen is increasingly being used for energy end uses as a chemical additive to fuels, though it continues to be primarily a chemical feedstock. The extent to which it is produced for use as a fuel except in aerospace awaits the introduction of widespread energy systems that can effectively utilize it.

Near-term Hydrogen Supply in Southern California

At NREL's request, the NHA also investigated the economic feasibility of piping excess or by-product hydrogen from the south central states to Southern California. The trade-off of such an approach was the low cost of by-product hydrogen versus the expense of transporting hydrogen from the southeast to California. As mentioned, the questionnaire included questions on hydrogen production and use in the southeast, specifically Alabama, Arkansas, Louisiana, Mississippi, Oklahoma, Texas, and Southern California. Pipeline costs were also included in the survey. Finally, the future hydrogen energy requirements in Southern California for auto, air, and power generation were estimated.

Hydrogen Pipeline Information

Although there are a number of hydrogen pipelines in the U.S., it is difficult to obtain a good estimate of the cost of a hydrogen pipeline. The survey did not yield complete responses, so the information on pipeline operations and costs was obtained in discussions with individuals in companies operating hydrogen pipelines. In these discussions, several rules of thumb were mentioned for performing back of the envelope calculations on pipeline costs. They are:

- For a 6" to 10" diameter pipeline, the cost of obtaining the right-of-way, the cost of installing the pipeline, valves, control, and sensing equipment is approximately $250,000 per mile;

- The pipeline is likely to be welded carbon steel with pressures of no more than 800 psi;
- Natural gas and other pipelines have been leased, modified and used for hydrogen pipelines in Texas;
- For long distance transport, compressor stations will have to be used to recompress hydrogen;
- Today either electrically driven or engine driven reciprocal compressors would be used for hydrogen compression;
- A compressor station using electrically driven compressors is estimated to cost about $1,000 per brake horsepower;
- A compressor station that uses engine driven reciprocal compressors, which could operate on natural gas but might be modified to operate on hydrogen gas, is estimated to cost about $1,500 per brake horsepower;
- The annual costs (O&M, taxes, insurance, capital recovery, profit) associated with a pipeline including an adequate return for a non-utility company is approximately 25%;
- Typical flows for a 6" to 10" hydrogen pipeline is about 50-100 cubic feet per second depending upon operating pressure;
- The cost of pipeline installation does not increase linearly with through put or pipe diameter.

Hydrogen Availability in the Southeastern Region

The survey shows that 95% of the gaseous hydrogen produced in the region is consumed in the region by chemical plants and refineries. There is 60 MMSFC/day of hydrogen that might be available to be shipped to Southern California; enough gaseous hydrogen to supply one 50 MMSCF/day pipeline. There is also a small amount of liquid hydrogen (~3 tons per day) available that might be made available. There could be significantly more if NASA recaptured boil-off at the Kennedy, Stennis, and Marshall facilities, where approximately 5 million to 7 million pounds of hydrogen is lost annually. As much as half could be recaptured, representing 350,000/MMBtu, or just under 1 million annual vehicle fill-ups.

Piping Hydrogen from the South Central Region to Southern California: A Case Study

In this case study, it is assumed that inexpensive hydrogen is available in Houston, Texas as a by-product of a petrochemical process. How much would the price of the hydrogen be affected if a 1,500 mile pipeline of 8", operating at pressures of 500 to 800 psig, with pipeline flows of 50 feet/second, were built from Houston to a site in Southern California?

Using the guidelines given in the previous section, the pipeline cost would be $375 million dollars (1,500 miles x $250,000 per mile). Compressor stations would add several million dollars more for each compressor station required. If the exit pressure leaving a compressor station is 800 psi, the pressure loss averages 1 psi per mile for the hydrogen, and the minimum pipeline pressure allowed is 500 psi, then a compressor station would be required every 300 miles. The carrying cost for the pipeline including debt service, O&M, insurance, taxes, and profit for a company in the hydrogen production business was given as 25%. The annual cost of such a pipeline, then, would be just under $100 million dollars.

These assumptions are optimistic. The pressure loss rate for hydrogen is likely to be 2 to 5 psi per mile. The 1.6 to 1 hydrogen compression required to compress hydrogen from 500 psi to 800 psi would probably be done in two stages. The cost information provided in the previous section is for single stage compression. Assuming that the speed of hydrogen flow in the pipeline is 50 feet per second, then the quantity of hydrogen moved is about 17.5 SCF per second, or just over 1.5 million SCF per day. This represents almost 415 MMBtu per day of hydrogen energy (lhv) delivered by pipeline, or over 151,000 MMBtu per year of hydrogen energy (lhv). The incremental cost per MMBtu is over $500 for the pipeline, excluding compression.

The costs do not improve substantially for pipelines with greater diameters. If sufficient hydrogen were available, a 24 inch diameter pipeline might be expected to carry 9 times the quantity of hydrogen that the 8 inch pipeline carries for perhaps 3 times the price. If all the other conditions remain constant, then the cost of installing the pipeline would be almost four hundred million dollars with annual carrying cost and profit estimated at almost $100 million. The quantity of energy delivered would be over 1.35 trillion Btus, and the incremental cost of the pipeline would be over $73/MMBtu. Again, the cost of compression has not been considered. Even a 48 inch hydrogen pipeline would add prohibitively expensive hydrogen transport costs for new hydrogen pipelines.

Energy Requirements in Southern California

Southern California has a number of environmental problems that could be mitigated if vehicles, planes, and power plants were operated on hydrogen. To estimate the amount of hydrogen that would be required, the number of vehicles, take-offs and landings, and megawatts of generation that could use hydrogen was estimated, and then the hydrogen requirements for each was calculated. A change from petroleum and natural gas would not occur overnight, but rather over several decades. Conditions at the time when such a change in energy sources occurs are likely to be different than they are today. Nonetheless, if today's energy requirements are estimated, it provides a useful planning target for the future.

There are approximately 10 million vehicles of all types in Southern California. For the purposes of this analysis, it is assumed that all the vehicles are passenger vehicles operating 15,000 miles per year, and all the vehicles meet new car mileage standards of 30 miles per gallon. The assumes that each vehicle uses 500 gallons of gasoline per year. Assuming that each gallon of gasoline is about 128,000 Btu/gallon, each vehicle consumes 64 MMBtu of gasoline each year. A rough estimate is that 640 million MMBtu of gasoline is used to operate vehicles in Southern California. This is .64 quads of annual energy use in Southern California. It takes 2.32 trillion SCF of hydrogen to supply that much energy, or almost 500 24-inch pipelines of the type discussed in the previous section to meet that requirement. If fuel cells are commercialized for vehicles, and the Partnership for a New Generation Vehicle goals are achieved, energy requirements would be reduced by over two-thirds. The vehicle fuel requirement could be supplied by just over .21 quads of energy annually with a huge reduction in infrastructure requirements.

In the mid 1980's, the Los Angeles International Airport averaged over 1,250 daily takeoffs and landings. These operations, along with similar activities at the four other major airports in the LA Basin represented a significant source of NO_x and particulate emissions. Aircraft activity has increased in the past decade, adding to emissions from buses, autos, service vehicles, and courtesy vans. If 20% of the flights leaving LAX involved refueling operations for an average size passenger aircraft (130 passengers), then the hydrogen per refueling would be about 4,400 lb. This would require 125 aircraft to be refueled each day, using 550,000 lbs. per day of liquid hydrogen. Assuming no losses, this refueling requires over 25,000/MMBtus of hydrogen per day. The pipeline described above could supply less than 450 MMBtus per day of hydrogen. A 275 ton per day liquefaction plant would be required to supply 550,000 lbs. per of liquid hydrogen to aircraft at LAX, assuming no losses. Experience at NASA with liquid hydrogen indicates that approximate 50% of the liquid hydrogen is lost due to boil-off. If liquefaction is done on site and a just-in-time production system is developed, this loss rate may be significantly reduced.

The opportunities for hydrogen powered plants in Southern California is significant. California has requirements for over 30,000 Mw of generation, and almost 67% of that power requirement is in Southern California. Hydrogen fueled fuel cells could supply at least 10% of that requirement. A 50% efficient fuel cell requires just 6,800 Btu of hydrogen fuel to supply one kilowatt-hour of electricity. If 5,000 hours of full load operation is assumed for each fuel cell, then each kilowatt of fuel cell capacity requires 340 MMBtu of hydrogen annually. This means that 1,000 Mw of generation operated in this manner requires 340 million MMBtu. If 10% of Southern California's power generation is hydrogen fueled fuel cells, then 680 million MMBtu of hydrogen would be required for those 2,000 Mw of generation (.68 quads). The hydrogen industry would be required to supply 1.23 trillion SCF of hydrogen annually to meet this requirement.

Conclusion

There are several points that are clear from this quick look at hydrogen pipelines and ultimate hydrogen requirements in Southern California. New long low pressure hydrogen pipelines using conventional pipeline materials cannot be economic in moving hydrogen between regions. Transport costs would have to decline by two orders of magnitude for hydrogen pipelines to be attractive. This confirms why today in the U.S. production, transport, and use of hydrogen gas is regional. In the future, hydrogen is likely to be produced locally and regionally. Given the regional nature of the hydrogen business, it is likely that the sources of hydrogen would be a combination of natural gas, biomass, by-product hydrogen, and electrolysis production.

Hydrogen producers are planning a major expansion of gaseous hydrogen production capacity of about 72 billion SCF per year in the next two years in California, enough fuel for over 150,000 cars/day. The hydrogen industry would require tremendous growth to supply the needs of Southern California; current production levels for merchant hydrogen would have to double.

Near-Term Venture Opportunities

A questionnaire on demonstrations was sent to seventeen organizations to assess what hydrogen-related demonstrations are on-going and planned in the U.S., and what role DOE could have, if any, in them. Each organization was also contacted. Based on those contacts, information in the literature, and survey responses, demonstration briefs on the following ten demonstration projects will be written in the task report.

- Phosphoric Acid Fuel Cell for SCAQMD
- The Xerox-CAN Plan Solar Hydrogen Project
- Fuel Cell Hydrogen Bus Demonstrations in the L.A. Basin
- Renewably Fueled Total Energy System for St. George Island, Alaska
- Green Car Demonstration Project
- Systems Definition Study on Fuel Cell Locomotives
- Photovoltaic-Hydrogen-Fuel Cell Energy System
- University of California, Riverside Solar-Hydrogen Research Facility
- Phosphoric Acid Fuel Cell Bus
- Hydrothane Vehicle Demonstrations

Some of the demonstrations are supported by federal funding from other parts of DOE. Many would be enhanced with additional DOE funding. The impact of additional funding would vary from demonstration to demonstration, and could enable such things as increased instrumentation and analysis of results, a technology program to address technical problems that might arise in the demonstration, and funding of follow-on phases of a demonstration.

Codes & Standards Workshop

In late January, the first of a series of planned workshops on codes and standards activities was conducted in Washington, DC. The *Codes and Standards for Safe Use of Hydrogen Energy* workshop attracted over forty participants, several from outside the hydrogen community, including participants from CGA, the natural gas vehicle industry, and the insurance industry. The Workshop presented current safe hydrogen handling practices, codes, standards, and regulations, and the need for continuing development as new applications for hydrogen emerge. The presentations covered three broad areas:

- Current and developing codes, standards and handling practices for hydrogen
- Field experience with safety, insurance, and codes and standards
- Codes, standards and safety requirements for existing commercial hydrogen products and infrastructure

Speakers described an array of different codes, standards & practices that must be addressed in utilizing hydrogen. There are no specific codes or standards for many commercial hydrogen products currently, and practices that have been developed through experience over time are followed. The process of getting new codes and standards accepted is slow. It can take the International Standards Organization (ISO) can take up to five years to get a standard adopted. One ISO Work Group is completing a standard on land vehicle fueling systems interface and fuel tanks for liquid hydrogen, and will meet in Quebec City in June 1995.

Current Codes and Standards

Industry design and operating practices were discussed. There are relatively few codes and standards that apply to hydrogen production, but customer facilities are well covered. The hydrogen industry mitigates risk by assuming that leaks will occur, and all leaks will find an ignition source. They do everything possible to prevent leaks from occurring.

NASA follows ventilation and personnel training and certification procedures that are similar to those of industry. They incorporate safety in their designs, and view every incident involving hydrogen as a design failure. The government is in the process of revising the explosion standards for hydrogen downward. Current development efforts at NASA are improved hydrogen and hydrogen flame sensors, and developing draft standards for slush hydrogen.

An insurance industry representative presented the general approach used to make underwriting decisions on property insurance. He indicated that the insurance industry had catalogued all the incidents concerning hydrogen. In every case that there was an indoor hydrogen release, there was ignition.

Hydrogen Demonstration Experience

Presentations on the codes & standards experience of hydrogen demonstration projects showed the difficulty associated with obtaining informed judgements from local permitting authorities on hydrogen technologies. In two of the demonstration cases presented, the implementation teams used the compressed natural gas experience as the starting point for demonstration system designs. In another case, local authorities were brought in from the beginning of the process. After extensive review by local permitting authorities, a 30 kW fuel cell demonstration using by-product hydrogen was allowed to operate. Ballard learned from their experience in the demonstration of their first fuel cell bus to use welded piping for the hydrogen fuel system. The Energy Technology Engineering Center (ETEC) indicated that in its full scale tests, current standards were inadequate in addressing high temperature cycling of hydrogen systems. The natural gas industry addressed codes and standards for compressed natural gas vehicles because of safety concerns. They recommended that the hydrogen industry should sponsor comprehensive product safety standards to protect the public and rely on natural gas standards for hydrogen applications.

Codes, Standards and Safety Requirements for Commercial Products

Several interesting points were raised in the commercial products presentations, including:

- There are no codes and standards for electrolysis equipment
- Hydrogen generator suppliers have established safety practices related to indoor machinery and outdoor storage that could be considered in developing hydrogen codes
- The hydrogen equipment supplier's concern is with foreseeable and controllable risks
- Electrical switches near hydrogen equipment is hermetically sealed to avoid ignition
- Trace oxygen analyzers should be placed at the hydrogen discharge of any system.

It was also mentioned that the overwhelming number of hydrogen incidents that occurred were due to inadequate purging of hydrogen systems or improper ventilation of indoor spaces for hydrogen. In discussion of infrastructure for hydrogen vehicles, two points worth noting are that the infrastructure will be largely determined by the form of on-board vehicle storage used, and that the transport costs of hydrogen are significant.

The following conclusions were reached in the workshop:

- Consensus must be reached by industry on codes and standards issues relating to hydrogen equipment
- Demonstrations are a way to identify codes and standards issues and the gaps in current standards
- A mechanism to inform and coordinate the hydrogen industry response on codes and standards is needed
- Codes and standards activities need to coordinated with the Department of Transportation

Subsequent activities will focus on identifying and prioritizing the most important hydrogen codes and standards issues that need to be addressed. It is anticipated that task groups will be formed with participants from the appropriate standards organizations to address these issues. The next workshop is being planned in late June.

In addition, the NHA is increasing its involvement and coordination with the International Standards Organization and the Canadian Hydrogen Association. A major issue that the U.S. hydrogen community must address is whether to adopt develop national standards or adopt international standards.

Westinghouse Savannah River Company Activities

The NHA is working with WSRC to establish an industry-directed hydrogen research center that addresses key but neglected areas of hydrogen research. The initial goals of the activity are to:

- Share with the hydrogen community existing in-house expertise
- Perform or support hydrogen-related demonstrations
- Develop expertise in emerging areas, such as codes and standards

The WSRC is working with the NHA to obtain industry input in developing the operating plans and activities for a hydrogen center. WSRC interests include use of metal hydrides for pump and compressor applications, operating a hydrogen bus for the 1996 Olympics in Atlanta, and utilizing the site's in-house capability for codes and standards testing and validation.

Future NHA Activities Related to DOE Activities

Markets for hydrogen technologies will not emerge until the technical and non-technical barriers are identified and resolved. Representatives from both industry and government will need to be involved in that process. The NHA is the focal point for a diverse group of industry, small business, government organizations, universities, and government laboratories with a specific interest in hydrogen as an energy source, and naturally facilitate technology transfer as a result of our activities.

The NHA is interested in seeing hydrogen-related technologies commercialized. It will be identifying those issues that its membership believes must be addressed to prepare for commercial products. There exists a consensus that hydrogen producers and manufacturers of hydrogen equipment must agree on codes and standards issues for hydrogen technologies to be compatible with each other as part of a hydrogen system. Plans must be developed and implemented for the first hydrogen vehicles to have available easy access to hydrogen fuel and experienced servicing. The NHA would be interested in working with industry to identify these needs and suggest approaches to addressing those needs. The NHA will act as a sounding board and poll its membership on demonstration programs suggested by HTAP. Future activities would include supporting HTAP in these areas.

References

Survey responses received from Air Products & Chemicals, Air Liquide, BOC Gases, (formerly Airco), and Praxair. October 1994. National Hydrogen Association Hydrogen Production and Use Survey.

Heydorn, Barbara. 1994. Hydrogen Product Review. *Chemical Economics Handbook.* Menlo Park, CA: SRI International.

Mohitpour, M. December 1988. "The Design and Engineering of Cross-Country Hydrogen Pipelines." *Journal of Energy Resources Technology.* Volume 110: 203-207.

Moore, R. B. & Nahmias, D. 1990. "Gaseous Hydrogen Markets and Technologies." *First Annual Meeting of the National Hydrogen Association Proceedings,.* 11-1 to 11-17. Washington, DC: National Hydrogen Association.

Appendix

Regions Used in Survey

New England: Connecticut, Maine, Massachusetts, New Hampshire, Rhode Island, Vermont

Middle Atlantic: New York, New Jersey, Pennsylvania

East North Central: Ohio, Indiana, Illinois, Michigan, Wisconsin

West North Central: Minnesota, Iowa, Missouri, North Dakota, South Dakota, Nebraska, Kansas

East South Central: Kentucky, Tennessee, Alabama, Mississippi

West South Central: Arkansas, Louisiana, Oklahoma, Texas

South Atlantic: Delaware, Maryland, District of Columbia, Virginia, West Virginia, North Carolina, South Carolina, Georgia, and Florida

Mountain: Arizona, Colorado, Idaho, Montana, Nevada, New Mexico, Utah, Wyoming

Pacific: Alaska, California, Hawaii, Oregon, Washington

SUPPORTING ANALYSES AND ASSESSMENTS

Jim Ohi
National Renewable Energy Laboratory
Golden, CO 80401

Abstract

Supporting analysis and assessments can provide a sound analytic foundation and focus for program planning, evaluation, and coordination, particularly if issues of hydrogen production, distribution, storage, safety, and infrastructure can be analyzed in a comprehensive and systematic manner. The overall purpose of this activity is to coordinate all key analytic tasks—such as technology and market status, opportunities, and trends; environmental costs and benefits; and regulatory constraints and opportunities—within a long-term and systematic analytic foundation for program planning and evaluation. Within this context, the purpose of the project is to help develop and evaluate programmatic pathway options that incorporate near and mid-term strategies to achieve the long-term goals of the Hydrogen Program. In FY 95, NREL will develop a comprehensive effort with industry, state and local agencies, and other federal agencies to identify and evaluate programmatic pathway options to achieve the long-term goals of the Program. Activity to date is reported.

Project Rationale

Supporting analysis and assessments can help establish a sound analytic foundation and focus for program planning, coordination, and evaluation through a strategic planning group (hereafter Group). NREL will organize and coordinate the activities of the Group with those of the other major elements of the DOE Hydrogen Program (hereafter Program) and with relevant activities and programs of industry organizations, other Federal agencies, state and local governments, and nongovernmental organizations. The overall purpose of this activity is to define and execute an analytic agenda to provide programmatic guidance to the Program. NREL will structure the analysis activities in the Program by extending the concept of energy pathways to that of *programmatic pathway* options that can help define a set of program trajectories. These trajectories, in turn, will provide templates for assessing where the Program wants to be and how fast the Program wants to get there in terms of hydrogen production, storage, and utilization. The Group must structure its agenda to keep industry and other key stakeholders involved in defining programmatic pathways. The major question that the Group must help answer is: is the Program doing what it should be doing? Furthermore, the Group must be able to communicate an answer in a way that key stakeholders in the Program (as defined by the industry and public outreach efforts) can understand. Analysis tasks must answer critical question about hydrogen technologies, such as technology and market status, market opportunities and trends, environmental costs and benefits, and regulatory constraints and opportunities. These questions must be asked within a comprehensive structure if analysis tasks are to help establish a long-term and systematic analytic foundation for program planning and evaluation. One key need under supporting analysis and assessments is defining and implementing a transition to long-term goals and objectives of the Program through near and mid-term initiatives, activities, and projects. Analysis and assessments must help ensure that near-term efforts are part of a cost-effective and coherent path to achieve the strategic and long-term programmatic goals.

NREL is also continuing work on the energy, economic, and environmental benefits of hydrogen technologies with emphasis on the transportation and utility sectors. This activity will contribute directly to Program evaluation and planning. As part of the supporting analysis and assessments work, hydrogen production, distribution, storage, safety, and infrastructure needs should be analyzed in comprehensive manner. This need will be met by integrating H-Scan (a project evaluation tool) and a decision analysis tool as described in another paper. In summary, Supporting Analysis and Assessments will establish an analytic foundation and focus for program planning, coordination, and evaluation to help achieve the long-term goals of the Program.

Approach

To establish the analytic framework for the Program, the Group will take all the inputs it is aware of on what the Program should do (e.g., legislation, recommendations from the Hydrogen Technical Advisory Panel, results of industry and public outreach efforts) and (1) map them against a set of programmatic pathway options, (2) identify the analytic tasks needed to draw and evaluate the pathways, and (3) set an analytic agenda of critical tasks. The agenda should establish the intellectual and organizational teamwork and resources needed to do the work and the schedule that must meet to contribute most effectively to the Program's strategic analysis needs. To begin sketching programmatic pathway options, inputs will be mapped against (at least) the following questions.

a. what are the axes of the trajectories? If the x-axis is most likely time (in calendar years, e.g., 2010), the y-axis is problematic. It could be hydrogen production in quads (or fractions of quads), cost of hydrogen per MMBtu, % hydrogen consumption in each end-use sector, ratio of renewable to fossil-derived hydrogen, % reduction of key air pollutants, etc. More than one set of axes may be needed. The larger question is what is the best way to set and frame the goals and progress of the Program in terms that are relevant to the national energy, economic, and environmental agenda? Such issues as the role of the Program in helping to meet nation's strategic goals and whether the Program should focus on long-term R&D for renewable hydrogen production can be addressed in this context.

b. how can the end points for each axis be set? What time span(s) is (are) appropriate for the Program? Why are specific time (and quantity) goals set? These questions set the larger analytic context where issues such as fossil fuel depletion, energy security, environmental impacts are relevant. How such issues are factored in when end points are set must also be evaluated.

c. how are the slope(s) between the start and end point(s) to be drawn? Here such issues as transition strategies (e.g., near-term hydrogen production from fossil fuels), technology diffusion projections, role of demonstrations, etc., are relevant and need to be incorporated.

d. how are program R&D elements correlated with a given trajectory? If production, storage, transport, and utilization are the correct set of program elements, how can these elements be integrated to achieve a given trajectory? Should separate trajectories for each element be established? Should separate trajectories for each end-use sector be established? Should priority elements and sectors be established? Issues such as the production of hydrogen from fossil energy sources for stationary and mobile applications as a transition to production from renewable energy sources can be discussed in this context.

e. how can the Program know where it is on a slope at any given time and how can the Program plot (measure) progress on a particular slope? Program metrics and evaluation procedures must be established and built into all four sub-paragraphs (a-d) above.

f. how can the total and incremental costs and benefits (C/B) of a given trajectory be measured? The total C/B is needed to justify Program approach while the incremental C/B is needed to justify annual budgets.

Key Results

Progress to date on developing the programmatic pathway options and on the quality metrics work is described below. Progress on H-Scan is described in another paper.

Analysis Agenda

An initial session to explore programmatic analysis needs was held as part of the annual Program review in April 1995. NREL drafted a short paper to initiate and guide discussion and facilitated the exchange of ideas during the working session. This meeting was useful in eliciting a variety of opinions on analysis issues and needs and in beginning to involve industry in defining an analysis agenda. Minutes of the meeting are available. In addition, initial meetings of working groups on production, storage, and utilization were also held at the same Program review. A second session for all of the working groups (production, storage, utilization, and systems integration) is scheduled in October and will be hosted by a major company.

After the initial meeting on programmatic analysis needs, NREL met with a small group of analysts representing the private sector, universities, and other national laboratories to discuss the results of the meeting. The initial activity of this group will be to draft a "white paper" on programmatic pathway analysis. A first draft of this white paper is under review by the group.

Analysis of Costs and Benefits

NREL also continued to define the costs and benefits of the Program, particularly in the transportation sector. Four major vehicle types were characterized: gasoline-powered conventional vehicles (GCV)—the benchmark technology—hydrogen-powered internal combustion engine vehicles (ICEV), hydrogen-powered hybrid-electric vehicles (HEV), and hydrogen-powered fuel-cell vehicles (FCV). The analysis considered the benefits of displacing gasoline technologies with hydrogen-fueled alternatives by studying reductions in criteria pollutant emissions, oil imports, and carbon emissions. Market penetration scenarios were constructed using the Alternative Vehicle Spreadsheet (AVS) model using the inputs discussed in more detail in a forthcoming report.[1] Market projections generally adhered to the following guidelines: (1) penetration is slow in the first years of development, increasing more rapidly as technologies are proven and fuel becomes available; (2) there is a general transition from the ICEV to HEV to FCV technology that permits storage technologies and fueling infrastructure to evolve incrementally; and (3) as a new hydrogen-powered technology becomes available, the market for the previous version (ICEV or HEV) diminishes rapidly as the niche of the older vehicles is subsumed under the improved technology. These estimates do not consider competition with other technologies beyond the GCV (e.g., battery-powered EVs) or other fuel options (e.g., a gasoline-powered HEV). Assumptions concerning fuel source for hydrogen, light-duty automobile (LDA) efficiencies, and market penetration are shown in Figure 1.

Emissions of the three regulated criteria pollutants from the hydrogen-powered ICEV, HEV, and FCV were estimated based on the benchmark GCV. The GCV is assumed to achieve the Tier II emissions standards of the 1990 Clean Air Act Amendments (CAAA). The FCV operating on hydrogen is a zero emissions vehicle. Because hydrogen contains no carbon, the HEV and ICEV have very low emissions of CO and NMOG, but tests have demonstrated considerable variability in achieving NO_x emission reductions (Schaper, et al. 1995). This analysis assumed that lean-burn technologies will be developed by 2010 that permit the vehicle to operate at a high air:fuel ratio, achieving NO_x reductions of 25% for the ICEV and 50% for the HEV relative to the GCV. Emissions savings and oil reductions are valued using estimates from OTT (1994). The value of criteria pollutant emissions reductions were based on the avoided-cost values implied by the CAAA, and the value of carbon is a middle-of-the-road estimate based on the range found in the literature (0-55 \$/ton CO_2) (Mark, Ohi, and Hudson 1994). The value of oil savings is equal to the national security benefits from lower oil

---

[1] AVS was developed by Dr. Lew Fulton, who is currently with the DOE Policy Office. AVS was used in the EPACT 2021 report (OTT 1994) and was adapted to include hydrogen vehicles for this analysis.

imports, and the $4/barrel value used is a middle estimate based on the cost of averting or weathering supply disruptions and market manipulation as well as military expenditures to maintain access to Persian Gulf oil (OTT 1994). This analysis assumed that all of the oil displaced by hydrogen technologies will be of imported oil. Hydrogen consumption, air emissions and oil savings, and the benefits of displacing criteria air and carbon emission and oil imports are shown in Figure 2.

Cost factors treated in this study included the purchase price of the vehicle and fuel costs and savings. These assumptions are shown in Figure 3. Figure 4 shows the overall results of this study. The net gains (of benefits studied) achievable through hydrogen usage in the transportation sector is very large, totaling a cumulative discounted value of $80 billion by 2030 ($320 billion undiscounted) in constant 1990 dollars. Details of the this study are available from NREL.

For the utility sector, NREL has completed a comprehensive mapping of a utility system to identify opportunities for hydrogen production, storage, distribution, and utilization. Figure 5 shows a block diagram of hydrogen production, storage, transportation, and end use potential in a utility system. Figure 6 maps the technology options available at each production, storage, transportation, and end-use "nodes." Based on such maps, NREL will compare hydrogen technologies against competing conventional technologies and evaluate the most feasible hydrogen technologies in detail for their potential operational and environmental benefits to a utility system.

Definition of Success

The project will be successful if NREL can (through the Group and the four working groups) identify, assess, and recommend programmatic pathway options to achieve the long-term goals of the Program. The programmatic pathway options will also provide measures of progress and success and help unify near and mid-term objectives with long-term goals. The work of the Group will be based on a partnership with industry, utilities, and government (local, state, federal) to develop long-range pathway options for near and mid-term hydrogen production, storage, distribution. A key measure of success will be the willingness of industry to participate in the Group, particularly in linking critical near-term transitional hydrogen technologies with the long-term technology development goals of the Program. The project can then, for example, make an important contribution toward linking near-term demonstration efforts with the long-term strategic goals of the Program. Other measures of success include helping to define the energy, economic and environmental benefits of the Program to industry and other stakeholders.

Proposed Future Work

Proposed future work will depend on the outcome of on-going work, but a number of follow-on efforts are possible. These include:

- a systematic method to identify and evaluate programmatic pathway options that incorporate potential near-term market opportunities, existing and projected market trends and industry activity, regulatory constraints and opportunities, and regional interests and development patterns into the long-term goals, objectives and funding strategies of the Program;

- comprehensive criteria to evaluate near-term demonstration opportunities based on industry perspectives and needs (H-Scan);
- a comprehensive programmatic costs and benefits analysis to develop metrics based on *strategic national goals* (such as economic strength, scientific and technical leadership, environmental quality, and energy security) and *comprehensive R&D portfolio criteria* (such as technology diversification, balance in time frame, cost, and return on investment) to help evaluate Program priorities and pathways.

Technology Transfer

The project incorporates technology transfer by including key industry representatives in the Working Group and by recognizing that close interaction with industry will be key to the success of this project.

Acknowledgments

The author would like to acknowledge the contributions of Jason Mark and Steve Adelman in preparing this paper.

References

Mark, J., J.M. Ohi, and D.V. Hudson, Jr. (April 1994). *Fuel Savings and Emissions Reductions from Light Duty Fuel Cell Vehicles.* Golden, CO: National Renewable Energy Laboratory. NREL/TP-463-6157.

Schaper, V., J. Mark, C.J. Hammel, T. Wheat. (January 1995). *Transportation Market Characterization.* National Renewable Energy Laboratory. Draft.

U.S. Department of Energy, Office of Transportation Technologies (OTT) (1994). *Five-Year Transportation Program Plan.* Draft.

FIGURE 1

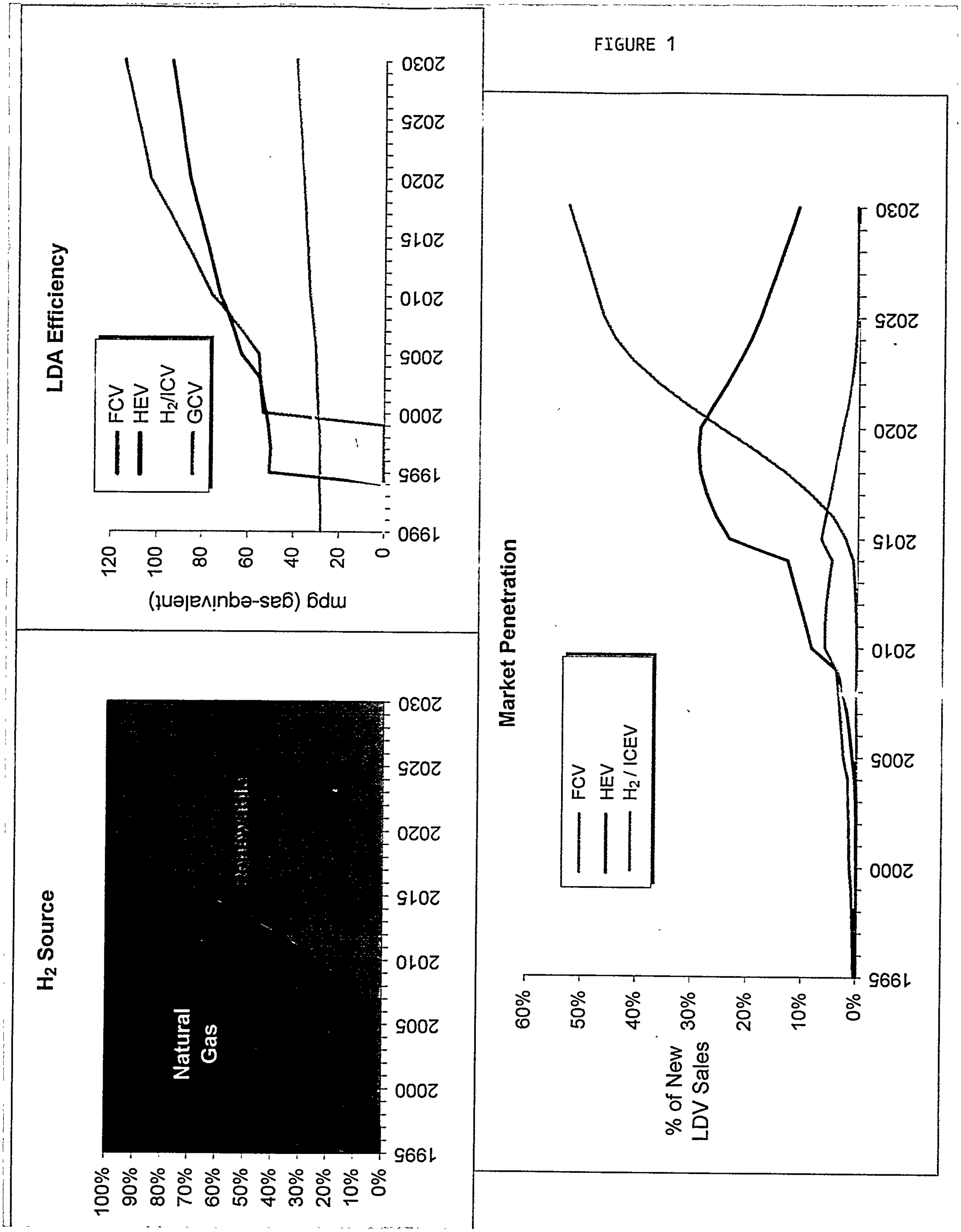

LDA Efficiency
mpg (gas-equivalent)
120
100
80
60
40
20
0
1990
1995
2000
2005
2010
2015
2020
2025
2030
FCV
HEV
H_2/ICV
GCV
H_2 Source
100%
90%
80%
70%
60%
50%
40%
30%
20%
10%
0%
Natural Gas
Renewable
Market Penetration
% of New LDV Sales
60%
50%
40%
30%
20%
10%
0%
FCV
HEV
H_2 / ICEV

FIGURE 2

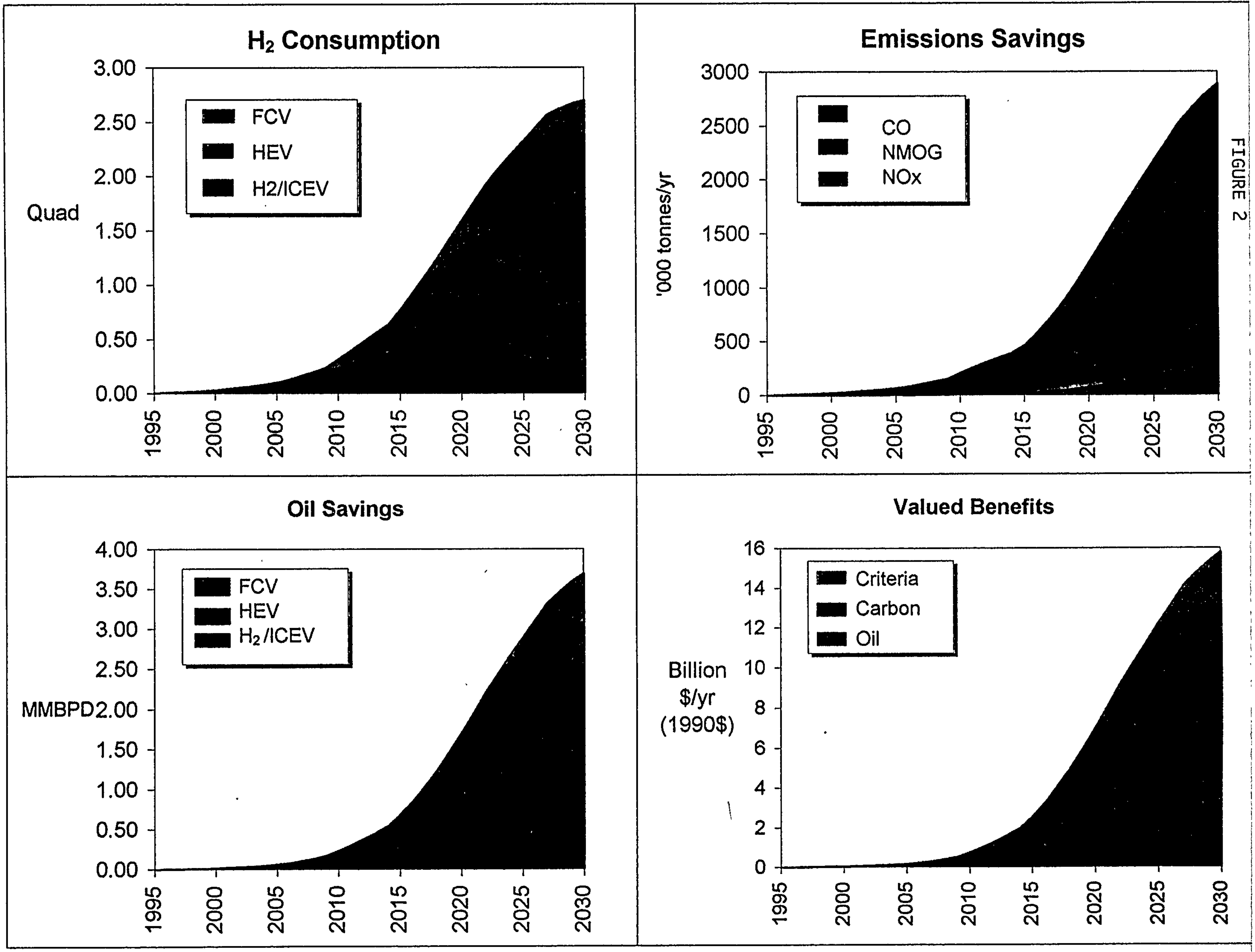
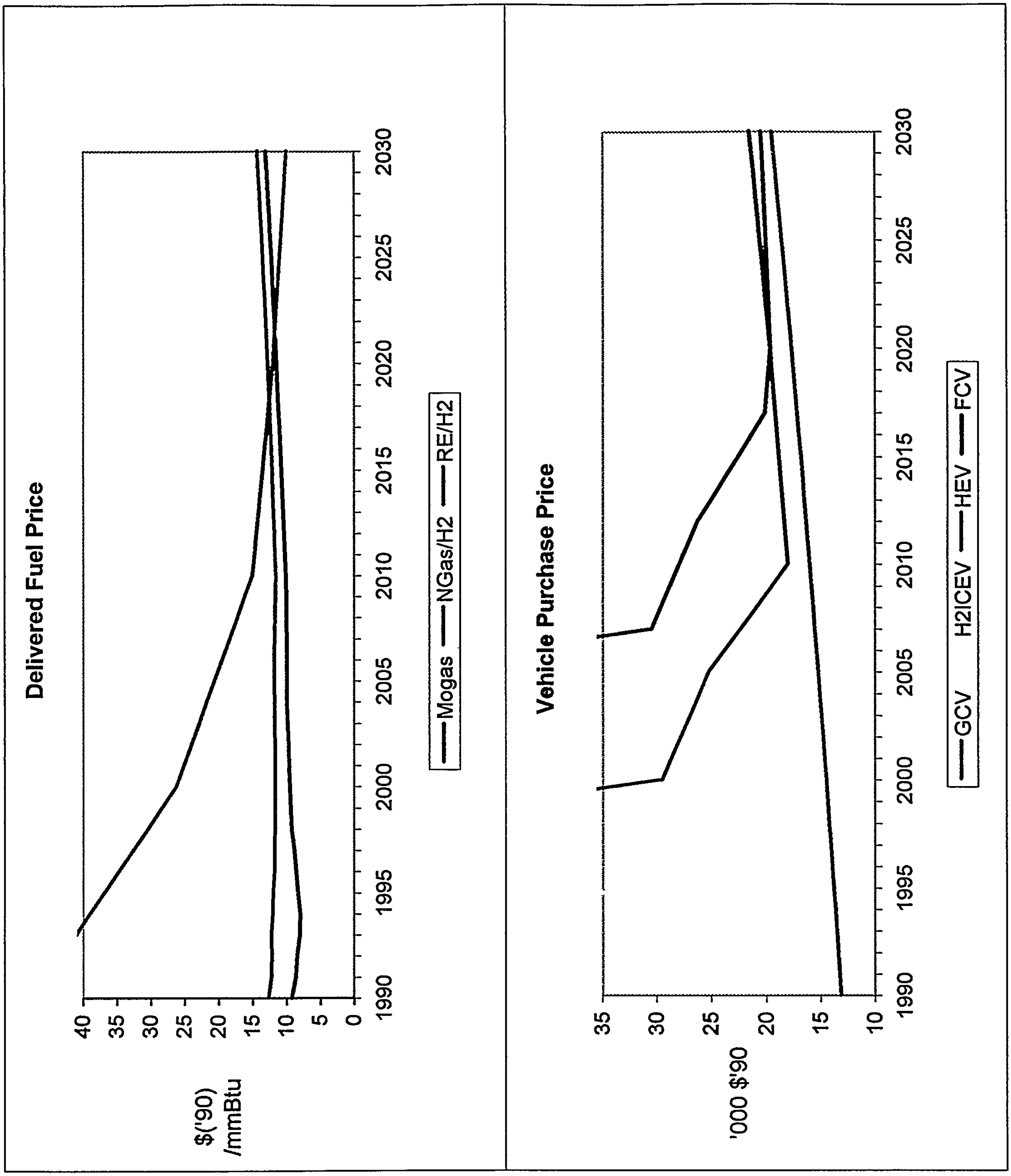
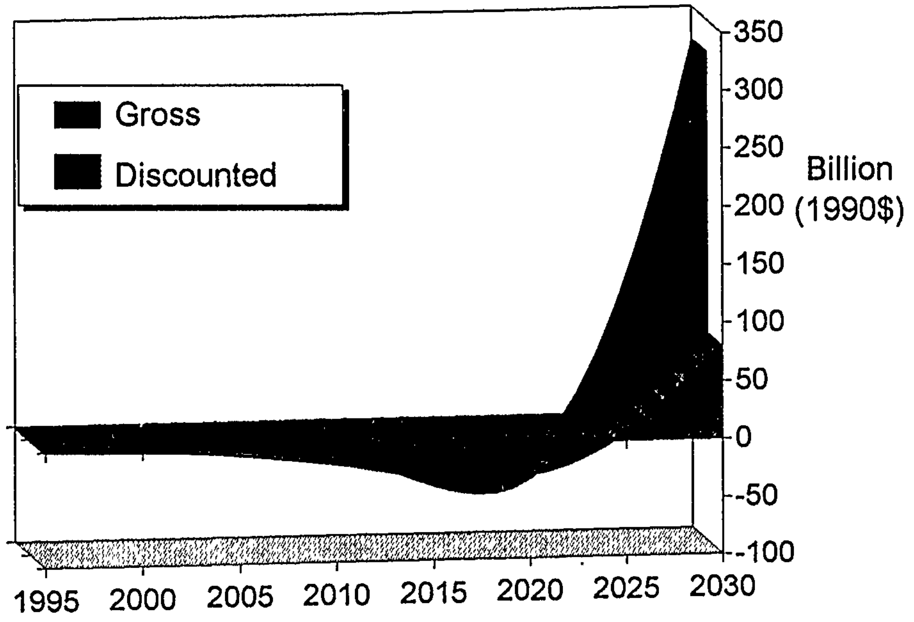

H$_2$ Consumption
Quad
3.00
2.50
2.00
1.50
1.00
0.50
0.00
FCV
HEV
H2/ICEV
1995
2000
2005
2010
2015
2020
2025
2030
Emissions Savings
'000 tonnes/yr
3000
2500
2000
1500
1000
500
0
CO
NMOG
NOx
1995
2000
2005
2010
2015
2020
2025
2030
Oil Savings
MMBPD
4.00
3.50
3.00
2.50
2.00
1.50
1.00
0.50
0.00
FCV
HEV
H$_2$/ICEV
1995
2000
2005
2010
2015
2020
2025
2030
Valued Benefits
Billion $/yr (1990$)
16
14
12
10
8
6
4
2
0
Criteria
Carbon
Oil
1995
2000
2005
2010
2015
2020
2025
2030

FIGURE 3



Delivered Fuel Price
$('90) /mmBtu
40
35
30
25
20
15
10
5
0
1990
1995
2000
2005
2010
2015
2020
2025
2030
Mogas
NGas/H2
RE/H2
Vehicle Purchase Price
'000 $'90
35
30
25
20
15
10
1990
1995
2000
2005
2010
2015
2020
2025
2030
GCV
H2ICEV
HEV
FCV

Cumulative Costs / Benefits



Total Annual Cost / Benefit (undiscounted)

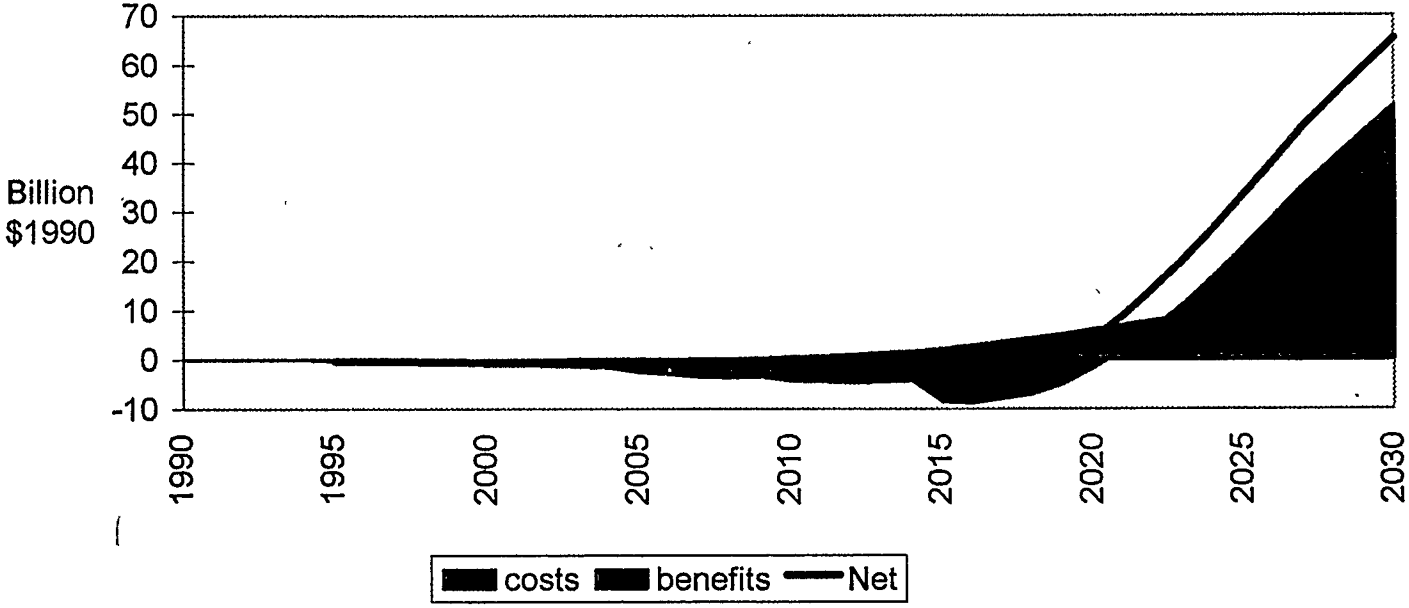


FIGURE 5

Hydrogen Production and Use within an Electrical Utility System

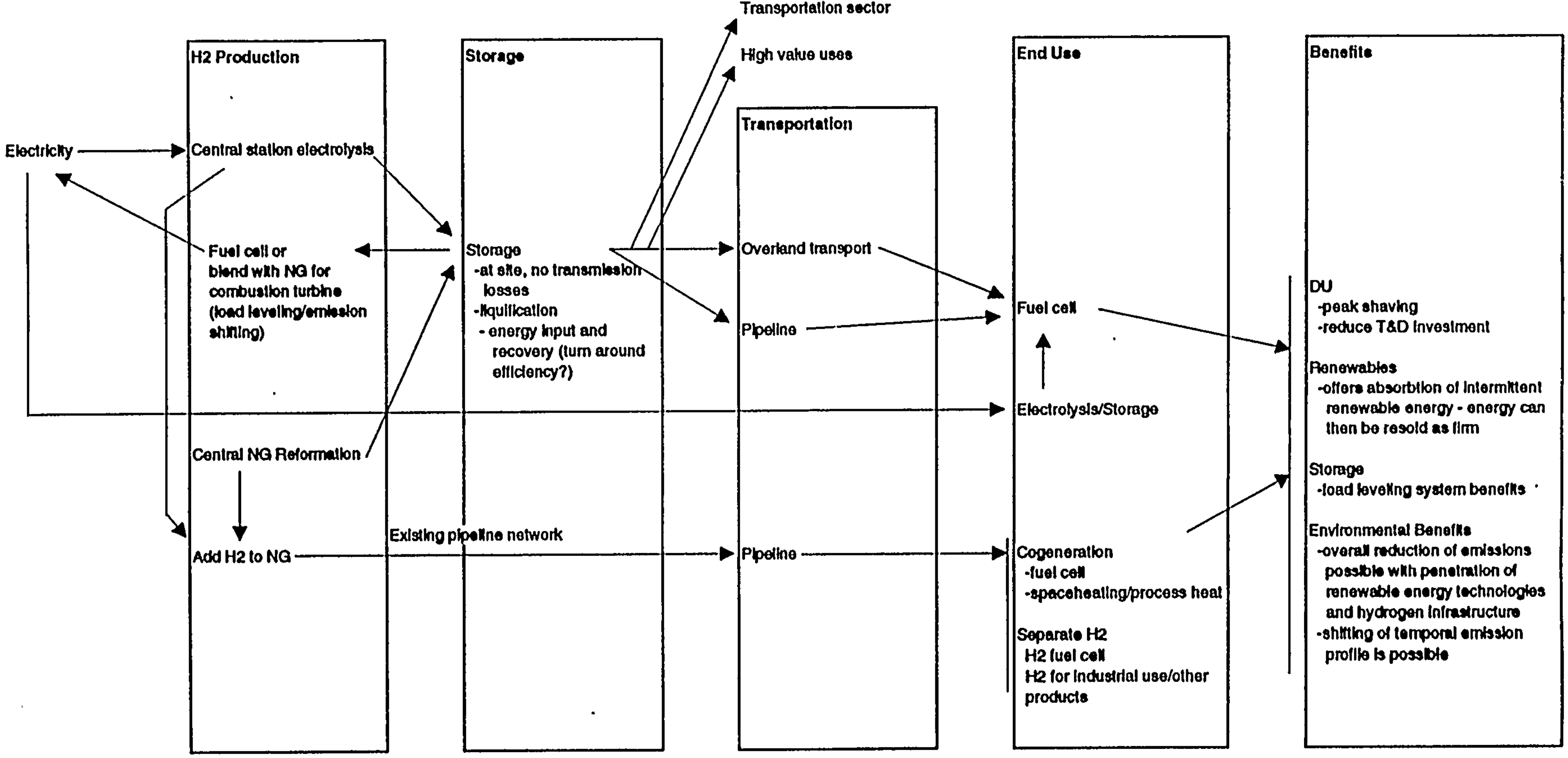
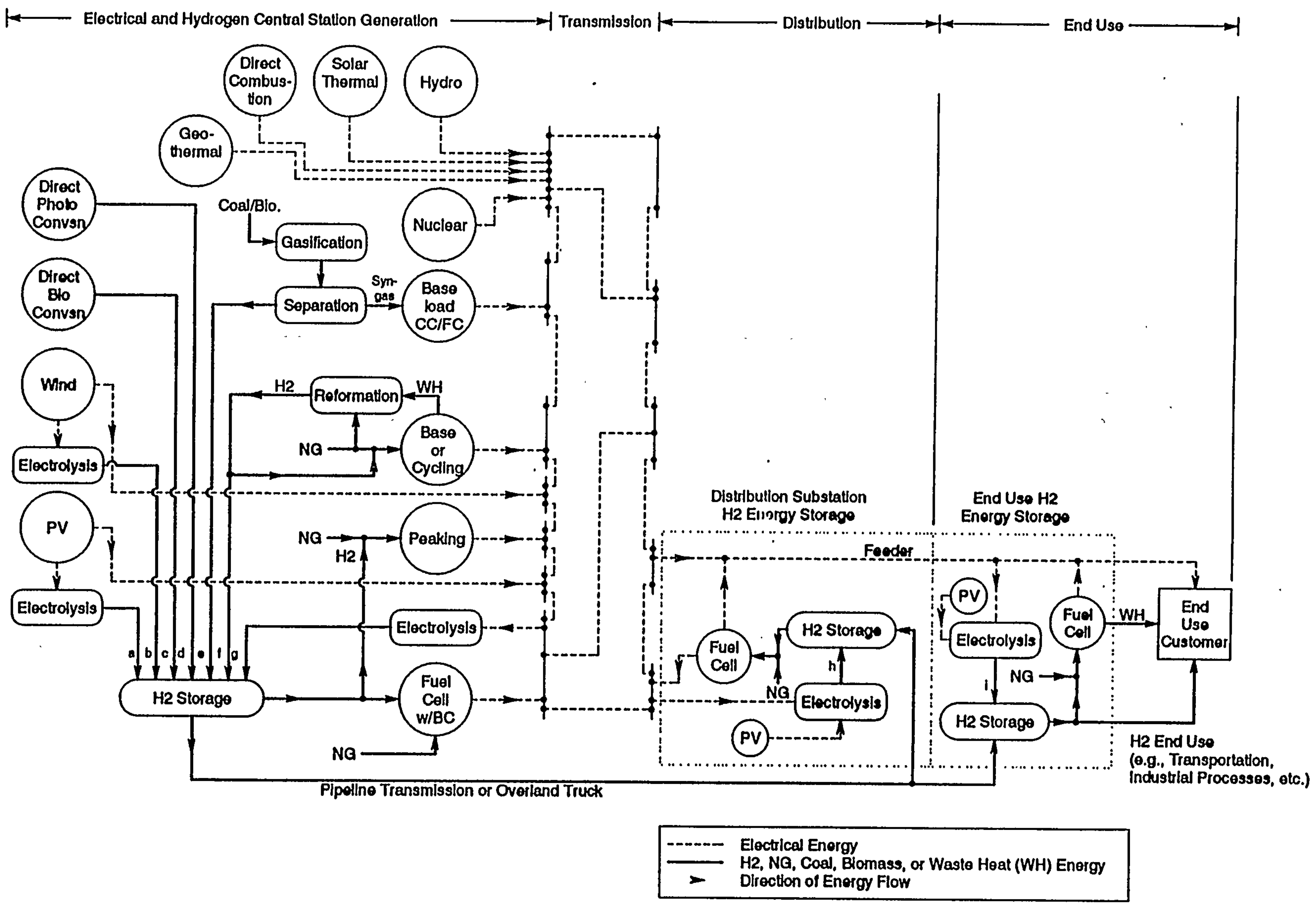


FIGURE 6


Electrical and Hydrogen Central Station Generation
Transmission
Distribution
End Use
Direct Combus-tion
Solar Thermal
Hydro
Geo-thermal
Direct Photo Convsn
Coal/Bio.
Gasification
Nuclear
Direct Bio Convsn
Separation
Syn-gas
Base load CC/FC
Wind
H2
Reformation
WH
NG
Base or Cycling
Electrolysis
PV
NG
Peaking
H2
Electrolysis
Electrolysis
a
b
c
d
e
f
g
H2 Storage
Fuel Cell w/BC
NG
Pipeline Transmission or Overland Truck
Distribution Substation H2 Energy Storage
End Use H2 Energy Storage
Feeder
PV
Fuel Cell
WH
End Use Customer
Fuel Cell
H2 Storage
h
NG
Electrolysis
PV
Electrolysis
i
NG
H2 Storage
H2 End Use (e.g., Transportation, Industrial Processes, etc.)
Electrical Energy
H2, NG, Coal, Biomass, or Waste Heat (WH) Energy
Direction of Energy Flow

H SCAN/AHP DECISION PROCESS PLANNING FOR EVALUATING AND RANKING OF PROPOSALS SUBMITTED TO THE DOE HYDROGEN PROGRAM

Mary-Rose Szoka de Valladares
National Renewable Energy Laboratory
409 12th St., S.W.
Washington, D.C. 20024

Stephen Mack
Energetics
501 School Street, S.W.
Washington, D.C. 20025

Introduction

We shape the world by the questions we ask. These questions help us to formulate and articulate our vision of the world. Science, in particular, exacts rigorous attention to the craft of asking questions.[1] Questions provide the framework for a sound analytic foundation and the careful development of plans for the future.[2]

---

[1] Robert MacFarlane. "Science, from one perspective, is the art of phrasing questions and identifying their attendant assumptions. Its basic tenet is that nature has no secrets. The obstacles to furthering knowledge lie in formulating the right questions and circumventing ambiguous answers, never an easy task. The best practitioners know that incisive questions and skillful analysis will ultimately yield their reward. Artful questions may require new technology, often from unrelated disciplines. New questions may require fresh insight, unencumbered by the baggage of past experience, and a probing mind to test old concepts. The importance of the proper question is often overlooked by experienced observer and novice alike."

[2] Ludwig Wittgenstein. "If a question can be put at all then it can also be answered."

Failure to frame and pose questions germane to the world we seek to order puts us at risk of forfeiting our future, either to chance or to those forces which have asked relevant questions and developed an agenda. The authors' position is that the process of asking "right questions" has implications of such importance for the DOE Hydrogen Program that it compels development of a framework to accommodate and encourage application of questions to proposals for Hydrogen funding. The clear intent of this undertaking is to enhance the present performance and future prospects of the DOE Hydrogen program.

The DOE Hydrogen Program offers a unique, "big picture" opportunity for good science and good business. Hydrogen is often referred to as the "energy carrier of the future" and the "forever fuel." The DOE Hydrogen Program includes research, development and demonstration -- a full range of activities that emphasizes state of the art science and engineering. Photochemical and photobiological processes as well as various storage technologies are examples of "state of the art" R&D.

And then there is the business side of the hydrogen equation. Hydrogen not only has a place in tomorrow's markets, it has a strong presence in the contemporary marketplace. The latter includes petroleum refining and chemical manufacturing as well as small volume production for metal fabrication, oil and fat hydrogenation and other of the so-called "merchant markets" for hydrogen. And unlike the early days of the solar energy industry, the contemporary hydrogen industry can count mature, sophisticated businesses within its ranks. This industry has considerable breadth and depth of capacity. Many of its members understand research, development and demonstration processes as well as the business process and the assessment of risks inherent in both.

Rationale

Purpose and Genesis

A method is needed to identify and evaluate opportunities in research, development and validation hydrogen production, storage, distribution and utilization technologies. In general, there is a need for a systematic evaluation of potential projects that is part of the greater program planning process for the Hydrogen Program. This evaluation process should be consistent with Hydrogen program planning documents.[3]

The present effort is part two of the NREL Supporting Analysis for Hydrogen as well as a part of Energetics' ongoing Systems Analysis work. The April 1994 Hydrogen Program Review identified *Ranking Systems Analysis* as a first priority in hydrogen research and development needs. The Program Review cited development of "energy significant, economically attractive roles for hydrogen" as a specific purpose of the Systems Analysis work. Later, the July 1994 Hydrogen Program Review suggested establishment of a framework with criteria to identify and evaluate near-

---

[3] These documents include: Hydrogen Program Plan, FY 1993-1997, The Hydrogen Program Implementation Plan, FY 1994-1998, The FY 1995 Annual Operating Plan, The Hydrogen Program Overview, and The Hydrogen Program Summary, FY 1994.

term opportunities for cost-effective hydrogen production, storage, distribution and use. The guidance that emerged from these Program Reviews was central to design of this planning and evaluation process.

Principal Drivers

Our sense is that the best interests of the Hydrogen Program are served by a selection strategy that seeks to balance the Hydrogen Program's portfolio of projects. A balanced portfolio would contribute to the Program's technical and market success. The balanced portfolio would consist of projects that are:

- Technically sound and consistent with Program goals and objectives
- Responsive to congressional guidance and the federal role
- Sensitive to private sector needs and concerns

The development of this kind of a project portfolio implies that the Hydrogen Program will receive a sufficient quantity of high quality proposals from which it can select projects for programmatic support. Consequently, there is a need to facilitate preparation of proposals that provide decision makers with a sufficient quality and quantity of information with which to perform effective evaluations. Further, and consistent with emergence of *Ranking Systems Analysis* as a first priority for the Hydrogen Program, there is a need for a logically defensible, transparent decision analysis mechanism for project selection.

Other Considerations

Beyond the concern for development of solid projects within the parameters of the current funding, there is a need to prepare for the opportunities associated with funding increases that might substantially expand current programmatic efforts. H.R. 655, *The Hydrogen Futures Act of 1995*, would authorize $25 million for FY '96, $35 million for FY '97 and $40 million for FY '98 for hydrogen research, development and demonstration.[4] These funding levels contrast sharply with the FY '95 level of $10 million and immediately prior fiscal years in which budgets hovered around the $2-4 million level.

Off of Capital Hill, Hydrogen has likewise drawn attention. The Galvin Commission, the advisory committee charged by Secretary of Energy Hazel O'Leary with examining the purpose and future of America's national laboratory structure, has a critical role in the Department of Energy's evolving realignment strategy. Their report calls out hydrogen -- "abundant in water, gas and biomass -- among fuel sources that must be considered in DOE's energy mix."[5]

---

[4] The *Hydrogen Futures Act of 1995* is sponsored by Rep. Robert Walker (R-PA). Sen. Tom Harkin (D-IA) has championed the companion Senate bill whose introduction is anticipated in early June of 1995.

[5] Task Force On Alternative Futures for the Department of Energy Labs - The Galvin Commission Report, Robert Galvin, Chairman of the Executive Committee, Motorola, Schaumburg, IL., p. 2.

The American Solar Energy Society's new platform statement incorporates solar-produced hydrogen among renewable energy technologies that must be "rapidly developed and selectively deployed wherever they may economically substitute for conventional energy sources."[6] In the recent past Hydrogen has also received national exposure through print media coverage in such distinguished national press as the *New York Times* and the *L.A. Times Magazine.*[7]

Approach

In this process, DOE Hydrogen Program Management defines evaluation and selection objectives that are collectively called "criteria." These criteria are then explicitly linked to the H Scan/AHP Decision Process. The criteria are intended to be the principal drivers for proposal identification, evaluation and selection.

The H Scan component of this process provides a framework in which a project proposer can fully describe their candidate technology system and its components. The H Scan complements traditional methods of capturing cost and technical information. It consists of a special set of survey forms designed to elicit information; these forms are described later on. The actual index of factors addressed in H Scan will, however, depend on the proposed technology and its level of development. Expert reviewers will assess the completed proposer H Scan relative to the DOE specified selection criteria and synthesize their conclusions. Management will then utilize the reviewer prepared H Scan Summary to further evaluate the proposals.

The Analytic Hierarchy Process (AHP) component of the decision process assembles the management defined evaluation and selection criteria into a coherent multi-level decision construct by which projects can be evaluated in pair-wise comparisons. The AHP model will reflect management's objectives and it will assist in the ranking of individual projects based on the extent to which each contributes to management's objectives. The evaluation construct of the process is a decision hierarchy in which the general objectives or criteria of the program are disaggregated into more specific sub-criteria. Pair-wise evaluation of both criteria importance and technology importance are conducted. Once proposals have been evaluated through H Scan, they can be scored and ranked against the weighted criteria in the AHP. Management can then choose to edit or modify the rankings to take into account special or unique circumstances such as funding and cross-project synergies. The selection process will consist of multiple steps that are logically connected by H Scan and AHP.

---

[6] Platform Statement of American Solar Energy Society, 1995.

[7] Weisman, Alan. March 19, 1995. "The Last Best Hope of Earth -- Harnessing the Big H," *Los Angeles Times Magazine*. "Hydrogen seems the ideal energy source -- plentiful efficient and clean. Can something this perfect be real? Just ask the Japanese . . . "

Leary, Warren E. April 16, 1995. "Use of Hydrogen as a Fuel Moving Closer to Reality." *The New York Times*. "Irresistible allure as a power source: low cost, simplicity and little pollution . . . 'if we can make it work it would fundamentally change the country.'"

Model management is maintained with supporting HP software called Expert Choice.[8]

What follows is a detailed description of the products and activities associated with the planning and evaluation process. The products consist of:

- Product #1 - Objectives or "Criteria"
- Product #2 - H Scan
- Product #3 - The Analytic Hierarchy Process (AHP)

Figure 1, *H Scan/AHP Decision Process*, illustrates the overall planning and decision process and displays the discreet activities on a step by step basis.

Products

Product #1 - Objectives or "Criteria"

The first product consists of objectives or criteria.[9] The criteria will be both quantitative and qualitative to account for technical and political issues. The objectives or "criteria" that will govern the selection process are actually developed by H_2 Program Management. These criteria will be further refined into sub-criteria so that finer distinctions can be made among the proposal candidates. H_2 Program Management then structures the criteria by determining the relative importance of the criteria in the decision hierarchy through a pairwise comparison process.

These criteria become the principal drivers for proposal identification, evaluation and selection. Upon adoption, the criteria are explicitly incorporated in both the H Scan and the AHP, linking the two essential parts of the decision analysis process.

Product #2 - H Scan

The Request For Proposal (RFP) will be finalized with a special section (H-Scan, Part 1) that is designed to facilitate proposal evaluation with the established selection criteria. H Scan provides a framework in which a project proposer can fully describe their candidate technology system and its components and expert project reviewers can assess the proposed project. This is a holistic effort to examine -- not just the technical merits, but the economic, business and environmental aspects of the proposal. H Scan (shorthand for "scanning" potential Hydrogen projects in the evaluation process) complements traditional methods of capturing cost and technical data, some of which will be utilized in other volumes of the project application process.[10]

---

[8] A Beta test version of Expert Choice software has been utilized for purposes of development of the H Scan/AHP courtesy of Expert Choice.

[9] The terms "objectives" and "criteria" are used interchangeably.

[10] The content and format of other volumes of the request for proposal process, while important, are beyond the scope of the H Scan/AHP Decision Process topic. They are, therefore, not treated here.

The complete H Scan is a tool that consists of two major parts. Complementary H Scan survey forms have been developed to capture both the proposer description and the expert assessment of the proposed project. H Scan survey forms gather information on:

- Relevant markets
- Energy efficiency
- Economics: cost and performance, together with other impacts
- Applicable law and regulations (including codes and standards)
- Operations and maintenance
- Proposer capacity and experience

In its present draft form H Scan Part I contains five sections which will be completed by the proposer according to a set of instructions and format provided by the DOE Hydrogen Program. The sections are listed below:

- *Section I - Candidate Technology System and Market*
- *Section II - Energy Efficiency and Economics*
- *Section III - Environmental Impacts*
- *Section IV - Regulation and Operation*
- *Section V - Capabilities, Experience and Commitment*

Part I, The Proposer H Scan

The presentation given at the Hydrogen Program Review featured the contents of three sections of the proposer H Scan: *Section I - Candidate Technology: System and Market*; *Section III - Environmental Impacts*; and *Section V - Capabilities, Experience and Commitment: Suitability of Proposers for Participation*. Highlights of these sections are likewise addressed in this paper. H-Scan Part I will be structured so that responses coincide with the criteria in the AHP decision hierarchy.

Section I - Candidate Technology: System and Market (see Figure 2) asks for classification of the candidate technology according to DOE pathway (production, storage, infrastructure and end-use) and market segment. There is space for comment on challenges and opportunities associated with these categories. Proposers are asked to classify the proposed technology as to maturity level and indicate how close it is in the relevant time frame (near, mid and long term) to realization of certain developmental milestones.

The issue of technology maturity level and developmental status is key to the planning and evaluation process. Ultimately, the classification of the candidate technology as to its research, development and validation status will help to determine the most appropriate type of evaluation exercise for a given proposal. The underlying implication is that evaluation will differ according to stage of development.[11] In-depth discussion of the distinctions and subtleties associated with various stages of development, however important, is beyond the scope of this paper. This topic will be addressed by H_2 Program Management as it resolves issues related to adoption of the H Scan AHP Decision process.

A description of the energy pathway for the components and the complete system is called for.[12] Proposers are asked whether this is a substitute product or process, in whole or part, and whether it is entails a redesign issue. Proposers are asked to establish whether it is an enabling technology. They are further queried as to the extent to which a systems approach was employed in analysis of the candidate technology. There are also questions about business issues and practices such as guaranties, warranties, services and financing.

Proposers are asked to provide a mini market profile of the market segment impacted by their candidate H_2 system. If the proposed technology is a substitute for an existing product they are asked to comment on the characteristics of the existing product market. Alternatively, if a new product is contemplated, they are asked to forecast the market potential. These descriptions are to include infrastructure and product distribution network considerations.

Section III - Environmental Impacts (see Figure 3) addresses emissions on a life-cycle basis and allows for accounting of other externalities, both institutional and social. Stakeholder impact is also included in this section. Stakeholder impact is examined from the standpoint of activities that might affect the proposed candidate technology/system. It is also explored from the standpoint of possible contribution to industrial collaboration and strategic alliances for the H_2 industry.

Section V - Capabilities, Experience and Commitment (see Figure 4) deals with the capacity of the proposer to successfully participate in the proposed project. There is an assumption that proposals might be jointly formulated by a team consisting of some combination of industry(ies), university (ies) and national laboratory(ies). Hence, this section deals with capability issues that could impact the suitability not only of potential individual collaborators, but also the quality of the team that would emerge from collaboration. Information on previous experience and present capabilities is called for, together with evidence of commitment. Relevant previous experience includes general background, management experience and specific experience with H_2. It also includes experience with commercialization, government partnerships and other cooperative ventures. Present capabilities include planning and management functions as well as financial and partnership capacities. Evidence of commitment is requested in the form of proposed investment and investment-to-date in debt, equity and in-kind contributions.

Part II, The Expert Reviewer's H Scan

---

[11] For example, proposals at the concept or early R&D phase may not reliably be able to estimate or forecast economic and environmental impacts.

[12] The Hydrogen Program Plan 1993-1997 defines an energy pathway as ". . a conversion chain linking primary resources to ultimate end-use consumption."

The second part of H Scan consists of the reviewer's assessment of the proposer's part of H Scan. Recognized experts in the field perform this function. The reviewer's expert knowledge and experience constitute the basis for their opinions about proposed work. The Hydrogen Program Management recognizes their expertise as valuable programmatic resource, critical to the evaluation process. An expert will review the proposer completed H Scan to assess the project's prospects for success. The expert will then synthesize this appraisal in the H Scan Reviewer Summary and Recommendations. The evaluation of a given proposal (see figure 5 *-Reviewer Summary and Recommendations*) will address the following topics:

- Technical and commercial challenges to DOE categories and relevant market sector
- Linkages with the Hydrogen Program and DOE
- Impact of success or failure and benefits of programmatic funding
- Appropriate types of near-term development
- Suggestions on the role for DOE and other participants
- Suggestions for level of additional analysis needed
- Assessment of technical and commercial risk

Each of these items may entail a subjective and an objective assessment of risk. Reviewers may assess certain subjective aspects of risk in narrative format. The criteria listed in Figure 5 are only preliminary and are subject to refinement as the H Scan/AHP process is fully developed. Ultimately, these criteria may be more expansive than Management developed criteria.

Then, reviewers would rate the proposals on an absolute basis against management developed criteria and sub-criteria on a scale that ranges from poor to outstanding, for example. As an example of the absolute ranking mode, see Figure 6 - *Evaluate Production R&D Proposals* for a graphic representation of the criteria and sub-criteria structured in a hierarchical format. Included are definitions of the following criteria and sub-criteria:

- Cost
  -DOE
  -Cost-sharing

- Quality
  -Staff
  -Facility
  -Experience
  -Commitment

- Technical
  -Insight
  -Approach
  -Outcome

Rating the proposal by sub-criteria and criteria will allow reviewers to quantify their subjective assessment of findings and recommendations for a given proposal.

Product #3 - Analytic Hierarchy Process (AHP)

The third component in the planning and evaluation process is the Analytic Hierarchy Process (AHP). The AHP is a relatively new judgmental modeling technique developed by Dr. Thomas Saaty, formerly of the Wharton School of Business, now with the University of Pittsburgh.[13] This method has proven valuable in assisting decision makers with evaluation and understanding of complex problems of choice.

The AHP is a multi-level decision construct that integrates management defined evaluation and selection criteria. AHP reflects management's objectives in supporting individual hydrogen technology categories during their full research and development cycles. This is critical inasmuch as the 1994 Hydrogen Program Review identified *Ranking Systems Analysis* as a first priority in hydrogen R&D needs for the specific purpose of "identifying energy significant, economically attractive roles for hydrogen."[14]

The AHP will be conducted in a two phase process. In Phase I, Hydrogen Program Management will pair wise compare the component technologies (production, storage, transmission and end-use) to determine their relative importance for programmatic purposes. (See figure 7 - *Determine Importance of Component Technologies in H_2 Program*). H_2 Program Management will then define the higher level global strategic and tactical objectives (criteria) that are important to Program success. These criteria will be assembled into a decision hierarchy that uses pair-wise comparison to determine their placement and relative value.

The actual candidates for evaluation will be technology families that are grouped according to some method of distinction. For example, grouping could come by stage of development (research, development, validation) as a sub-category to technology component (production, storage, transport, end-use). Within the technology component type, families to be evaluated will then be set out. See Figure 8 -*Evaluate H_2 Technology Families* for a breakdown within all hydrogen component technologies.

The results of phase I will provide a global strategic context for proposal evaluation.

In Phase II, the AHP will establish criteria of a more specific, or "local" nature that will directly relate to the technologies being evaluated. The results of this phase of the AHP analysis will provide a specific economic, technical and environmental context for proposal evaluation. The local criteria will be constructed to allow for refinement and accommodation of sensitivity analyses.

---

[13] "Saaty, Thomas. 1982. *Decision Making for Leaders*. California: Wadsworth.

[14] *Hydrogen Program Review*, 1994.

Two examples currently being tested are used here to illustrate the local nature of the sub-criteria. Figures 9 - *Evaluation of Hydrogen Production Research Technologies* and Figure 10 - *Demonstration Evaluation* contain hierarchies with technical and economic sub-criteria. Figure 9 would apply to the research stage of the development process; this hierarchy would evaluate particular technology families by sub-criteria. Figure 11 would apply to the validation or demonstration stage of development; that hierarchy would evaluate proposed demonstrations by pertinent criteria and sub-criteria. The latter hierarchy may be further expanded to accommodate sub-system evaluations by technology family. This is important because proposals will be scaled by the relative strategic importance of the particular technology family.

The results of Phase II will provide a local strategic context for proposal evaluation.

Activities

The second element in the H Scan/AHP decision process is activities. The activities entailed in this process are illustrated in Figure 1, the *H Scan/AHP Decision Process* flow chart that numbers each step and indicates who is responsible for what actions. For all activities, the Hydrogen Technical Advisory Panel (HTAP), a statutory creation of the Matsunaga Act, may participate in an advisory capacity.[15]

It should be emphasized that this process is not meant to be rigid or overly prescriptive. Rather the intent of developing the H Scan/AHP decision process is to facilitate reasonable, analytically defensible decision-making that reflects programmatic goals and incorporates the full array of variables that may impact project success. The process is also intended to allow for communication about proposals between DOE H_2 Program Management and project proposers during the review and evaluation process.

The eight steps in the H Scan/AHP Decision Process are listed below:

<u>Step 1</u> DOE H_2 Program Management:

- Defines programmatic criteria for incorporation in the decision model
- Integrates criteria into the H Scan
- Integrates criteria into the AHP
- Solicits requests for proposals with cost and technical data as well as H Scan Part I, the proposer prepared H Scan

<u>Step 2</u> Industry/Proposers:

- Complete and return proposals with cost and technical data as well as proposer H

---

[15] See Public Law 101-566, 101st Congress, "Spark M. Matsunaga Hydrogen Research, Development and Demonstration Act of 1990," Sec. 108. Technical Panel, for the enabling act's language creating the Hydrogen Technical Advisory Panel.

Scan forms; all data sources used in proposal are referenced and utilized consistently unless otherwise specified

Step 3 DOE H_2 Program Management:

- Accepts proposals, screens for completeness; in the event that a proposal is incomplete, coordinates with proposer to finish proposal wherever possible
- Forwards to DOE experts for review

Step 4 H_2 Experts:

- Review proposals; communicate requests for clarification and more information with DOE H_2 Program Management; verify data sources where appropriate (in conjunction with DOE H_2 Program Management if necessary)
- Prepare H Scan Summaries of findings and recommendations
- Score proposals in absolute ranking using DOE H_2 Program criteria and sub-criteria for H Scan
- Return proposals to DOE H_2 Program Management

Step 5 DOE H_2 Program Management:

- Reviews H Scan Summaries of findings and recommendations as well as absolute ranking of proposals
- Selects proposals deemed suitable for further evaluation

Step 6 DOE H_2 Program Management:

- Proceeds with AHP evaluation and ranking of proposals using H Scan Summaries as guidance and data sources

Step 7 DOE H_2 Program Management:

- Reviews results of AHP evaluation and ranking
- Modifies results to reflect management concerns, as appropriate

Step 8 Doe H_2 Program Management:

- Completes proposal selection process
- Notifies industry of proposal status

Data Reference Requirements

Relevant Findings from 1994 Program Review

The data requirements associated with completion of the H Scan and application of the AHP are challenging. Certain findings from the 1994 Program Review provide parameters for establishing data reference requirements. Key findings are listed below:

- Creation of a universal data base to clarify pathway input assumptions would be helpful
- Economic analysis should be performed with every technology development program
- Use of systems analysis would be helpful to evaluate technologies not currently included in the H_2 Research and Development Program

Apart from these considerations, it is clear that data reference requirements vary with the stage of technology development and the nature of the proposal. Data reference requirements correspond with particular levels of techno-economic analysis. In ascending order of complexity, techno-economic analysis includes literature search, cost boundary analysis and detailed cost analysis. A literature search might be the most (or perhaps only) appropriate form of analysis for a technology at the concept stage. In contrast, a detailed cost analysis might be essential for a mature technology at the validation phase. To maximize effectiveness of the decision analysis process it is critical to appropriately identify data requirements and analysis needs, both present and future.

Other kinds of support analysis that might be required to supplement the basis techno-economic study include market analysis, life analysis and environmental analysis.

A large literature consisting of various kinds and levels of relevant analysis already does exist. There is no central repository for this information, however. It is dispersed throughout universities and industry as well as the Department of Energy and its laboratories. The Energetics *Technology Characterization for the E3 (Energy, Economics, Environment) Pathway Analysis* can be considered a major resource for the H Scan/AHP decision process, especially for the DOE H_2 Program and its expert reviewers. It is not inconceivable that this tool would be made available to project proposers in the future. Use of this resource by project proposers would help to assure a higher level of consistency in assumptions and approach and thereby facilitate the planning and evaluation process.

Preliminary Milestones for Development of H Scan/AHP Decision Process

A preliminary schedule with major milestones has been developed for the H Scan/AHP decision process. The schedule covers the period from spring into the fall of 1995. Milestones appear below:

● Development of DOE H_2 Program goals and objectives by H_2 Program Management	Summer '95
● Development and testing of H Scan	Fall '95
● Development and testing of AHP	Fall '95

Conclusion

Hydrogen has begun to capture the imagination of the world. The challenge now is to hold that interest. The H Scan/AHP decision process can contribute to retention and enhancement of the world's interest in and stakeholder support of hydrogen by facilitating planning and selection of successful projects for the Hydrogen Program portfolio. This is a significant step toward a world in which hydrogen will play an important role.[16]

Acknowledgments

Michael Antal, Ph.D., University of Hawaii
For sharing his philosophical approach to planning in science, and in particular, his favorite quotations on the nature of questions in science.

Joe Badin, Energetics
For review of the Analytic Hierarchy Process (AHP) and suggestions on integration with AHP in his capacity as Principal Investigator of the Energetics Systems Analysis work.

Joan Ogden, Ph.D., Princeton University
For assistance on the topic of data reference requirements in her capacity as hydrogen expert and contractor for the DOE H_2 Program.

Jim Ohi, Ph.D., NREL
For his guidance and assistance on development of the H Scan process in his capacity as Principal Investigator of the NREL Supporting Analysis task.

Sandy Thomas, Ph.D., Directed Technologies, Inc.
For his review and suggestions on H Scan.

---

[16] The process brings to mind the famous admonition of turn-of-the-century architect Sanford White: "Make no small plans. They have no power to move men's minds."

References

American Solar Energy Association (ASES), 1995. "Platform Statement of American Solar Energy Society." Denver: ASES.

DiPietro, J. Philip, Badin, Joseph S. for Energetics, Inc. 1994. *Technology Characterizations for the E3 (Energy, Economics, Environment) Pathway Analysis*. Washington, D.C.: U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy.

Galvin, Robert. 1995 Task Force On Alternative Futures for the Department of Energy Labs - The Galvin Commission Report. Washington, D.C.: U.S. Department of Energy.

Golden, B.L., Wasil, E.A., and Harker, P.T., editors. 1989. *The Analytic Hierarchy Process: Applications and Studies*. New York: Springer-Verlag.

Hamalainen, Raimo P. June 1992. "Politics and Policy: Decision analysis makes its way into environmental policy in Finland." *OR/MS Today*, 40-43.

International Energy Agency. 1991. *Renewable Energy Technology Applications*. Paris, France: OECD/IEA.

International Energy Agency. 1991. *Choosing Priorities in Science and Technology*. Paris, France: OECD/IEA.

Leary, Warren E. April 16, 1995. "Use of Hydrogen as a Fuel Moving Closer to Reality." *The New York Times*.

Liberatore, Matthew J. 1988. "A Decision Support System Linking Research and Development Project Selection with Business Strategy." *Project Management Journal*, XIX, Number 5:14-21.

McFarlane, Robert. From *Professor Michael Antal's personal collection of quotations*. University of Hawaii.

Saaty, T.L. 1980. *The Analytic Hierarchy Process*. New York: McGraw Hill.

Saaty, T.L. 1982. *Decision Making for Leaders*. California: Wadsworth.

Saaty, T.L. and Kearsn, K.P. 1985. *Analytical Planning: The Organization of Systems*. Pergamon Press.

Short, Walter, Packey, Daniel J., and Holt, Thomas. 1995. *A Manual for the Economic Evaluation of Energy Efficiency and Renewable Energy Technologies*. DE-AC 36-83CH10093. Golden, CO: National Renewable Energy Laboratory.

U.S. Department of Energy, Office of Conservation and Renewable Energy. 1992. *Hydrogen Program Plan, FY 1993-1997.* DOE/CH10093-147. Golden, CO: National Renewable Energy Laboratory.

U.S. Department of Energy, Office of Conservation and Renewable Energy. 1993. The Hydrogen Program Implementation Plan, FY 1994-1998. Washington, D.C.: U.S. DOE.

U.S. Department of Energy, Office of Conservation and Renewable Energy. 1994. The FY 1995 Annual Operating Plan. Washington, D.C.: U.S. DOE.

U.S. Department of Energy, Office of Conservation and Renewable Energy. The Hydrogen Program Overview. Washington, D.C.: U.S. DOE.

U.S. Department of Energy, Office of Conservation and Renewable Energy. The Hydrogen Program Summary, FY 1994. Washington, D.C.: U.S. DOE.

Walker, Robert A. (The Honorable). 1995. *Hydrogen Futures Act of 1995.* Washington, D.C: legislation pending before the U.S. Congress.

Weisman, Alan. March 19, 1995. "The Last Best Hope of Earth -- Harnessing the Big H," *Los Angeles Times Magazine.*

Wittengenstein, Ludwig. From *Professor Michael Antal's personal collection of quotations.* University of Hawaii.

Figures

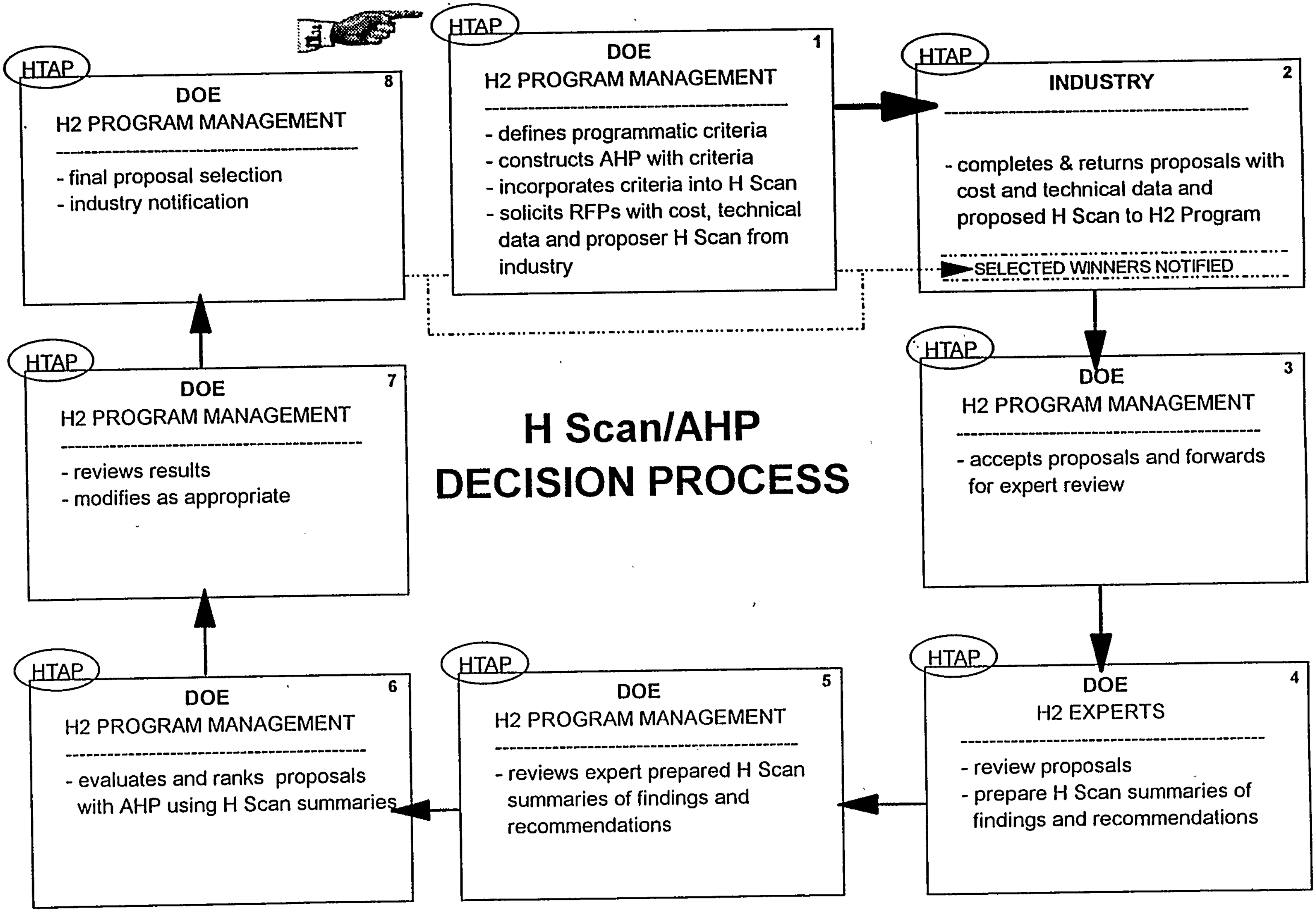
HTAP
DOE
H2 PROGRAM MANAGEMENT
1
- defines programmatic criteria
- constructs AHP with criteria
- incorporates criteria into H Scan
- solicits RFPs with cost, technical data and proposer H Scan from industry
HTAP
INDUSTRY
2
- completes & returns proposals with cost and technical data and proposed H Scan to H2 Program
SELECTED WINNERS NOTIFIED
HTAP
DOE
H2 PROGRAM MANAGEMENT
3
- accepts proposals and forwards for expert review
HTAP
DOE
H2 EXPERTS
4
- review proposals
- prepare H Scan summaries of findings and recommendations
HTAP
DOE
H2 PROGRAM MANAGEMENT
5
- reviews expert prepared H Scan summaries of findings and recommendations
HTAP
DOE
H2 PROGRAM MANAGEMENT
6
- evaluates and ranks proposals with AHP using H Scan summaries
HTAP
DOE
H2 PROGRAM MANAGEMENT
7
- reviews results
- modifies as appropriate
HTAP
DOE
H2 PROGRAM MANAGEMENT
8
- final proposal selection
- industry notification
H Scan/AHP
DECISION PROCESS

Figure 1

H SCAN
Draft 3/15/95

Section 1 - Sheet 1

DATE ____
PROPOSER ____

Section I - THE CANDIDATE TECHNOLOGY: SYSTEM AND MARKET

Description

1a DOE Classification
Production ____
Storage ____
Infrastructure ____

End-Use
Transportation ____
Utilities ____
Industry ____
Building ____

1b Relevant Technical and Commercial Challenges faced by DOE Categories and End-Use Sectors

2a Affected Segment of Market Place
Petroleum Refining ____
Chemical Manufacting ____
Small Volume ____

Metal Fabrication ____
Oil & Fat Hydrogenation ____
Rocket Propulsion ____
Government ____
Public Utilities ____
Other ____
(Specify) ____

2b Relevant Challenges, Opportunities, Threats Faced by Market Segment

3a MATURITY LEVEL OF PROPOSED TECHNOLOGY SYSTEM

CONCEPT ____
LAB R&D ____
PROCESS ENGINEERING ____
PILOT PLANT ____
COMMERCIAL PLANT
ENGINEERING ____
COMMERCIAL PLANT ____

3B COMMENTS

4A HOW CLOSE (NEAR TERM -5); MID TERM (15), LONG-TERM (15+ YEARS)] TO DEVELOPMENTAL MILESTONES:
POC (TECHNICAL FEASIBILITY) ____
TECHNICALLY PROVEN (PRE-COMMERCIAL) PROTOTYPE ____
SUBSEQUENT COMMERCIAL PROTOTYPES ____

4b) COMMENTS

5 PATHWAY - Description of components and complete pathway for technology

____

____

____

____

5a Is H2 Technology/System a Substitute for an Existing Product?
YES ____ NO ____

5b If yes, describe the existing product

H SCAN
Draft 3/15/95

Section 1 - Sheet 1

DATE __________
PROPOSER __________

Is it an enabling technology? Explain.

YES____ NO______

5c If yes, is it a whole ____ or a partial _____ substitute?

5d Is this a "redesign" issue? Explain.

5e Is there a systems approach to the analysis?

5f What are the terms of guarantees, warranties and service? What kind of financing is offered?

6a If a substitute, identify and briefly characterize competition.

6b Is/are Existing Products/Processes Challenged?
YES __ NO __
NO ____
If yes, describe

6c Possible Competitive Advantages of Candidate Technology:

7a MARKET SEGMENT IMPACTED BY H_2 TECHNOLOGY SYSTEM

Size $__________ units______
Location ____________________
Domestic ______________
Local ______________
Regional ______________
National ______________
International ______________
Infrastructure ______________

Other ________________________
____

7b COMMENTS

7c IF PROPOSED H_2 TECHNOLOGY IS A SUBSTITUTE PRODUCT, CHARACTERISTICS OF SPECIFIC EXISTING PRODUCT MARKET; IF A NEW PRODUCT, FORECAST OF MARKET POTENTIAL:

Size $____________ units________
Location ____________________
Domestic
Local
Regional
National
International
Product Distribution Network

Other ________________________
____

Attach Assumptions

7d COMMENTS
____
____
____
____
____
____

Figure 2

H SCAN Sheet3 DATE ________

Draft 3/15/95 PROPOSER ________

Section III - ENVIRONMENTAL IMPACTS

1) Emissions displacement

-Carbon units ________ $________ aggregate

-Other pollutants:

type ______________ units _______ $/unit_______ $______aggregate

type ______________ units _______ $/unit_______ $______aggregate

type ______________ units _______ $/unit_______ $______aggregate

2) Other externalities

-Institutional ____

-Social ____

3) Stakeholders ____

Figure 3

H SCAN
Draft 3/15/95

DATE ________
PROPOSER ________

Section V - CAPABILITIES, EXPERIENCE, COMMITMENT:

Suitability of Proposers for Participation

PREVIOUS EXPERIENCE

1) GENERAL ______________________________

2) MANAGEMENT ______________________________

3) WITH H2 RELATED APPLICATIONS ______________________________

4) WITH COMMERCIALIZATION ______________________________

5) WITH GOVERNMENT PARTNERSHIPS ______________________________

6) WITH OTHER KINDS OF COOPERATIVE VENTURES ______________________________

Figure 4

H SCAN
Draft 3/15/95

DATE ________
PROPOSER ________

b) PRESENT CAPABILITIES

1) PLANNING CAPACITY ________________________________

2) FINANCIAL CAPACITY ________________________________

3) PARTNERSHIP CAPACITY ________________________________

c) FINANCIAL COMMITMENT

1) TOTAL ESTIMATED COST: $______

2) PROPOSED INVESTMENT: $_____ DEBT _____ EQUITY_____ IN-KIND ________
COMMENTS: ________________________________

3) PROPOSER INVESTMENT-TO-DATE: $_____ DEBT _____ EQUITY_____ IN-KIND ________
COMMENTS: ________________________________

Figure 4

DATE ________
PROPOSER ________

H SCAN
Draft 3/15/95

REVIEWER SUMMARY & RECOMMENDATIONS

1a DOE Classification
Production ________

Storage ________
Distribution ________
Utilization
End-Use
Transportation ________
Utilities ________
Industry ________
Building ________

2a Affected Segment of Market Place

Petroleum Refining ________
Chemical Manufacting ________
Small Volume ________
Metal Fabrication ________
Oil & Fat Hydrogenation ________
Rocket Propulsion ________
Government ________
Public Utilities ________
Other ________
(Specify) ________

1b TECHNICAL AND COMMERCIAL CHALLENGES TO DOE CLASSIFICATIONS AND END-USES
nature and importance

2B CHALLENGES, OPPORTUNITIES, THREATS TO MARKET SECTOR: nature and importance

3) COMPLETED H SCAN VOLUMES

ATTACHED: Section I CANDIDATE TECHNOLOGY SYSTEM AND MARKET

Section II ENERGY EFFICIENCY AND ECONOMICS: PERFORMANCE, COST AND BENEFIT IMPACTS

Section III ENVIRONMENTAL IMPACTS

Section IV REGULATION AND OPERATION

Section V CAPABILITIES, EXPERIENCE, COMMITMENT

4 COMPONENTS OF THE PATHWAY: focus on innovative components

5 - WHAT IS LINKAGE OF PROPOSAL WITH LONG-TERM STRATEGIC PROGRAM GOALS FOR H_2 PROGRAM? Comments:

6 - WHAT IS LINKAGE WITH DOE COMMERCIALIZATION, GLOBAL CLIMATE CHANGE AND EXPORT OBJECTIVES? Comments:

Figure 5

H SCAN
Draft 3/15/95

DATE ________
PROPOSER ________

7 RISK

a) Probability of technical success

b) Probability of commercial success

i. experience and qualifications of proposer

ii. proposer's investment (to-date and proposed)

iii. proposer's financial condition

iv. type of other participation

v. cooperation/support from other stakeholders

vi. viability of product/process to be "substituted" or redesigned

vii. market analysis findings and forecast - is the market opportunity real? is the proposal realistic relative to the market analysis?

viii. environmental impact

ix. energy efficiency impact

x. economic impact

xi. public perception of risk association with H2

viii. Insurance (Type, requirements)

c) Impact of success or failure on DOE Program

8a WHAT TYPE OF DEVELOPMENT ACTIVITY WOULD BE APPROPRIATE IN THE NEAR-TERM FOR THE PROPOSED TECHNOLOGY/SYSTEM?
- POC (TO ESTABLISH TECHNICAL FEASIBILITY) ________
- PRE-COMMERCIAL (CLEARLY TECHNICALLY PROVEN) PROTOTYPE ________
- INITIAL COMMERCIAL PROTOTYPE ________
- SUBSEQUENT COMMERCIAL PROTOTYPE ________
- R&D TECHNOLOGY TRANSFER ARRANGEMENT ________

8b PRELIMINARY SUGGESTION ON ROLE OF H_2 PROGRAM IN THIS ACTIVITY:
TECHNICAL ADVISOR ________
FINANCIAL PARTICIPANT ________
SUPPORT FOR R&D TECH TRANSFER ________

8c WHAT LEVEL OF ANALYSIS WOULD BE SUITABLE FOR ASSESSMENT
PRE-FEASIBILITY ________
FEASIBILITY ________
DETAILED ENGINEERING ________
PROJECT ENGINEERING ________

Figure 5

H SCAN
Draft 3/15/95

DATE ________
PROPOSER ________

8d SUGGESTED ROLE OF OTHER POTENTIAL PARTICIPANTS IN THIS ACTIVITY:

TECHNICAL ADVISOR ____________
FINANCIAL PARTICIPANT ____________ SUGGESTED LEVEL $______
SUPPORT FOR TECH TRANSFER ____________ SUGGESTED LEVEL $______
OTHER ____________
____
____

8e IDENTIFY POTENTIAL PARTICIPANTS

9 DESCRIBE BENEFIT OF PARTICIPATION TO H2 PROGRAM

10 FINDING

Significant Challenges

Significant Impacts

Value Added to H_2 Program

Other

RECOMMENDATION

Type of Development Activity

Role of H_2 Program

Associated Level of Analysis

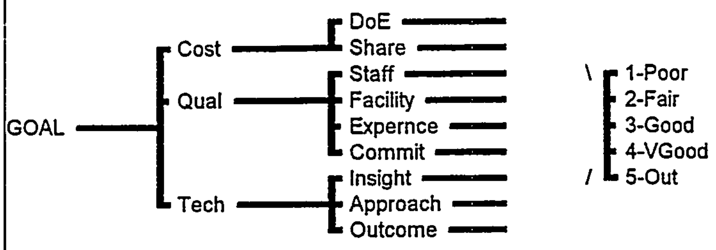
H_2 Program Investment

Investment Priority

Other

Figure 5

Evaluate Production R&D Proposals

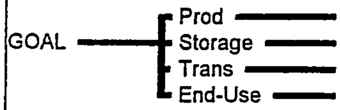


Abbreviation	Definition
Cost	Proposal Cost
Qual	Quality of the proposers
Tech	Technical Aspects
DoE	DoE Cost
Share	Cost share from the proposer
Staff	Qualifications of the technical staff
Facility	Suitability of proposers facilities
Expernce	Experience in this project area
Commit	Commitment to the work
Insight	Technical insight in the statement of work
Approach	Feasibility of the technical approach
Outcome	Projected improvement on existing BAT

Figure 6

Beta Tester

Determine Importance of Component Technologies in H2 Program

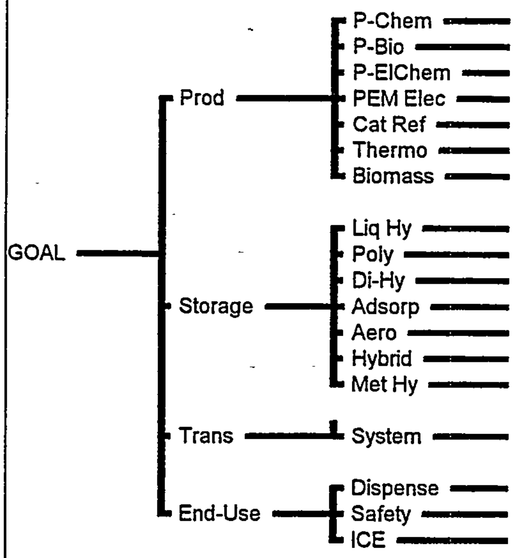

GOAL
Prod
Storage
Trans
End-Use

Abbreviation	Definition
Prod	Hydrogen Production
Storage	Hydrogen Storage
Trans	Hydrogen Transmission
EU	Hydrogen Utilization
End-Use	Hydrogen Utilization
External	External Support for Component Technologies
R&D?	Lack of R&D by other Investigators
Cost	Cost to Research and Develop Component Technologies
Feasible	Feasibility (technical and economic) of best technologies

Figure 7

Beta Tester

Evaluate H2 Technology Families



Abbreviation	Definition
Prod	H2 Production
Storage	H2 Storage
Trans	H2 Transmission
End-Use	H2 End-Use
P-Chem	Photo-Chemical Processes
P-Bio	Photo-Biological Processes
P-ElChem	Photo-ElectroChemical Processes
PEM Elec	PEM Electrolysis
Cat Ref	Catalytic Reforming
Thermo	Thermo--Chemical Cycles
Biomass	Biomass Conversion
Liq Hy	Liquid Hydrides, Methyl Cyclohexane
Poly	Non-Classical Polyhydrides
Di-Hy	Di-Hydrides
Adsorp	Adsorption
Aero	Aero-Gels
Hybrid	Liquid Gas Hybrid
Met Hy	Metal Hydride
System	System Studies
Dispense	H2 Dispensing Station
Safety	Safety and Leak Detection

~~Figure 8~~

Beta Tester

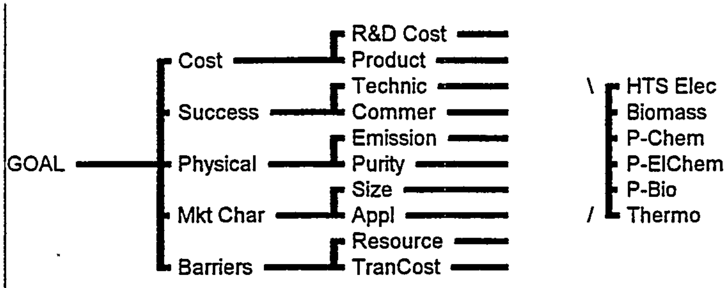
Evaluate H2 Technology Families

ICE	ICE Performance Improvement

Figure 8

Beta Tester

Evaluation of Hydrogen Production Research Technologies

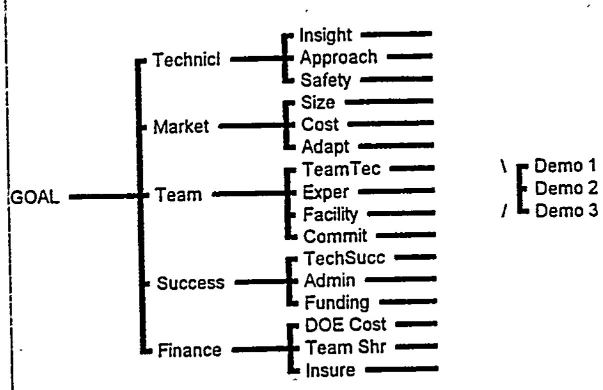


Abbreviation	Definition
Cost	Projected cost of produced hydrogen
Success	Probability of success
Physical	Physical characteristics of technology process
Mkt Pot	Projected Market for the Technology
R&D Cost	R&D cost to fully develop the technology
Product	Projected unit hydrogen cost after full development
Technic	Probability of technical success
Commer	Probability of commercial success
Emission	Emissions from the production process
Purity	Purity of the untreated produced hydrogen
Mkt Char	Projected market characteristics for the technology
Size	Potential market size for the produced hydrogen
MakeProd	Production Constraints
Resource	Constraints on available resources
TranCost	Transmission cost to storage, end-users
Barriers	Barriers to large scale production
Appl	Scope of applications
HTS Elec	High temperature steam electrolysis
Biomass	Biomass gasification
P-Chem	Photochemical processes
P-ElChem	Photoelectrochemical processes
P-Bio	Photobiological processes
Thermo	Thermochemical cycles

Figure 9

Beta Tester

Rank Hydrogen Demonstration Proposals

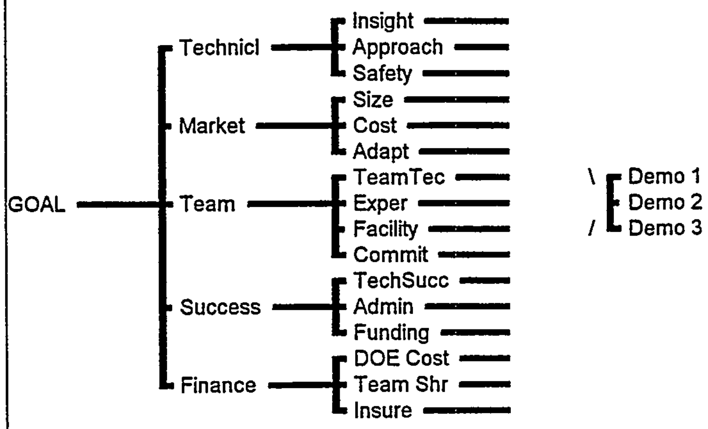


Abbreviation	Definition
Technicl	Technical aspects of the demonstration proposals
Market	Market aspects of the demonstration proposals
Team	Team qualifications of the proposers
Success	Success probabilities of important factors
Finance	Financial aspects of the demonstration proposals
Insight	Techical insight evidenced by proposed component integration
Approach	How well the approach conforms to the statement of work
Safety	The real and perceived safety of the operating demonstration
Size	The size of the potential market directly targeted by the demo
Cost	The relative cost of of the pathway vs conventional technologies.
Adapt	The potential adaptability of the pathway to other applications
TeamTec	The technical qualifications of the team members
Exper	Experience of the team with the proposed technologies
Facility	Quality of proposer facilities to build and conduct the demo
Commit	Level of commitment by the team to the project
TechSucc	Probability of the project's technical success
Admin	Probability that the team can meet all administrative hurdles
Funding	Probability that the project will remain funded to completion
DOE Cost	DOE's financial outlay in absolute dollars
Team Shr	Percent cost share by the proposing team
Insure	Availability and cost of insurance for the project
Demo 1	
Demo 2	
Demo 3	

Figure 10

Beta Tester

Rank Hydrogen Demonstration Proposals



Abbreviation	Definition
Technicl	Technical aspects of the demonstration proposals
Market	Market aspects of the demonstration proposals
Team	Team qualifications of the proposers
Success	Success probabilities of important factors
Finance	Financial aspects of the demonstration proposals
Insight	Techical insight evidenced by proposed component integration
Approach	How well the approach conforms to the statement of work
Safety	The real and perceived safety of the operating demonstration
Size	The size of the potential market directly targeted by the demo
Cost	The relative cost of of the pathway vs conventional technologies.
Adapt	The potential adaptability of the pathway to other applications
TeamTec	The technical qualifications of the team members
Exper	Experience of the team with the proposed technologies
Facility	Quality of proposer facilities to build and conduct the demo
Commit	Level of commitment by the team to the project
TechSucc	Probability of the project's technical success
Admin	Probability that the team can meet all administrative hurdles
Funding	Probability that the project will remain funded to completion
DOE Cost	DOE's financial outlay in absolute dollars
Team Shr	Percent cost share by the proposing team
Insure	Availability and cost of insurance for the project
Demo 1	
Demo 2	
Demo 3	

Figure 10

Beta Tester

SYSTEMS ANALYSIS -
INDEPENDENT ANALYSIS AND VERIFICATION

J.S. Badin and J.P. DiPietro
Energetics, Incorporated
Columbia, MD 21046

Abstract

The DOE Hydrogen Program is supporting research, development, and demonstration activities to overcome the barriers to the integration of hydrogen into the Nation's energy infrastructure. Much work is required to gain acceptance of hydrogen energy system concepts and to further develop them for implementation. A systems analysis database has been created that includes a formal documentation of technology characterization profiles and cost and performance information. Through a systematic and quantitative approach, system developers can understand and address important issues and thereby assure effective and timely commercial implementation. This project builds upon and expands the previously developed and tested pathway model and provides the basis for a consistent and objective analysis of all hydrogen energy concepts considered by the DOE Hydrogen Program Manager. This project can greatly accelerate the development of a system by minimizing the risk of costly design evolutions, and by stimulating discussions, feedback, and coordination of key players and allows them to assess the analysis, evaluate the trade-offs, and to address any emerging problem areas. Specific analytical studies will result in the validation of the competitive feasibility of the proposed system and identify system development needs. Systems that are investigated include hydrogen bromine electrolysis, municipal solid waste gasification, electro-farming (biomass gasifier and PEM fuel cell), wind/hydrogen hybrid system for remote sites, home electrolysis and alternate infrastructure options, renewable-based electrolysis to fuel PEM fuel cell vehicle fleet, and geothermal energy used to produce hydrogen. These systems are compared to conventional and benchmark technologies. Interim results and findings are presented. Independent analyses emphasize quality, integrity, objectivity, a long-term perspective, corporate memory, and the merging of technical, economic, operational, and programmatic expertise.

Introduction

The methodology being applied in this analysis task builds upon the developed Energy, Economics, Emissions (E3) Pathway Model to construct a complete representation of the proposed hydrogen energy system concept, encompassing all aspects from primary energy source to end-use. All the data inputs (i.e., capital cost, efficiency, useful life) required to determine the total delivered cost of the energy carriers and the final energy service cost are researched and incorporated into the model. Consistent macro-economic and standard equipment cost and performance assumptions are employed across all pathway analyses. A technology cost and performance database has been developed to serve as the program's technology characterization reference book. Where necessary, the standard input assumptions are adjusted to concept-specific conditions (i.e., the marginal cost of off-peak electricity). All input data are presented to the system proposers to ensure concurrence. For each hydrogen energy concept, several alternate pathways are constructed that represent systems that can provide the same energy services. These pathways serve as competitive benchmarks to which the proposed concept can be compared. For example, a novel hydrogen production concept would be compared to both conventional steam reforming of natural gas and water electrolysis using off-peak electricity. Environmental impacts in terms of physical quantities of emissions such as CO_2, SO_2, NO_X are included in the comparisons. Certain states have prescribed a set of dollar values per ton of emissions. This option is also available. Sensitivity analyses are performed to achieve the following objectives: 1) identify what technologies in the proposed concept drive the total cost of the energy commodity and services provided; 2) determine what improvements (if any) are needed to make the concept competitive with the benchmark technologies; and 3) determine the effect that changes in the macroeconomic assumptions will have on the life-cycle cost of both the proposed concept and benchmark technologies. The system proposer and other system study investigators review the draft final report and all reasonable efforts are made to achieve concurrence. This process allows for coordination of on-going systems analysis studies within the program.

Technical Approach

This effort will result in a uniform set of thorough, defensible and objective published analyses of proposed hydrogen research and demonstration concepts. This work will enable the DOE Hydrogen Program Manager to set priorities in the implementation of hydrogen energy systems and allocate limited resources accordingly. Moreover, a complete analysis will expedite commercialization of meritorious concepts and focus system developers' and principal investigators' efforts on areas where advancements are required. The hydrogen energy system concepts under evaluation are listed below and grouped by competing energy options (benchmark technologies).

Figure 1 presents a schematic of the independent analysis and verification process. As shown, the following steps are involved:

Proposed System Concept. A hydrogen energy system or technology proposal is received by the DOE Program Manager. The system is described with a certain level of technical

Table 1. System Analyses

Benchmark	Hydrogen Energy System	Status
Fossil-Based Options (turbines, fuel cells, steam reforming)	An integrated peak electricity and merchant hydrogen production process using a solar reactor and a reversible hydrogen bromine cell (Solar Reactor Technologies Inc.)	Draft Complete
	Hydrogen production via municipal solid waste gasification (Lawrence Livermore National Laboratory, Texaco)	Draft in Progress
	Switchgrass electro-farm using biomass gasifier and PEM fuel cell for electric power market (Electro-Farming, Inc, H Power, and Auburn University)	Draft Complete
	Geothermal energy used to both displace fossil-based electricity generation and produce hydrogen during off-peak hours (Stanford University and General Electric Company)	Draft in Progress
Diesel Generator/ Stationary Battery Storage	Wind-based electricity generation system using hydrogen energy storage (Aleut Corp, Alaska Global Hydrogen, ADL, Lawrence Livermore National Laboratory)	Draft Complete
Gasoline Vehicles, Battery Electric Vehicles	Home electrolysis used to supply hydrogen to residential customers without the investment in hydrogen transport infrastructure (Lawrence Livermore National Laboratory)	Draft Complete
	PEM fuel cell vehicle fleet fueled by hydrogen from renewable-based electrolysis (Schatz Energy Research Center/Humboldt State, Lawrence Livermore National Laboratory, and the City of Palm Desert, CA.)	Draft in Progress

specifications, operating profile, and cost estimates. If the system is deemed potentially feasible and appropriate for inclusion into the program, then a comprehensive analysis begins.

Pathway Representation. The system is represented as a set of linked technology process nodes from production through utilization. In this way, delivered hydrogen costs and levelized cost of energy services can be determined. Each technology node is analyzed using the given data. This information is then verified through conversations with other vendors, a literature search, and consultation with the Technology Characteristics Database compiled for the DOE Hydrogen Program. This database covers a wide range of technologies from generation, production, storage, transport, and utilization. The cost and performance information is regularly updated.

Baseline Results and Sensitivities. The analysis is run and parameters such as capital cost, efficiency, capacity factor, discount rate, and system life are varied and their impacts on the delivered energy costs are noted.

Comparison to Benchmark and Conventional Technologies. Each proposed system can be considered a competing alternative that provides energy services that are being served by conventional technologies. Other emerging technologies are also competing for market share. Hydrogen systems need to be economically competitive and offer environmental and other advantages over other options in order to reach the marketplace. These benchmark analyses combined with the sensitivity studies result in competitive threshold targets for cost and performance.

Report. A draft report is sent to the original system proposers and other principal investigators for review, comments, and interaction. When a common understanding is reached, a final report is issued. This project will result in a set of such analyses.

DOE management will consider the results of these analyses along with other program-oriented factors in its decision making process. Proposed hydrogen systems that are developed or proceed to demonstrate will be re-analyzed by incorporating additional data and operating experience into the verification process.

Results and Discussion

In this section the following results will be discussed:

- Technology Cost and Performance Database
- Representative Analysis Example
- Base Case Comparisons
- Representative Analysis Summary Sheets

Technology Cost and Performance Database. In order to ensure consistent input values to this analytical effort, a database was created to document completely all relevant technologies under consideration. Technology characterization sheets are provided. The following technology categories are included: electricity generation; hydrogen production; hydrogen and electricity storage, for both stationary and on-board applications; and hydrogen utilization. The database has been made widely available and is periodically updated.

Representative Analysis Example. The St. George Alaska Wind Turbine/Fuel Cell Project can serve as a typical example of the system analysis activities. The system consists of fourteen 50-kW wind turbines for a total plant capacity of 700-kW, alkaline electrolyzers, gaseous hydrogen storage in cylinders (500 psi), and a 200-kW phosphoric acid fuel cell.

This system is to serve a small remote island off the coast of Alaska with about 180 people that are getting their electricity by diesel generator at an average residential rate of 39.5 ¢/kWh. After collecting and analyzing cost and performance data for this system, the cumulative cost of energy through each process step is determined and shown in Figure 2. Figure 3 presents results from a typical parametric sensitivity study. The base case wind/hydrogen system delivers electricity at 46.5 ¢/kWh, however, reasonable adjustments to parameters such as capacity factor, fuel cell efficiency and wind turbine capital cost will bring this system into the competitive range. Figure 4 shows the impact of capital cost and fuel cell efficiency on delivered electricity cost.

Base Case Comparisons. Figure 5 presents the base case results of the systems listed in Table 1. It should be noted that these are interim results and further analysis is underway. As with the wind example, parametric studies indicate the level of cost reductions and system improvements needed to meet the cost of the benchmark technology. In all cases, conditions can be established where the hydrogen systems are competitive to the benchmark systems.

Representative Analysis Summary Sheets. The summaries of the home electrolysis and the hydrogen bromine electrolysis systems are highlighted. For the home electrolysis concept, Figure 6 illustrates the pathway representation of the system concept and of competing alternatives. Figure 7 shows a comparison of delivered energy costs from each alternative. Figure 8 comprises the summary sheet which details a system synopsis, quantitative results, advantages, disadvantages, and technology development needs. Similarly, Figures 9 and 10 depict pathway representations of the hydrogen bromine electrolysis concept and its alternatives as well as the analysis summary sheet.

Conclusions and Future Work

Figure 11 shows how this project and its products fit into the overall Hydrogen Program. The proper execution of this task requires extensive coordination with other system analysis investigators funded through the program. The review and iteration cycle of the system analysis result in concurrence and an updated and expanded Hydrogen Program Technology Cost and Performance Database. The published set of system studies will be used as a means to involve industrial participants at the System Analysis Working Group and also to be distributed at other industry outreach meetings. These and future studies will be coordinated with the International Energy Agency (IEA) Hydrogen Agreement Task 11 - Integrated Systems. Synergies will be fully realized between this effort and the industry outreach activities in terms of data and information exchanges and discussions of results and their implications.

Acknowledgements

This work has been funded by the U.S. Department of Energy and was performed under subcontract to R.K. Sen & Associates, Inc. (No. 94 DE-CE001-ENI001). The authors wish to thank the principal investigators of the system study analyses for their cooperation and helpful feedback.

References

Badin, J.S., G. Kervitsky, S. Mack, 1994. "Energy Pathway Analysis," In *Proceedings of the 1994 DOE/NREL Hydrogen Program Review*, 51-65, Livermore, CA.

Badin, J.S., J.P. DiPietro, 1994. *Technology Characterizations for the E3 (Energy, Economics, Environment) Pathway Analysis - Cost and Performance Database*, Energetics, Incorporated.

Badin, J.S., S. Tagore, 1994. "Energy Pathway Analysis - A Fuel Cycle Framework for System Studies," In *Hydrogen Energy Progress X*, 117-126, Cocoa Beach, FL.

Energy Information Agency, 1994. *Annual Energy Outlook*, U.S. Department of Energy.

Deluchi, Mark, Hydrogen Fuel-Cell Vehicles, Research Report UCD-ITS-RR-92-14, September 1992.

Smith, J. Ray, "The Hydrogen Hybrid Option," presented at the Workshop on Advanced Components for Electric and Hybrid Electric Vehicles, October 27-28, 1992.

Parker, Robin, Solar Reactor Technologies, Inc., Solar and Electrochemical Hydrogen and Electrical Energy Storage System, May 1994.

Ogden, Joan, et al., "A Technical and Economic Assessment of the Role of Natural Gas in a Transition to a Hydrogen Economy," presented at the 10th World Hydrogen Energy Conference, July 1994.

Blazek, C., and R. Biederman, Preliminary Assessment of the Technical and Economic Feasibility of Hydrogen Enrichment of Natural Gas, September 1992.

Figures and Tables

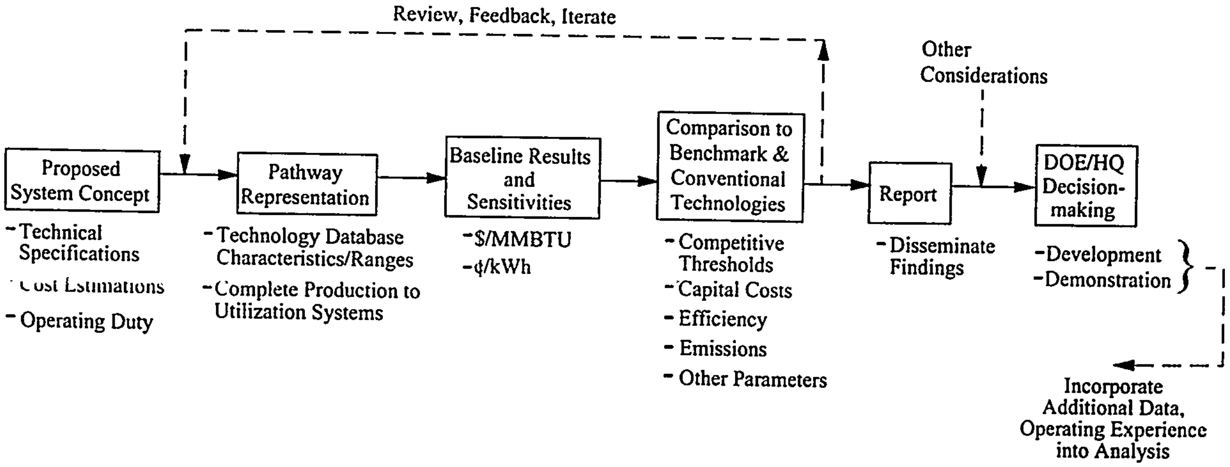


Figure 1. Independent Analysis and Verification Process

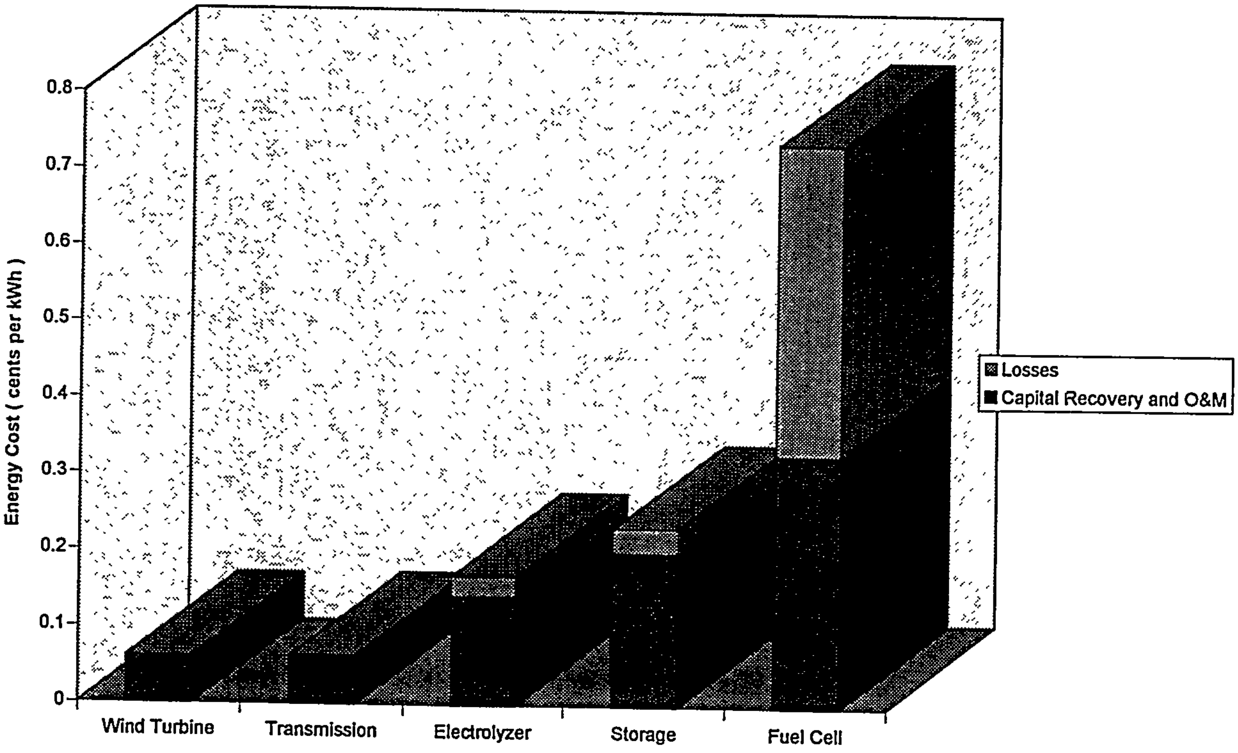


Figure 2. Cumulative Levelized Cost of Energy Across the Alaska Wind Load Matching System

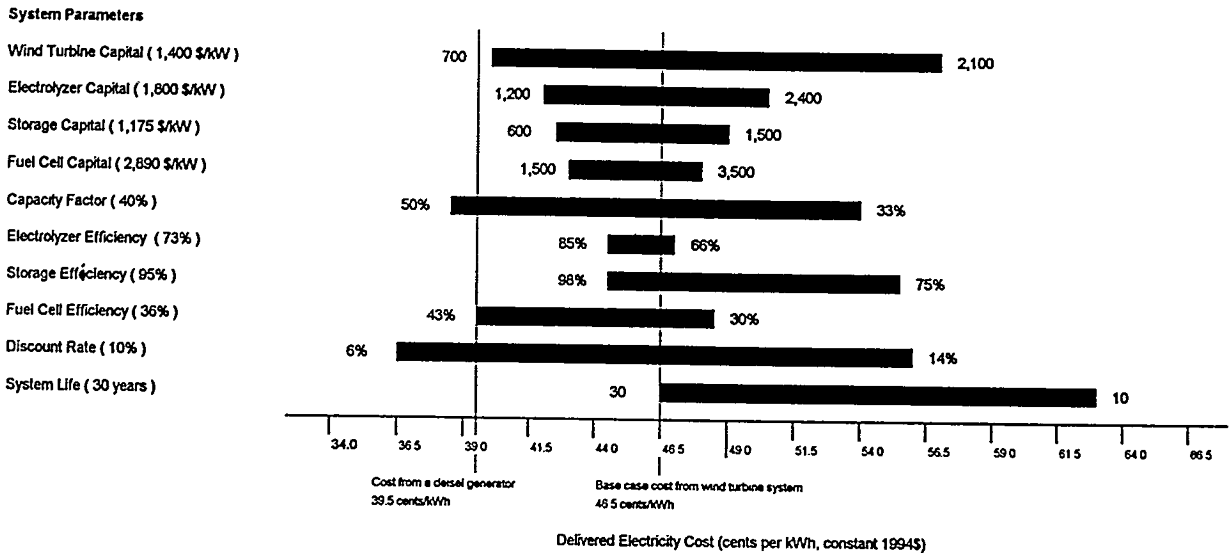


Figure 3. System Sensitivity Analysis

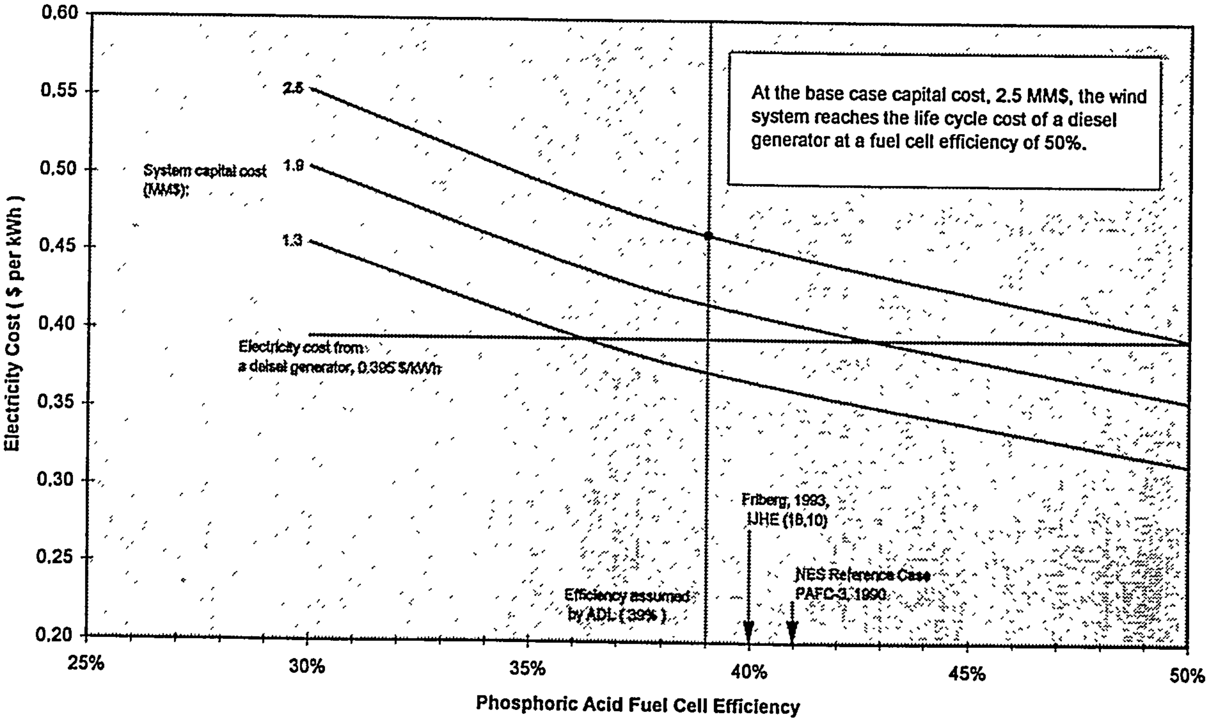
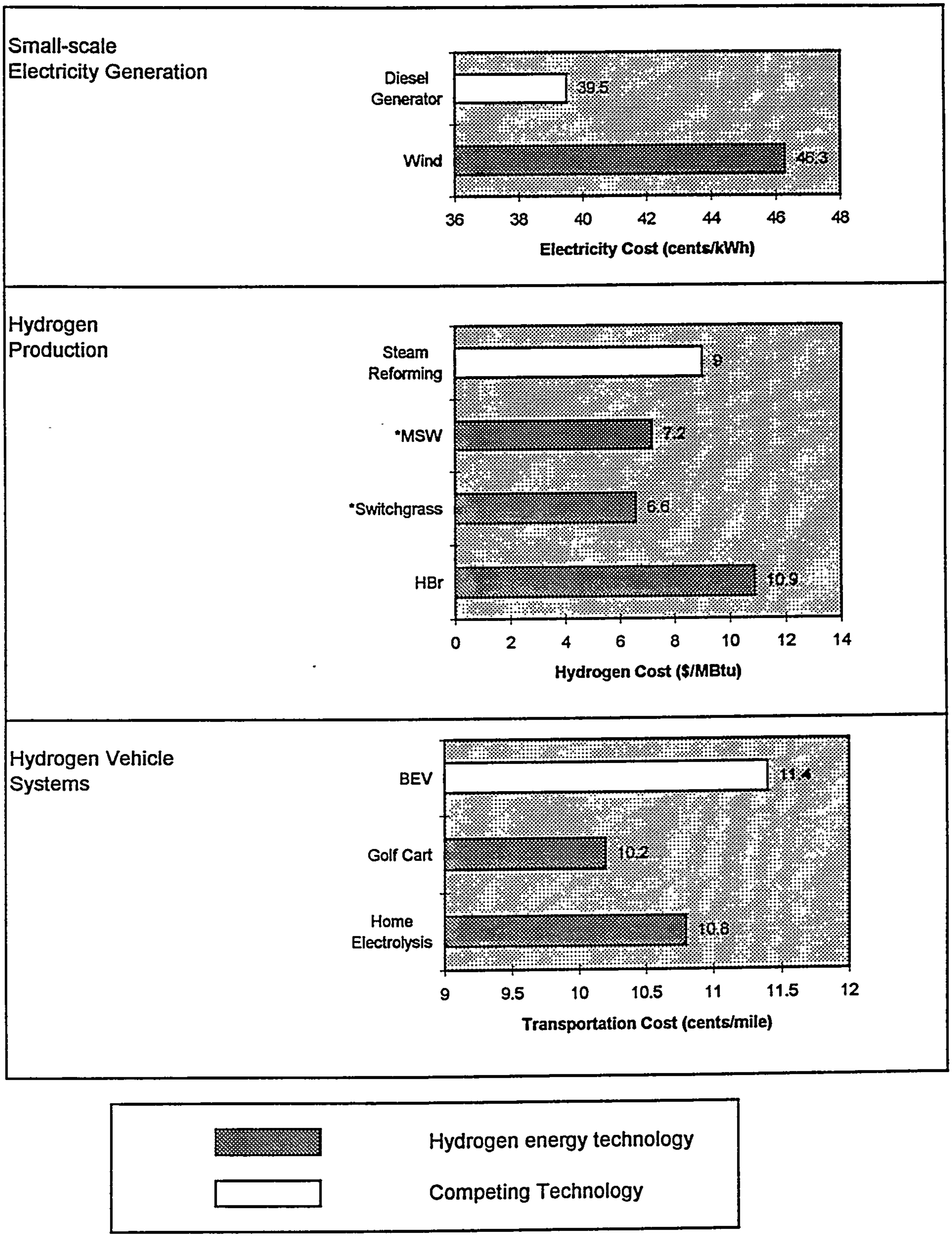


Figure 4. Electricity Cost as a Function of Fuel Cell Efficiency and System Capital Cost



* Analysis in Progress

Figure 5. Summary Comparisons of Base Case Hydrogen Energy Concepts

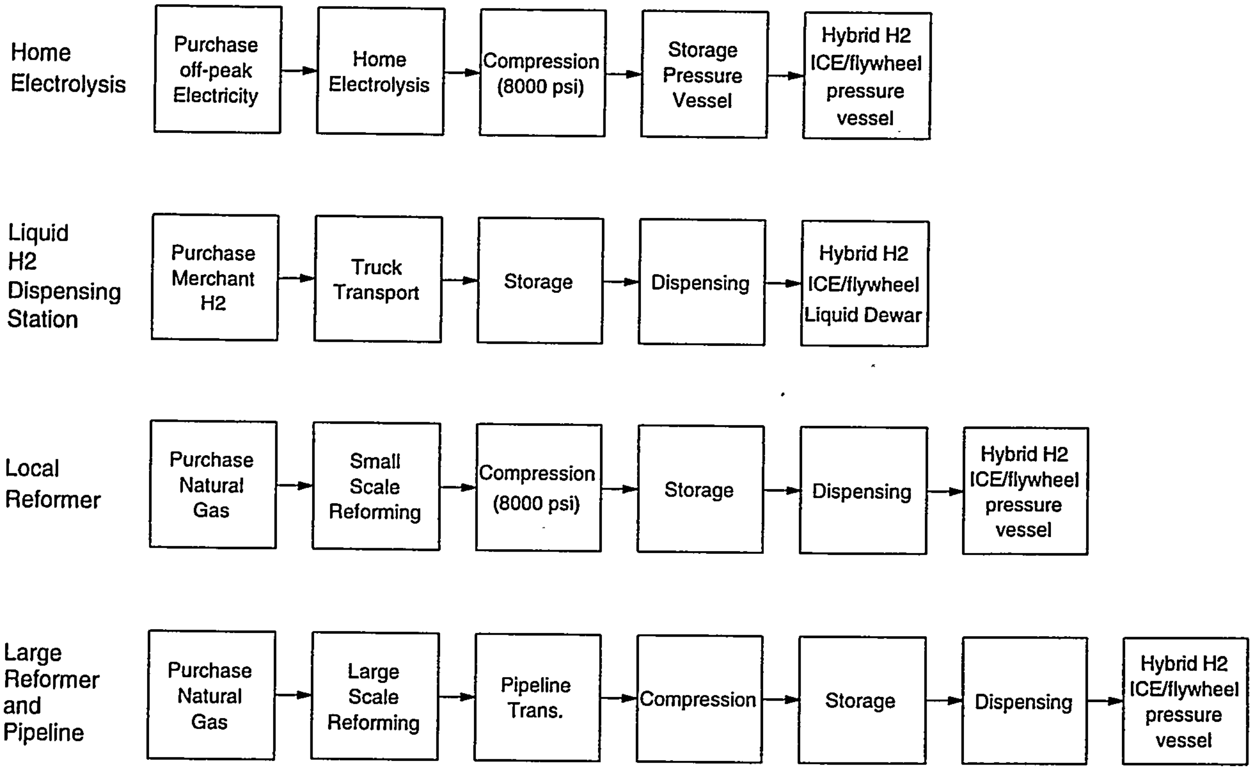


Figure 6. Pathway Analysis of the Home Electrolysis Concept

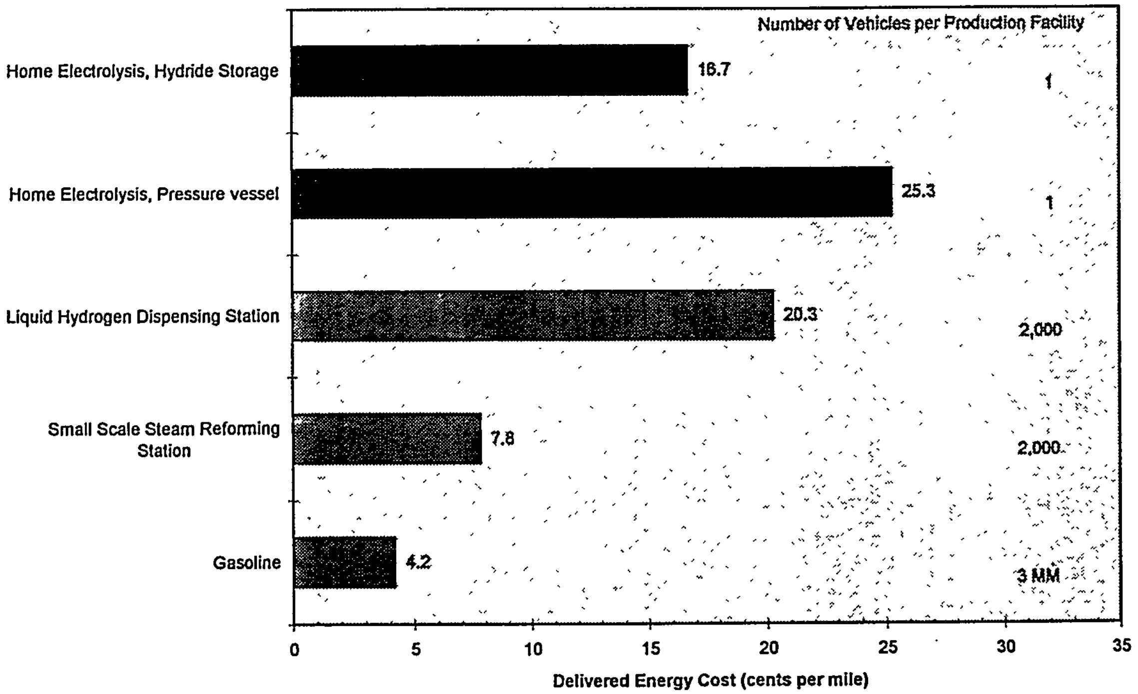


Figure 7. Delivered Energy Cost for Hydrogen Vehicle Systems

Figure 8. DOE Hydrogen Program. Systems Analysis Summary Sheet

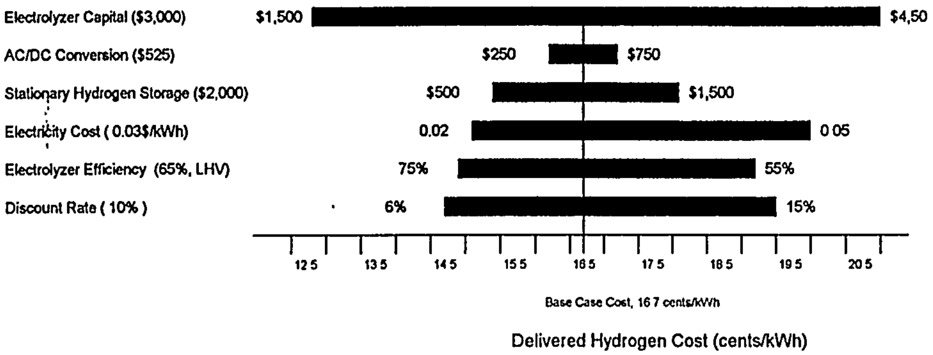
April 14, 1995

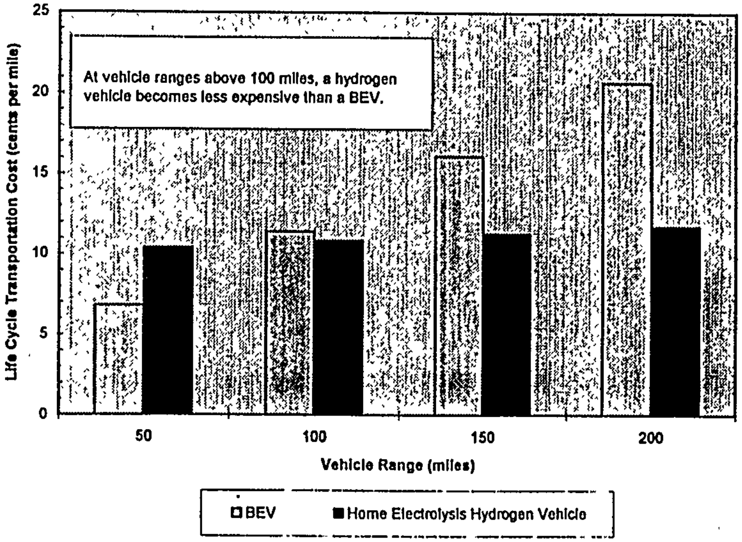
Concept Title: Home Electrolysis
Originator: LLNL
Analysis: Energetics, Incorporated

Concept Synopsis: A small scale electrolysis unit (2 kW) is located at a home to supply fuel for a commuter vehicle.

Competing Technologies: BEVs
Key Base Case Results: Delivered H_2 Cost: 16.7 cents/kWh
Transportation Cost: 10.8 cents/mile

Sensitivity Analysis:





Advantages	Disadvantage	Technology Development Needs
• Can be deployed without large investments in hydrogen transport infrastructure. • Amenable to a small number of geographically dispersed end-users. • Because refueling is convenient, vehicle range can be lower.	• No mass produced, small-scale electrolyzer exists, must be developed. • Applicability is limited to second car, commuter-like situations in which the vehicle is not driven more than 100-150 miles per day. • High cost per hydrogen delivered compared to larger systems (e.g., small scale reformer, 7.8 cents/kWh).	• Low-pressure (50-100 psi) on-board H_2 storage system offering 100-150 mile range and costing less than $800. • Low-cost, small-scale electrolyzer. 2 kW DC input, $3,000. • Hydrogen ICE/turbine/flywheel engine 100 $/kW, 0.4 kWh/mile.

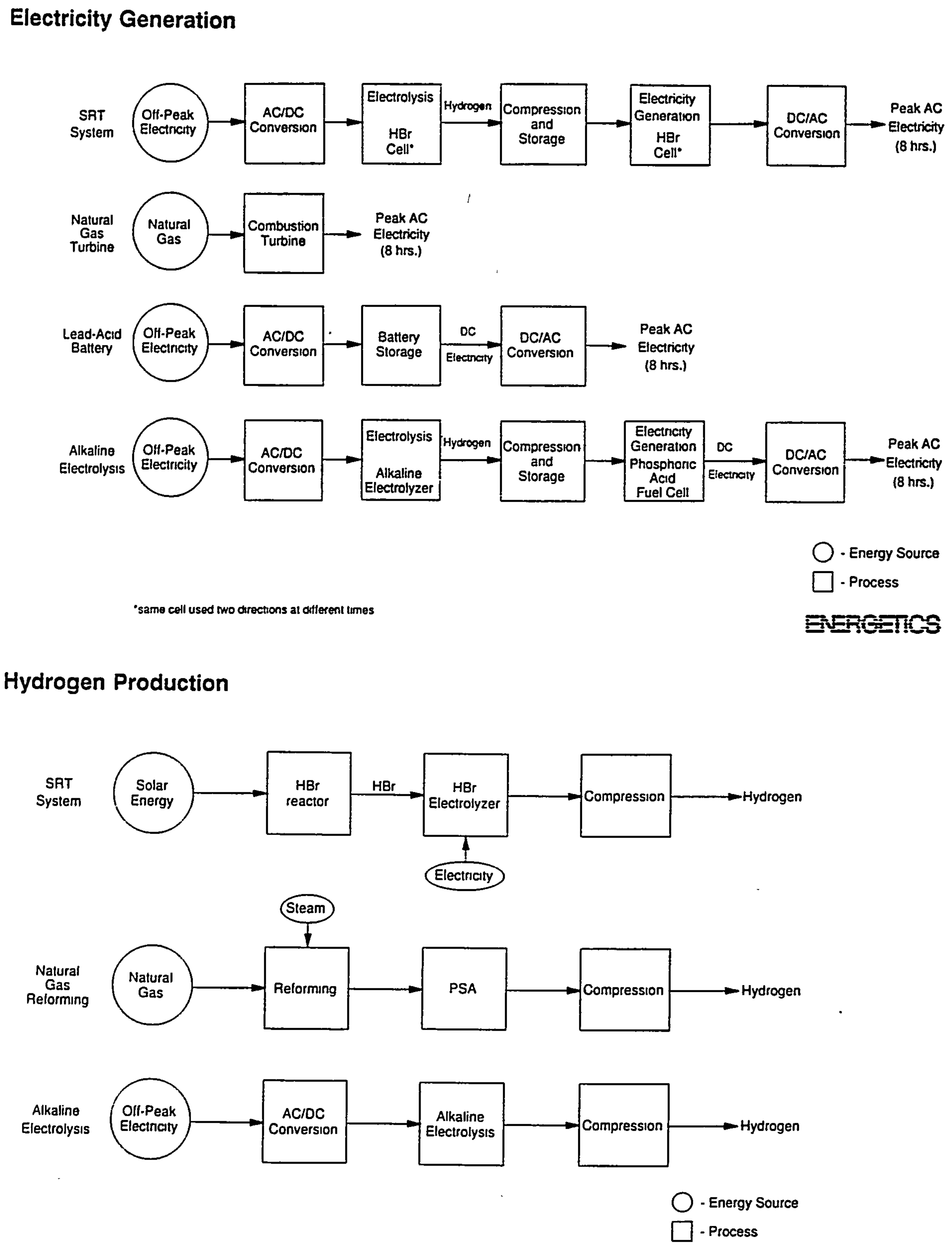


Figure 9. Pathway Analysis of the HBr-Based Electrolysis Concept

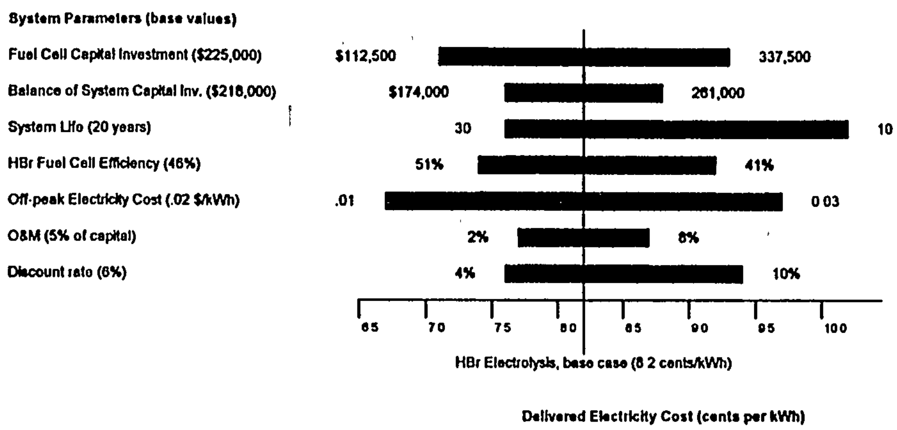
Figure 10. DOE Hydrogen Program. Systems Analysis Summary Sheet

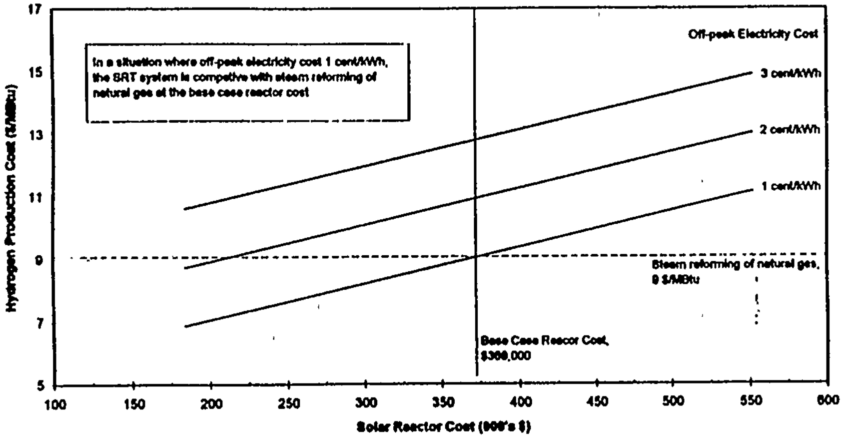
April 14, 1995

Concept Title: HBr Electrolysis
Originator: Solar Reactor Technologies
Analysis: Energetics, Incorporated

Concept Synopsis:	A reversible HBr cell is based at an industrial facility to store off-peak electricity as hydrogen and produce electricity during peak demand hours to lower the facility's electricity charges. During idle time the cell dissociates Hbr produced in a solar reactor to generate hydrogen for use within the facility.
Competing Technologies:	Natural Gas Turbines, Steam Reforming of Natural Gas
Key Base Case Results:	Peak Electricity Cost: 8.2 cents/kWh Hydrogen Cost: 10.9 $/MBtu

Sensitivity Analysis:





The solar reactor is sized to produce 43 MBtu of hydrogen per day (136,000 scf per day), at a 40% capacity factor

Advantages	Disadvantage	Needed Technology Developments
• High utilization of capital equipment compared to other renewable-based systems. • High efficiency energy storage (76% AC/AC) and low electricity consumption per hydrogen produced (.46 kWh/kWh HHV). • HBr, a liquid, is easier to handle than HCl.	• Natural gas turbine and steam reforming of natural gas are formidable competition.	• Solar-based hydrogen production process must be proven, efficiency and cost estimates must be firmed up. • 40% reduction from base case reactor cost needed to compete with steam reforming (2 ¢/kWh off-peak electricity cost).

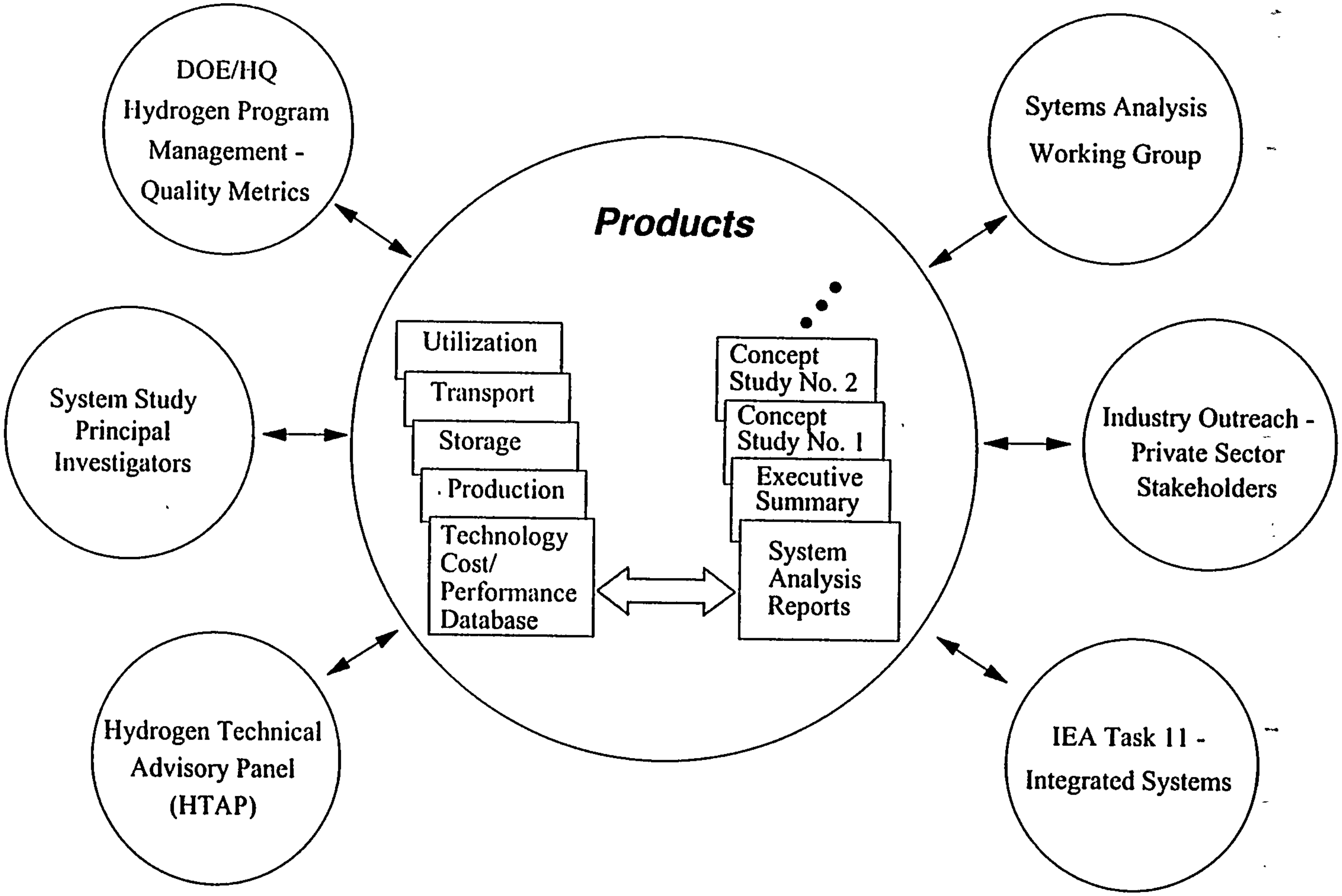


Figure 11. How This Project Fits Into the Overall Program

ELECTROLYTIC PRODUCTION AND DISPENSING OF HYDROGEN

C.E. (Sandy) Thomas
Ira F. Kuhn, Jr.
Directed Technologies, Inc.
4001 North Fairfax Drive, Suite 775
Arlington, Virginia 22203

Abstract

The fuel cell electric vehicle (FCEV) is undoubtedly the only option that can meet both the California zero emission vehicle (ZEV) standard *and* the President's goal of tripling automobile efficiency without sacrificing performance in a standard 5-passenger vehicle. The three major automobile companies are designing and developing FCEV's powered directly by hydrogen under cost-shared contracts with the Department of Energy.

Once developed, these vehicles will need a reliable and inexpensive source of hydrogen. Steam reforming of natural gas would produce the least expensive hydrogen, but funding may not be sufficient initially to build both large steam reforming plants and the transportation infrastructure necessary to deliver that hydrogen to geographically scattered FCEV fleets or individual drivers. This analysis evaluates the economic feasibility of using small scale water electrolysis to provide widely dispersed but cost-effective hydrogen for early FCEV demonstrations.

We estimate the cost of manufacturing a complete electrolysis system in large quantities, including compression and storage, and show that electrolytic hydrogen could be cost competitive with fully taxed gasoline, using existing residential off-peak electricity rates.

Introduction

Fuel cell electric vehicles (FCEV's) have the potential of increasing energy efficiency by a factor of 2.5 or more compared to the gasoline-powered internal combustion engine, while virtually eliminating urban smog precursors and carbon monoxide. The President's Partnership for a New Generation of Vehicles (PNGV) has set a goal of increasing vehicle efficiency by a factor of three. Replacing the internal combustion engine with a fuel cell plus electric motor drive train would achieve 83% to 90% of that goal. The small efficiency boost needed to reach the full 3X goal can be achieved relatively easily with some combination of reduced drag coefficient, reduced rolling resistance, or reduced weight. While battery powered EV's may also be able to achieve the 3X efficiency goal, most analysts concede that they will fall short of the required PNGV performance goals in terms of acceleration, range or possibly refueling time, and the extra weight of batteries will increase the difficulty of achieving the 3X goal.

To capitalize on the virtues of FCEVs, the nation must also develop a reliable source of hydrogen and the infrastructure to refuel vehicles. The Department of Energy is funding two analytical studies to evaluate the production of hydrogen based on steam reforming of natural gas. This approach has great merit, since the U.S. has large domestic reserves of natural gas, which is the least expensive transportation fuel and produces the least carbon dioxide -- the main greenhouse gas -- per unit of energy output.

Steam reforming of natural gas could eventually be the dominant mode of producing hydrogen for the next few decades, generating a robust hydrogen infrastructure that would provide a smooth and seamless transition to solar hydrogen as renewable energy became cost effective in the 21st century. Hydrogen produced from renewable sources would simply supplement natural gas-derived hydrogen when and where renewable hydrogen became economic. The market would decide. As natural gas prices inevitably rise, the cost of hydrogen from wind and biomass might cost less in the Midwest within a decade. Hydrogen from photovoltaics might be less expensive than natural gas in the southwest somewhat later. Renewable hydrogen would enter the market when and where it could compete economically with hydrogen derived from fossil fuels.

While steam reforming of natural gas may be the intermediate bridge to a renewable hydrogen future, it might have two limitations during the early years of such a transition: steam reformers may not scale down in size to the smaller units that might be needed initially, and natural gas is not available in all parts of the country. Large hydrogen production plants could utilize liquid hydrogen delivery trucks to provide service to remote areas, but the market will not support such an infrastructure initially.

As an alternative to steam reforming of natural gas, small quantities of hydrogen can be produced by electrolyzing water. Water and electricity are available virtually anywhere a vehicle might travel, and electrolyzers can be scaled down to very small sizes, including units to supply just one or two vehicles in a home. Small electrolyzers might even be mounted on trucks or vans that could accompany early FCEV prototype vehicles as they were demonstrated across the country. These mobile, van-mounted hydrogen generators could be plugged in to the local electrical grid in each city, generating the hydrogen while the FCEV was being driven around the city. The purpose of this study is to explore the economic viability of water electrolysis as a near-term alternative or complement to steam reforming of natural gas.

At first glance, using electricity to produce hydrogen instead of inexpensive natural gas might seem uneconomic. As shown in Figure 1, electricity is the most expensive source of energy for transportation, primarily because two-thirds of the energy is lost at the utility generating station. Per unit energy delivered, residential electricity at 8.5 cents/kWh is 3.9 times more expensive than natural gas and 2.6 times more expensive than gasoline, including gasoline taxes.

However, DTI has estimated that a midsized passenger vehicle powered by fuel cells would have 2.68 times greater energy efficiency (LHV) on the Federal Urban Driving Schedule (FUDS) than that same vehicle powered with gasoline[1]. On a per mile basis, then, electricity and natural gas used to produce hydrogen would have a 2.68 times energy advantage over gasoline, as illustrated in Figure 2, assuming that gasoline fuels an internal combustion engine, while electricity and natural gas are used to produce hydrogen for FCEVs.

Figure 2 is based on the average U.S. residential electrical rate of about 8.5 cents/kWh. If we can obtain off-peak power in the range of 2 to 4 cents/kWh, then electricity could become competitive with natural gas as a feedstock for hydrogen generation, as shown in Figure 3. This figure shows only the potential fuel feedstock cost. The eventual hydrogen price will have to include capital recovery for the electrolyzer system, as discussed below.

The purpose of this study is to explore this potential of off-peak electricity to produce competitively priced hydrogen. The study concentrated on two tasks: an initial conceptual design of small electrolyzer systems including estimates of their efficiencies and costs, and a survey of off-peak electrical rates. The primary output from this analysis was the definition of system costs and electrical rates necessary to make electrolytic hydrogen cost competitive with gasoline for transportation[2].

---

[1] This efficiency gain of 2.68 is based on the lower heating value (LHV) of hydrogen, to correspond to the customary use of LHV to rate internal combustion engines. A Taurus-class vehicle with 19 mpg energy efficiency consumes 6,050 BTU/mile (LHV), while we estimate that the same vehicle powered by a fuel cell system would consume 15 pounds of hydrogen to cover 342 miles on the Federal Urban Driving Schedule, or 2,260 BTU/mile.

[2] For those drivers who base their decision on life cycle costs of owning and operating a vehicle, it may not be necessary for hydrogen costs be competitive with gasoline. Fuel accounts for less than 10 to 15% of life cycle costs, and the longer lifetime and reduced maintenance expected from fuel cell vehicles may offset higher hydrogen costs. Nonetheless, we assume conservatively here that many drivers will insist on comparable fuel prices at the pump.

Electrolyzer System Definition

An electrolytic hydrogen fuel dispensing system would have at least six components as shown in Figure 4: the electrolyzer itself, a compressor, several storage tanks, the dispensing hose and coupling, plus controls and safety equipment. We are assuming that the unit would be contained in a shed outside the home garage or fleet vehicle facility.

We have sized two systems for this evaluation: a two-car FCEV family and a 50-car fleet. We assume a Taurus-like FCEV that would consume 526 pounds of hydrogen each year, or 1.44 pounds per day. But the electrolyzer must be capable of producing hydrogen at rates above this average to meet weekly, seasonal or other variations in driver habits. We have arbitrarily chosen a surge factor of 1.5 for a two-car family. The home electrolyzer must therefore produce at least 4.3 pounds of hydrogen per day.

For a 50-car fleet operator, the electrolyzer would need to provide enough fuel for an average of 18,000 miles per car per year, or 790 pounds per vehicle. The surge factor could be reduced to 1.28, or a total electrolyzer capacity requirement of 140 pounds of hydrogen per day.

We assume onboard compressed hydrogen storage at 5,000 psi. The refueling station must therefore supply hydrogen at pressures above 5,000 psi, say at 6,000 to 8,000 psi. In theory the electrolyzer itself could provide the high pressure. The electrochemical loss for operating an electrolyzer at high output pressure is not large. The electrolyzer cell voltage required increases with the logarithm of the pressure ratio[3]:

$$\Delta E = \frac{3RT}{4F} \times \log P_r \qquad (1)$$

where P_r = ratio of output pressure to ambient pressure,
R = gas constant,
T = temperature (°K), and
F = Faraday constant.

This equation predicts a voltage increase of about 36 mv at 100 psi and 25 °C, rising to 94 mv at 2,000 psi and 115 mv at 6,000 psi. In terms of voltage efficiency, an electrolyzer operating with 100 psi output at 1.55 volts might need only 1.63 volts to operate at 6,000 psi output. This would correspond to a voltage efficiency drop from 95.5% to 90.8%. For a PEM electrolyzer, the back diffusion through the membrane at high pressure would cause some recombination of hydrogen and

---

[3] A.P. Fickett and Fritz R. Kalhammer, "Water Electrolysis," Chapter 1 of Hydrogen: Its Technology and Implications, Edited by Kenneth E. Cox and K.D. Williamson, CRC Press, Cleveland, Ohio, 1977, pg. 9.

oxygen, or a current density drop of four to eight percent[4]. The net energy efficiency drop might be from 80% to 70% (HHV).

A six to ten percent drop in energy efficiency might be worth the elimination of a compressor from the refueling system. However, higher pressure, especially up to 6,000 psi, would probably place other mechanical constraints on the electrolyzer. One manufacturer has designed a PEM electrolyzer that operates with a hydrogen output pressure of 2,000 psi.[5] This design evolved from an electrolyzer that produced oxygen on board a submarine, where the higher hydrogen pressure was required for overboard disposal of hydrogen, considered a waste product in this application![6]

If the electrolyzer cannot be built to operate at 6,000 psi, there still may be economic merit in providing high electrolyzer output pressure, say 2,000 psi, to reduce the burden on the compressor. A single stage compressor could then boost the pressure from 2,000 to 6,000 psi.

The theoretical pumping power required is quite small for the electrolyzer flow rate of about 69 SCF/hour.[7]. Assuming adiabatic compression, the power required would be:

$$P_a = M_f \times R \times T \times \frac{\gamma}{(\gamma - 1)} \times \left[\left(\frac{P_o}{P_i} \right)^{\frac{\gamma - 1}{\gamma}} - 1 \right] \tag{2}$$

where M_f = hydrogen mass flow rate (moles per second),
R = gas constant (8.314 J/mol-°K),
T = absolute temperature (°K),
P_i = inlet pressure to compressor,
P_o = outlet pressure, and
γ = the ratio of specific heats (1.42 for hydrogen).

For the home refueling system with a flow rate of 69 SCF/hr (0.045 g/sec), the theoretical compressor power required would be 0.6 kW (0.8 hp) for compressing 100 psi to 6,000 psi assuming

---

[4] Private communication with Jim McElroy of Hamilton Standard, January 6, 1995.

[5] The Hamilton Standard "SPE Hygen-90 Automotive Hydrogen Fuel Generating System" generates up to 12 pounds of hydrogen per day at 2,000 psi.

[6] Private communication, Jim McElroy, December 21, 1994.

[7] We assume here that "Standard Cubic Feet" (SCF) is defined at 70°F and one atmosphere, or a density of 0.00521 pounds per cubic foot, as summarized by the Compressed Gas Association publication CGA G-5-1991, Table 1, pg.5.

75% efficient adiabatic compression. If the electrolyzer output pressure was increased to 2,000 psi, then the theoretical compression power required would fall by a factor of 6.1. A 75% efficient mechanical compressor would then need to supply only 0.1 kW (0.13 hp) to boost the hydrogen from 2,000 to 6,000 psi.

The recommended characteristics of the electrolyzer system components are summarized in Table 1.

Cost Estimates

System Capital Cost Estimates

While a detailed cost analysis of an electrolytic hydrogen refueling station was beyond the scope of this small study contract, we surveyed the literature and talked with a limited set of hardware suppliers to estimate the possible capital costs, assuming high volume manufacturing.

Electrolyzer Capital Cost

Most cost studies reported in the literature are limited to very large, single electrolyzer plants with outputs ranging from 30 to 300 tons of hydrogen per day, whereas the hydrogen refueling systems considered here only require 4.3 pounds (home system) to 138 pounds (50-car fleet) of hydrogen per day. We must therefore extrapolate down by factors of 400 to as much as 140,000 in hydrogen output capacity to provide capital cost data for our model.

The results of our literature review are summarized in Table 2 and illustrated in Figure 5 as a function of hydrogen output. In all cases, the reported cost data have been converted to dollars per kilowatt output of hydrogen, using the lower heating value (LHV) of hydrogen -- $\$/kW_{out}$ -LHV. Some authors specify the capital costs per unit of input electrical energy to the plant, which neglects the efficiency of the plant. We have used the estimated plant efficiency, if available. Otherwise we have assumed an electrolyzer efficiency of 67.5% (LHV, or 80% HHV). All cost estimates have been converted to 1995 dollars using the GNP implicit price deflator.

As shown in Figure 5, there are only two electrolyzer cost estimates in the small hydrogen output range of interest to this study. The Lawrence Livermore National Lab estimated costs of $\$1480/kW_{out}$ for the small home electrolyzer in very small production quantities, based on discussions with electrolyzer suppliers. Hamilton Standard estimated that home electrolyzers could be built at a cost of $\$330/kW_{out}$, assuming that they manufactured 100,000 units per year. The manufacturing cost estimate was made by the Carrier Division of United Technologies that makes home air conditioners in very large quantities.

These two estimates can be reconciled by referring to historic "learning curves" for other home electronic products as shown in Figure 6. Reduction in cost by this factor of 4.5 is similar to actual experience with television sets. We have therefore used the capital cost estimate of $\$300/kW_{out}$ for small electrolyzers in large volume manufacturing.

Table 1. Recommended Specifications for a Conceptual Electrolytic Hydrogen Refueling System

		Residential		Fleet	
Number of Vehicles		2		50	
Miles per year per vehicle		12000		18000	
H_2 Consumption (lbs/mile)		0.04386		0.04386	
Surge Factor		1.5		1.28	
Operating Time (hours/day)		12		12	
H_2 Production	(lbs/day)	4.33		138	
	(SCF/day)	830		26,570	
	(SCF/hour)	69.2		2,214	
	(kW$_{out}$ - LHV)[8]	5.67		174	
Storage Pressure (psi)		6,000		6,000	
Electrolyzer Output Pressure (psi)		100	2000	100	2000
Compressor Power (75% eff. & adiabatic)	(kW)	0.6	0.1	19.2	3.2
	(hp)	0.8	0.13	25.7	4.3
Storage Capacity	(lbs of H_2)	36		276	
	(SCF)	6,900		53,000	
	Actual Vol (ft^3)	21.5		165	
Number of Storage Tanks		>3		>5	

Compressor Cost

Capital costs for compressors in most studies in the literature are also based on low volume

---

[8] The term "kW$_{out}$" refers to the output lower heating value (LHV) of hydrogen, using a heat of combustion of 268.8 BTU/ft^3, Ibid. CGA Table 1.

manufacturing. For home electrolyzers, the emerging natural gas refueling industry may provide a better estimate for our purpose. For example, FuelMaker of Toronto, Canada is marketing a small compressor for home refueling of natural gas vehicles. This unit delivers 1.7 SCFM of natural gas at pressures up to 3,000 psi. We need twice the pressure but 70% of this flow rate.

The FuelMaker is selling for $4,000 now, but the manufacturer estimates that the price could be cut to $2,000 in quantities of 10,000, and to $1,120 in quantities of 100,000[9]. This corresponds to about $115/kW$_{out}$, which we use in our economic analysis for compressor cost.

Storage Cost

High pressure storage vessels are generally custom made, so that commercial prices are not indicative of high volume manufacturing rates. Tank cost estimates are shown in Figure 7 for 6,000 psi steel tanks and for 3,600 psi composite reinforced aluminum tanks in small quantities. The DTI datum point is our estimate for a nine cubic foot tank made from carbon filament composites, based on large scale production of tanks for a hydrogen vehicle. Clearly the stationary tank does not need to be made out of very expensive carbon fibers, when weight is of no concern and less expensive steel or aluminum tanks will suffice. But we use the high manufacturing volume carbon price estimate of $50 per pound of stored hydrogen for the economic analysis since we were not able to find an estimate for high volume manufacturing of aluminum or steel tanks.

Hydrogen Cost

To estimate the cost of hydrogen produced electrolytically using off-peak electricity, we assume that the total annual expenses are:

$$E = (CRF + o + i + t_p) \times C + C_e \tag{3}$$

where CRF = annual capital recovery factor:

---

[9] Private communication with Matthew Fairlie of Electrolyser Corporation, December 5, 1994.

Table 2. Electrolyzer Cost Comparison

	Date of Estimate	Cell Type	Efficiency	Plant Size		Cost ($94) ($/kW$_{out}$ - LHV)	
Organization			(HHV)	Input (MW$_e$)	Output (MW)	Alkaline	PEM
Fluor Daniel	1991	Alk.	0.716	100	60.5	770	
Electrolyser		Alk.	(0.80)	100	67	590	
Princeton	1994	Alk.	0.81	10	6.8	580	
Lawrence Livermore	1994	Alk.	0.81	2.5	1.7	1275	
Los Alamos	1986	Alk.	(0.80)	530	360	1350	
Stone & Webster	1984	PEM	0.675	17.5	10		850
Lawrence Livermore	1994	PEM	(0.80)	0.0025	0.00169		1480
General Electric	1977	PEM	(0.80)	50	34		210
Los Alamos	1986	PEM	(0.80)	530	360		410
Hamilton Standard	1994	PEM	(0.80)	0.011	0.00755		330
DTI Projection	1994	PEM	0.80	0.004	0.003		300
DOE/Energetics Projection	1994	Alk.	0.88	?	?	355	

$$CRF = \frac{d}{1 - \left(\frac{1}{1+d}\right)^N} \quad (4)$$

o = operating and maintenance costs (% of capital)
I = annual insurance (% of capital),
t_p = annual property taxes (% of capital),
d = discount rate,
N = the lifetime of the component in year (or economic recovery period),
C = total *installed* capital cost of electrolyzer, compressor, tanks and associated controls, and
C_e = annual cost of electricity to run both the electrolyzer and the compressor.

We calculated the hydrogen cost under three different financing scenarios: a business with 10% expected real ate of return over 15 years (after taxes and after correcting for inflation), a utility with 9% discount rate (6.3% corrected for inflation) and 15-year lifetime, and a third analysis assuming that the electrolyzer system would be included in a 30-year, 9% home mortgage.

For the home mortgage case, we assumed that the home-owner would deduct interest payments from both state and federal income tax, so the effective discount rate becomes:

$$d = i_m \times [1 - T_f - T_s \times (1 - T_f)] \quad (5)$$

where i_m = mortgage interest rate (9%)
T_f = federal marginal income tax rate (31% for couple with \$89K to \$140K income), and
T_s = state income tax rate (5.75%).

For the business case, we assume that the company demands an after tax real rate of return of 10%. The price of hydrogen is set so that the net annual revenues minus the net annual expenses yields zero present worth for the investment.

To account for inflation, the discount rate for the business becomes:

$$d = r + i + i \times r \quad (6)$$

where r = after-tax real rate of return on the investment in constant dollars, and
I = general inflation rate.

To account for corporate income tax, we must choose a depreciation schedule. The IRS currently specifies the Modified Accelerated Cost Recovery System (MACRS), which allows somewhat accelerated depreciation for the first five years of a 15-year recovery period. But MACRS also delays the first year depreciation by six months, which almost offsets the value of the accelerated recovery schedule from a net present value perspective. As a result, straight-line depreciation is a sufficiently accurate surrogate for MACRS on a zero present worth basis.

Including depreciation and federal income tax (property taxes are included in fixed expenses), the total business expenses become:

$$E_b = \left[\frac{\left(CRF - \frac{T_b}{n} \right)}{(1 - T_b)} + o + i + t_p \right] \times C + C_e \tag{7}$$

where T_b = the corporate income tax rate.

The resulting cost of hydrogen per pound is shown in Figure 8 as a function of the price of electricity for the three different financing arrangements. For comparison, we have also plotted the effective retail cost of gasoline converted to $/lb of hydrogen as a horizontal line on Figure 8, assuming 19 mpg for the internal combustion engine vehicle and crude oil selling at $20/barrel (about 78 cents/gallon retail). Since 18 gallons of gasoline yields the same range as 15 pounds of hydrogen, the conversion factor is 1.2 -- 78 cents/gallon is equivalent to 93.6 cents per pound of hydrogen as plotted as the lower horizontal line in Figure 8.

We have also plotted the retail price of gasoline, including federal, state and local excise taxes[10] on Figure 8. Normally this comparison would not be valid, since any motor fuel would eventually be taxed at the same rate as gasoline to raise money for highway construction. By this reasoning, we should only compare wholesale costs of alternative fuels without taxes. But, in this case, the home owner would have a choice between paying for retail gasoline with taxes, or using electricity to produce hydrogen at home. Initially, there would be no road tax on this source of fuel.

There is precedent for hydrogen not being taxed as heavily as gasoline or not being taxed at all, at least initially. For example, natural gas vehicles currently are taxed at a lower rate than gasoline at the federal level, and some states have reduced their highway taxes for natural gas to encourage the use of this cleaner burning fuel, as indicated in Table 3.

---

[10] The federal excise tax on gasoline is currently 18.4 cents per gallon, while the average state road tax on gasoline is about 22.9 cents per gallon, varying from a low of 8 cents in Alaska to a high of 28 cents per gallon in Connecticut. We have added 41 cents per gallon as an average of all gasoline taxes.

More importantly, electric vehicles at this time have *no* highway tax burden at either the federal or state level. This may change as electric vehicles become more plentiful, and as tax revenues for highway funds decrease. But governments may also decide to shift more of the tax burden to the more polluting fuels through "carbon taxes" to encourage the use of clean fuels such as hydrogen. In any case, we do not anticipate any highway taxes initially for electrolytic hydrogen, if for no other reason than collecting them would be complex, particularly with mobile hydrogen refueling vans roaming the countryside and home owners plugging electrolyzers into their home electrical outlets. Therefore we consider the fully taxed retail gasoline price to be an appropriate benchmark to compare with early hydrogen production costs.

Returning to Figure 8, electrolytic hydrogen is cost-competitive with fully taxed gasoline as long as electricity costs less than 3 to 4.5 cents/kWh, depending on the economic assumptions. If hydrogen-powered FCEVs take over a large market share and *if* governments begin to tax hydrogen at the same rate as gasoline, then electricity prices would have to be less than 1 to 2.5 cents/kWh for electrolytic hydrogen to remain competitive with gasoline. By that time, however, the reduced operating and maintenance costs and the longer life time of FCEVs may more than offset any increased cost of fuel taxes.

The cost components in the electrolytic hydrogen price are shown in Figure 9 for each economic case, assuming electricity at 2.5 cents/kWh. For the utility type 15-year loan, electricity accounts for just over half of the estimated cost. Surprisingly, storage accounts for more than the cost at the electrolyzer itself. Operation and maintenance (which includes taxes and insurance on this chart) is almost as expensive as the electrolyzer capital cost recovery.

Cost of Electricity

Our main thesis for this study is that utilities have considerable excess generating capacity, particularly during off-peak periods in the evening and early morning hours, and they can increase their profits by selling electricity at very low rates during periods of low demand. Typical utility daily load profiles are shown below, followed by a summary of current marginal operating costs and current off-peak residential retail rates.

Electrical Demand Profiles

To survey current utility load profiles, we downloaded a large database from the Federal Energy Regulatory Commission. Each utility supplies FERC with a "Form 714" each year, listing the hourly power output and system marginal cost for every hour of the year. We have plotted representative load profiles in Figures 10 through 18 to illustrate general utility load requirements across the country. The difference between night and day power consumption gives some

Table 3. Motor Fuel Tax Rates as of January, 1993[11]
(Cents/gallon)

	Gasoline	Natural Gas	Electricity
Federal	18.4	5.9	0
Alabama	18	17	0
Arizona	18	1	0
Arkansas	18.7	0	0
California	17	7	0
Colorado	22	20.5	0
Iowa	20	16	0
Kansas	18	17	0
Kentucky	15.4	12	0
Maryland	23.5	21.75	0
Montana	21.4	7.49	0
Nevada	24	20.5	0
New Jersey	10.5	5.25	0
New Mexico	17	16	0
New York	22.89	8	0
Oklahoma	17	16	0
Oregon	24	22	0
Pennsylvania	22.4	12	0
Tennessee	20	13	0
Virginia	17.5	16	0
Wyoming	9	0	0

---

[11] Source: the Natural Gas Vehicle Association, Arlington, Virginia. Only states which have lower tax on natural gas than on gasoline are shown.

indication of the excess generating capacity available if we can generate hydrogen during the night.

For each utility in our small sample, we averaged the electrical load over each 24-hour period for the months of January and February, 1993, as representative of the winter utility load. We averaged and plotted weekdays and weekends separately. We then repeated the same process for the months of July and August to represent typical summer load profiles. On each plot, we included the absolute peak load for the year, along with the calculated ratio of the minimum average load (averaged over the two-month period) to the peak load.

Beginning in the eastern U.S., Figure 10 shows the load profiles for the Central Maine Power Company. This is a typical winter-peaking utility. The winter load profile is characterized by a double peak -- one around 8 to 9:00 am, the other between 5:00 and 7:00 pm as workers arrive home. The peak load of 1629 MW is well above the average winter peak, and the minimum average load (which occurs for summer weekends for this utility) is only 46% of the peak load. During summer nights, the Central Maine Power Company only needs 46% of the electricity it supplied during the peak hourly period for the year. However, this under estimates their excess capacity, since they are required to provide reserve margin above their expected peak load.

Figures 11 through 15 show a sampling of utilities in the midsection of the country, running from Northern States Power Company through the Houston Lighting and Power Company. Similarly, Figures 16 through 18 show a sampling of utilities on the west coast.

In general, the average minimum to peak ratios run from 40% to 50%, with the separation between summer and winter peaks growing as one moves south. Almost all utilities are characterized by a large gap between peak load and night-time load, often approaching 50% even for the largest off-peak periods. We conclude that almost all utilities have excess off-peak capacity, and infer that most could recover capital costs if they could sell extra electricity above their marginal costs during these periods.

Marginal Operating Costs

In addition to hourly load data, most utilities are required to provide FERC with hourly data on "system lambda." System lambda is essentially a measure of a utility's marginal operating cost -- the cost of fuel and other maintenance costs associated with adding extra electrical output at any instant of time -- in mils/kWh. Utilities use these system lambda data to provide for virtually instantaneous dispatch of electrical power in response to demand within a given region[12]. If the load increases in a region, then the utility will turn on the idle generator with the lowest system lambda, thereby minimizing system operating costs. The most costly generators are saved for last, operating rarely if at all. Not all generators are required to follow this method of economic dispatch, however.

---

[12] Private communication with William C. Booth of the Federal Energy Regulatory Commission on October 31, November 4 and December 19, 1994.

In particular, hydroelectric plants with very low marginal costs are managed to optimize their storage contributions to shaving the peak load, or sold as baselaod if storage is not an option. Some utilities also belong to a larger power pool, and are not required to report their individual system lambda data.

A sampling of system lambda data are plotted in Figures 19 through 25. In general, system lambda data fluctuate much less than load profiles on either an hourly or seasonal basis. Most utilities sampled have an average system lambda below 2 cents/kWh. Nighttime rates are consistently below 2 cents/kWh (except for the west coast), and sometimes below 1.5 cents/kWh, particularly in the winter months.

Based on these data, we conclude that many utilities could recover some of their capital investment and still provide home electrolyzers with electricity below 3 cents/kWh during off-peak periods.

At least two utilities have applied for and received permission to provide "real time pricing" rates to selected customers: Florida Power & Light and the Southern California Edison Company. These rates would be tied to the hourly system lambda marginal costs, fluctuating in response to the utilities' real costs. The SCE rate structure is for large industrial or commercial users, and provides at best a rate around 7 to 8 cents/kWh in the early morning hours, depending on the previous day's temperature. This rate rises to as much as \$3.05/kWh (dollars, not cents/kWh!) during the afternoon if the previous day's maximum temperature exceeded 95°F. Clearly this rate will not be conducive to cheap electrolytic hydrogen.

Florida Power & Light's real time pricing experimental rate tariff went into effect on February 1, 1995, and extends until December 1998[13]. This tariff essentially adds from 1 to 1.5 cents/kWh to the system lambda operating cost. During those rare periods when the load actually approaches the peak generating capacity, extra reliability charges could push these rates as high as several dollars per kWh, but these extraordinary rates might only occur once every few years. During off-peak periods, the rates would be only 1.0 to 1.5 cents/kWh above system lambda.

Florida Power & Light does have system lambda costs somewhat higher than other utilities that we sampled in this brief study, averaging 2.12 cents/kWh as shown in Figure 25. Higher operating costs may be due to the heavy reliance on oil generated electricity: about 43% of FPL electricity comes from oil, 35% from nuclear, and 23% from natural gas[14]. FPL paid an average of

---

[13] Private communications with Bob Bergstrom (October 31, 1994), Bob Suggs (December 19, 1994) and Tom Tramutola (December 19, 1994) of the Florida Power & Light Company.

[14] Ibid., EIA, p. 195.

$2.21/MBTU for oil in 1993,[15] which is equivalent to about 2.1 cents/kWh assuming 35% efficiency for an oil burning utility plant, while natural gas cost $2.22/MBTU or 1.89 cents/kWh at 40 percent efficiency.

Adding 1 to 1.5 cents/kWh to the system lambda cost of 2.12 cents/kWh would raise the price to the owner of a home electrolyzer to the 3.1 to 3.6 cent/kWh range, which would meet our goal of less than 4 to 5 cents/kWh for initial introduction of electrolytic hydrogen. However, the Florida Power & Light tariff apparently applies only to existing industrial customers with established energy use patterns. It is not clear how a home owner or a fleet operator would qualify for their real time pricing as currently written.

Nonetheless, this tariff does suggest that other utilities might benefit from selling electricity at rates 1 to 1.5 cents/kWh above system lambda. If Northern States Power Company, with an average annual system lambda of only 1.03 cents/kWh, offered a similar rate structure to encourage hydrogen production by electrolysis to new customers, then we could expect rates in the range of 2 to 2.5 cents/kWh.

Residential Off-Peak Rates

We do not, however, have to wait for new rate structures to begin producing electrolytic hydrogen at competitive prices in some sections of the country. Many utilities already offer off-peak rates below 4 to 5 cents/kWh.

Of 154 utilities listed in a publication of rate structures, 58% had some type of residential off-peak or "time of use" (TOU) rate, ranging from 1.4 cents/kWh[16] up to as much as 8 cents/kWh (see Figure 26)[17].. Seventy one utilities offered off-peak rates below 4.5 cents/kWh, and 27 offered rates below 3 cents/kWh, as summarized in Figure 27.

While off-peak TOU rates are low, the utilities generally raise the rates substantially during peak use hours. Virginia Power, for example, offers residential customers electricity at 2.92 cents/kWh off-

---

[15] Ibid, EIA, p. 255.

[16] Alabama Power Company offered the lowest off-peak rate listed in the Electric Rate Book: from 9:00 pm until 10:00 am during summer weekdays, from 9:00 pm until 7:00 am during winter weekdays, and all day on weekends, Alabama Power Company offers a base rate of 1.25 cents/kWh, plus an energy charge that was 0.15 cents/kWh at the time of the report (March 31, 1994), or a total of 1.4 cents/kWh. The energy charge will vary, depending on fuel costs, which allows the utility to pass on increased marginal costs to the customer.

[17] Electric Rate Book: Comprehensive Rate Information on Investor-Owned Electric Utilities, published by Casazza, Schultz & Associates, Inc., Arlington, Virginia.

peak, but the rate jumps to 17.516 cents/kWh from 11:00 am until 10:00 pm on summer weekdays, and from 7:00 am to 11:00 am plus 5:00 pm until 9:00 pm on winter weekdays, well above their standard rate of 8.17 cents/kWh. If the homeowner had to pay 17.5 cents/kWh to run his air conditioner in the summer time, then the effective cost of electrolytic hydrogen would be excessive. However, Virginia Power already has several thousand customers who continue to use regular rates for their household while installing a separate time of use rate for a garage or machine shop function.[18] We assume that a home electrolyzer would be treated the same as an electric vehicle, and would qualify for the TOU rates without affecting the rest of the household.

Many utilities also charge an additional monthly fee for the TOU rate, primarily to cover the costs of a separate meter. For example, Virginia Power charges an extra $5.00 per month for their TOU off-peak rates. For a two-car family consuming an average of 88 pounds of hydrogen per month, this would amount to an additional cost of about 5.7 cents per pound, which amounts to a 6% increase in cost for $1/lb hydrogen -- a manageable charge.

The geographic distribution of utilities with low off-peak rates is not uniform. Over half were located in the Midwest, as illustrated in Figure 28. Only eight utilities in the western region offered residential off-peak rates below 4.5 cents/kWh.

Impact of Electrolyzers on Utility Excess Capacity

Some observers have questioned whether increased use of electricity to produce hydrogen would eventually consume the excess utility generating capacity, requiring the addition of more power plants. We calculated the increased demand for electricity under the following demanding assumptions. First, we assumed that all the zero emission vehicle (ZEV) requirements mandated in California would be supplied by fuel cell electric vehicles (FCEVs.) Second, we assumed that all FCEVs would be fueled with electrolytic hydrogen. Third, we assumed that ZEV sales would continue at 10% per year after the California ZEV requirements expire. Finally, we assumed that six states (Massachusetts, New York, Maine, Maryland and New Jersey) opted into the ZEV program, further increasing the demand for electrolytic hydrogen.

Under these optimistic assumptions regarding hydrogen vehicle market penetration, the cumulative FCEV fleet would amount to about 2.5 million vehicles in 2010, or about 2 percent of the US car fleet. These 2.5 million FCEVs would consume about 2.7 billion kWh of electricity per month, which corresponds to about 5.9 percent of the electrical generation in the six states, or about 1 percent of the total U.S. electrical consumption.

Given that many utilities have excess capacity exceeding 50 percent of their output during half the day, an additional load of 1 to 6 percent by the year 2010 would have negligible impact.

A similar calculation was made by John Caskey of the Virginia Power Company. He estimated that

---

[18] Private communication, Brett Crable, Virginia Power Company, March 27, 1995.

if 10 percent of all new cars sold in Virginia each year were electric vehicles, then it would take 50 years before their existing excess nighttime generation capacity would be utilized.[19] Clearly the utility industry has sufficient excess capacity to supply FCEVs for several decades without adding any new generating equipment.

Conclusions

Based on this brief study of small electrolyzer systems and off-peak electrical rates, we come to these conclusions:

1. Home electrolyzer systems could produce hydrogen for fuel cell electric vehicles that is cost competitive with fully taxed gasoline on a per mile basis, provided that electrolyzers can be mass produced at less than $\$300/\text{kW}_{out}$, with compressors less than $\$115/\text{kW}_{out}$, and storage tanks less than \$50/pound of hydrogen stored at 6,000 psi, and provided that electricity can be purchased for less than 4.5 cents/kWh.

2. Seventy-one utilities currently sell off-peak electricity to residential customers at retail prices less than 4.5 cents/kWh.

3. Most utilities have excess generating capacity most of the time, often exceeding 40 to 50 percent of their total capacity during the night and early morning hours.

4. Many utilities have marginal operating costs below 1.5 to 2 cents/kWh, and could recover some capital costs by selling off-peak electricity at rates below 3 cents/kWh.

5. Utilities currently have sufficient excess nighttime capacity to supply electrolytic hydrogen to all fuel cell electric vehicles for several decades without building any new generation equipment, even if 10 percent of all new cars sold were fuel cell vehicles.

Recommendations

Based on these positive findings, we recommend that the concept of small hydrogen electrolyzer systems for hydrogen refueling stations be extended to the next level of detail. Capital costs of the main system components need to be determined as a function of manufacturing volume, and our assumptions regarding possible off-peak electrical rates need to be firmed up with representative electric utilities. We need to develop a feasible transition strategy for implementing a cost effective electrolyzer infrastructure to support early FCEV fleet and single owner demonstrations.

---

[19] Elaine Gaither and Mark Hopkins, Expanding the Markets for Alternative Fuel Vehicles in the Mid-Atlantic Region, The Alliance to Save Energy, December 1994, p. 8.

Specifically, we recommend a two-step program to more fully explore the small scale electrolytic hydrogen option. In the first phase of this program, the system would be designed and costed in detail, and the off-peak electrical rates would be discussed in detail with one or more utilities. Two key issues are the type of electrolyzer (alkaline or PEM) and whether high pressure electrolysis is cost effective for either replacing or reducing the pressure ratio needed from the compressor. In the second phase, one or more prototype electrolyzer systems would be built and tested, with the goal of having such a refueling capability in place by the time prototype fuel cell vehicles are ready for demonstration. These early demonstration projects would probably be sited in urban areas with excessive ozone smog.

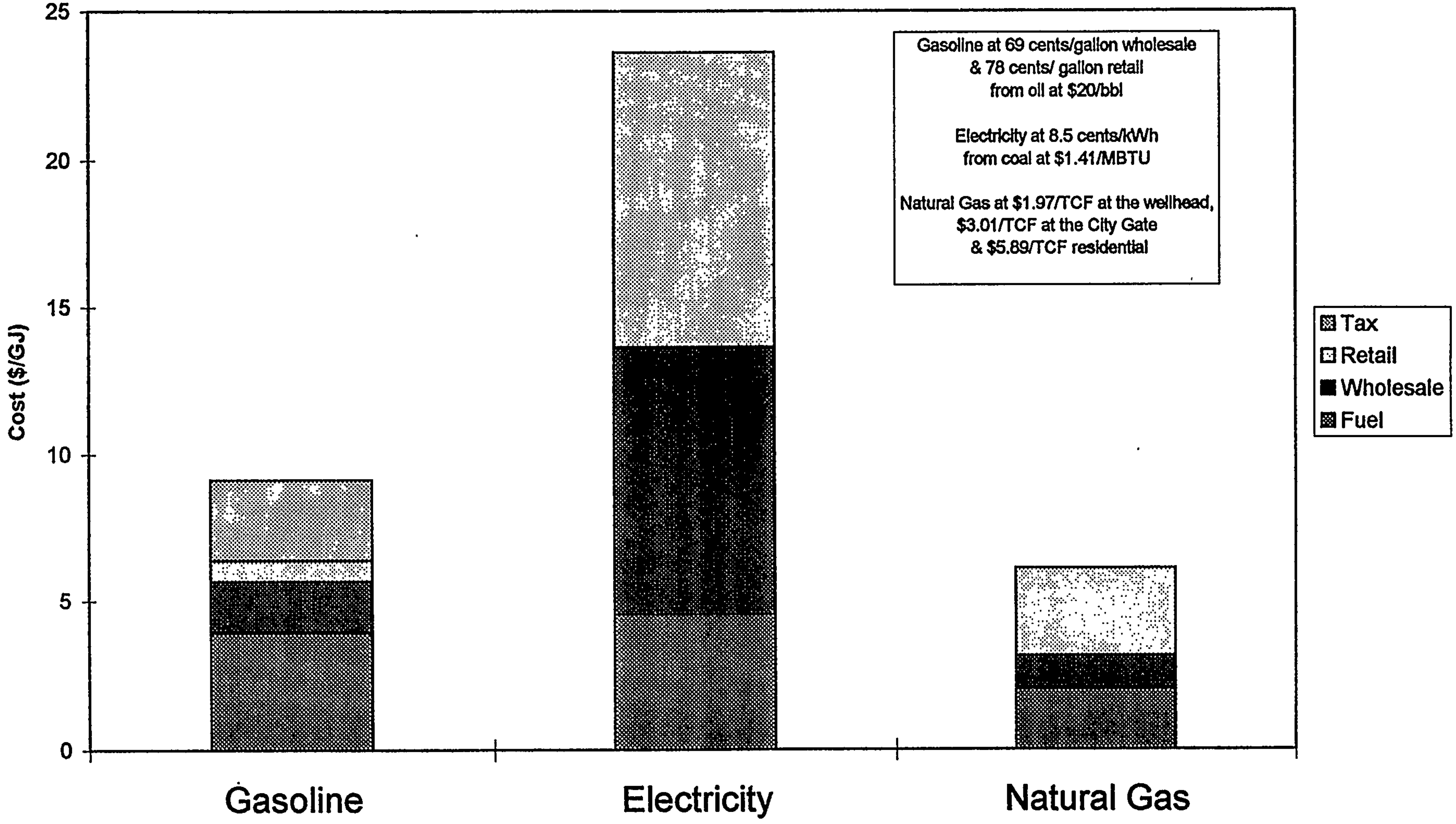
Acknowledgments

This work was funded by the National Renewable Energy Laboratory under subcontract ACF-4-14266-01 to the prime DOE contract No. DE-AC02-83CH10093. We thank Jim Ohi, the NREL Technical manager and Cathy Gregoire-Padró, the hydrogen program manager, for their valuable assistance. We also appreciate the guidance of numerous utility representatives and electrolyzer manufacturers including Matthew Fairlie of Electrolyser, Bill Kincaide and Jay Laskin of Teledyne Brown, and Jim McElroy of Hamilton Standard. Finally, we acknowledge the comments from reviewers of the draft final report including George Baum (DTI), Bob Bergstrom (Florida Power & Light), Jim Birk (EPRI), Tom Halvorson (Praxaire), Brian James (DTI), Fred Mitlitski (Lawrence Livermore National Laboratory), Dave Nahmias, Djong-Gie Oei (Ford Motor Company), Joan Ogden (Princeton University), Bob Schock (Lawrence Livermore National Laboratory), and Suman Singh (Oak Ridge National Laboratory).

Figure 1

Fuel Cost Comparison

per unit energy



Gasoline at 69 cents/gallon wholesale
& 78 cents/ gallon retail
from oil at $20/bbl

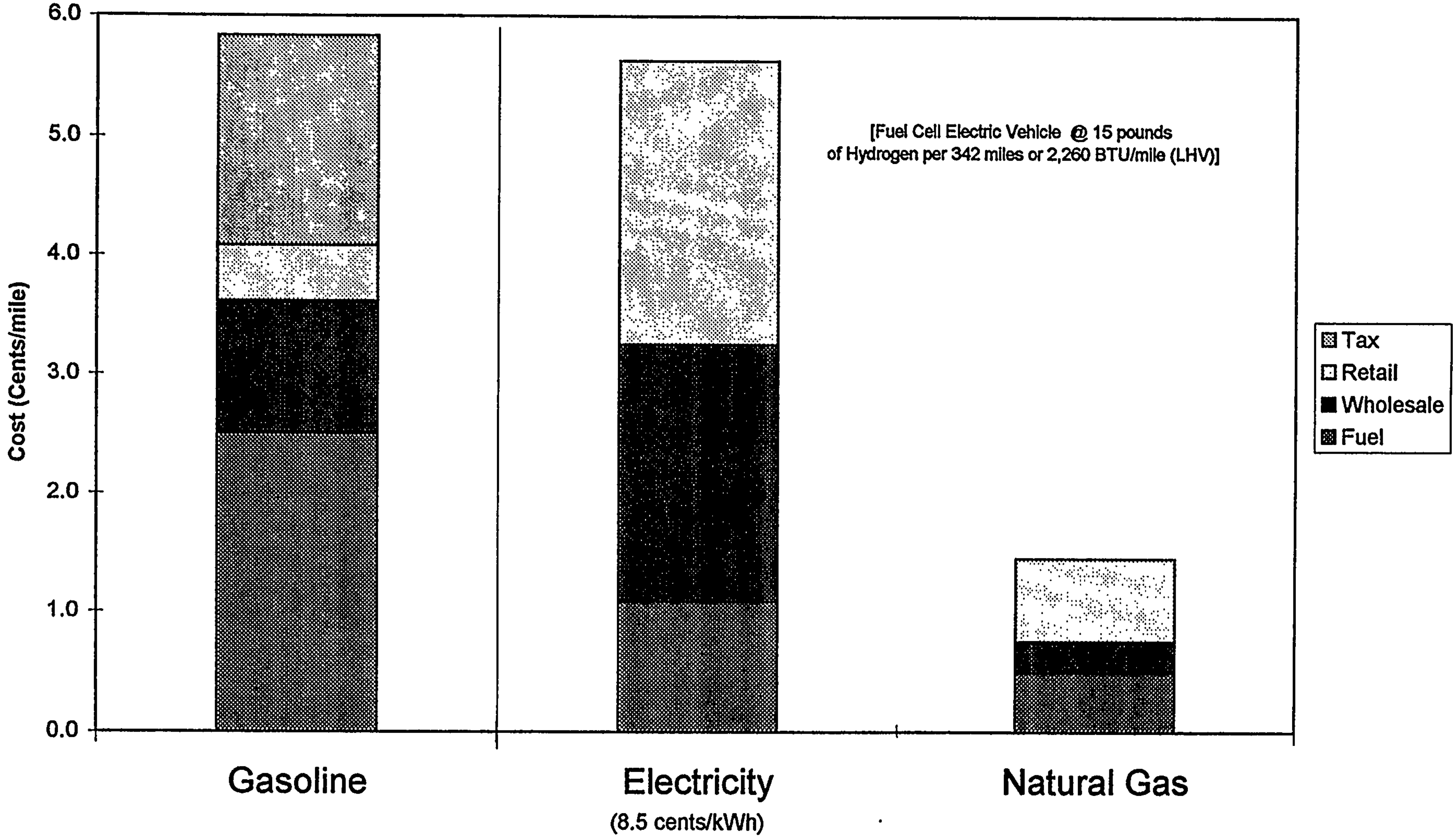
Electricity at 8.5 cents/kWh
from coal at $1.41/MBTU

Natural Gas at $1.97/TCF at the wellhead,
$3.01/TCF at the City Gate
& $5.89/TCF residential

Figure 2.
[Internal Combustion Engine
@19 mpg = 6,050 BTU/mile (LHV)]

Fuel Costs on a Per-Mile Basis

(Assuming 2.68 Times Greater Efficiency (LHV) with Fuel Cell Electric Vehicle)



[Fuel Cell Electric Vehicle @ 15 pounds
of Hydrogen per 342 miles or 2,260 BTU/mile (LHV)]

Figure 3

[Internal Combustion Engine
@19 mpg = 6,050 BTU/mile (LHV)]

Fuel Costs on a Per-Mile Basis

(Assuming Off-Peak Electricity)

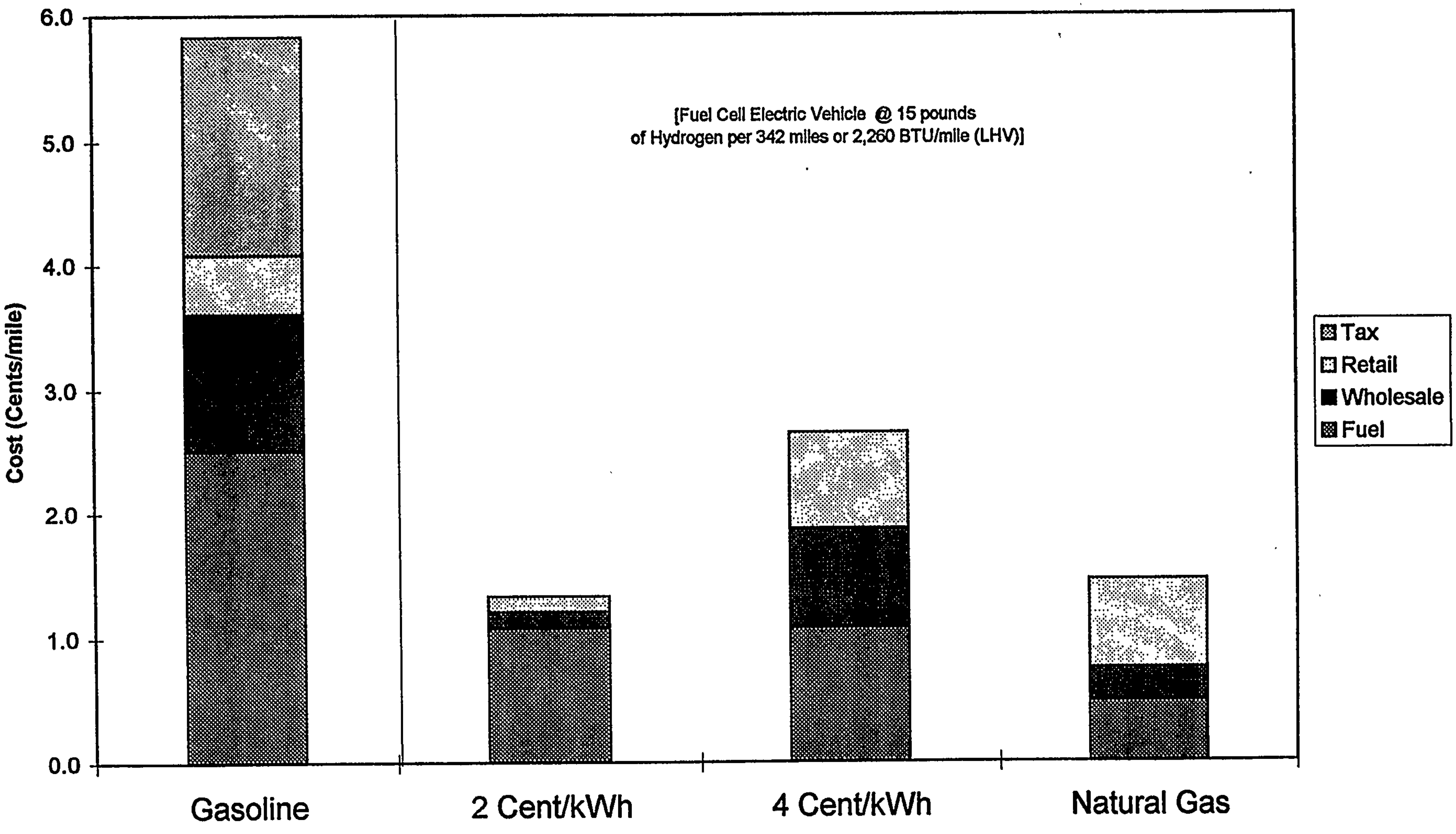


Figure 4

Electrolytic Hydrogen Dispensing Station

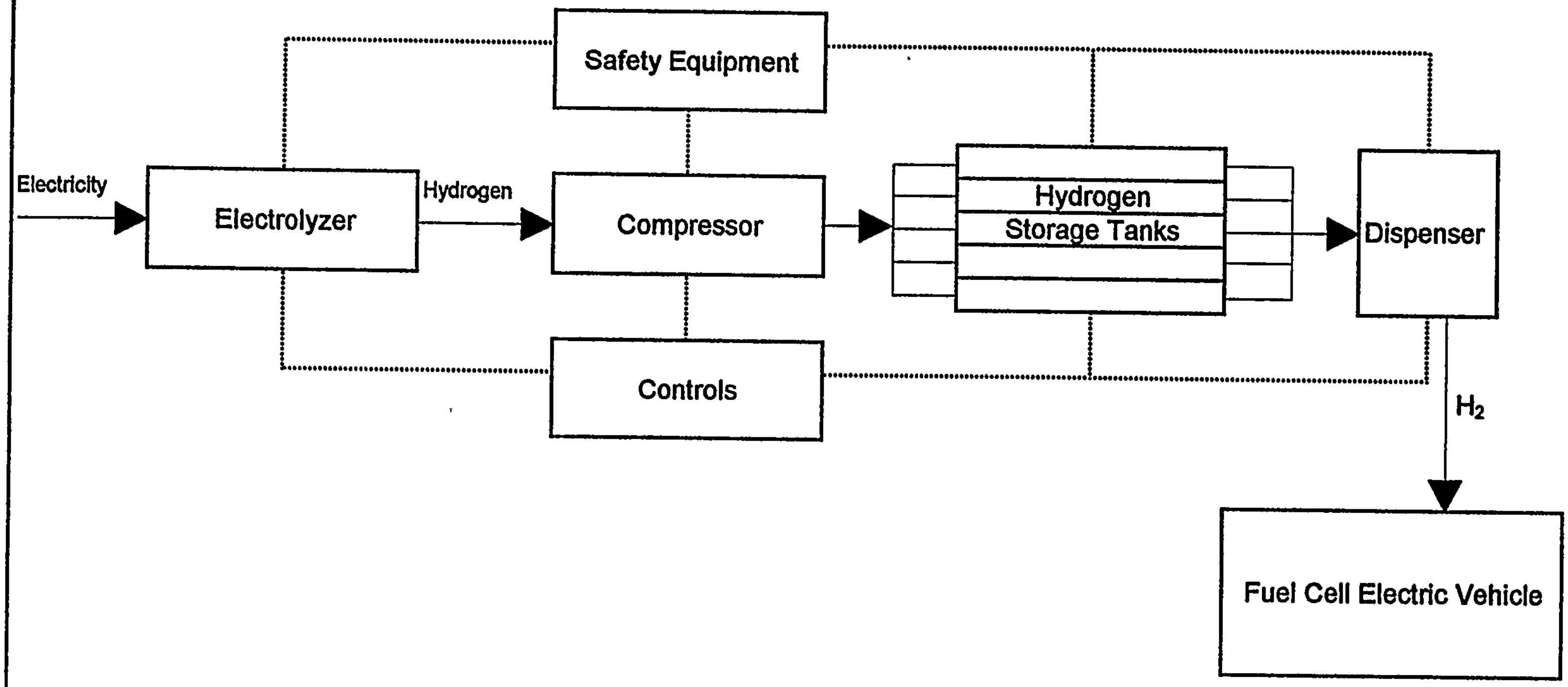


Figure 5

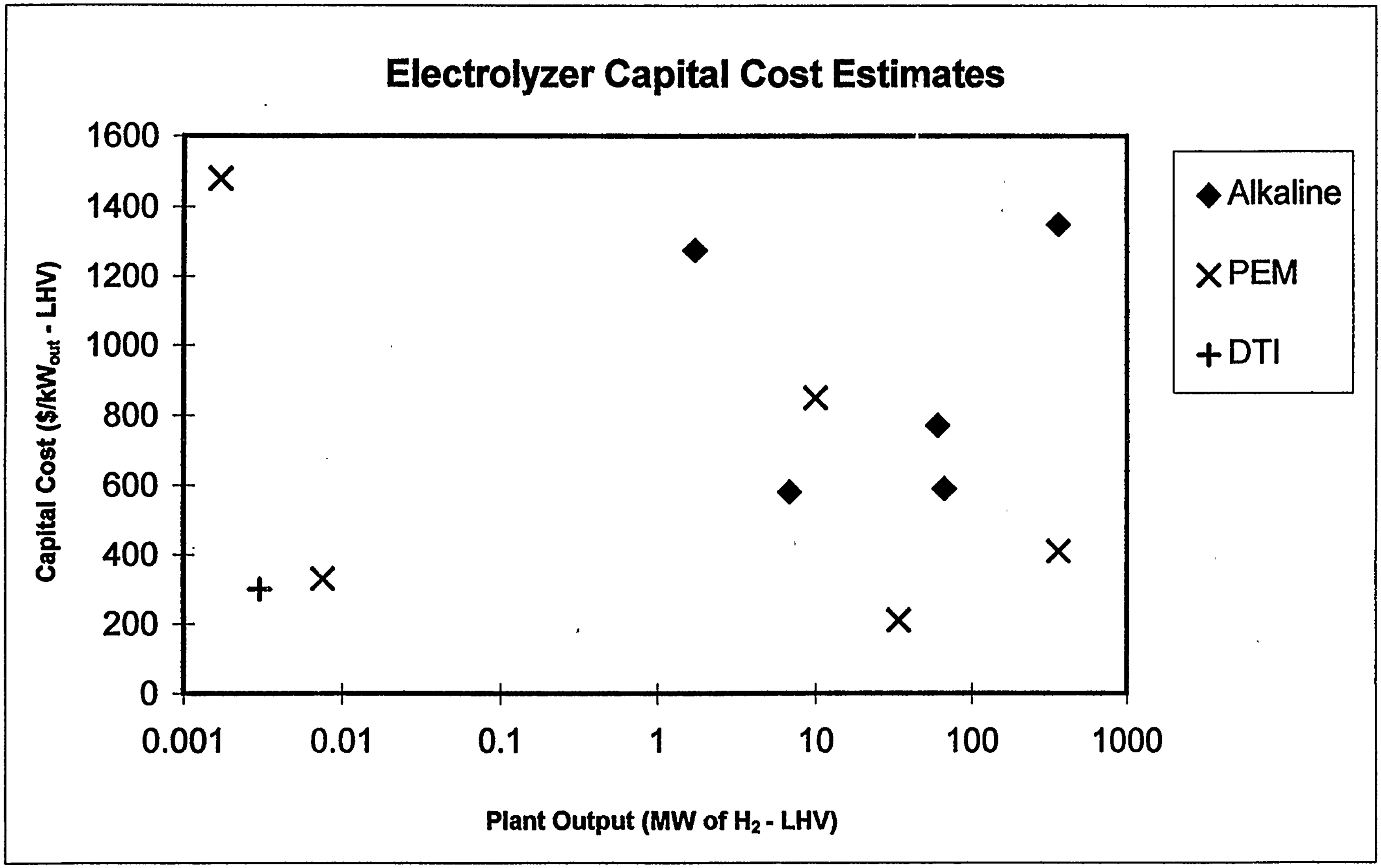
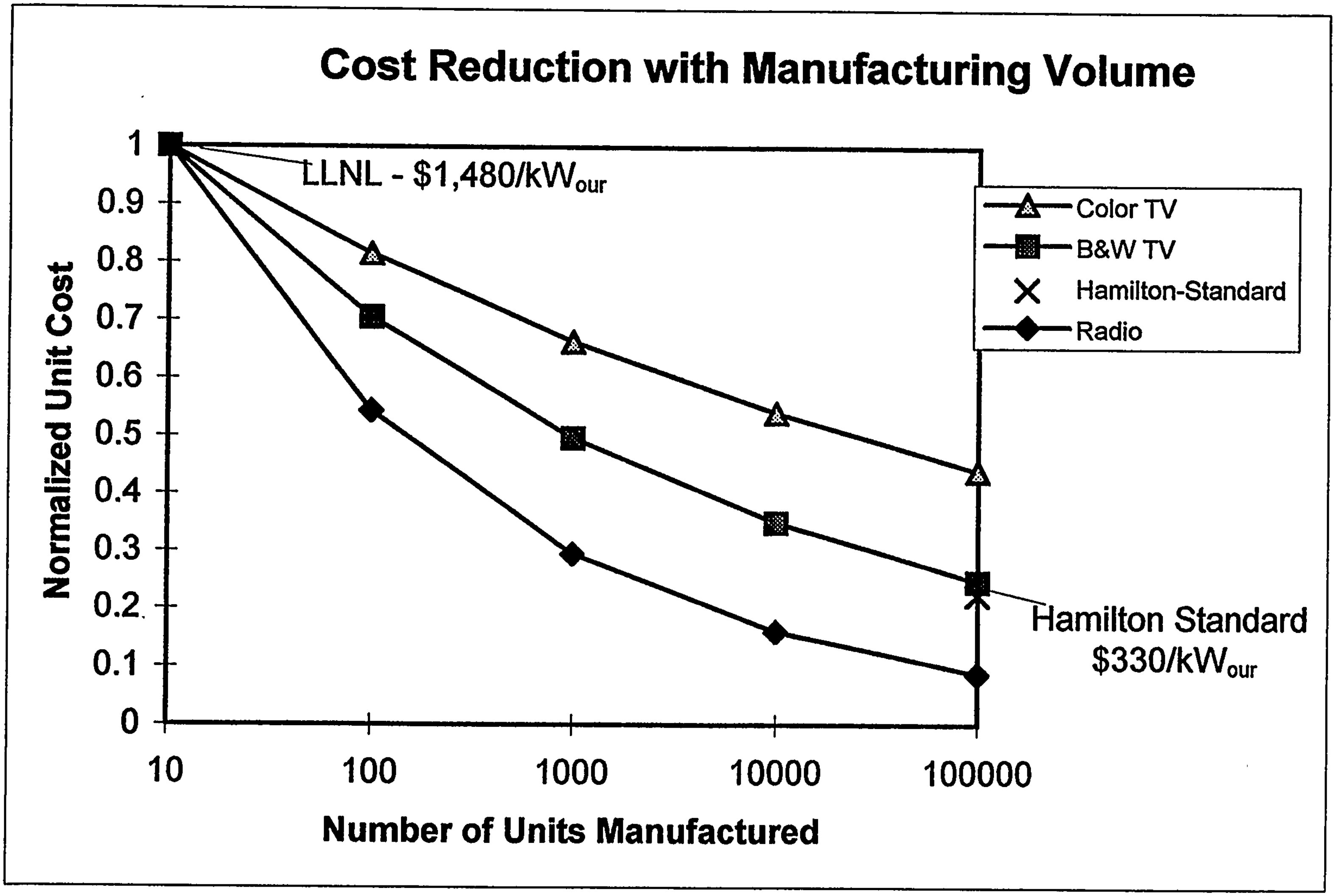
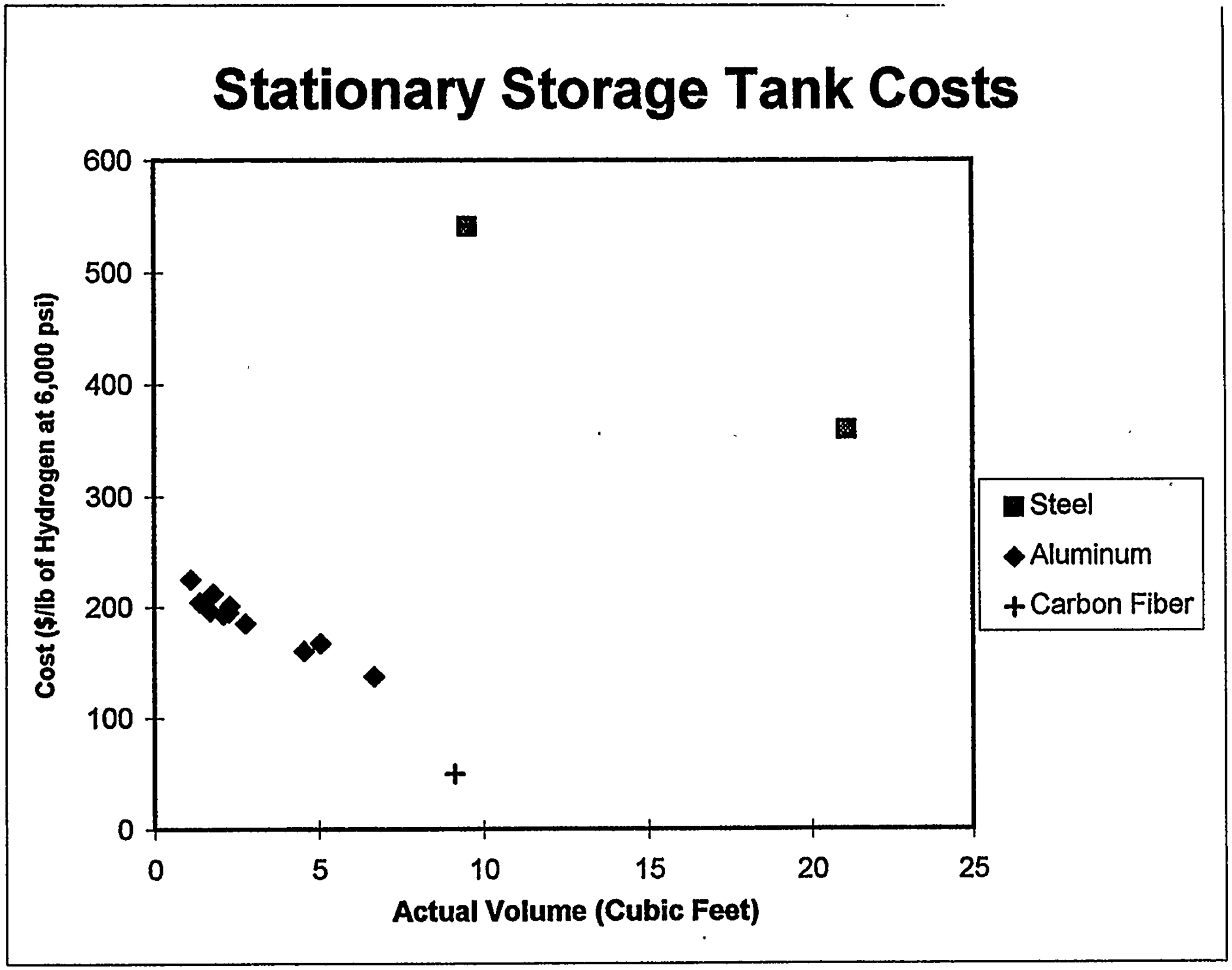

Electrolyzer Capital Cost Estimates
Capital Cost ($/kW$_{out}$ - LHV)
1600
1400
1200
1000
800
600
400
200
0
0.001
0.01
0.1
1
10
100
1000
Plant Output (MW of H_2 - LHV)
◆ Alkaline
× PEM
+ DTI

Figure 6

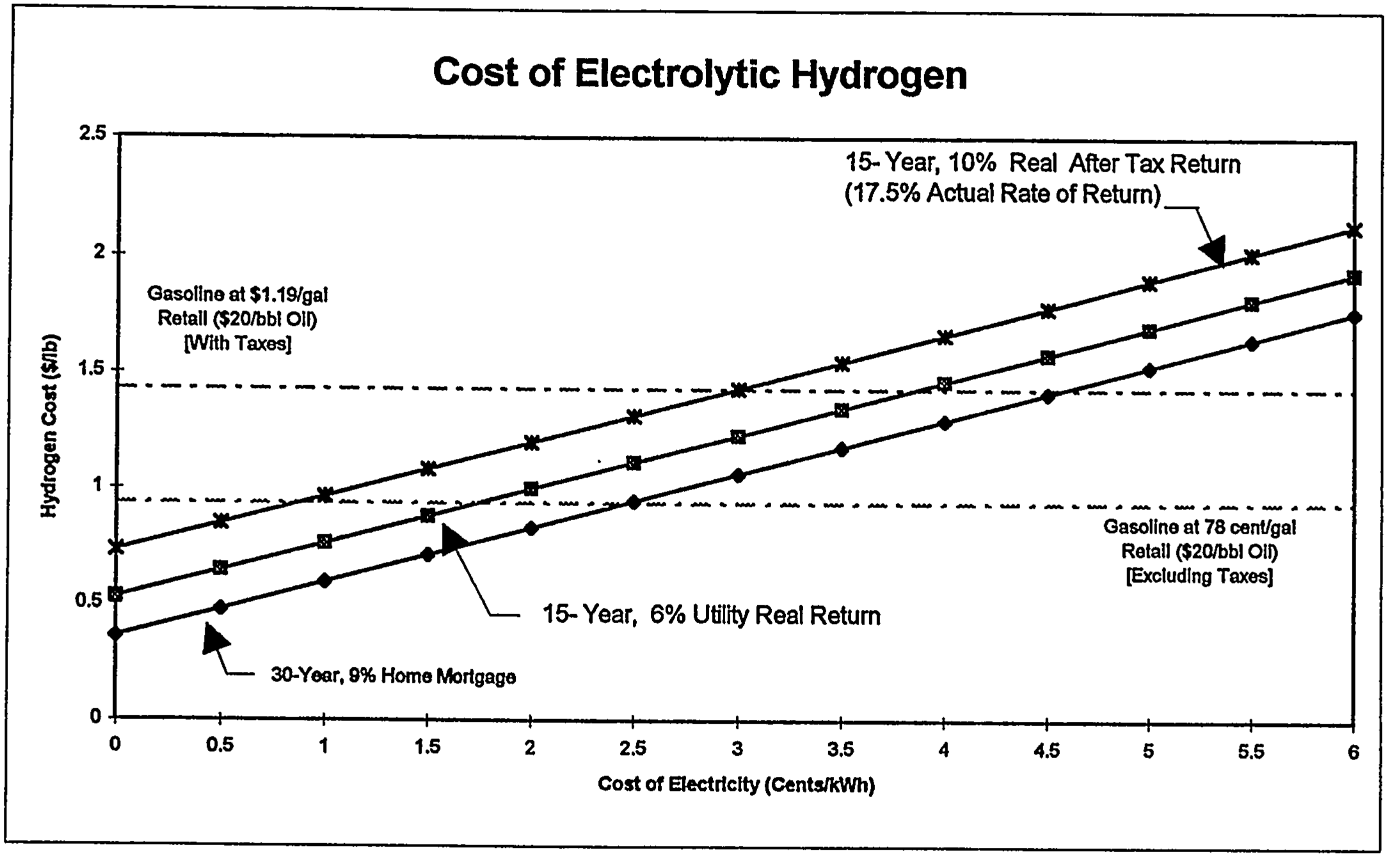

Cost Reduction with Manufacturing Volume
Normalized Unit Cost
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
10
100
1000
10000
100000
Number of Units Manufactured
LLNL - $1,480/kW$_{our}$
Hamilton Standard
$330/kW$_{our}$
Color TV
B&W TV
Hamilton-Standard
Radio



Steel Quote from CP Industries, Inc of McKeesport, Pennsylvania
For 6,000 psi ASME steel tanks, 16 " OD x 1.416" wall.

Aluminum Quote from NGV Systems, Inc of Long Beach, California
For 3,600 psi composite reinforced aluminum cylinders

Carbon Fiber tank is DTI projection for 2004, based on 6,000 psi
carbon fiber wrapped plastic tanks with metalized liner.



Cost of Electrolytic Hydrogen

		Home	Utility	Business
Capital Cost				
Electrolyzer	$/kW out	300	300	300
H2 Storage	$/lb	50	50	50
Compressor (8kpsi)	$/kW out	115	115	115
Total Capital Cost	$	$3,413	$3,413	$3,413
Hydrogen for 342 mile	lbs	15	15	15
Number of Vehicles		2	2	2
Miles/year/vehicle	miles	12,000	12,000	12,000
Storage capacity	[# of tanks/vehc.	1.2	1.2	1.2
H2 Production X Ave		1.5	1.5	1.5
Days to Produce One Tank:		3.5	3.5	3.5
ICE Mileage	mpg	19		
Cost of Crude Oil	$/barrel	20		

		Home	Utility	Business
Lifetime	Years	30	15	15
Discount Rate	% / 100	0.0585	0.089	0.1297
CRF	[calc]	0.0715	0.1230	0.1854
Capacity Factor	Ratio	0.7	0.7	0.7
Electrolyzer Efficiency	HHV%/100	0.675	0.675	0.675
Compressor Electr.	kWh/kWh H	0.065	0.065	0.065
O&M	% of Capital	0.02	0.02	0.02
Insurance	% of Capital	0.005	0.005	0.005
Property Taxes	% of Capital	0.015	0.015	0.015
Real Interest Rate	%/100	0.09	0.06	0.1
Fed. Marg. Inc. Tax	%/100	0.31	0	0.26
State Income Tax	%/100	0.058		

Figure 9

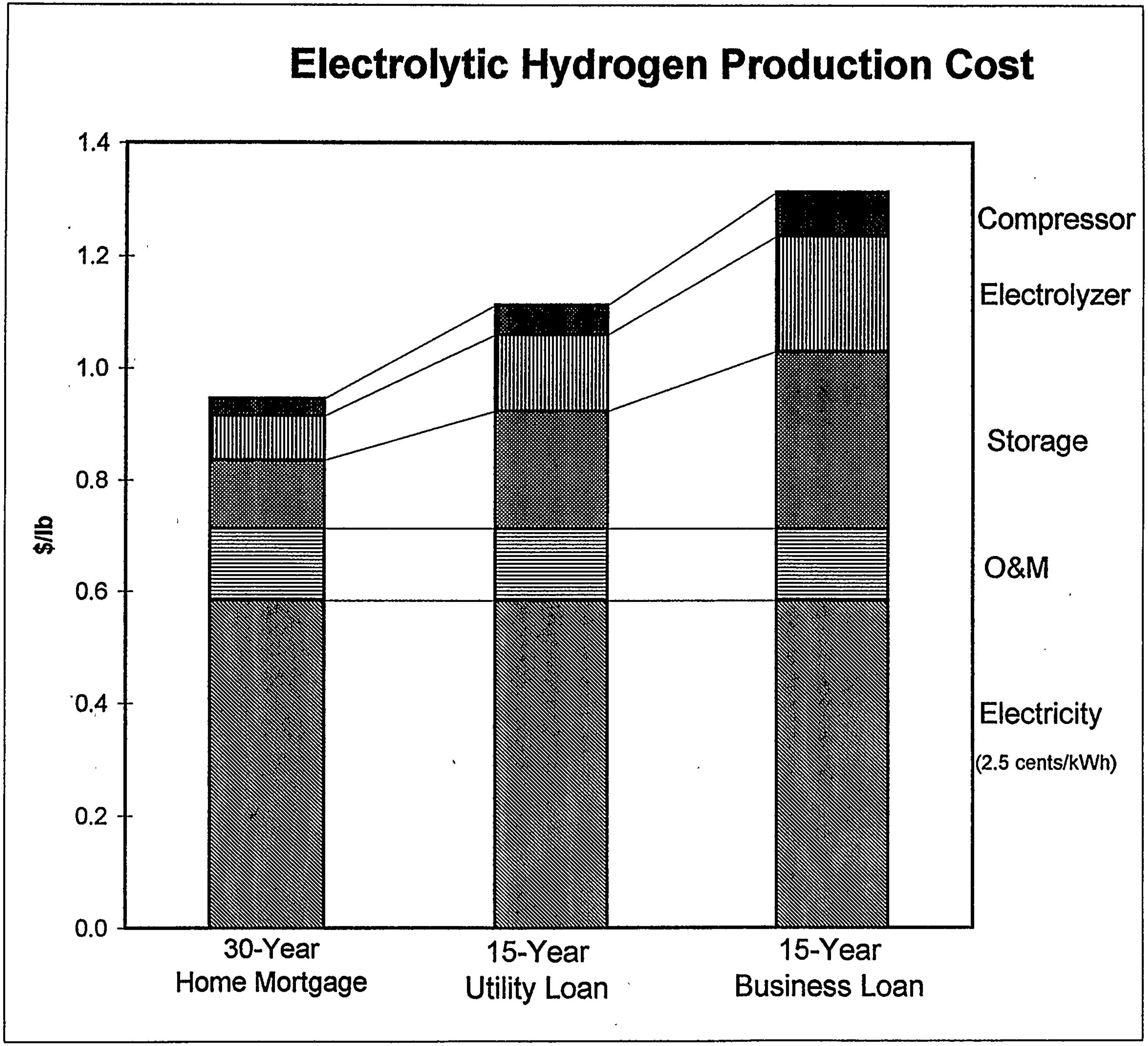

Electrolytic Hydrogen Production Cost
$/lb
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
30-Year Home Mortgage
15-Year Utility Loan
15-Year Business Loan
Compressor
Electrolyzer
Storage
O&M
Electricity
(2.5 cents/kWh)

Figure 10

Central Maine Power Company

Seasonal Load Profiles (1993)

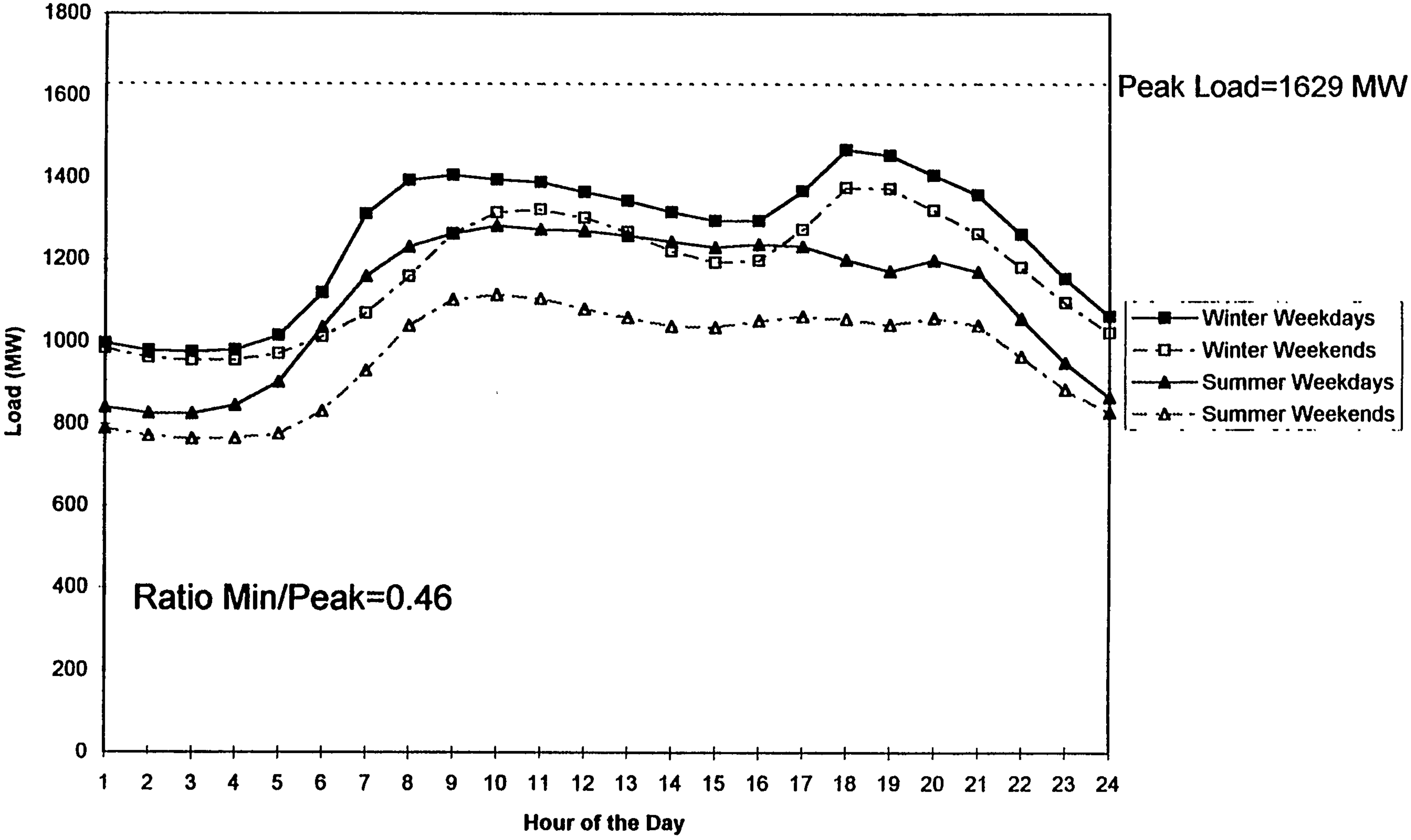


Figure 11

Northern States Power Company

Seasonal Load Profiles (1993)

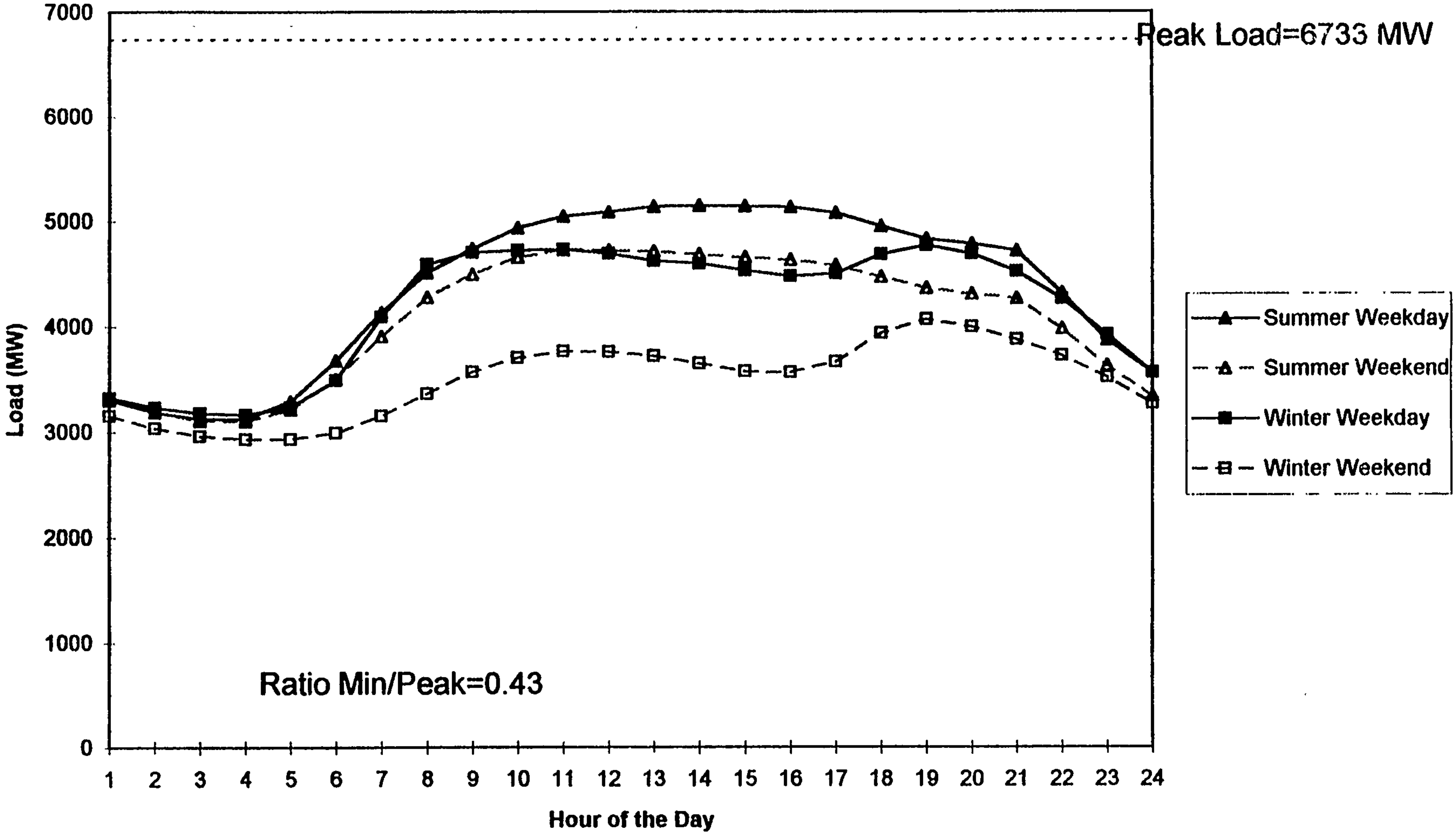


Figure 12

Springfield City Water, Light & Power

Seasonal Load Profiles (1993)

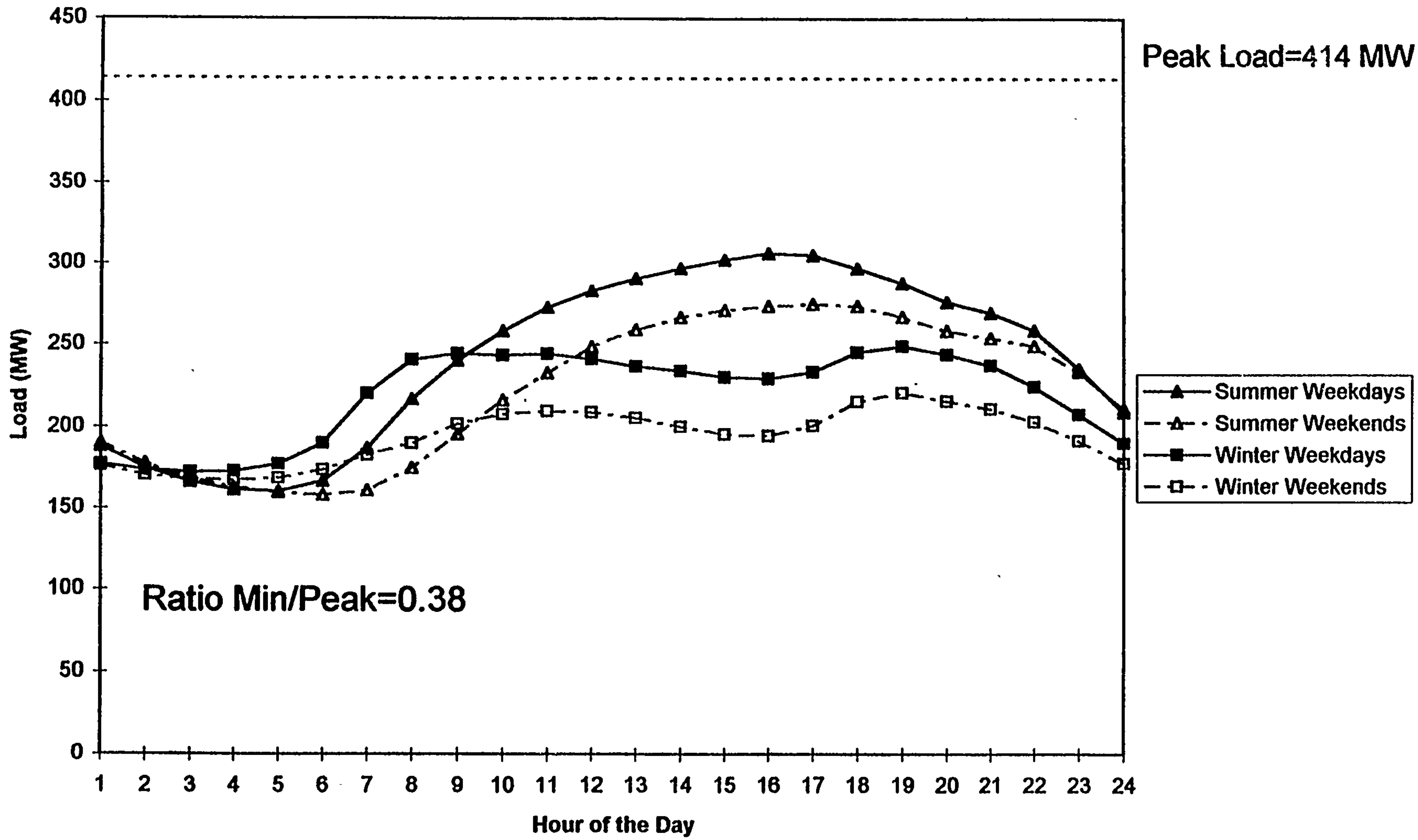


Figure 13

Cincinnati Gas & Electric

Seasonal Load Profiles (1993)

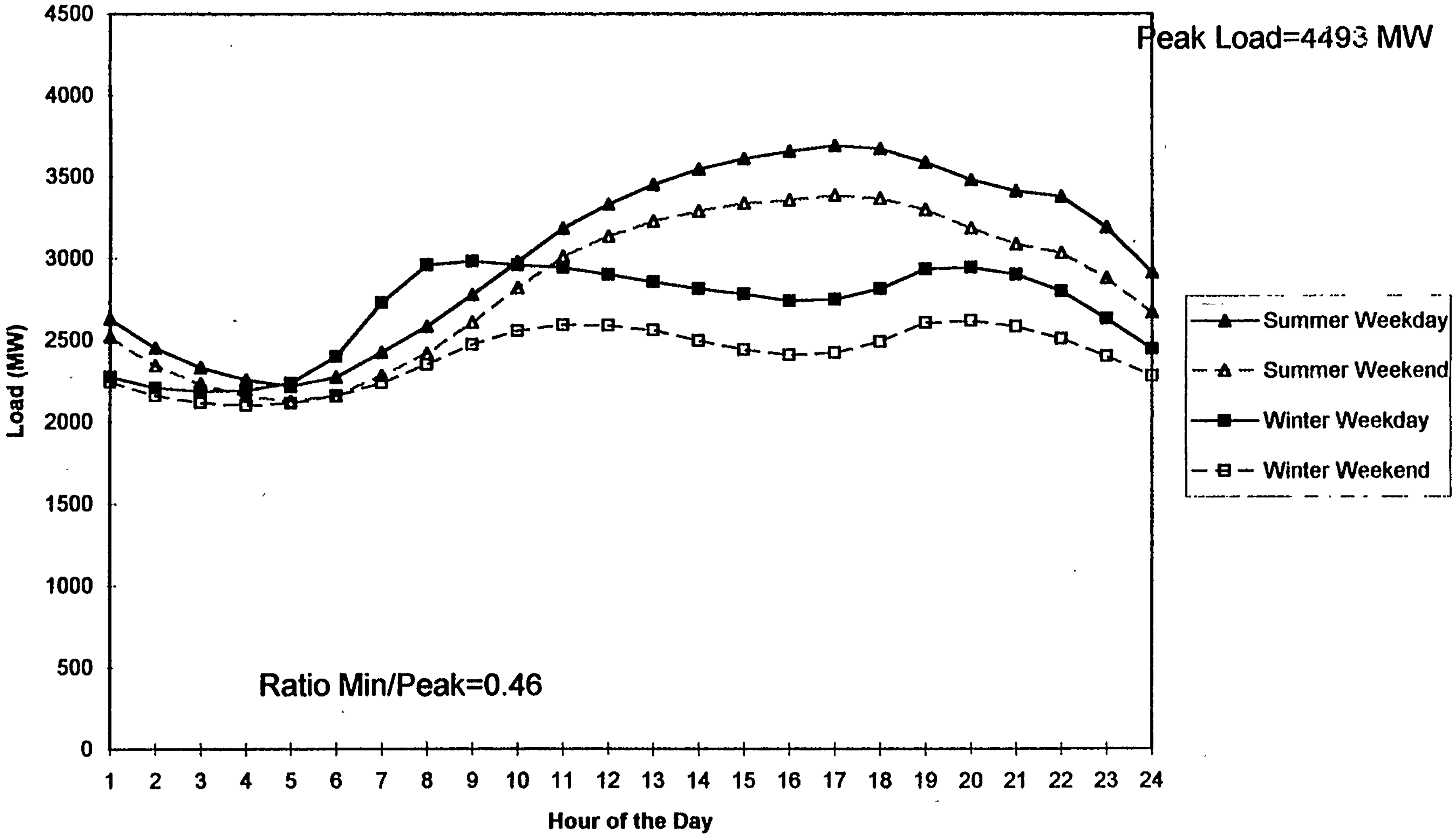


Figure 14

Tennessee Valley Authority

Seasonal Load Profiles (1993)

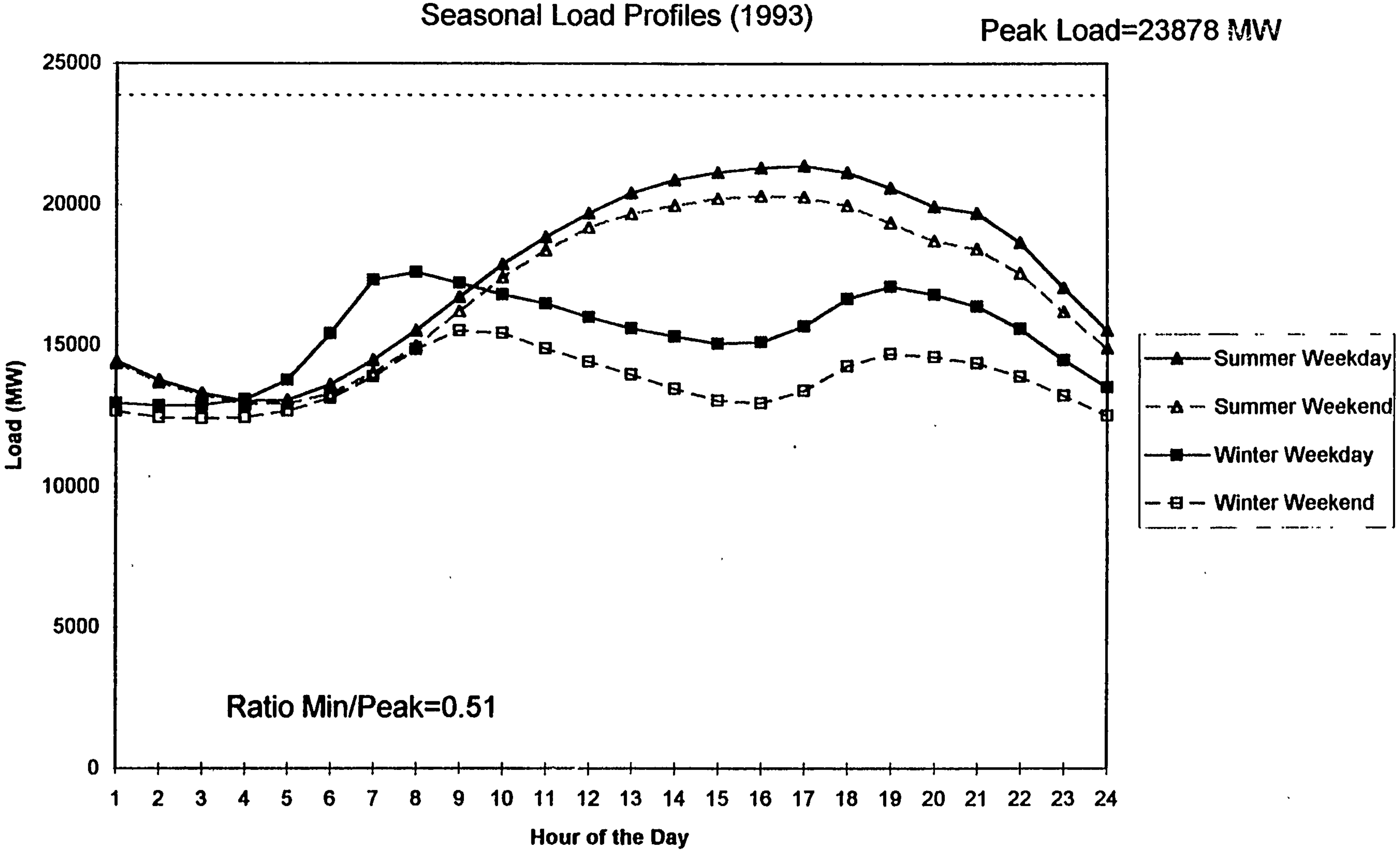


Figure 15

Houston Lighting & Power

Seasonal Load Profiles (1993)

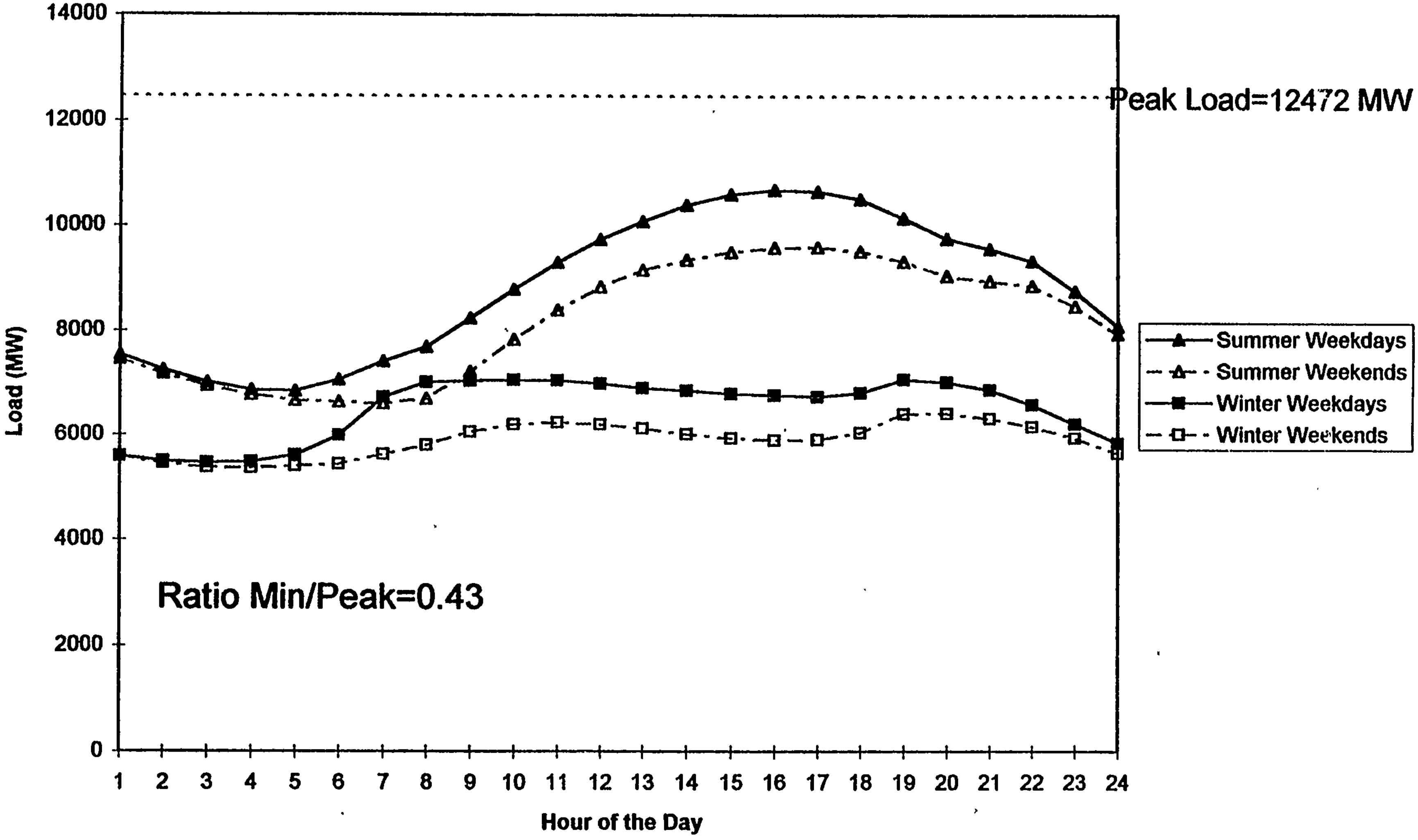


Figure 16

PacifiCorp (Pacific Northwest)

Seasonal Load Profiles (1993)

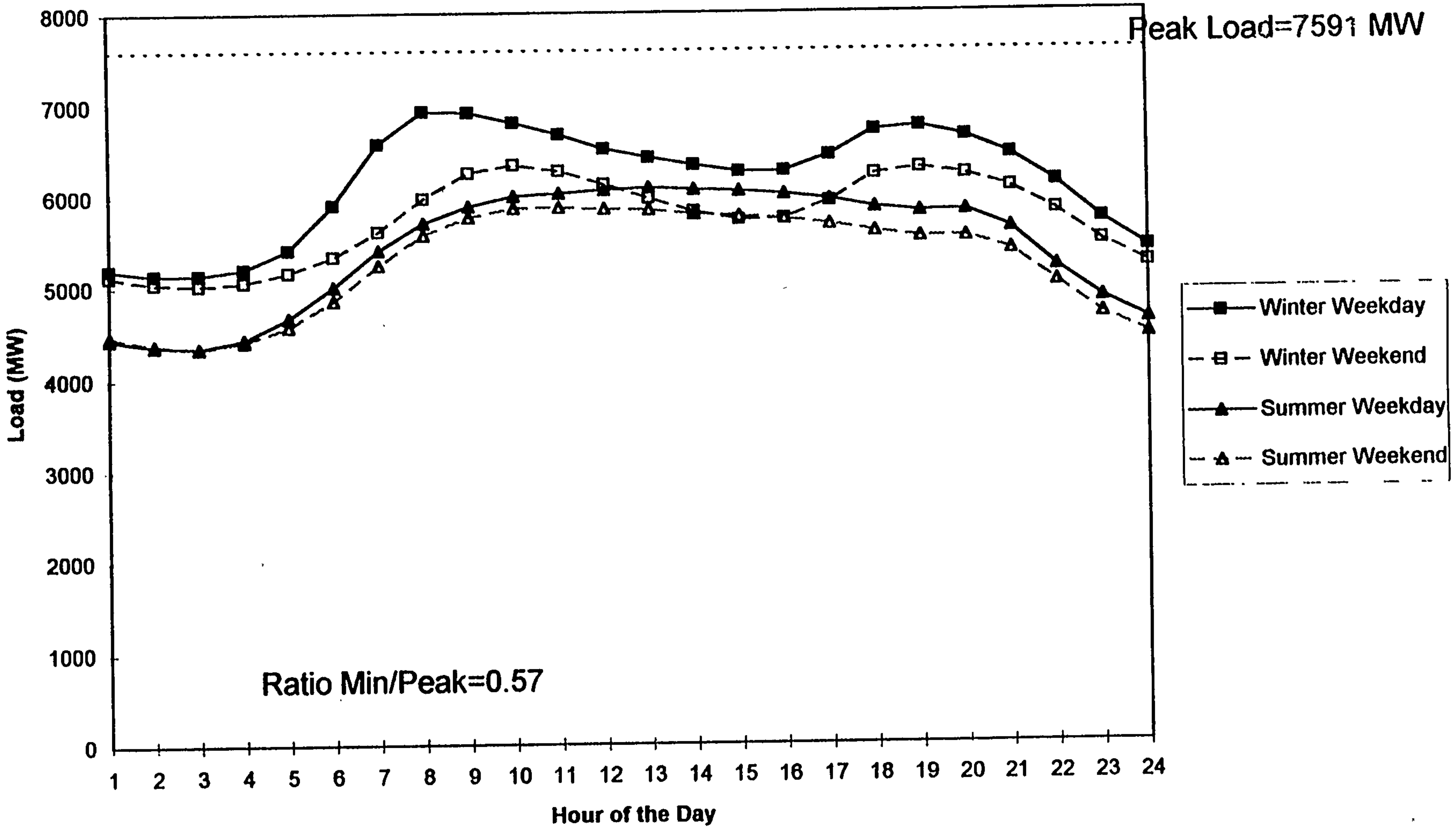


Figure 17

Sierra Pacific Power Company

Seasonal Load Profiles (1993)

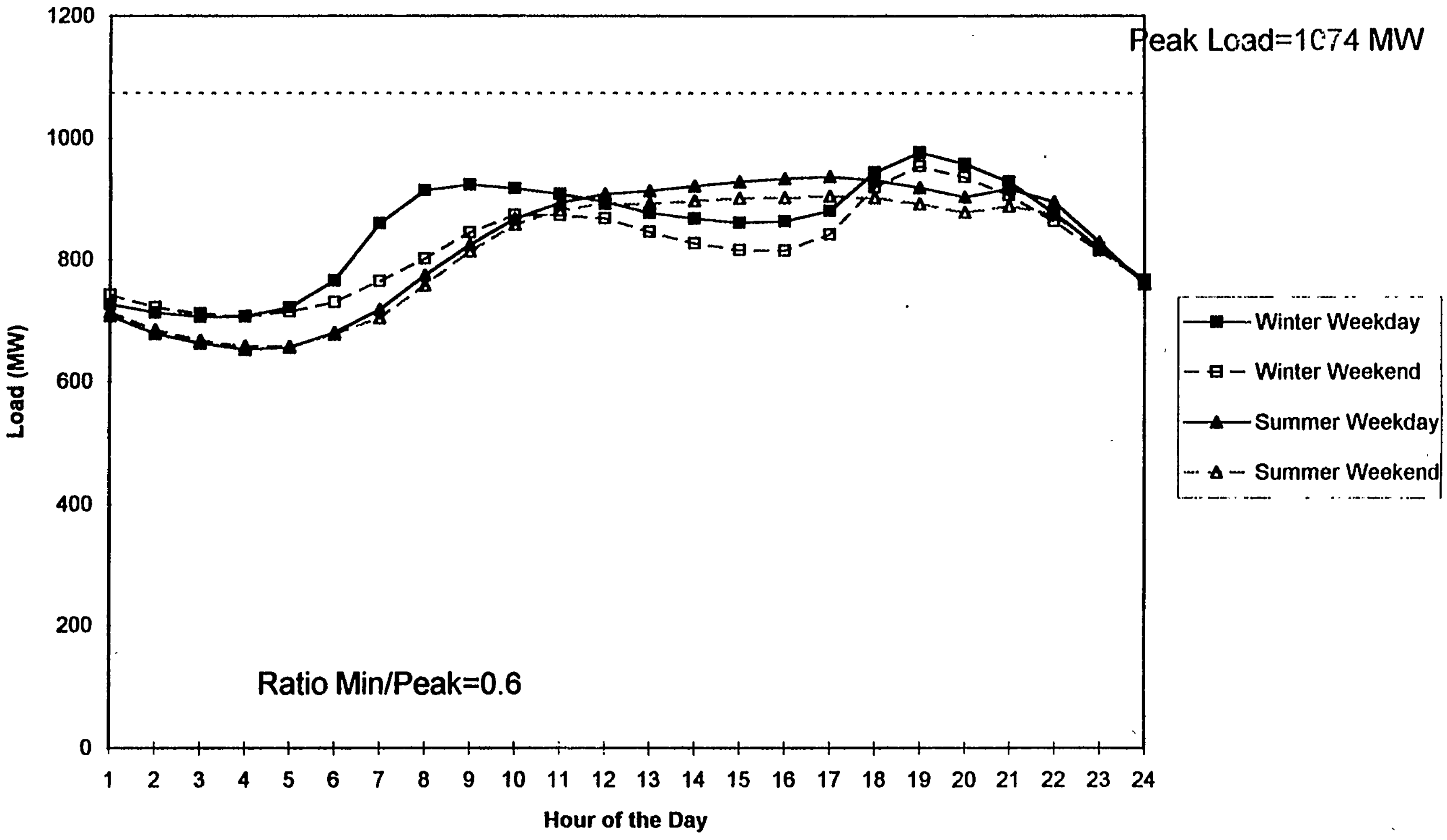


Figure 18

Pacific Gas & Electric

Seasonal Load Profiles (1993)

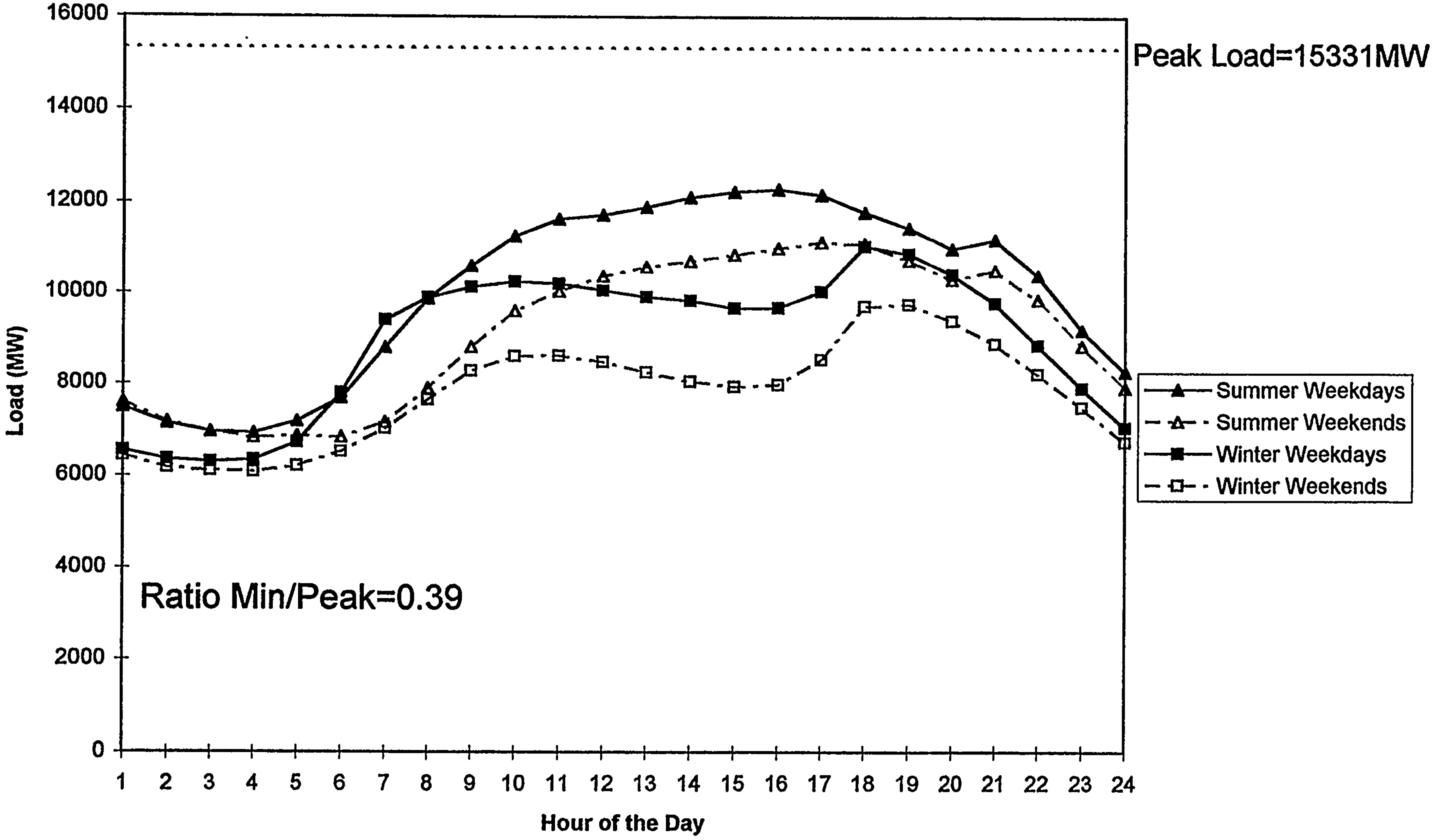


Figure 19

Northern States Power Company

Average System Lambda or Marginal Operating Cost

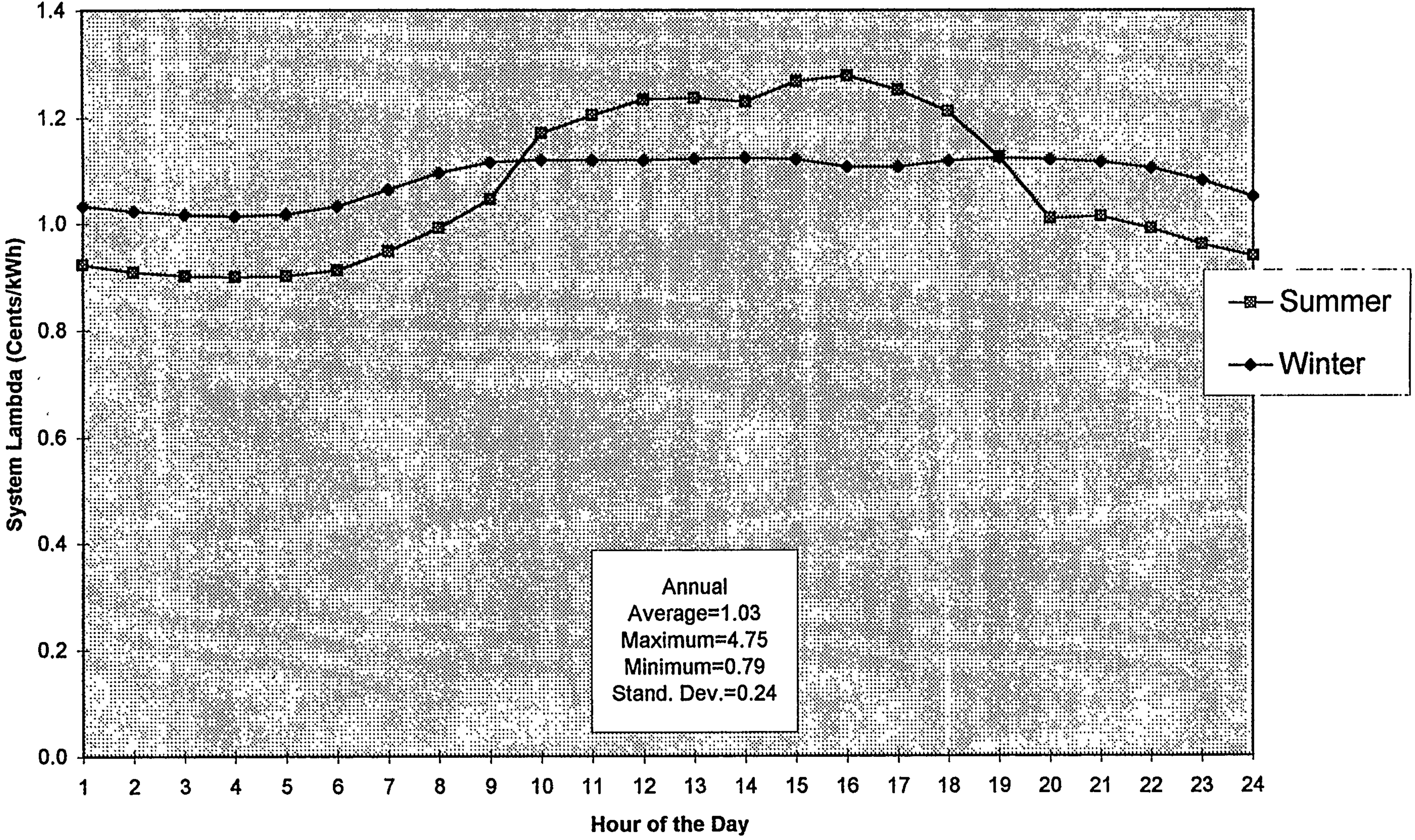


Figure 20

Cincinnati Gas & Electric

Average System Lambda or Marginal Operating Cost

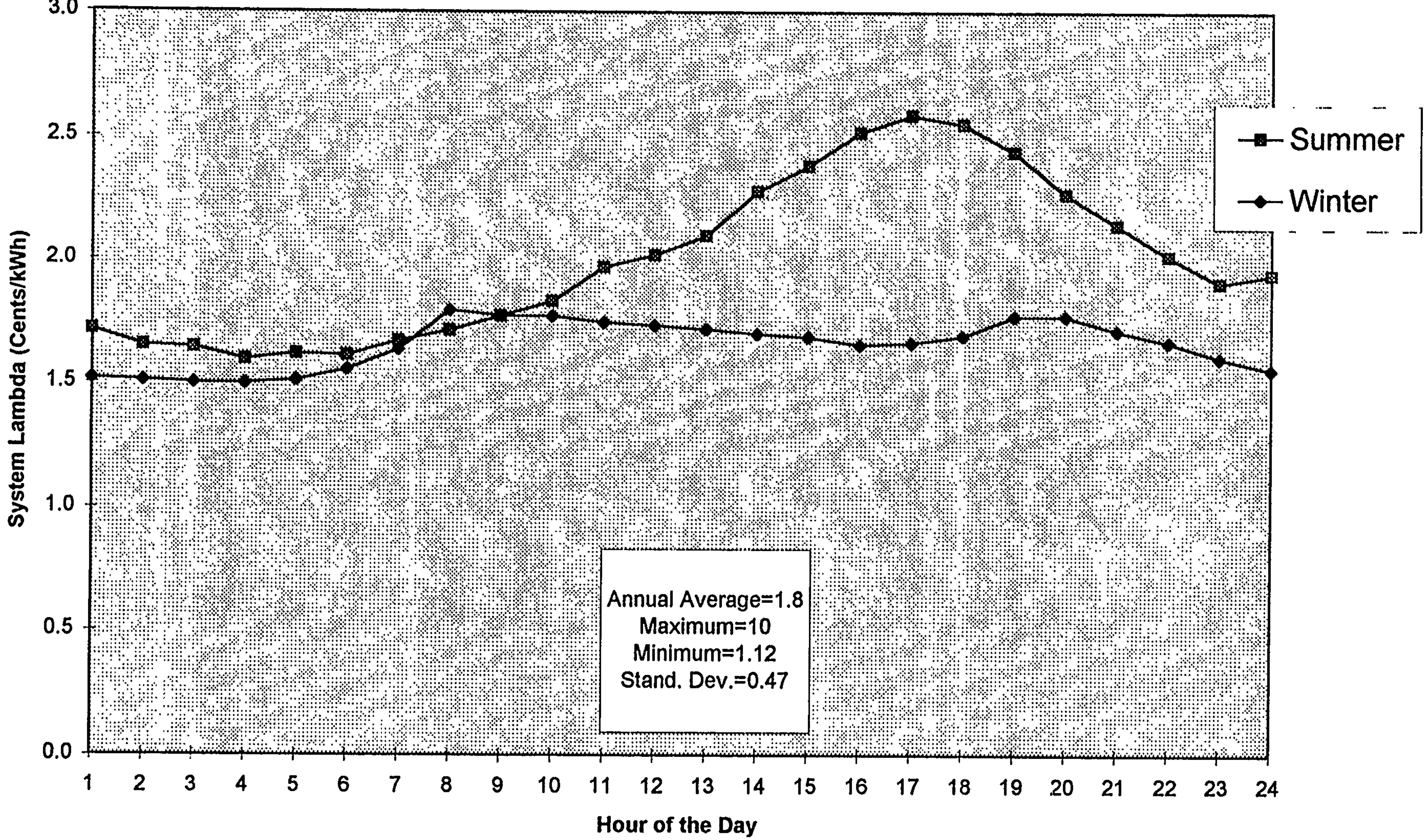


Figure 21

Tennessee Valley Authority

Average System Lambda or Marginal Operating Cost

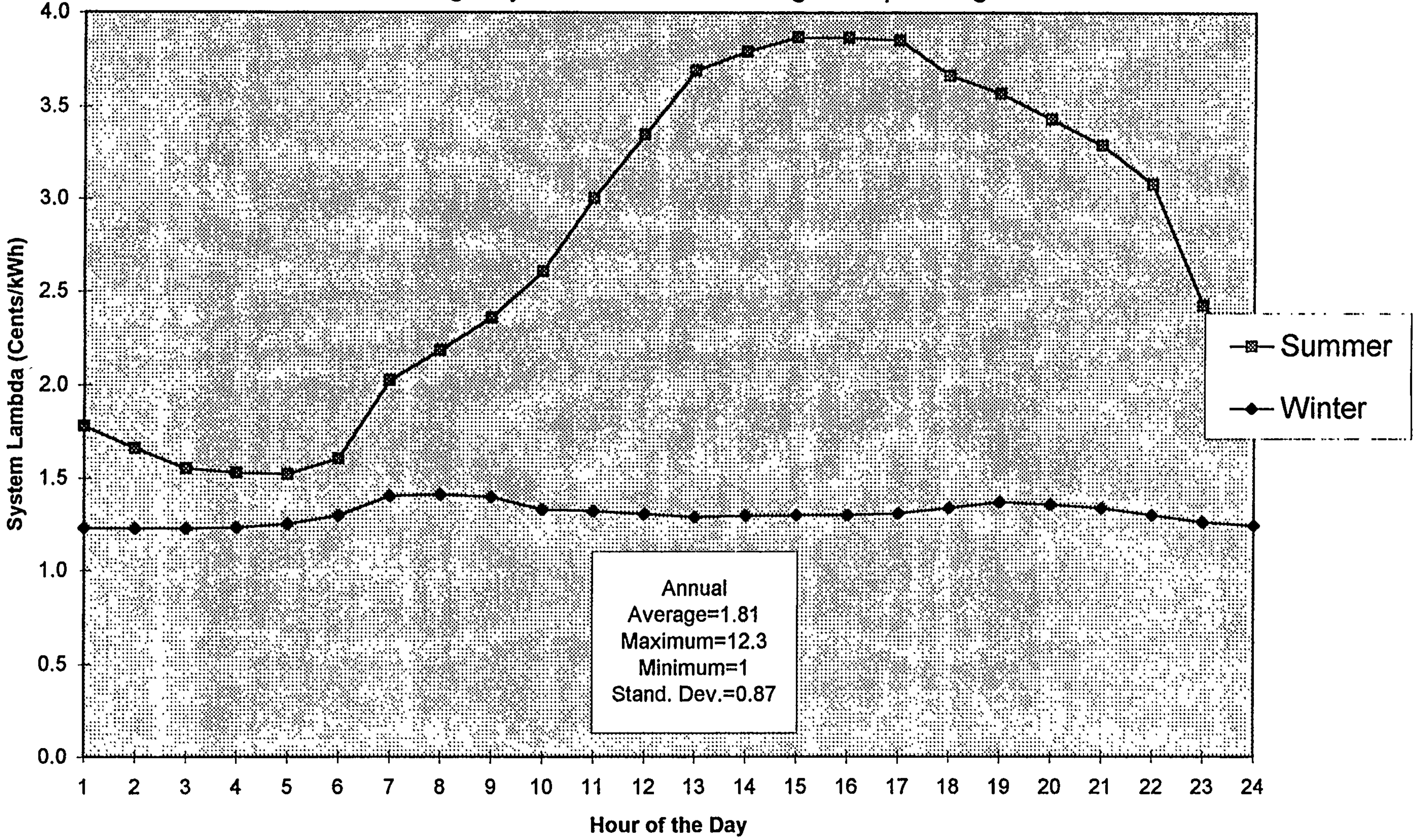


Figure 22

Houston Lighting & Power

Average System Lambda or Marginal Operating Cost

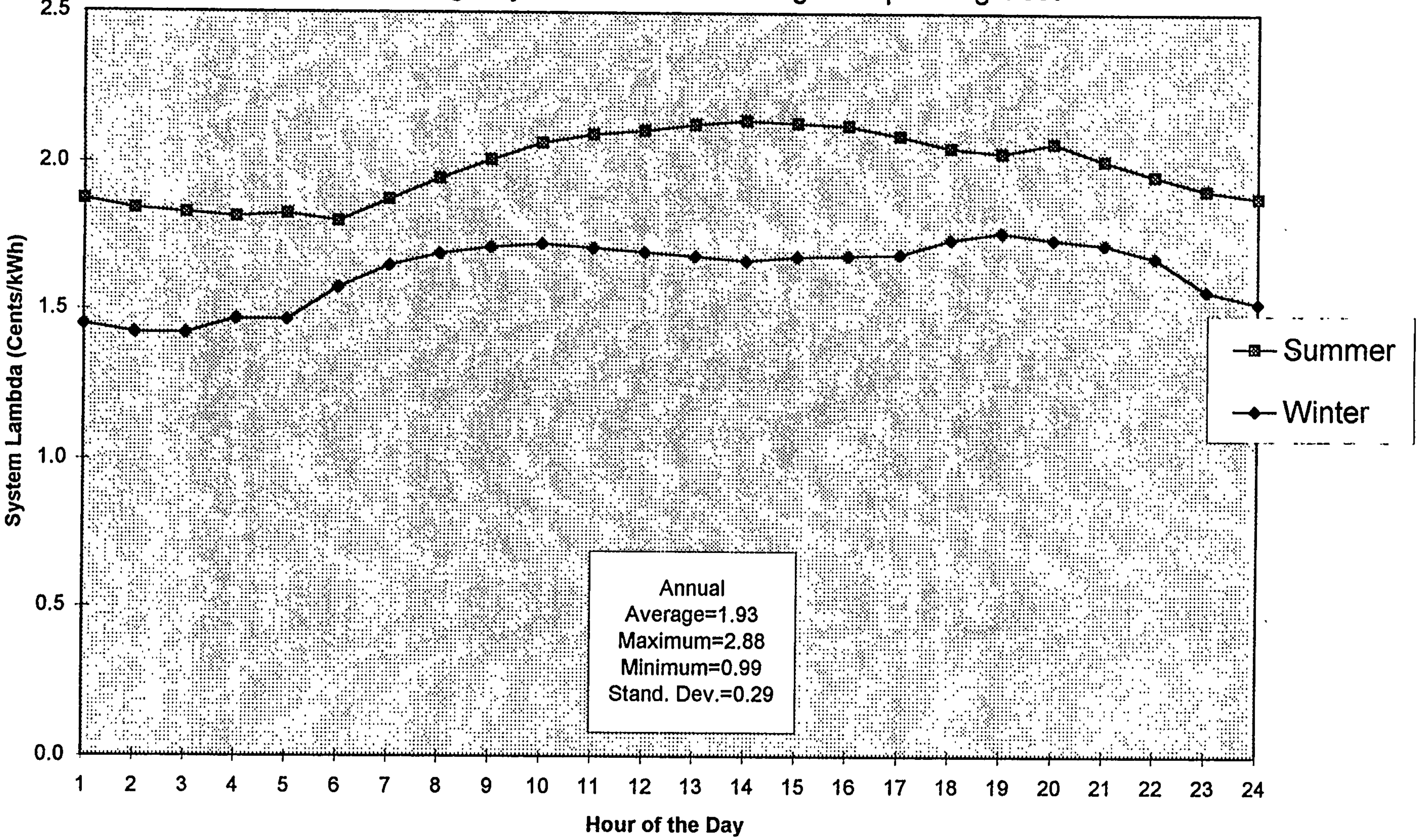
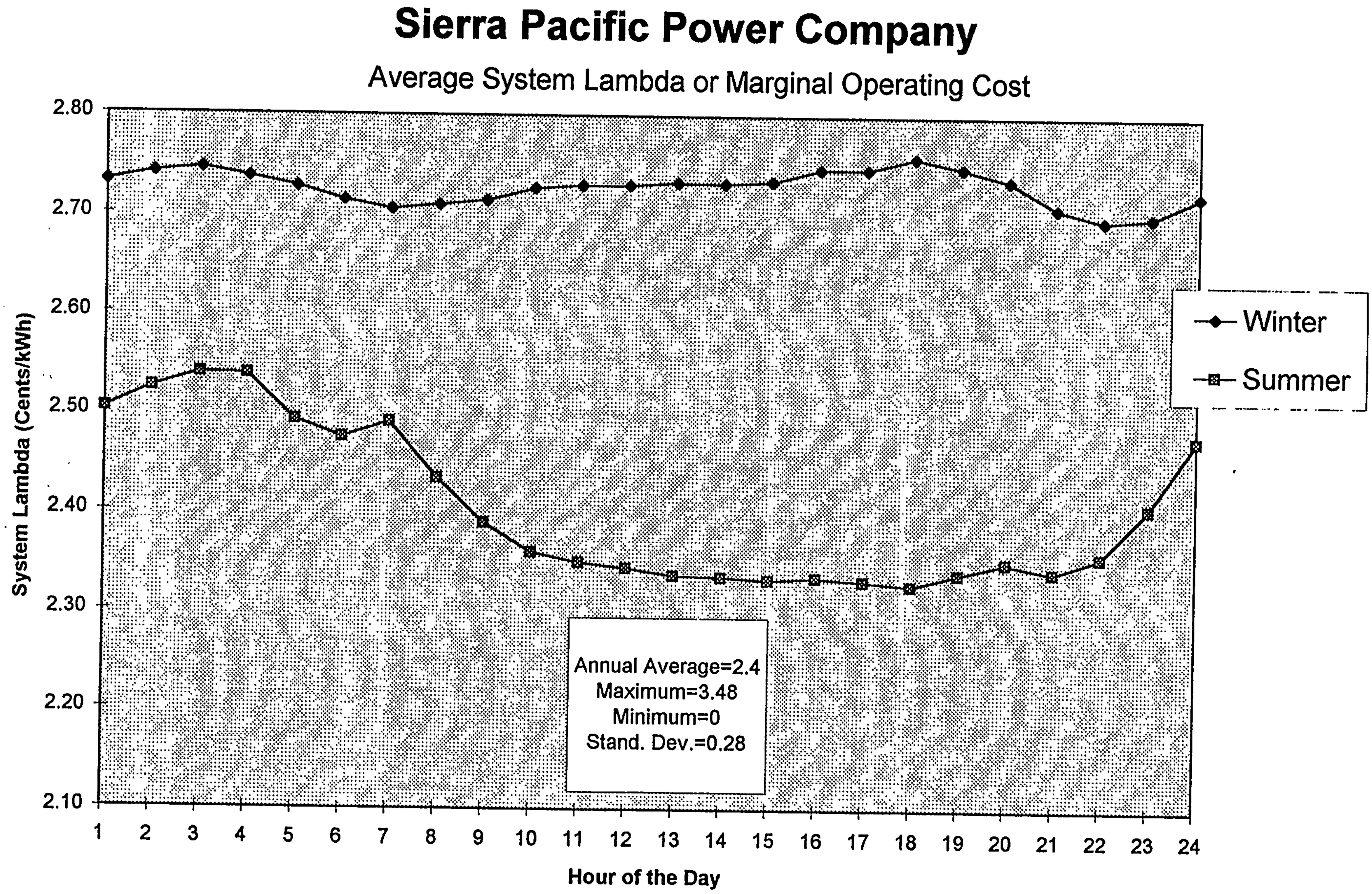


Figure 23



Sierra Pacific Power Company

Average System Lambda or Marginal Operating Cost

Figure 24

Southern California Edison

Average System Lambda or Marginal Operating Cost

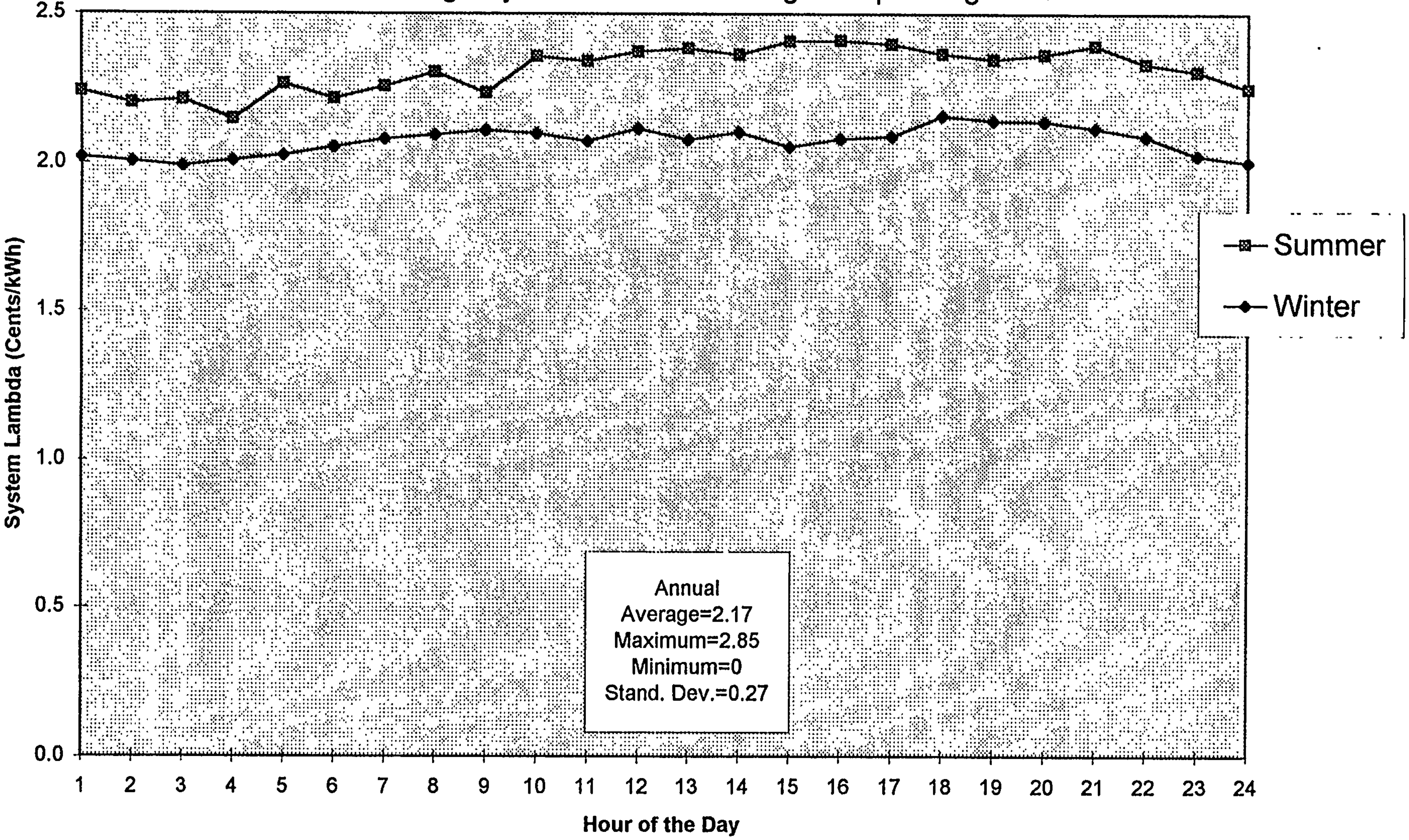


Figure 25

Florida Power & Light Company

Average System Lambda or Marginal Operating Cost

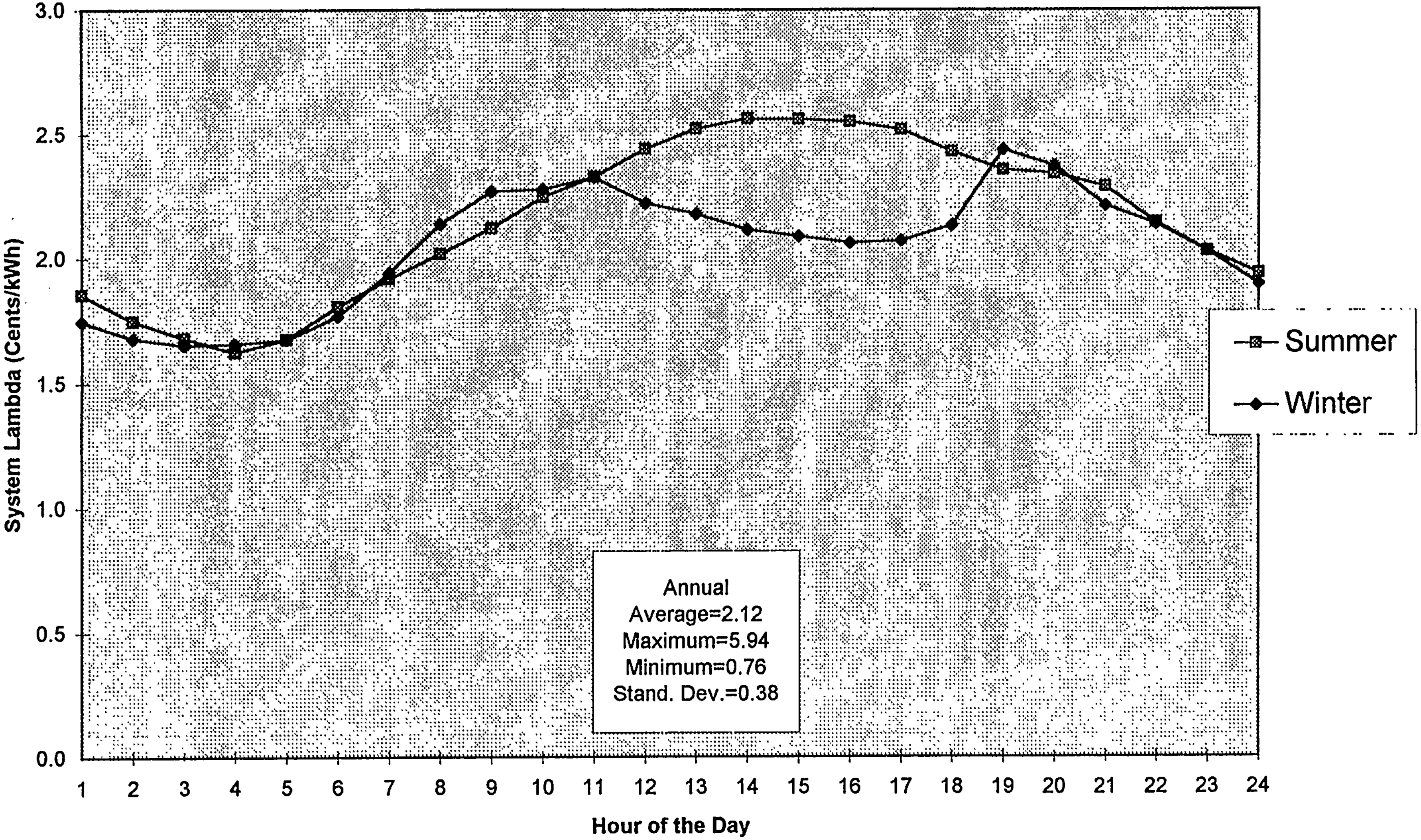


Figure 26

DIRECTED TECHNOLOGIES, INC.

Off Peak Residential Electrical Rates

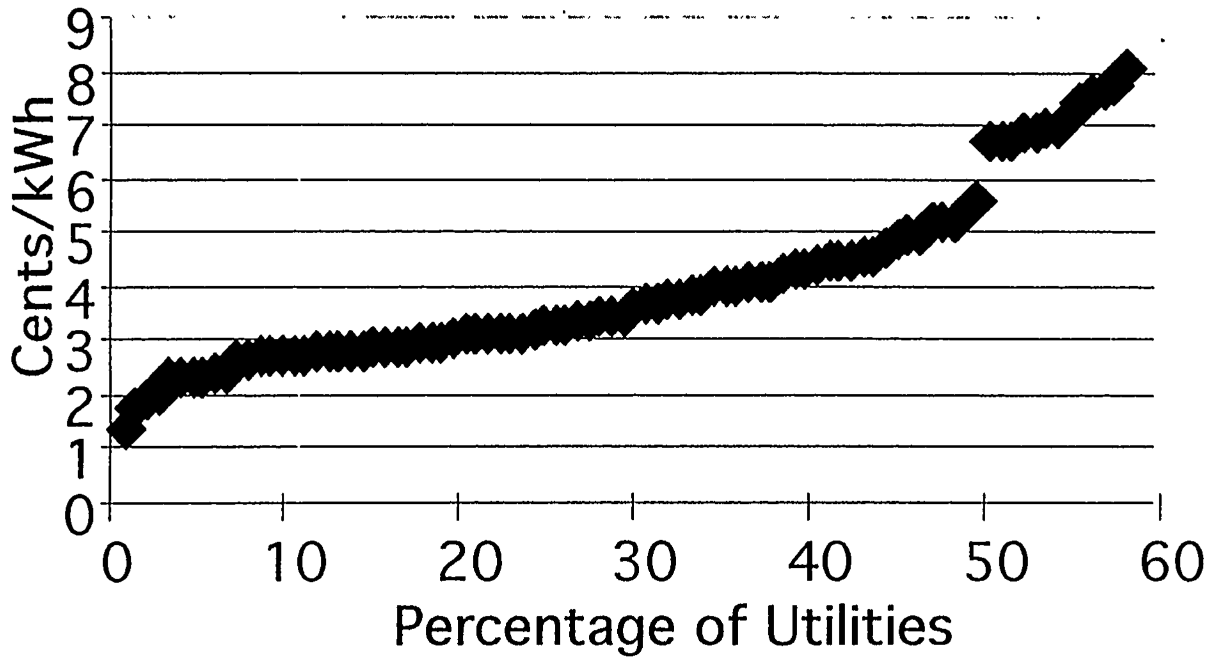
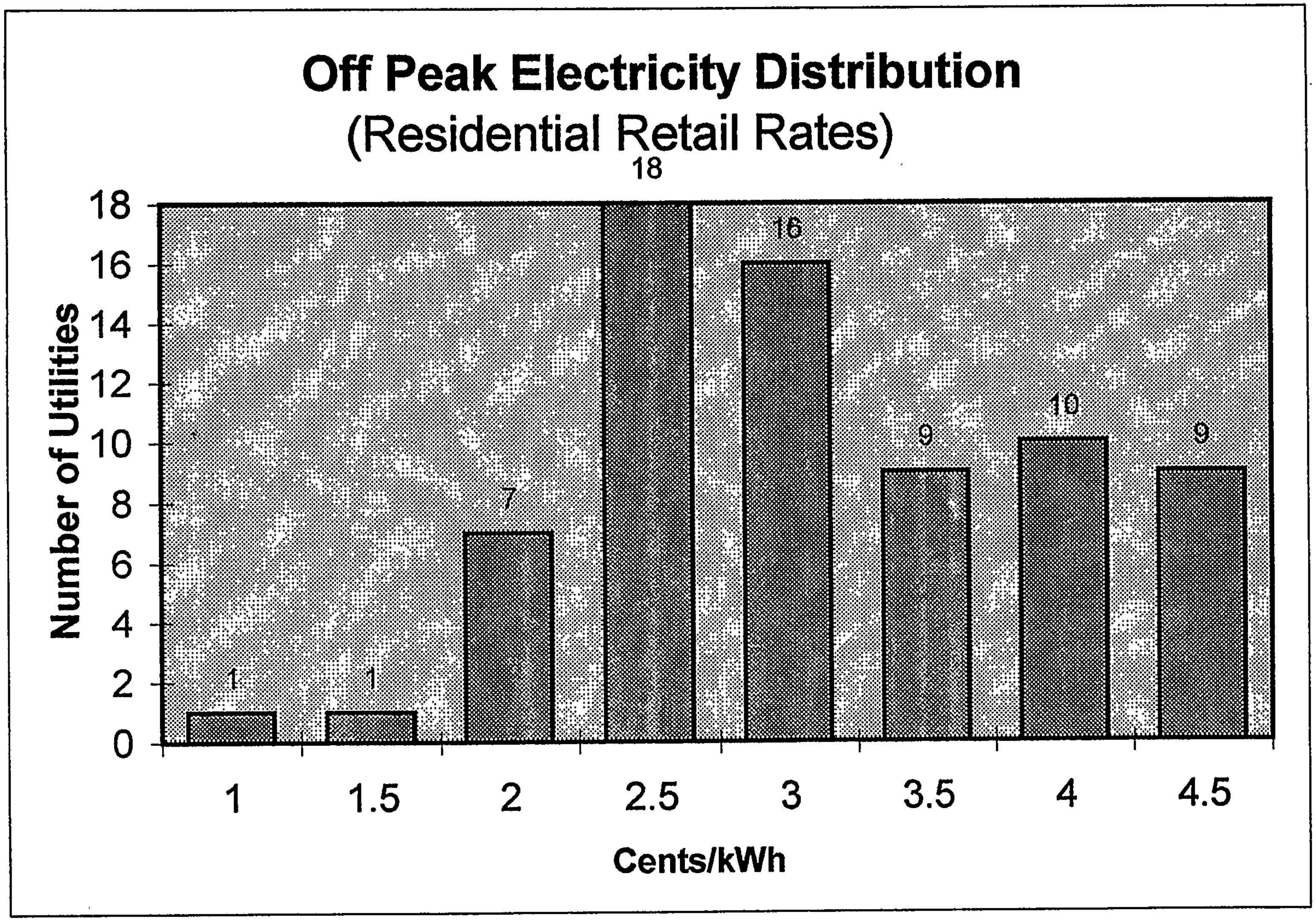


Figure 27

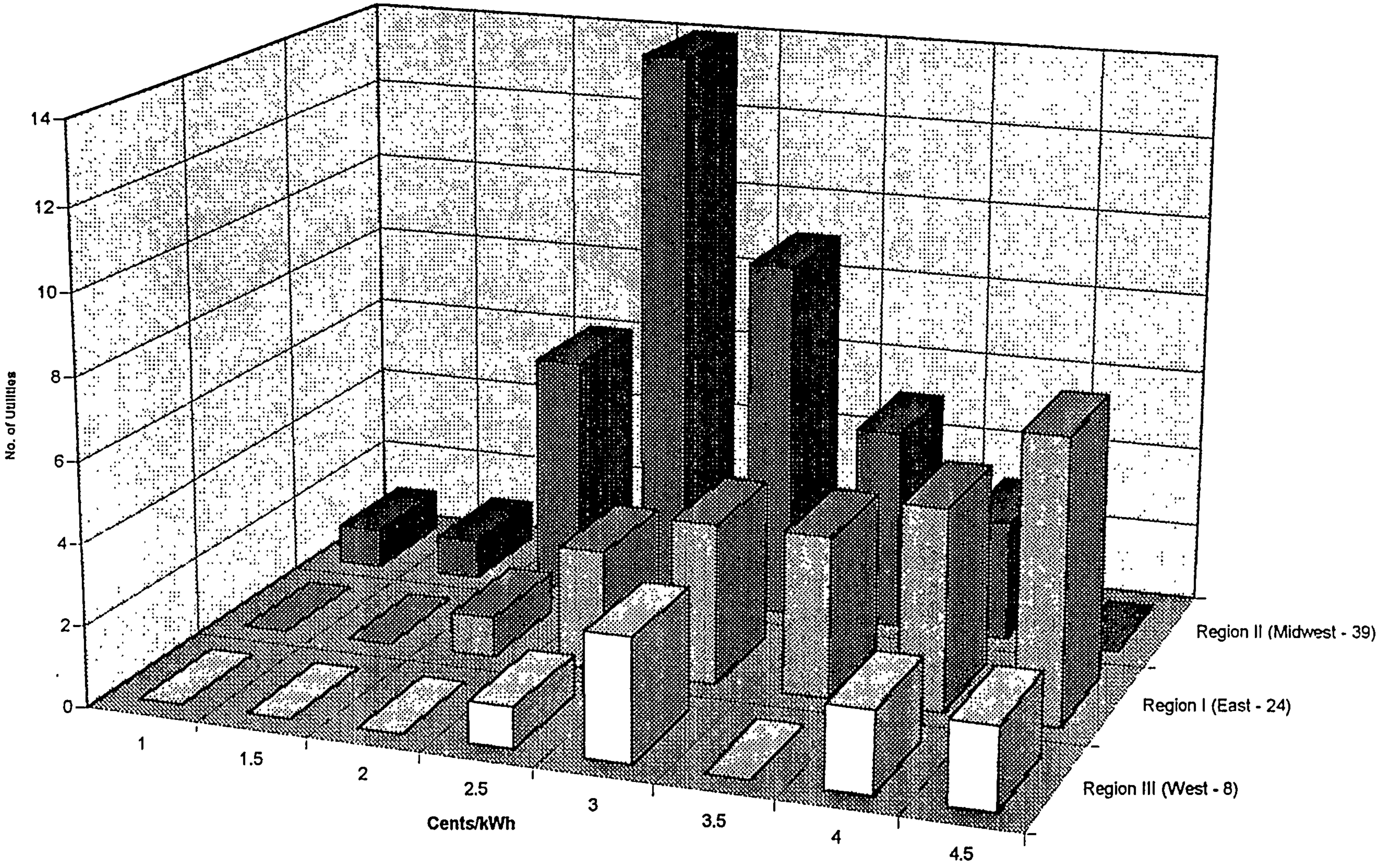


Off Peak Electricity Distribution
(Residential Retail Rates)

Figure 28

Off-Peak Electricity Cost Distribution

(Retail Residential Rates)



A SMOOTH TRANSITION TO HYDROGEN TRANSPORTATION FUEL

Gene D. Berry, J. Ray Smith and Robert N. Schock
Lawrence Livermore National Laboratory
Livermore, CA 94550

Abstract

The goal of this work is to examine viable near-term infrastructure options for a transition to hydrogen fueled vehicles and to suggest profitable directions for technology development. We have focused in particular on the contrasting options of decentralized production using the existing energy distribution network, and centralized production of hydrogen with a large-scale infrastructure. Delivered costs have been estimated using best available industry cost and deliberately conservative economic assumptions. The sensitivities of these costs have then been examined for three small-scale scenarios: 1) electrolysis at the home for one car, and production at the small station scale (300 cars/day), 2) conventional alkaline electrolysis and 3) steam reforming of natural gas. All scenarios assume fueling a 300 mile range vehicle with 3.75 kg.

We conclude that a transition appears plausible, using existing energy distribution systems, with home electrolysis providing fuel costing 7.5 to 10.5¢/mile, station electrolysis 4.7 to 7.1¢/mile, and steam reforming 3.7 to 4.7¢/mile. The average car today costs about 6¢/mile to fuel. Furthermore, analysis of liquid hydrogen delivered locally by truck from central processing plants can also be competitive at costs as low as 4¢/mile. These delivered costs are equal to $30 to $70 per GJ, LHV. Preliminary analysis indicates that electricity transmission costs favor this method of distributing energy, until very large (10 GW) hydrogen pipelines are installed. This indicates that significant hydrogen pipeline distribution will be established only when significant markets have developed.

These analyses have benefited from extensive interactions with a wide range of industrial and university experts, including Teledyne, Princeton University, Hamilton-Standard, Humboldt State University, University of California at Riverside, and Xerox.

Background

Hydrogen has been suggested as a convenient, clean-burning fuel for more than a century (Verne 1874). Hydrogen made from sustainable energy can ultimately replace fossil fuels, resolving the environmental, political, and resource concerns of their use. As a fuel, hydrogen can benefit automobiles, aircraft, and utilities, while enhancing environmental quality, energy security, and strengthening the domestic economies of energy-importing countries worldwide. The case for hydrogen-powered transportation depends broadly on being the most desirable solution to the transportation impacts on urban air pollution, energy supply insecurity, the risk of global climate change, and other environmental impacts.

Developing this case requires an assessment of the myriad methods, present and prospective, for producing, storing, and delivering hydrogen. Promising pathways are those which offer acceptable costs, while remaining consistent with a rationale under which hydrogen is among the best alternatives. Such pathways must offer reasonable costs while achieving maximum benefit from hydrogen's competitive advantages. This paper examines one of the most promising options: on-site production of hydrogen to fuel light-duty vehicles.

Introduction

Hydrogen's Competitive Advantages

Broadly speaking, hydrogen has two dominant characteristics. First, hydrogen is more expensive to produce and store than today's fuels. Second, hydrogen has unparalleled cleanliness, flexibility, and potential as a secure, sustainable transportation fuel. In these two characteristics lie the challenge and promise of hydrogen energy.

Hydrogen's high cost means that effective hydrogen use will require a high value end-use with an efficient production, delivery, and utilization structure. Hydrogen's high cost and desirability share a common root. Hydrogen is high cost because it must be manufactured, not simply discovered. This fundamental distinction is the basis of any sustainable fuel and a powerful advantage of hydrogen: it can be manufactured at or near the point of use. If small scale hydrogen production equipment can be built at reasonable cost it would allow an unprecedented level of decentralization and flexibility in the use of energy resources. Along with sustainability and potential versatility, hydrogen has additional competitive advantages over other fuels: efficiency and cleanliness in use. Its very high flame speed allows the highest efficiencies, lowest operating temperatures, and lowest emissions in internal combustion engines of any fuel. Hydrogen can achieve even higher efficiencies, and zero emissions, when used in fuel cells to produce electricity.

Hydrogen's Most Effective Role: Fueling the Light Duty Fleet

Given hydrogen's competitive advantages, its most effective large scale end-use is in the transportation sector, and specifically the light-duty vehicle fleet. There are detailed reasons for this, but, in essence, it is because the light-duty fleet accounts for the lion's share of the economic, environmental, and energy security problems associated with transportation and energy use (Office of Technology Assessment 1991). Also, the light duty fleet is relatively inefficient and has high capital stock turnover (American Automobile Manufacturers Association 1993) so hydrogen can make the most rapid and significant impact there. From a strictly economic perspective, hydrogen will make the most sense in the light duty fleet because:

- the light duty fleet places the highest value on useful energy delivered
- energy represents the smallest share of total costs (Sachs 1992)

Supporting Premises for Hydrogen Vehicles

The hydrogen vehicle itself will play the most significant role in determining the desirability of various hydrogen pathways. Vehicle efficiency determines allowable hydrogen costs and, in combination with vehicle range requirements, the feasibility of various onboard storage technologies. The choice of onboard storage technology(s) in turn may place different requirements on the delivery infrastructure. The range and efficiency of the hydrogen vehicle are constrained by three premises.

First, the vehicle must use much less fuel than today's vehicles, not only to reduce fuel and onboard storage costs, but also to minimize total fuel cycle emissions. In order for hydrogen to be economically feasible at today's or even future gasoline prices ($1.25-$1.50/gallon), vehicles must do two things:

- require less energy to travel than today's vehicles
- produce useful energy more efficiently than today's vehicles

Two proposed options are fuel-cell electric vehicles (FCEV's) (Deluchi 1992) and hybrid electric vehicles (HEV) using an internal combustion engine (Lovins 1993, Smith 1993). A critical element of both of these approaches is onboard peak power electrical storage. Another element is reduction of vehicle mass and drag to levels near those demonstrated in prototype battery electric vehicles.

A second premise of economically competitive hydrogen vehicles is that they compete with battery-powered electric vehicles (BPEV's) on the basis of range. A minimum range for hydrogen vehicles should probably be on the order of 200 miles, easily achievable with hydrogen, but well above near or intermediate term BPEV's (at least for similar costs).

The third premise necessary for hydrogen vehicles is that hydrogen is desirable over other alternative fuels such as methanol or natural gas. Hydrogen cannot compete on delivered fuel cost or vehicle range with these alternative fuels because of their higher energy density. Hydrogen probably cannot compete as the lowest cost solution to urban air pollution either, without strict zero-emission vehicle (ZEV), or "near ZEV" regulations.

In order for hydrogen to compete in the marketplace, it must offer what other alternative fuels cannot: a single, smooth, flexible and ultimate transition, for the light duty fleet; a transition that allows diversification of primary energy sources, but retains the potential for sustainability and almost negligible environmental impact, wherever and whenever the costs become worth the benefits. More so than any other fuel, powering the light duty fleet with hydrogen would give the United States greater versatility to respond (through changes in production method), without much disruption, to future changes in the importance and relative priority of oil imports, urban air pollution, greenhouse gas emissions, land and water use, and environmental quality. Pathways to fuel hydrogen vehicles must preserve these competitive advantages (a single, smooth, flexible transition) or hydrogen loses a significant edge over other alternative fuels.

Methods and Assumptions

Economic Assumptions and Approach

Throughout our assessment, we have used relatively conservative economic assumptions. If a particular strategy makes sense under conservative assumptions, then it should be relatively robust in the marketplace. Specifically, we have used commercial discount rates of 20% and consumer discount rates of 10%. Equipment lifetimes were 20 years for production plant equipment, 10 years for other capital equipment. No salvage value was assumed. Energy prices were relatively high. Off-peak electricity was assumed to be available at $0.05/kwh for 128 hrs per week. Lower rates may be available in some areas and seasons (Thomas 1995). Natural gas was assumed at $4.00/GJ. Hydrogen from central plants was $9/GJ (Korentz 1992). The lower heating value of hydrogen was used throughout. Gasoline reference costs were $1.25/gallon in a 25 mpg vehicle. Capital costs of electrolyzers were somewhat higher than other estimates (Ogden 1994, Thomas 1995) as well.

Hydrogen Vehicle Characteristics

Various hydrogen vehicle designs are possible. For our calculation we posit a 5-passenger hydrogen hybrid vehicle detailed elsewhere and shown in Fig. 1. The characteristics of this vehicle are drawn from GM Impact III, with allowance for the differences between hydrogen and battery-powered drivetrains. Such a vehicle is capable of good performance: accelerating (0-60 mph) in 10 seconds, with a 380 mile range and 80 mpg equivalent fuel economy on the mixed EPA Federal Urban/Highway Driving Cycle. To achieve a 380 mile range 4.75 kg of onboard hydrogen storage is needed (Aceves and Smith 1994). We use a more conservative range of 300 miles (and 3.75 kg H_2 onboard) for our base case calculations. A wide range of onboard hydrogen storage technologies are possible (Robinson 1994). Liquid hydrogen seems most desirable for long range. Although good progress has been made in Germany (Peschka 1992, Rudiger 1994) hydrogen filling stations delivering LH_2 to vehicles are still in development. We chose a basis of comparison with less cost uncertainty and greater compatibility with other recent analyses. We assume hydrogen onboard vehicles are stored in a carbon fiber wrapped vessel at high pressure (6000-8000 psi). The weights, volumes and storage cycle energy penalties associated with compressed gas and other various onboard hydrogen storage technologies are presented in Fig. 2.

Hydrogen Filling Stations

Most scenarios of interest assume hydrogen delivery to vehicles at a filling station as gasoline is delivered today. We did not examine filling station economics in detail, but instead assumed a flat operating overhead rate of $720/day ($263,000/yr.) to account for labor and capital charges associated with any filling station operation. These costs were assumed independent of fuel choice. Hydrogen dispensers sized for peak demand (15% of an entire day's vehicles in one hour). Operating and maintenance costs of $1000/yr for each compressed hydrogen (CH_2) dispenser were added to flat overhead costs (Ogden 1995).

Hydrogen filling stations were assumed to serve 300 cars/day. A gasoline station serving 300 cars per day with an average fillup of 10 gallons would take in about $3,750 per day. Our assumed overhead charge of $720 per day would correspond to 19.2% of gross revenues in this case, somewhat high, but reasonable. High overhead is especially likely considering the relatively high cost of stations in high urban air pollution hotspots, where hydrogen vehicles are likely to appear first. Quoted costs for installing a large gasoline station can be $750,000 in such areas (Ryan 1993).

Results

Truck Delivery to Filling Stations or On-Site Production?

In considering hydrogen filling station scenarios, we asked whether there was a clear cost difference between hydrogen delivery by truck and on-site hydrogen production options. First estimates of delivered hydrogen costs by truck using liquid hydrogen and alternative storage methods were made, and then compared to estimates of on-site production costs.

Hydrogen by Truck

The hydrogen transport technologies considered for delivery by truck were: liquid hydrogen, a magnesium-based hydride, a cryogenic (K) composite pressure vessel storing hydrogen at 3600 psi, and a microsphere storage bed storing hydrogen at 9000 psi. Estimated delivered hydrogen costs are shown in Fig. 3 (broken down by storage energy, transport energy, mobile hydrogen storage, personnel, etc). The technical assumptions and cost characteristics for each technology are detailed in Table 1. Fig. 3 shows that each of the technologies can deliver hydrogen approximately 250 miles for approximately $20/GJ. This cost is consistent with prices quoted for large, regular LH_2 deliveries today (Ogden 1994). Slightly lower costs may be achievable *if* alternative mobile storage technologies can meet or exceed the assumptions used in Table 1 *and* shorter delivery distances reduce the high variable costs of H_2 transport by methods other than LH_2. Significant improvements and cost reductions for alternatives to LH_2 transport would be required, however, since the majority (50-75%) of delivered hydrogen costs are fixed (i.e., hydrogen production and storage energy) for all technologies.

Hydrogen Produced On-Site

On-site production costs of hydrogen by three technologies were estimated: natural gas steam reforming, alkaline electrolysis, and steam electrolysis. The first two are relatively mature technologies, although alkaline electrolyzer markets have been relatively small and production costs for electrolyzers at the filling station scale may come down with increased demand. Steam electrolysis is still in the development stage, and estimated costs were taken from studies in Germany (Quandt 1986) and SOFC stack development goals of the Gas Research Institute (GRI). Other costs and efficiencies calculated for hydrogen stations are shown in Table 2 (Korenz 1992, Ogden 1994). Compressed gas storage costs used at the station were those collected by Ogden for her recent detailed examination of steam reforming at hydrogen filling stations (Ogden 1994, 1995), and represent current industrial equipment prices. Hydrogen delivery pressure was 6000 psi. The results of these estimates are given in Fig. 4. LH_2 delivery by truck, using the costs presented in Fig. 3, and a home electrolysis case for a single hydrogen vehicle are included for comparison. The fuel cost of gasoline was also included (for a 25 mpg vehicle). Figure 4 shows that on-site production technologies (at the station scale) achieve costs roughly similar to those for liquid hydrogen delivery. Alkaline electrolysis is somewhat more expensive, but the electricity and capital costs used for this case are conservative (Korentz 1992).

Compressed gas storage accounts for a large amount of the cost differential between the on-site production options and liquid hydrogen delivery. This gap could narrow considerably when hydrogen storage equipment is mass produced for filling stations. On-site production technologies might also reduce costs if delivery scale was increased. This would involve longer range hydrogen vehicles, or larger stations serving more cars per day. Figure 4 also shows that on-site hydrogen production at stations is competitive with gasoline costs today. On-site production at much smaller scales (e.g., home electrolysis) is cost-competitive with battery-powered electric vehicles, (especially considering the range advantage of hydrogen).

Table 1. Estimated Technical and Cost Parameters for Truck Transport of Hydrogen as Liquid Hydrogen and Alternative Methods

Truck and Delivery Schedule Parameters

Annual Mileage of Truck:	100,000 miles per year
Delivery Distance (round-trip)	500 miles
Trips per year:	200
Capital Cost of Truck Cab	$60,000
Life of Cab	10 years
Personnel Costs:.	$100,000/yr.
Fuel Cost	$10/GJ ($1.25/gallon gasoline)
Discount Rate	20%

Technical Parameters

Storage System	Cryogenic Gas	LH_2	Microspheres	Hydride
Temperature (to store or deliver)	80K	20K	250°C	250°C
Pressure (psi)	3600	<100	9000	<200
H_2 mass fraction of mobile storage	.12	.20	.10	.04
H_2 density (kg/m3) (alone)	53	70.8	36	100
H_2 density (kg/m3) (system)	40	50	20	50
Storage energy penalty (fraction of stored H_2 required for storage cycle)	25%	35%	10%	Waste Heat

Capital Cost of Mobile Hydrogen Storage System

	Cryogenic Gas	LH_2	Microspheres	Hydride
$/GJ	4000	1000	3000	3333
$ per kg of storage system (full)	60	22.5	3	16
$ per kg H_2 stored	480	112	360	400

H_2 Trailer Characteristics

Trailer Capital Cost (millions of dollars)	1.3	0.39	0.49	0.48
H_2 stored on 1 truck (kg)	2704	3479	1352	1200
Cargo weight (kg)	22500	17400	13520	30000
Cargo volume (m^3)	67.6	67.6	67.6	30
Fuel economy(mpg)	6.0	6.0	6.0	6.0

Table 2. Estimated Technical and Cost Parameters for Hydrogen Stations

Hydrogen Vehicle		
Vehicle Range	300 miles	
Vehicle Efficiency	80 mpg	
Onboard H_2 storage	3.75 Kg (6000 psi)	
Economic Assumptions		
Discount Rate	20% (Commercial)	
Electricity (off-peak 128 hrs/wk).	$0.05/kwh	
Natural Gas (at station)	$4.00/Gigajoule	
Hydrogen (at central plant)	$9.00/Gigajoule	
Generic Station Parameters		
Cars per day	300	
Daily Overhead	$720/day or $2.40 per fillup	
H_2 throughput per day	1125 kg (0.47 MMscf/day)	
On-site storage	1.0 days (1125 kg H_2)	
Station Storage Costs (compressed gas)	Dollars or Dollars/yr	Dollars/Fillup
Compressors (multi-stage from 200-6000 psi)	$350,000	
Storage Tanks (6000 psi)	$570,000	
Dispensers	$100,000	
Total Capital	$1.02 million	
Storage Capital Life	10 years	
Annual Levelized Capital Costs	$243,000	2.22
Annual Operating and Maintenance Costs	$8800	0.08
Storage Electricity (0.11 kwh/kwh H_2)	$0.05/kwh	0.69
Total		2.99
Station Storage Costs (LH_2)	Dollars or Dollars/yr	Dollars/Fillup
Storage Tank	$105,000	
Pumps and vaporizers	$ 72,000	
Total Capital	$277,000	
Annual Levelized Capital Costs	$ 66,000	0.60
LH2 Pump Electricity (0.04 kwh/kwh H_2)		0.27
Annual Operating and Maintenance Costs	$ 7,000	0.06
Total		0.93

Hydrogen Production Costs at Stations

Steam Reforming Costs (1125 kg H_2 per day)	Dollars or Dollars/yr	Dollars/Fillup
Reformer Capacity	0.47 MMScf/day	
Reformer Capital Cost	$2.39 million	
Reformer Life	20 years	
Annual Levelized Reformer Cost	$491,000	4.48
Reformer Ops costs	$0.35/kg H_2	1.31
Reformer Efficiency	68%	
Reformer Output Pressure	200 psi	
Natural Gas	$4.00/GJ	2.65
Total Reforming Costs per 300-mile Fillup		8.44

Alkaline Electrolyzer Costs (1125 kg H_2 per day)	Dollars or Dollars/yr	Dollars/Fillup
Electrolyzer Capacity	0.62 MMScf/day	
Electrolyzer Capital Cost	$2.85 million	
Electrolyzer Life	20 years	
Annual Levelized Electrolyzer Cost	$584,000	5.33
Electrolyzer Ops costs	$0.21/kg H_2	0.78
Electrolyzer Efficiency (LHV)	68%	
Off-peak availability	128 hrs/wk (76%)	
Electrolyzer Output Pressure	200 psi	
Electricity	$0.05/kwh	9.19
Total Alkaline Electrolysis costs per 300-mile Fillup		15.30

Steam Electrolyzer Station Costs (1125 kg H_2 per day)	Dollars or Dollars/yr	Dollars/Fillup
Electrolyzer Capacity	0.62 MMScf/day	
Electrolyzer Capital Cost	$1.61 million	
Electrolyzer Life	20 years	
Annual Levelized Electrolyzer Cost	$330,000	$3.01
Electrolyzer Ops costs	$0.12/kg H_2	$0.44
Electrolyzer Efficiency (LHV)	92% (exothermic operation)	
Off-peak availability	128 hrs/wk (76%)	
Electrolyzer Output Pressure	200 psi	
Electricity	$0.05/kwh	$6.68
Total Steam Electrolysis costs per 300-mile Fillup		$10.13

Of the mature technologies, LH_2 delivery can be the lowest cost source of H_2, but only by a narrow margin. This margin is contingent on travel distance from a central plant (there are only a few hydrogen liquefaction plants operating in the country today) and the amount of hydrogen stored on vehicles. Steam reforming offers hydrogen costs competitive with gasoline with widespread availability. Where off-peak electricity rates are lower than our conservative $0.05/kwh to alkaline electrolysis would approach LH_2 delivery or steam reforming costs. All the on-site station technologies appear cost competitive with gasoline in today's vehicles, and the cost differences are within the range of variability to make each preferred in certain cases.

The Impact of Delivery Scale on Hydrogen Costs

The cost comparisons and estimates above are dependent on the scale of hydrogen delivery, which is determined by the number of cars per day and the fuel requirement of each vehicle. To determine how the relative cost of hydrogen technologies varied with scale, the costs for the three station technologies (steam reforming, alkaline electrolysis, and steam electrolysis) were calculated as a function of delivery scale and compared with liquid hydrogen delivery in Fig. 5. Delivery scale was varied from 50 to 500 cars per day. Two scenarios were used to examine the impact of hydrogen storage onboard the vehicles. In the first case each car filled up with 3.75 kg H_2 (enough for a 300 mile range). In the second case fillups were 4.75 kg (enough for a 380 mile range - consistent with PNGV goals).

Daily overhead costs are omitted from Fig. 5 since these are identical for each filling station option and are uncertain at very small scales. Capital cost scaling data gathered by Ogden (Ogden 1994) was used for the steam reforming case. Electrolysis capital costs were scaled from point cost estimates from various sources (Korentz 1992, Kincaide 1994, Thomas 1995, Quandt *et al.* 1986, Krist 1995), and are more approximate than the steam reforming data. Liquid hydrogen station costs were adjusted for scale, but liquid hydrogen delivery costs were assumed constant at $21.30/GJ for illustrative purposes.

Figure 5 shows that under a 300 mile assumed vehicle range (the solid lines) the breakpoint between steam reforming and liquid hydrogen delivery is about 400 cars per day (1500 kg H_2 per day). Above this scale steam reforming is slightly lower cost. Below approximately 150 vehicles per day steam electrolysis (when further developed) could offer lower costs than steam reforming. Without the advance of steam electrolysis, steam reforming is lower cost than electrolysis until scales of about 65 cars per day. Increasing onboard storage to 4.75 kg H_2 (the dashed lines in Fig. 5) to achieve a 380 mile range, shifts the breakpoints to smaller scales. LH_2 delivery becomes cheaper than steam reforming below 310 cars per day. Steam electrolysis becomes cheaper than steam reforming at 115 cars per day, and alkaline electrolysis becomes cheaper than steam reforming at 50 cars per day.

Figure 5 also shows that LH_2 delivery can suffer large cost increases and remain competitive with on-site production at small scales: as much as $40/GJ for 50 cars per day and $30/GJ for 100 cars per day. In the longer term, if steam electrolysis is developed, allowable costs decrease to roughly $30/GJ at both scales. These costs are 50-100% higher than those given (Ogden 1994) for larger delivery rates, but are probably achievable, since the variable costs of LH_2 delivery are only a fraction of total costs (see Fig. 3).

Cost Breakdowns and Delivery Scale from 100-500 cars/day.

The relative importance of various portions of the total delivered hydrogen cost is a function of delivery scale. Capital and operating costs become more important at small scales, for example, while energy costs remain steady. The cost breakdowns as a function of delivery scale (from 100-300 cars/day) for on-site production are shown in Figs. 6-8. Costs are subdivided into capital, energy, and operating costs for production, storage, and overhead. Vehicles were assumed to have a 300 mile range and store 3.75 kg of H_2 onboard (80 mpg equivalent). Station related overhead was essentially a flat $720/day.

Figures 6-8, show that at large scales (300-500 cars/day) delivered hydrogen costs from on-site production are from 4.5-6.5 cents per mile (gasoline is roughly 5 cents/mile today). Steam reforming is the lowest cost, with cheaper energy inputs and low capital cost, but steam electrolysis has even lower capital costs and is competitive with steam reforming. Alkaline electrolysis costs 6.5 cents per mile, 2 cents/mile more than steam reforming. Notably, this difference is not entirely due to electricity costs. The additional capacity required because of limited off-peak availability increases the electrolysis capital investment. The investment for alkaline electrolysis is so high that it roughly equals the combined capital *and* energy costs for steam reforming. Figs. 6-8 also show that compressed storage costs are dominated by capital costs which don't scale very much and are roughly 1.0 cents per mile.

At smaller scales delivered H_2 costs rise to 7.5-9.0 cents per mile at 100 cars/day. Capital costs for steam reforming increase much faster than for electrolysis, as implied in the earlier discussion of Fig. 5. However, simple overhead costs (non-H_2 related costs of the station) rise faster than any other portion of total costs at small scales, accounting for roughly 2.0 cents per mile at 100 cars/day. The essential conclusions from Figs. 6-8 are:

1) Compressed H_2 Storage costs are capital dominated and are not a strong function of scale in the range of 100-500 cars/day (in comparison to capital costs). Storage costs are in the range of 1.0 cents per mile. Therefore the delivered fuel cost benefits of alternative onboard storage technologies to compressed gas would be $120/year at most (i.e., if station storage were zero cost for other onboard vehicle storage options).

2) Reduced capital costs would be necessary for alkaline electrolysis to achieve lower costs than steam reforming at large scales (300-500 cars/day). This not unlikely given the maturity differences between the two industries.

3) At small scales steam reforming costs rise quickly due to increasing capital costs, but operating costs rise even faster for all on-site technologies. Any technology that would allow lower labor and overhead costs at small scales could have a significant advantage.

4) Total hydrogen fueling costs are 4.5-6.5 cents per mile for 300 cars/day and 7.5-9 cents per

mile at 100 cars/day. For electrolysis technologies over half of the cost increase is overhead. For steam reforming the increase is mostly the capital cost of the reformer.

Figures 4-8, in combination, show that hydrogen can be delivered for total costs in the range of 4.5-7 cents per mile (in an 80 mpg equivalent hydrogen electric vehicle) by any of a number of conventional options: LH_2 delivery from a central plant, steam reforming, or off-peak alkaline electrolysis. Steam electrolysis could reduce future electrolysis costs significantly. All technologies are within the cost range necessary to be competitive with gasoline in cars today. At small scales (50-100 cars per day) the lowest cost on-site production technology shifts from steam reforming to electrolysis. However, it is possible that LH_2 truck delivery, if available, could compete with any on-site production technology except large stations (300-400 cars/day) using steam reforming.

Home or Commercial Electrolysis

There is a scale below which H_2 delivery is not feasible. Introducing hydrogen vehicles at this scale may be crucial to beginning a smooth transition to hydrogen vehicles either at home or small fleets, such as taxis or postal service vehicles. We have therefore estimated costs for producing hydrogen by electrolysis at the individual vehicle level. Informal estimates from electrolyzer manufacturers suggest that an electrolyzer sufficient for a single vehicle (around 2 kW H_2 output) could cost about \$2400/kW of H_2 output with somewhat higher production rates than today. Electrolyzer efficiency would be around 50% (LHV) (Kincaide 1994). For the home electrolysis case off-peak electricity was assumed available on weekends and 8 hours/night on weekdays (50% availability) for \$0.05/kwh. On-site storage of low pressure (200-300 psi) hydrogen was estimated to conservatively cost \$1500 for 3.75 kg of H_2. The technical feasibility of a system similar to the one proposed has been investigated and demonstrated for more than a year at Humboldt State University, using a small electrolyzer and low pressure storage to power a PEM fuel cell (Lehman *et al.* 1994). They achieved electrolyzer efficiencies of 60-65%. The costs for home electrolysis as well as the other larger scale options was shown previously in Fig. 4. We assumed hydride storage onboard the vehicle to avoid home high pressure storage issues. Recently, however, home electrolysis using high pressure PEM electrolyzers (at least 2000 psi) and compressed H_2 on vehicles has been advanced. Home electrolysis could compete with today's gasoline costs (i.e., delivered H_2 for less than 5 cents per mile) *if* electrolyzer, compressor, and storage tank capital costs were reduced sharply (from the values we used) through economies of mass production (Molter 1994, Thomas 1995).

Summary

The costs of delivered hydrogen using centralized production and delivery and on-site hydrogen steam reforming or electrolysis have been estimated for station and smaller scales. 80 mpg equivalent hydrogen electric vehicles were assumed, using compressed gas onboard storage. Hydrogen delivery by truck was found to have similar costs for a variety of mobile storage technologies (\$20-25/GJ). None appear to have a strong cost advantage over liquid hydrogen. Delivered hydrogen costs at stations (300 cars/day) are in the range of 4.5-7 cents per mile and 8-9 cents per mile at smaller scales 50-100 cars per day. Compressed H_2 storage at stations accounts for about 1.0 cents per mile of delivered H_2 costs and was not as strongly affected by scale as other components of delivered H_2 costs. At small scales (below 80 cars/day) alkaline electrolysis offered lower costs than steam reforming. The breakpoint between electrolysis and steam reforming would rise to 125 cars/day if steam electrolysis research results and cost estimates can be translated to commercial reality. Hydrogen refueling from very small electrolyzers (2 kW) at home or work had conservative costs of 10 cents per mile using low pressure home storage and hydride storage onboard the vehicle.

Conclusions

All hydrogen delivery and on-site production pathways were competitive with fuel costs for gasoline cars today, at station scales (300 cars/day). The cost differences between various methods were about 1-2 cents per mile or $120-240/yr. for a hydrogen vehicle driven 12,000 miles/yr. Such cost differences are small compared to the life cycle cost of hydrogen electric vehicles ($0.40/mile or $4800/yr.) and suggests that costs of LH_2 truck delivery and/or on-site production by reforming or electrolysis are low enough to allow a smooth hydrogen transition. A transition strategy using any or all of these options can be formulated without the hard constraint of fuel costs.

The critical issues surrounding a transition to hydrogen vehicles may lie outside the realm of fuel cost (given the high efficiency vehicles used here). Issues for future consideration should include vehicle capital cost and operating life, development of small-scale hydrogen technologies to begin a smooth transition, emissions and environmental impact of various transition strategies, and whether hydrogen pathways complement or compete with the existing energy system.

Acknowledgments

We would like to especially thank Sandy Thomas, Jim Birk and Joan Ogden for their helpful constructive criticisms, Bill Kincaide and Michael Miller of Teledyne-Brown Engineering, and Peter Lehman of Humboldt State University, for helpful conversations on small scale electrolyzers.

Work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

References

Aceves, S. M. and J. R. Smith. 1994. "A Hybrid Vehicle Evaluation Code and its Application to Vehicle Design." SAE International Congress and Exposition, Detroit, Michigan. February 27-March 2, 1995 (SAE # 950491); Lawrence Livermore National Laboratory Report UCRL-JC-117918.

American Automobile Manufacturers Association. 1993. *AAMA Motor Vehicle Facts & Figures 1993*, American Automobile Manufacturers Association Government Affairs Division.

DeLuchi, M. *Hydrogen Fuel-Cell Vehicles*. 1992. Research Report UCD-ITS-RR-92-14. Institute of Transportation Studies, Univ. of California, Davis. Davis, California 95616. (916)-752-1914

Kincaide, W. C. Teledyne Brown Engineering, Energy Systems. 1994. Personal Communication July 1994. Hunt Valley, Maryland 21031-1311.

Korenz, N. 1992. "Economics of Hydrogen Manufacture," Report by SFA Pacific Inc. for Texaco and others.

Krist, K. Gas Research Institute. 1995. Personal Communication. February 22.

Lehman, P.A. C.E. Chamberlin, G. Pauletto, M.A. Rochleau. 1994. "Operating Experience with a Photovoltaic-Hydrogen Energy System." in proceedings of *Hydrogen '94: The 10th World Hydrogen Energy Conference*. Cocoa Beach, Florida, June 20-24, 1994.

Lovins, A. J. Barnett, L. Lovins. 1993. "Supercars: The Coming Light-Vehicle Revolution." Presented at the *Summer Study of the European Council for an Energy-efficient Economy*, Rungstedgard, Denmark, June 1993. Rocky Mountain Institute, Snowmass, Colorado 81654-9199.

Molter, T. 1994. Hamilton Standard Division of United Technologies, Space and Sea Systems "SPE Water Electrolyzers for Commercial Hydrogen Production" Windsor Locks, CT.

Ogden, Joan. November 2, 1994. Personal Communication.

Ogden, J. E. Dennis, J. Strobehn. 1994. "A Technical and Economic Assessment of the Role of Natural Gas in a Transition to Hydrogen Transportation Fuel." *Hydrogen '94: The 10th World Hydrogen Energy Conference*. Cocoa Beach, Florida, June 20-24, 1994.

Ogden, J. 1995. Draft Report "Hydrogen Energy System Studies" Center for Energy and Environmental Studies, Princeton University, Princeton, New Jersey 08544.

Peschka, W. 1992. *Liquid Hydrogen: Fuel of the Future* . Springer-Verlag, New York, 1992.

Quandt, K.H., R. Streicher. 1986. "Concept and Design of a 3.5 MW Pilot Plant For High

Temperature Electrolysis of Water Vapor." *International Journal of Hydrogen Energy.* Volume 11, Number 5, pp. 309-315.

Ryan, Pat, ARCO. July 1993. Personal Communication.

Robinson, S. L. and J. L. Handrock. 1994. *Hydrogen Storage for Vehicular Applications: Technology Status and Key Development Areas*, Sandia National Laboratories report SAND94-8229 UC-406.

Rudiger, H. *et al.* 1994. "Liquid Hydrogen Storage System For an Urban Bus. "Hydrogen *'94: the 10th World Hydrogen Energy Conference*, Cocoa Beach, Florida, 20-24 June 1994. pp. 967-973.

Sachs H.M., J. Decicco, M. Ledbetter, U. Mengelberg. January 1992. *Heavy Truck Fuel Economy: A Review of Technologies and the Potential for Improvement*, TRB Paper No. 920619 71st Annual Meeting of the Transportation Research Board. Washington, D.C.: American Council for an Energy-Efficient Economy.

Smith J.R. 1993. "The Hydrogen Hybrid Option" presented at *NIST Workshop on Advanced Components for Electric and Hybrid Electric Vehicles*, Gaithersburg, MD, Oct. 1993; Lawrence Livermore National Laboratory Report UCRL-JC-115425 Livermore, CA 94550.

Thomas, S. January 27, 1995. Personal Communication, draft Technical Report. Directed Technologies, Inc. Arlington, Va 22203.

U.S. Congress, Office of Technology Assessment. 1991 *Improving Automobile Fuel Economy: New Standards, New Approaches,* OTA-E-504 Washington, DC: U.S. Government Printing Office, October 1991.

Verne, Jules. 1874. *The Mysterious Island*.

Figure Titles

Figure 1:	Conceptual Hydrogen Powered Vehicle.
Figure 2:	Storage Systems for 3.75 kg hydrogen (300 mile range at 80 mpg). Energy penalties are as follows: 9000 psi tank - 10%; Mg hydride - 25%; Liquid hydrogen - 32%; Cryotank - 25%; Carbon aerogel - 25%; Methanol reformer - 20%.
Figure 3:	Estimated Costs of Truck Delivery of Hydrogen for Liquid Hydrogen, Magnesium-Based Hydride, LN_2-Cooled Pressure Tank, and Microspheres (250 miles).
Figure 4:	Refueling Costs (3.75 kg H_2 per car/300 mile range) of LH_2 Truck Delivery, On Site Production at Filling Stations, and Home Electrolysis.
Figure 5:	Impact of Scale on Delivered Hydrogen Cost (3.75 & 4.75 kg) / Personnel and Non-Fuel related Overhead Omitted.
Figure 6:	Delivered Cost of H_2 for On-Site Steam Reforming.
Figure 7:	Delivered Cost of H_2 for On-Site Alkaline Electrolysis.
Figure 8:	Delivered Cost of H_2 for On-Site Steam Electrolysis.

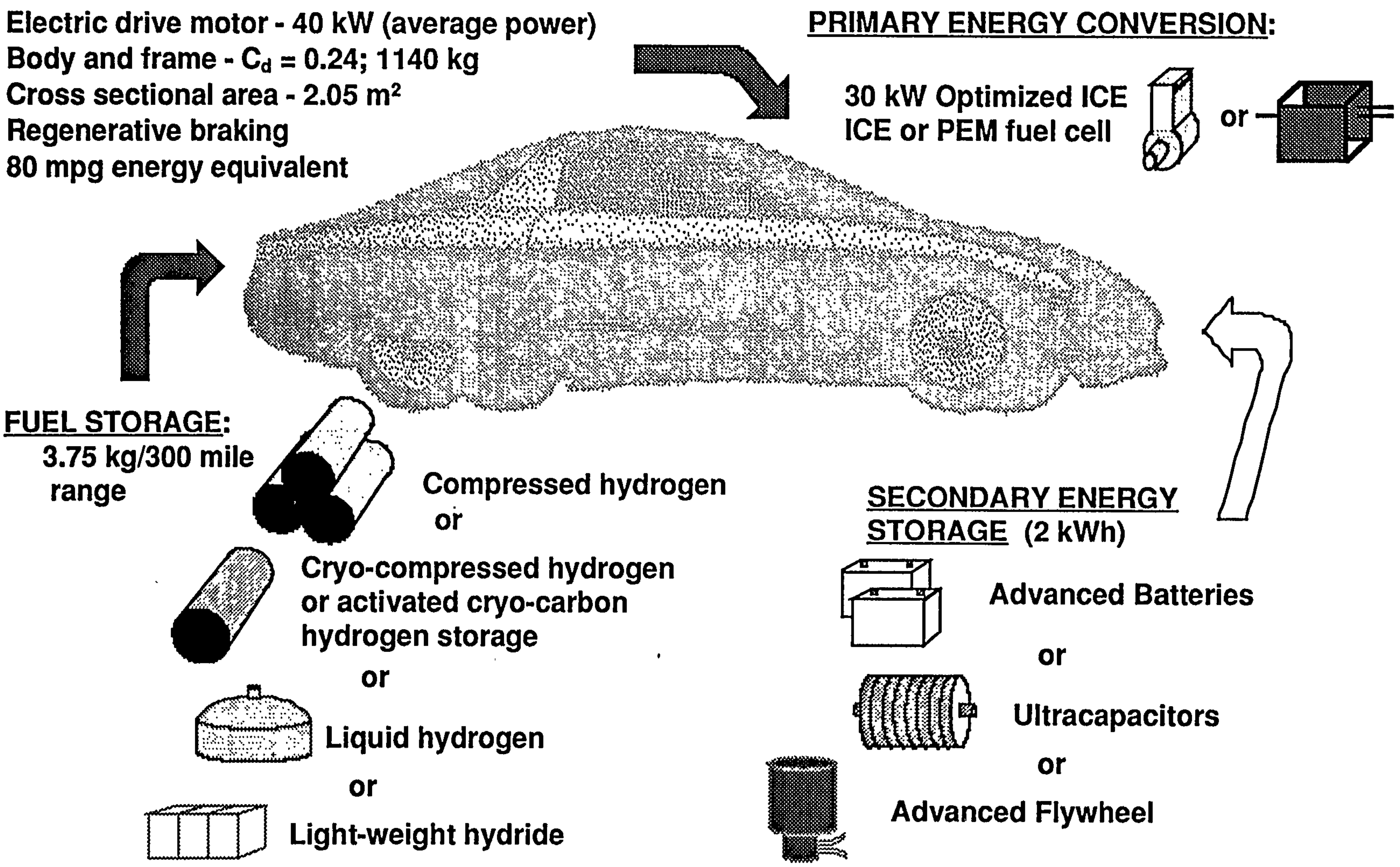

Electric drive motor - 40 kW (average power)
Body and frame - $C_d = 0.24$; 1140 kg
Cross sectional area - 2.05 m^2
Regenerative braking
80 mpg energy equivalent
PRIMARY ENERGY CONVERSION:
30 kW Optimized ICE
ICE or PEM fuel cell
or
FUEL STORAGE:
3.75 kg/300 mile range
Compressed hydrogen
or
Cryo-compressed hydrogen or activated cryo-carbon hydrogen storage
or
Liquid hydrogen
or
Light-weight hydride
SECONDARY ENERGY STORAGE (2 kWh)
Advanced Batteries
or
Ultracapacitors
or
Advanced Flywheel

Figure 1

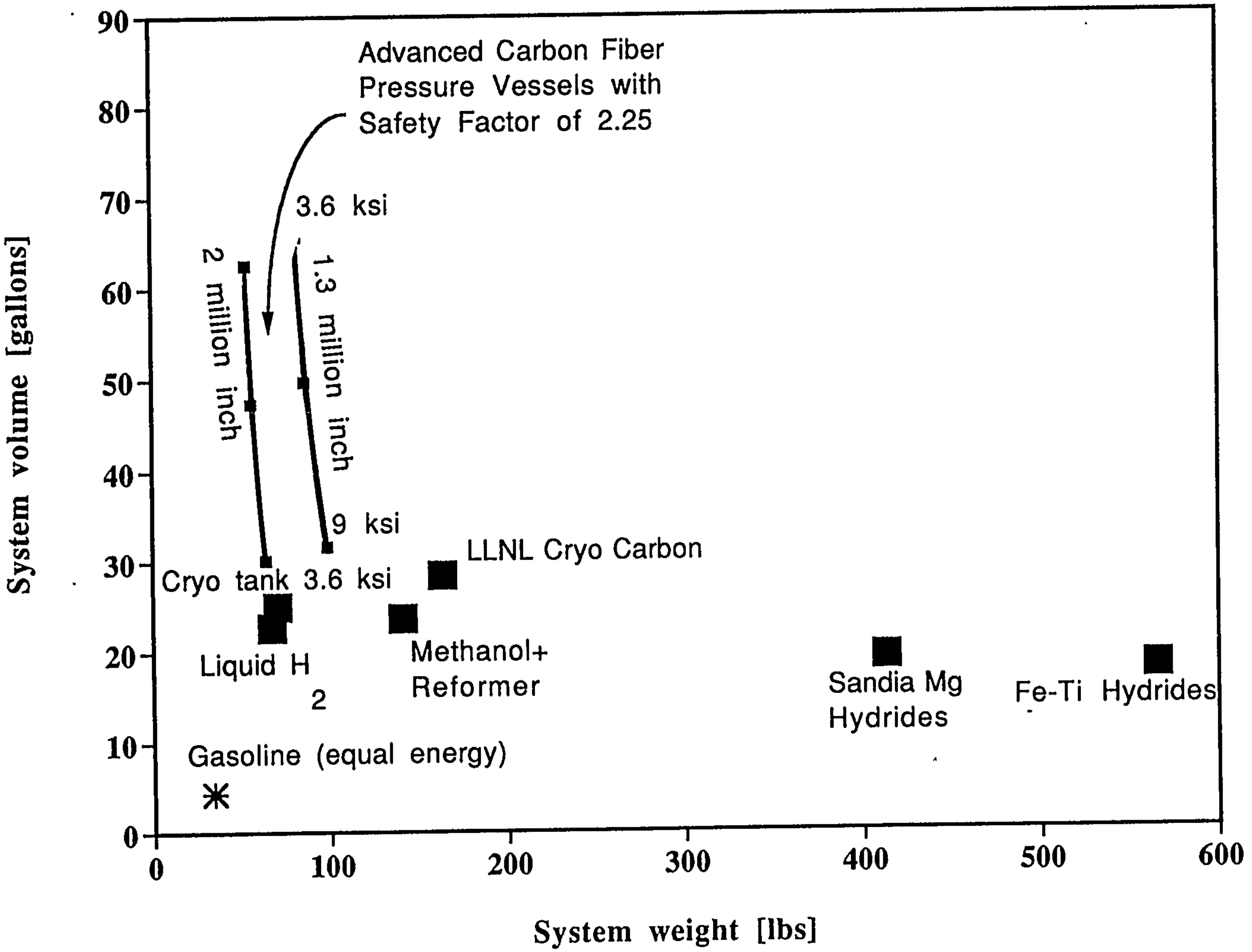

System volume [gallons]
90
80
70
60
50
40
30
20
10
0
System weight [lbs]
0
100
200
300
400
500
600
Advanced Carbon Fiber Pressure Vessels with Safety Factor of 2.25
3.6 ksi
2 million inch
1.3 million inch
9 ksi
Cryo tank 3.6 ksi
LLNL Cryo Carbon
Liquid H 2
Methanol+ Reformer
Sandia Mg Hydrides
Fe-Ti Hydrides
Gasoline (equal energy)

Figure 2

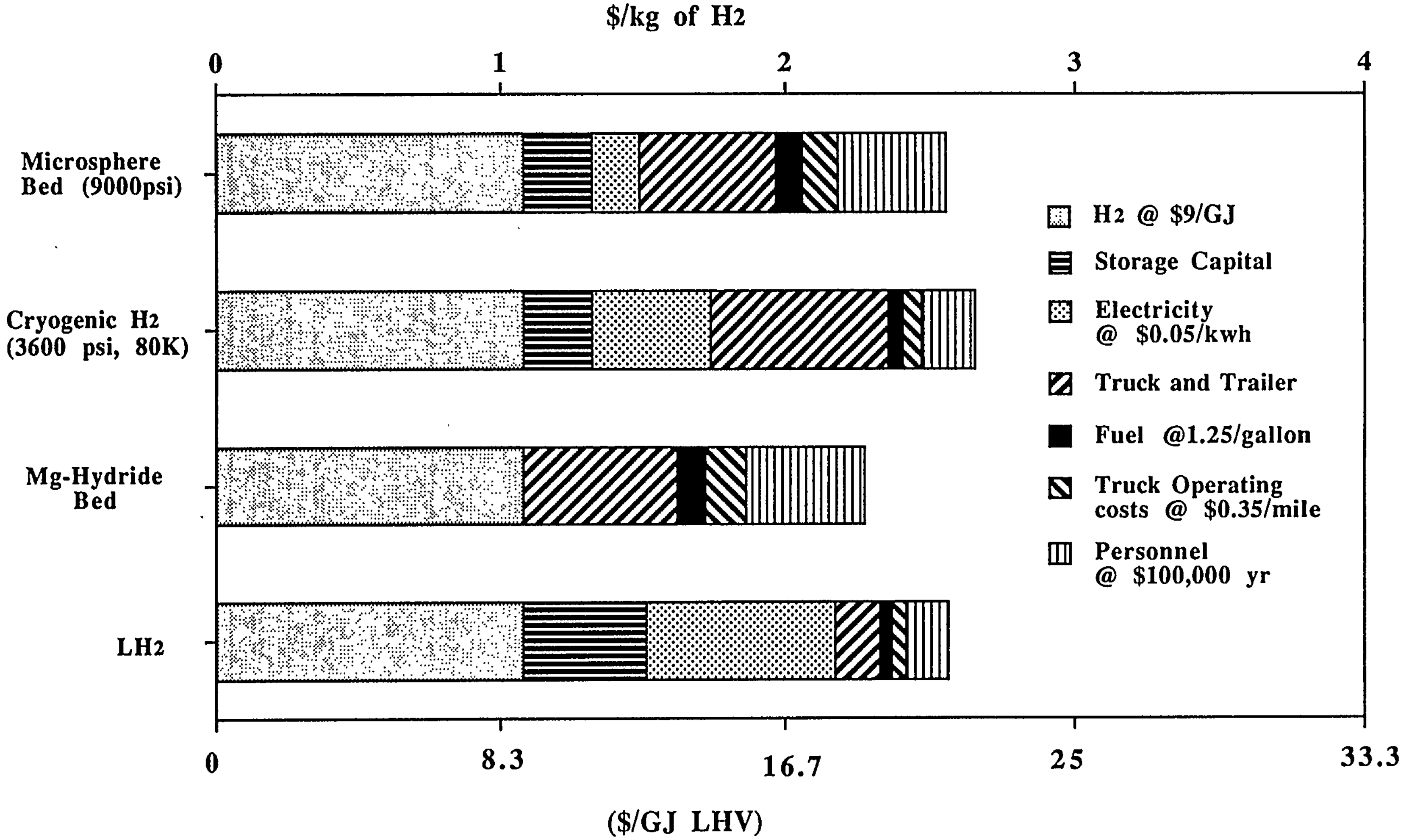

$/kg of H2
0
1
2
3
4
Microsphere Bed (9000psi)
Cryogenic H2 (3600 psi, 80K)
Mg-Hydride Bed
LH2
H2 @ $9/GJ
Storage Capital
Electricity @ $0.05/kwh
Truck and Trailer
Fuel @1.25/gallon
Truck Operating costs @ $0.35/mile
Personnel @ $100,000 yr
0
8.3
16.7
25
33.3
($/GJ LHV)

Figure 3

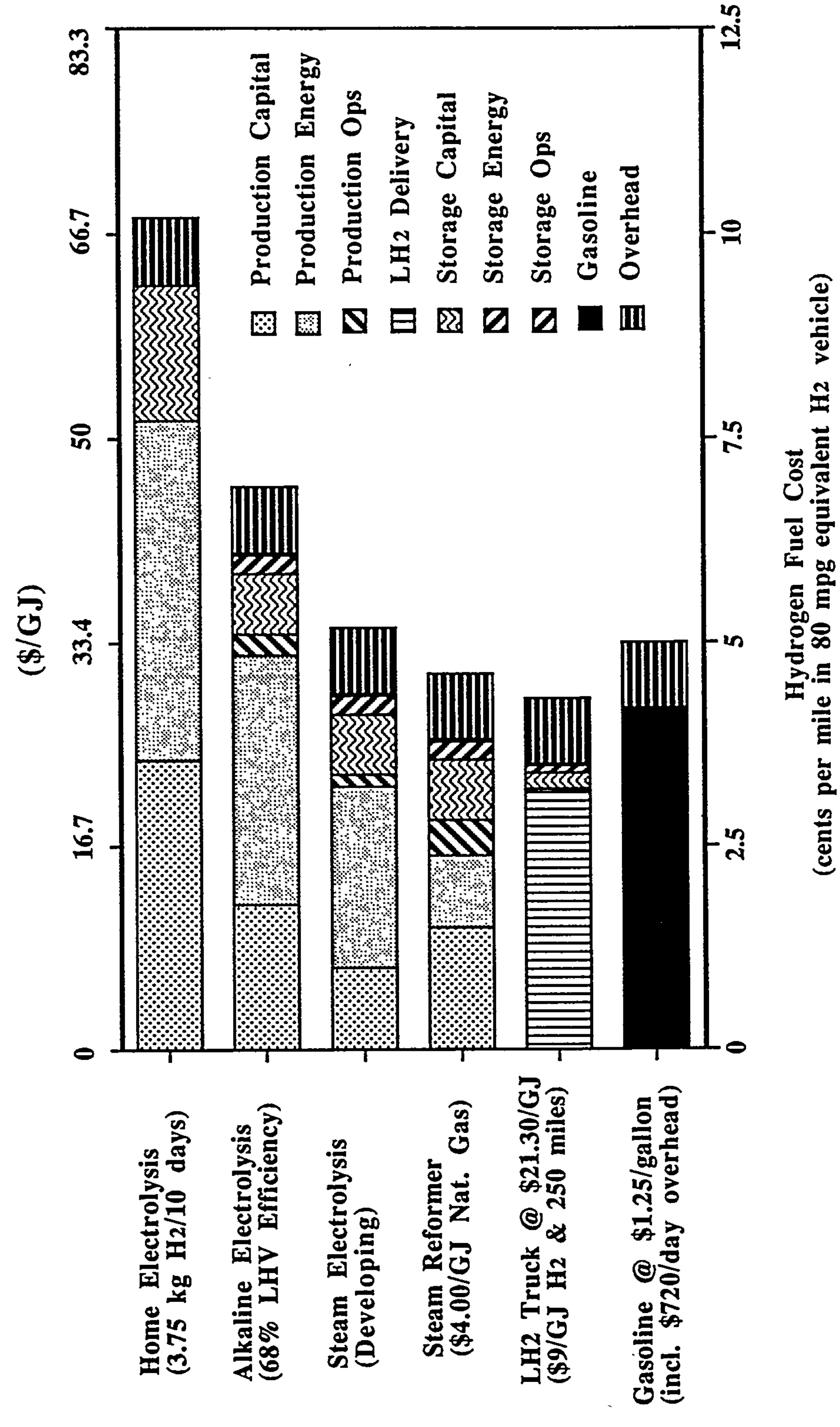

($/GJ)
0
16.7
33.4
50
66.7
83.3
Hydrogen Fuel Cost
(cents per mile in 80 mpg equivalent H2 vehicle)
0
2.5
5
7.5
10
12.5
Production Capital
Production Energy
Production Ops
LH2 Delivery
Storage Capital
Storage Energy
Storage Ops
Gasoline
Overhead
Home Electrolysis (3.75 kg H2/10 days)
Alkaline Electrolysis (68% LHV Efficiency)
Steam Electrolysis (Developing)
Steam Reformer ($4.00/GJ Nat. Gas)
LH2 Truck @ $21.30/GJ ($9/GJ H2 & 250 miles)
Gasoline @ $1.25/gallon (incl. $720/day overhead)

Figure 4

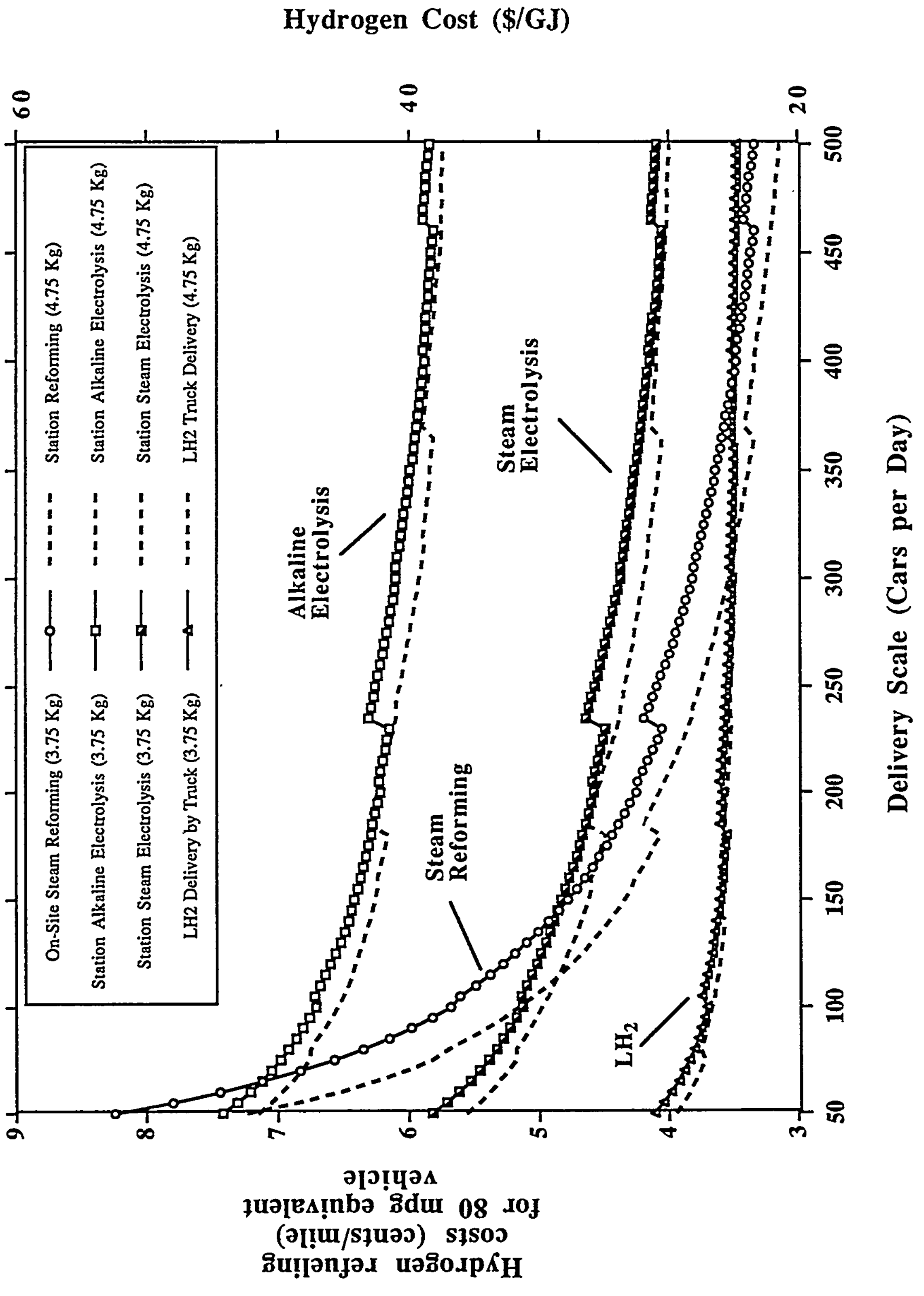

Hydrogen Cost ($/GJ)
20
40
60
Hydrogen refueling costs (cents/mile) for 80 mpg equivalent vehicle
3
4
5
6
7
8
9
50
100
150
200
250
300
350
400
450
500
Delivery Scale (Cars per Day)
On-Site Steam Reforming (3.75 Kg)
Station Alkaline Electrolysis (3.75 Kg)
Station Steam Electrolysis (3.75 Kg)
LH2 Delivery by Truck (3.75 Kg)
Station Reforming (4.75 Kg)
Station Alkaline Electrolysis (4.75 Kg)
Station Steam Electrolysis (4.75 Kg)
LH2 Truck Delivery (4.75 Kg)
Alkaline Electrolysis
Steam Electrolysis
Steam Reforming
LH$_2$

Figure 5

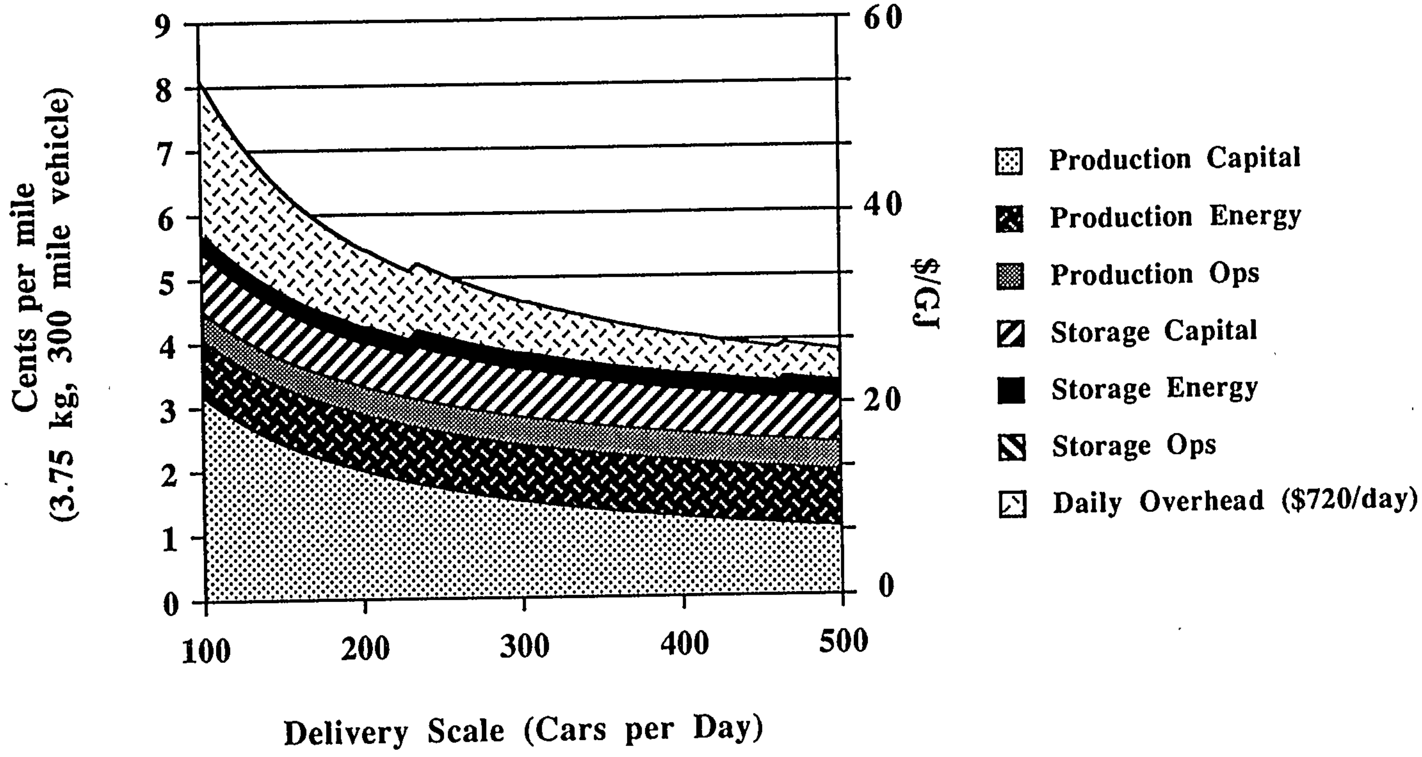

9
8
7
6
5
4
3
2
1
0
Cents per mile
(3.75 kg, 300 mile vehicle)
100
200
300
400
500
Delivery Scale (Cars per Day)
60
40
20
0
$/GJ
Production Capital
Production Energy
Production Ops
Storage Capital
Storage Energy
Storage Ops
Daily Overhead ($720/day)

Figure 6

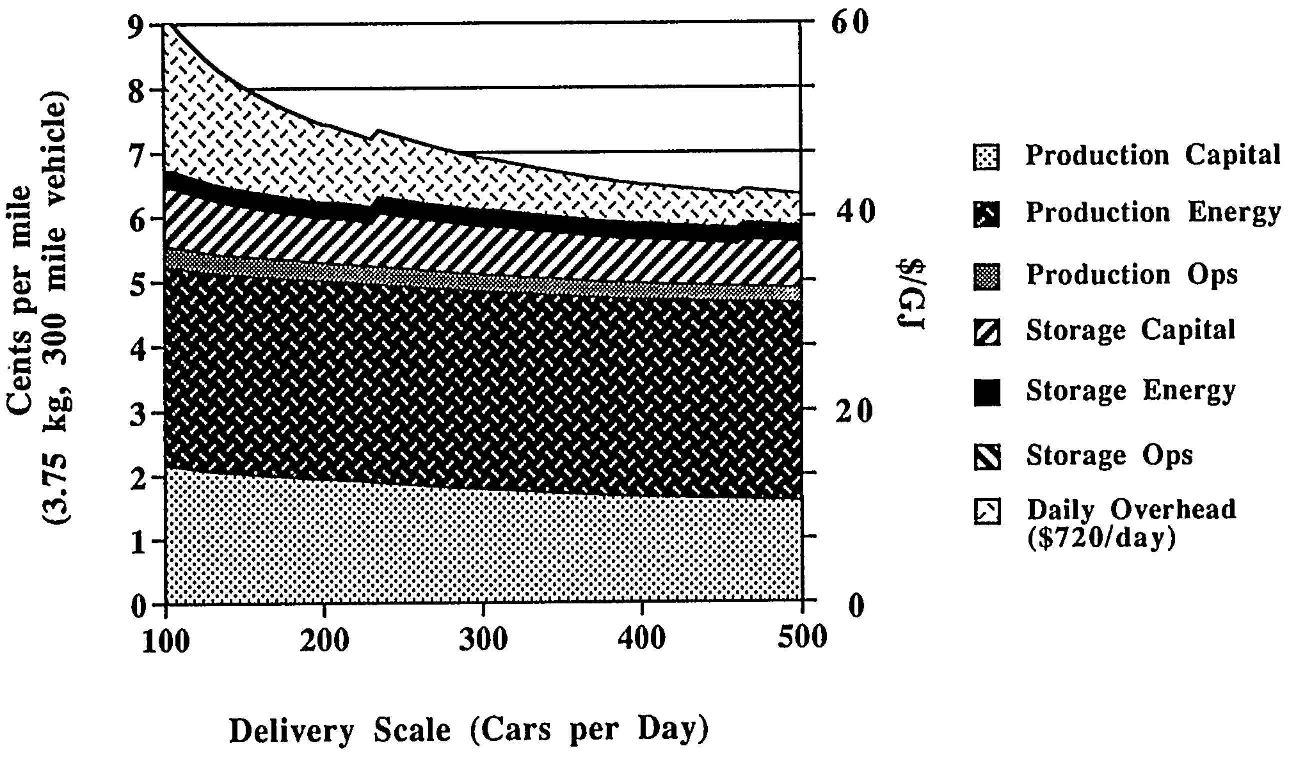

Cents per mile
(3.75 kg, 300 mile vehicle)
9
8
7
6
5
4
3
2
1
0
100
200
300
400
500
Delivery Scale (Cars per Day)
60
40
20
0
$/GJ
Production Capital
Production Energy
Production Ops
Storage Capital
Storage Energy
Storage Ops
Daily Overhead
($720/day)

Figure 7

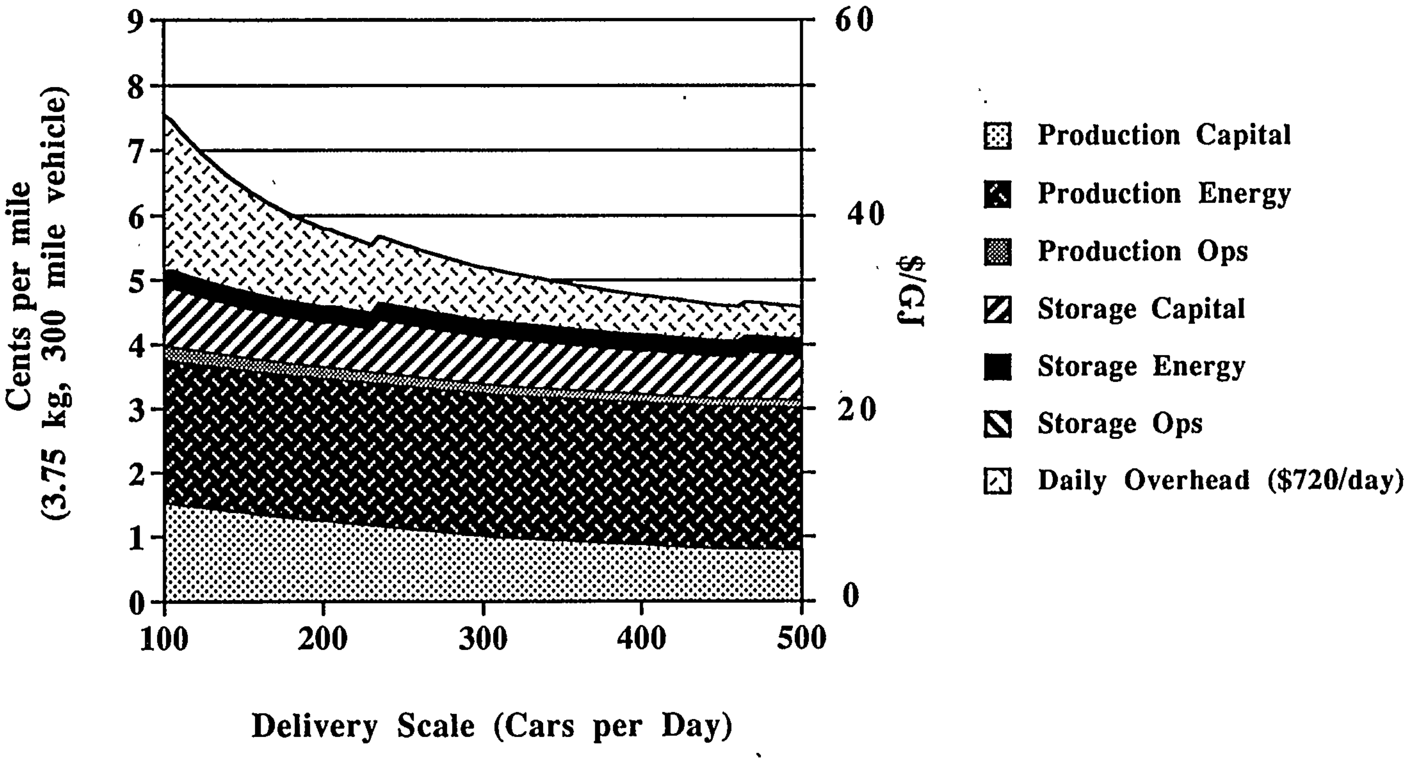

9
8
7
6
5
4
3
2
1
0
Cents per mile
(3.75 kg, 300 mile vehicle)
100
200
300
400
500
Delivery Scale (Cars per Day)
60
40
20
0
$/GJ
Production Capital
Production Energy
Production Ops
Storage Capital
Storage Energy
Storage Ops
Daily Overhead ($720/day)

Figure 8

INDUSTRY OUTREACH A STATUS REPORT

Ms. Debbie Surek
Dr. Rajat Sen
R.K. Sen & Associates, Inc.
4733 Bethesda Avenue, Suite 608
Bethesda, MD 20814

Abstract

The Outreach Project was initiated in October 1994 with the objective of developing a multi-year plan for the U.S. Department of Energy (DOE) for targeted outreach activities for stakeholders in industry and the general public. This status report summarizes the work on industry outreach that has been completed since the inception of the project in October 1994.

A three-pronged approach was taken to ascertain issues related to industry outreach. First, there was a review of on-going and past industry outreach activities at DOE and NHA. Next, a series of meetings with industry decision makers was arranged to get a better understanding of industry interests and concerns, and to discuss how DOE and industry could work collaboratively to develop hydrogen energy systems. Third, a workshop is scheduled where representatives from industry, DOE and other federal agencies can identify issues that would enhance partnering between the federal government and industry in the development of hydrogen energy systems.

At this time, the review of on-going and past activities has been completed. Industry interviews are in progress and a majority of meetings have been held. Analysis of the information gained is in progress. The preliminary analysis of this information indicates that for appropriate near-term demonstration-type projects, the level of interest for collaboration between DOE and industry is high. The data also identifies issues industry is concerned with which impact the commercialization of

hydrogen energy systems.

Introduction

The Matsunaga Hydrogen Research, Development & Demonstration Act of 1990, the underlying authorizing legislation for the DOE Hydrogen Program, mandated that DOE undertake an aggressive industry outreach program to promote partnerships between DOE and industry and thus facilitate technology transfer. The same Act also directed DOE to initiate educational activities that would inform the American Public about the merits of hydrogen as an energy carrier in sustainable energy systems. In response to this mandate, DOE requested us to develop a multi-year plan for targeted industry and public outreach activities. The project was initiated in October 1994 and this paper presents an overview of the current status.

It is important to have close collaboration between industry and public outreach programs since specific activities in one area can significantly affect the other. For example, a successful public outreach campaign that generates enthusiasm for hydrogen will also encourage industry to invest in hydrogen energy systems and to work with DOE in a sustained long-term effort to develop and deploy critical technologies. Although we recognize this synergy and the plans will be developed keeping this in mind, for purposes of developing the plan we treat the industry and public outreach activities separately. It is in that perspective that we discuss the status of only the industry outreach plans in this paper. Progress on the public outreach plan will be presented at following meetings.

Objectives & Approach

The objective is to develop an Industry Outreach Plan that will facilitate a closer partnership between DOE and U.S. Industry to develop and deploy the components of a hydrogen energy system in the near to mid-term.

In order to develop this plan, the approach we have taken includes the following steps:

- A thorough review of current and past industry outreach activities. These include activities by DOE and the National Hydrogen Association (NHA).
- A series of meetings with industry decision makers to discuss the DOE Hydrogen R&D Program and to solicit their opinions on issues pertaining to hydrogen energy systems and avenues for collaboration between DOE and industry.
- A workshop with attendees from industry, the DOE laboratories, and other federal agencies to identify and prioritize issues that could improve collaboration between DOE and industry on hydrogen energy systems.

Current Status

In the six months since the inception of the project, the review of past and current activities by DOE and NHA has been completed and based on that review a detailed work plan for the industry outreach activities was prepared. The work plan discusses in detail the industry visits and the workshop. We are currently implementing the industry visits.

How are the organizations selected for these visits? The criteria that was used include the following factors:

- Visits should encompass a diversity of industry stakeholders in terms of organizational size, industry sectors and geographic location.
- Candidates should have either a current or a potential future interest in hydrogen energy technologies and/or markets.
- Companies should be U.S. owned and operated. If foreign owned, they must have a sizable manufacturing base in the U.S.
- Senior-level technical or business decision-makers from the company must agree to participate in the approximately two-hour long meetings.

Based on these criteria, a list of organizations were chosen for site visits. As Table I shows, to date we have visited 16 companies. The organizations that are expected to be scheduled for the remaining visits are also shown in Table I.

Table I. Industries Selected for Outreach Interviews

Industry Sectors	Name of Companies	Visit Schedule
Automotive	U. S. Car (Chrysler, GM, Ford)	March 23, 1995
	Detroit Diesel	March 23, 1995
	U. Of California-Davis Campus	February 15, 1995
Chemical	Air Products	March 3, 1995
	Du Pont	TBD
	Dow Chemical	March 21, 1995
	Monsanto	April 4, 1995
A&E Firms	Bechtel	February 13, 1995
	Foster Wheeler	March 2, 1995
OEM's	Aerojet	February 15, 1995
	Energy Conversion Devices	March 22, 1995
	H Power	February 15, 1995
	Teledyne Brown	March 15, 1995
Refining	National Petroleum Refiners Association	January 9, 1995
	TEXACO	TBD
Utilities	ENRON	January 20, 1995
	U.S. Generating	January 11, 1995
	New York Power Authority	TBD
	Northern States Power	February 16, 1995
	Pacific Gas & Electric	February 14, 1995
	SMUD	February 15, 1995
Trade Associations	American Gas Association	February 8, 1995
	National Hydrogen Association	November 16, 1994
	American Institute of Chemical Engineers	TBD
Regulatory Authority	California Energy Commission	February 15, 1995

A team of professionals representing DOE, NREL, Energetics, Inc., and R.K. Sen & Associates, Inc. visited these companies. Table II lists the individuals that represented each organization at these meetings. It should be pointed out that not all of the persons were at every outreach meeting. It was customary for the team to consist of one individual from DOE and/or NREL and two individuals from the two contractors. The preparation that went into each meeting included sending the company to be visited a detailed briefing book describing the DOE Program, important background material and a discussion agenda listing the issues that were to be covered at the meeting.

Table II. Industry Interview Team Members

DOE	NREL	Energetics, Inc.	R.K. Sen & Associates
Dr. Russell Eaton	Ms. Cathy Gregoire Padró	Mr. Joseph Badin	Mr. David Nahmias
Mr. Neil Rossmeissl	Ms. Margaret Mann	Dr. Ed Skolnik	Ms. Debbie Surek
		Mr. Phil Di Pietro	Dr. Rajat Sen

Findings

Although many of the scheduled meetings have been completed, the analysis of the information acquired at the meetings is yet to be complied into a finished document. However, we have drawn some preliminary conclusions and these are categorized below:

Enabling Factors

- Industry will pursue hydrogen and other energy options as a result of or in anticipation of environmental mandates.
- Hydrogen's long-term prospects are viewed favorably by industry.
- Industry is interested in participating in appropriate demonstration projects.

Barriers to Commercialization

- High cost of production & storage.
- Perception of safety problems and risk of liability.
- Infrastructure issues.

- Perception of hydrogen as a competitor to natural gas.

Outreach Issues

- Industry is not familiar with DOE Program.
- Coordination of activities within DOE is not apparent to industry.
- Industry is interested in participating in the DOE working groups as well as NHA activities.

TECHNICAL AND ECONOMIC ANALYSES OF HYDROGEN PRODUCTION VIA INDIRECTLY HEATED GASIFICATION AND PYROLYSIS

Margaret K. Mann
National Renewable Energy Laboratory
1617 Cole Blvd
Golden, CO 80401

Abstract

Technoeconomic analyses have been conducted on two processes to produce hydrogen from biomass: indirectly-heated gasification of biomass followed by steam reforming of the syngas, and biomass pyrolysis followed by steam reforming of the pyrolysis oil. The analysis of the gasification-based process was highly detailed, including a process flowsheet, material and energy balances calculated with a process simulation program, equipment cost estimation, and the determination of the necessary selling price of hydrogen. The pyrolysis-based process analysis was of a less detailed nature, as all necessary experimental data have not been obtained; this analysis is a follow-up to the preliminary economic analysis presented at the 1994 Hydrogen Program Review. A coproduct option in which pyrolysis oil is used to produce hydrogen and a commercial adhesive was also studied for economic viability.

Based on feedstock availability estimates, three plant sizes were studied: 907 T/day, 272 T/day, and 27 T/day. The necessary selling price of hydrogen produced by steam reforming syngas from the Battelle Columbus Laboratories indirectly heated biomass gasifier falls within current market values for the large and medium size plants within a wide range of feedstock costs. Results show that the small scale plant does not produce hydrogen at economically competitive prices, indicating that if gasification is used as the upstream process to produce hydrogen, local refueling stations similar to current gasoline stations, would probably not be feasible.

For many positive biomass feedstock costs, the selling price of hydrogen produced by reforming the entire biomass pyrolysis oil falls within the current market price of hydrogen. The economic position of this process depends on whether the pyrolysis oil can be produced in-house or must be purchased. If an adhesives coproduct can be made, the necessary hydrogen selling price is competitive with hydrogen produced from conventional processes and is lower than when no coproduct is produced. Because biomass pyrolysis oil is similar to petroleum crude oil in that many fuels and chemicals can be derived from it, further coproduct options will be studied according to current economic and market conditions. The coproduct option was not studied to economically justify the pyrolysis-based process, but is meant to be an example of the opportunities available from biomass pyrolysis oil once a system of coproducts is developed.

Summary

The process studied to produce hydrogen by steam reforming biomass syngas or pyrolysis oil is very similar to that used to reform natural gas. All necessary unit operations are commercially available, and should require no special engineering design. The estimated capital costs for the most profitable gasification-based scenario studied are \$6.08 million for the 27 T per day (30 ton/day) plant, \$34.5 million for the 272 T/day (300 ton/day) plant, and \$90.4 million for the 907 T/day (1000 ton/day) plant. At the same scales, for the pyrolysis-based process where all of the pyrolysis oil is reformed, the capital costs are \$3.07 million, \$20.2 million, and \$58.7 million. These costs do not include the capital for the pyrolysis operation as the oil is assumed to be purchased from outside producers. Capital costs for the hydrogen/adhesives coproduct option are slightly lower because of the decreased flowrates throughout the process.

The necessary selling price for hydrogen produced by steam reforming BCL biomass syngas or biomass pyrolysis oil falls within the current market values (\$5 - \$15/GJ) for many of the cost scenarios studied. If the pyrolysis oil is purchased rather than produced in-house, the pyrolysis-based process is more likely to be economically feasible than the gasification-based process at reasonable biomass costs. However, it should be noted that the analysis of the pyrolysis-based process contains a higher degree of uncertainty than that of the gasification-based process. Error will be reduced as further experimental data become available and are incorporated into the analysis. Even if this process turns out to be less economically feasible than the gasification-based process, the added flexibility of pyrolysis offers many opportunities for pyrolysis-based processes to be viable options for renewable hydrogen production. As expected, the most feasible process is the hydrogen/adhesives coproduct option. Further coproduct options will be studied to take advantage of the diverse product opportunities of pyrolysis oil.

Of the three plant sizes studied, the most economically feasible configuration depends upon the availability of waste biomass at a lower price than biomass from a DFSS. If waste biomass can be obtained for the medium size plant, this scale yields the lowest hydrogen price. If the medium size plant must use biomass from a DFSS, the large plant is the most economic. Results show that the small scale plant using any of the process schemes studied does not produce hydrogen cheaper than the medium size plant. However, if the small plant is the only size for which cheaper waste biomass can be obtained, local refueling stations, similar to current gasoline stations, would be feasible.

Introduction

This study addresses two thermochemical routes to produce hydrogen from biomass. The two processes studied were biomass gasification and biomass pyrolysis, each followed by steam reforming to produce hydrogen. Biomass is considered to be anything that has participated in the growing cycle recently. Agriculture waste, forest residue, urban wood waste, and trees and grasses grown as energy crops, are commonly the process feedstocks referred to as biomass. Because biomass consumes as much CO_2 in its growing cycle as is produced when it is transformed to energy, the net$_2$ CO contribution from biomass-derived fuels to the atmosphere is much less than from petroleum-derived fuels. Furthermore, producing biomass on a sustainable basis by growing energy crops supports the U.S. agriculture sector and potentially reduces our oil and gas imports.

The gasification system used for this study was the Battelle Columbus Laboratory (BCL) indirectly heated gasifier. The heat necessary for the endothermic gasification reactions is supplied by circulating sand from a char combustor to the gasification vessel. The product syngas, containing primarily CO, H_2, CH_4, CO_2, and some higher hydrocarbons, is then steam reformed to produce H_2 and CO_2 in a process based on that used for natural gas reforming. The H_2 can be purified and sold as an energy carrier to be used in vehicles, power plants, or refinery applications.

The second process studied was fast pyrolysis of biomass followed by steam reforming of the pyrolysis oils. Fast pyrolysis differs from gasification and combustion in that only heat is added to the reactor vessel with the biomass. Thus, instead of reacting with steam or oxygen, the biomass thermally decomposes to produce an oil. This oil is composed of oxygenated compounds such as acids and aldehydes derived from the carbohydrate portion of the biomass, phenolic compounds derived from the lignin portion of the biomass, and water. The same reforming operation studied for the gasification-based scenario was used in this analysis.

The pyrolysis-based process has greater flexibility than the gasification-based process, thus offering more opportunities for successful commercialization. Two scenarios for the production of hydrogen from pyrolysis oil can be envisioned. One would involve a regionalized system of hydrogen production with small and medium-sized pyrolysis units (<500 Mg/day) providing pyrolysis oil to a centralized reforming operation. The alternative is to pyrolyze biomass in a large unit and directly reform the uncondensed vapors. In the first case, it is more likely that biomass can be obtained at cheaper costs, perhaps through the use of biomass waste. Transportation costs will also be lower because an oil is cheaper to transport than biomass and has a higher energy density than biomass. Most importantly, the similarity of biomass pyrolysis oil to petroleum crude oil makes a multitude of fuels and chemical products in addition to hydrogen possible. An appropriate combination of these coproducts can increase the economic feasibility of pyrolysis-based processes and make a significant contribution to markets that are currently dominated by petroleum-derived products.

The purpose of this study was to assess the technical and economic feasibility of these processes. Enough experimental data were available for the gasification-based process to conduct a detailed analysis including a process design and mass and energy balances. Because experimental work for the pyrolysis-based process is incomplete, hydrogen yield estimations were made based on the gasification study and a preliminary economic analysis was performed. As more experimental data become available, this analysis will be updated to more accurately reflect the process feasibility.

From available data, a gasification and reforming plant was simulated in ASPEN Plus™, and used to perform material and energy balances. For the gasification-based process, these balances were used to size and cost major pieces of equipment, from which a capital cost estimation was made. The capital cost estimation for the pyrolysis-based process was made by using the same overall hydrogen yield from the syngas reforming operation to estimate hydrogen production and equipment size. Using discounted cash flow rate of return (DCFROR) and return on investment (ROI) analyses, the economic positions of these biomass-derived processes relative to conventional processes to produce hydrogen were assessed.

Process Descriptions

Gasification Using the BCL Indirectly Heated Gasifier

Biomass, obtained either from a dedicated feedstock supply system (DFSS), or as agricultural, urban, or industrial waste, is fed to a rotary dryer system to reduce the moisture content from approximately 50% to 11%. The biomass is then gasified in the BCL gasifier which is heated indirectly by sand circulating between a char combustor and the gasification vessel. The product syngas is cooled and compressed to the appropriate conditions for reforming.

A schematic of the BCL gasifier is shown in Figure 1. This system was simulated in ASPEN Plus™ using run data from Battelle Columbus Laboratories. According to the ultimate analyses shown in Table 1, biomass and char were simulated as non-conventional components. The biomass composition used for this study is typical of woody biomass such as hybrid poplar.

Table 1: Elemental Analysis of Biomass and Char

	Ultimate Analysis (Weight percent, dry basis)	
	Biomass	Char
Carbon	50.9	65.2
Oxygen	41.9	3.03
Hydrogen	6.04	3.70
Nitrogen	0.17	2.47
Sulfur	0.09	28.65
Chlorine	0.00	0.00
Ash	0.92	3.04

After drying, the biomass is fed to the fluidized bed gasifier, where hot sand from the char combustor is used as the bed material and source of heat for the gasification reactions. This reactor operates at nearly atmospheric pressure and 825°C (1517°F). Steam rather than air or oxygen is added to the gasifier to produce a syngas of medium quality: 18.35 MJ/m^3 (493 Btu/scf). After a cyclone separator removes the char, it is expected that the syngas will be cleaned using the hot-gas cleanup processes currently being developed by the Department of Energy (DOE) and Westinghouse; the current technology uses a water quench system. Hot-gas cleanup would consist of ceramic candle filters to remove particulates from the syngas prior to downstream operations such as reforming. The resultant syngas composition is shown in Table 2.

Table 2: Syngas Composition After Cleanup

Component	Volume%
CO	43.17%
H_2	21.22%
CH_4	15.83%
CO_2	13.46%
C_2H_4	4.62%
C_2H_6	0.47%
tar	0.40%
C_2H_2	0.37%
NH_3	0.37%
H_2S	0.08%

After cleanup, the syngas is cooled to 91°C (195°F) so that it can be compressed to the pressure required for the PSA system plus the expected pressure losses in the reactors. During this cooling, the water and higher hydrocarbons (tars) remaining in the syngas will most likely condense and must be removed and pumped before being re-added to the compressed syngas. The syngas compressor outlet pressure is 3,654 kPa (530 psi).

Pyrolysis

Because experimental work for the reforming of biomass pyrolysis oil is not complete, a rigorous process design was not performed in ASPEN Plus™. Data such as yields and composition of the pyrolysis operation were taken from earlier work (Gregoire 1992). A more thorough analysis will be conducted as information becomes available from current experimental efforts.

Fast pyrolysis consists of converting biomass into low molecular weight oxygenated compounds (pyrolysis oil), noncondensible gases, and a carbonaceous residue (char) through an intense heating process. Several fast pyrolysis technologies exist and are the result of intense research activities in biomass conversion during the 1980's. Many of these technologies, such as circulating fluid beds, bubbling fluid beds, and fluid transport reactors, are similar to reactors used for other purposes.

Ablative or cyclonic pyrolysis reactors and vacuum pyrolysis reactors were designed specifically for biomass. Despite the different designs, operating conditions in each reactor are similar. Temperatures range between 400°C and 600 °C and residence times of less than one second are common. Pyrolysis oil yields as high as 78 wt% of dry biomass are possible (Chornet et al 1994).

Experimental work and the literature available on pyrolysis processes indicate that essentially total equilibrium conversion of oxygenates to H_2 and CO_2 can be achieved by an appropriate combination of steam to carbon ratio and temperature. Furthermore, experimental work has confirmed that commercially available catalysts can improve the kinetics of converting oxygenated compounds to hydrogen. Based on thermodynamic simulations for this process and the desire for a conservative estimate, the yield of oil from biomass was assumed to be 65% of the weight of the biomass. From the simulation of the gasification-based process, 74.2% was used as the percentage of the stoichiometric maximum amount of hydrogen that could be obtained from steam reforming the pyrolysis oil. Once experimental results have been obtained from reforming actual pyrolysis oil, this analysis will be updated with the correct yield. It should be noted that the results of the pyrolysis-based process analysis are probably optimistic.

Because biomass pyrolysis oil is similar to petroleum crude oil in that many useful chemicals can be derived from it, a proven co-product option was analyzed. Before the reforming operation, the lignin-derived portion of the biomass can be extracted from the pyrolysis oil using ethyl acetate (Chum and Black 1990). The extracted material is known as phenolics/neutrals and has been found by NREL researchers to have properties comparable to phenolic resins. The remaining portion of the oil, primarily carbohydrate-derived oxygenates, can be steam reformed to produce hydrogen after this extraction step.

Steam Reforming

The reforming process, shown in Figure 2, is nearly identical to that used for production of hydrogen from natural gas, and is not expected to change much for either of the biomass conversion processes studied. Based on the available literature, the steam reforming of gasification syngas was simulated in ASPEN Plus™. The calculated yields from this simulation were used to estimate how much hydrogen would be produced in the reforming of biomass pyrolysis oil. The reactions governing the reforming process are shown in the following equations:

$$C_nH_m + nH_2O + \text{heat} \Rightarrow nCO + (m/2 + n)H_2 \tag{1}$$

$$CO + H_2O \Rightarrow CO_2 + H_2 + \text{heat} \tag{2}$$

The primary reformer, a reactor similar to a process furnace with catalyst-filled tubes, converts the methane and higher hydrocarbons to CO and H_2 (Reaction 1), and performs a significant portion of the water-gas shift reaction to convert CO and water to H_2 and CO_2 (Reaction 2). Nearly all of the CO left after the primary reactor is consumed via this reaction in the subsequent high temperature and low temperature shift reactors. A pressure swing adsorption (PSA) system is used to produce hydrogen pure enough for use in fuel cell applications.

Reaction 1 typically takes place at temperatures between 800°C and 850°C (1472°F and 1561°F) in the primary reformer, although laboratory work has shown that it may be possible to operate this reactor at 700 °C for pyrolysis oil reforming. The heat necessary for the endothermic reactions taking place within the primary reformer is supplied by combusting the PSA offgas outside of the reactor tubes through which the reactants and products are flowing. According to results from operating plants, the primary reformer was simulated as an equilibrium reactor with a 20°F approach temperature (Tindall and King 1991).

Reaction 2 is the water-gas shift reaction. A substantial portion of the CO that was originally in the syngas as well as that produced by Reaction 1 from CH_4 and the higher hydrocarbons is converted to H_2 in the primary reactor. According to the thermodynamics of the reforming process, practically all of the tar and C_2H_x species are consumed, 60 mol% of the CH_4 is converted, and there is a 22 mol% net conversion of CO.

Since Reaction 2 is exothermic, it is beneficial to convert the remaining CO at a temperature lower than the temperature of the primary reformer. Nearly complete conversion of CO is accomplished in the subsequent high and low temperature shift reactors. The feed to the high temperature shift reactor is cooled to 370°C (698°F) and increases to 435°C (814°F) as the water-gas shift reaction proceeds. The product of this reactor is then cooled to 200°C (392°F) and fed to the low temperature shift reactor which produces a gas at 220°C (430°F) with a dry-basis composition of 61.9% H_2, 34.1% CO_2, 2.9% CH_4, and 1.1% CO for the gasification-based process.

A steam to carbon ratio of three was used in the simulation of the reforming operations. This is consistent with that used for natural gas reforming; however, higher hydrocarbon feedstocks may require additional steam (Tindall and King 1991). The higher percentage of CO in syngas should improve the kinetics of this process over steam reforming natural gas. However, reforming the C_2 and higher compounds could prove more difficult, especially in reforming biomass pyrolysis oil. Actual experimental data will dictate the appropriate steam to carbon ratio. The process studied has a great deal of excess heat available from which steam will be produced for export, so a higher reforming steam requirement will not greatly affect the economics of the process.

Before the reformer product stream can be purified in a PSA unit, it must contain at least 70 mol% hydrogen (Ahmad 1995). Feeding streams more dilute than this to a PSA unit decreases the purity and recovery of the hydrogen. Therefore, part of the PSA product stream is recycled back into the PSA feed to increase the hydrogen fraction to 70 mol%, at which point the hydrogen recovery is 85%. The incorporation of the recycle loop decreases the overall separation recovery to 77%. The operating pressure of the PSA unit is 2,500 kPa (363 psi) (Gerhartz 1989, V A13).

Three process configurations, or schemes, were studied. Scheme 1 utilizes all reforming operations typically used in natural gas reforming: the primary reformer, the high temperature shift reactor, and the low temperature shift reactor. Scheme 2 uses only the primary reformer, and Scheme 3 uses the primary reformer and the high temperature shift reactor. All schemes use a PSA purification process. Schemes 2 and 3 were studied in order to assess the profitability if the capital requirements could be lowered at the expense of producing less hydrogen. Because these process configurations are referred to throughout the report as Schemes 1, 2, and 3, Table 3 gives a description of each for easy reference. The configurations tested in Schemes 2 and 3 were not analyzed for the pyrolysis-based process because they were not found to improve the economics of the gasification-based process.

Table 3: Summary of Unit Operations Used in Different Process Configurations

Scheme	Reforming operations used
1	primary reformer, high temperature shift reactor, low temperature shift reactor
2	primary reformer
3	primary reformer, high temperature shift reactor

Steam Generation

In the ASPEN Plus™ simulation, gasification and reforming were integrated such that heat available from the reforming operation could generate the steam necessary for gasification as well as a substantial amount of export steam. The process gas was cooled as it moved between the primary reformer, the shift reactors, and the PSA unit, generating steam in each step. Steam was also generated by cooling the primary reformer flue gas. The majority of the steam produced was superheated at 690 kPa (100 psig); the steam produced by cooling the process gas between the high and low temperature shift reactors was at 3,450 kPa (500 psig).

Conversion Efficiencies

Two methods were used to estimate the efficiency of producing hydrogen from biomass by indirectly heated gasification and fast pyrolysis. The first method looks at the ratio of the amount of hydrogen that was produced to the stoichiometric maximum amount of hydrogen possible according to Reactions 1 and 2. The second method calculates the ratio of the energy value of the product hydrogen and export steam to the energy value of the biomass feed plus purchased electricity. The amount of hydrogen produced for each plant size and scheme is shown in Table 4.

Table 4: Hydrogen Produced in Each Scenario Analyzed (scmd)

Plant size (T biomass/day)	Gasification-based process			Pyrolysis-based process	
	Scheme 1	Scheme 2	Scheme 3	Scheme 1	coproduct option
27	21,600	16,850	20,440	30,415	24,332
272	215,940	168,500	204,390	304,152	243,322
907	719,800	561,650	681,280	1,013,842	811,073

Stoichiometric Maximum Efficiency Calculation

In order to calculate the stoichiometric maximum efficiency of the gasification-based process, the "molecular formula" of biomass was approximated as $CH_{1.47}O_{0.67}$ on a dry basis. Completely steam reforming this biomass yields 2.07 moles of hydrogen per "mole" of biomass as shown by the following stoichiometry:

$$CH_{1.47}O_{0.67} + 1.33H_2O \Rightarrow CO_2 + 2.07H_2$$

This hydrogen yield is equivalent to 2.02 scm hydrogen/kg biomass (32.38 scf/lb). In Scheme 1, with all reforming operations used, 0.79 scm hydrogen / kg biomass (12.71 scf/lb) is produced. This corresponds to a 39.3% conversion and recovery efficiency.

From the ASPEN Plus™ simulation, the stoichiometric conversion efficiency of the reforming operation by itself was found to be 74.2%. This efficiency was applied to the process of steam reforming pyrolysis oil to estimate how much hydrogen would be produced. From this, and the assumption that 65% of the dry biomass could be recovered as pyrolysis oil, the stoichiometric conversion and recovery efficiency of producing hydrogen by steam reforming the entire biomass pyrolysis oil is 55.3%. The "molecular formula" of biomass pyrolysis oil was assumed to be $CH_{1.33}O_{0.53}$, giving the maximum stoichiometric amount possible as 2.14 moles of hydrogen per "mole" of oil.

The calculation of the stoichiometric efficiency of the coproduct option was made by assuming that 20% of the original weight of the biomass is recovered as the phenolic resin and 65% of the remaining biomass is converted to pyrolysis oil. The resultant efficiency is 39.4%.

Energy Conversion Efficiency Calculation

The efficiency on an energy in, energy out basis can be calculated by the following formula:

$$\frac{(H_2)(HHV_{H2}) + (stm_{ex})(\Delta H_{sh})}{(B_f)(HHV_b) + e}$$

where:

H_2 = hydrogen recovered (kg)
HHV_{H2} = higher heating value of hydrogen (GJ/kg)
ΔH_{sh} = difference in enthalpy between incoming water and steam produced (GJ)
stm_{ex} = steam produced to be sold (kg)
B_f = biomass fed to process (kg)
HHV_b = higher heating value of biomass (19.75 MJ/kg = 8,500 Btu/lb)
e = electricity imported for process requirements (GJ equivalent)

The efficiencies calculated for the three schemes are shown in Table 5. The efficiencies for the pyrolysis-based process are higher than for the gasification-based process primarily because more char is produced in gasification than in pyrolysis. Approximately 19% of the carbon in biomass is rejected as char in this gasification process, and for every mole of carbon rejected, two moles of hydrogen cannot be obtained in steam reforming.

Table 5: Process Conversion Efficiencies

	Gasification-based process			Pyrolysis-based process	
	Scheme 1	Scheme 2	Scheme 3	Scheme 1	coproduct option
Stoichiometric Efficiency	39.3%	30.6%	37.2%	55.3%	39.4%
Energy Conversion Efficiency	79.0%	69.7%	76.5%	86.5%	62.8%

Economic Analysis

The current market value of hydrogen is between \$5/GJ and \$15/GJ. The potential profitability of the process being studied can be assessed by comparing economic results to current hydrogen selling prices. Possible sources of error in this analysis are in equipment cost estimation, feedstock and product market predictions, and invalid economic assumptions. The total error can be reduced by looking at ranges of profitability, such as the range of hydrogen selling price versus a range of biomass feedstock costs. As more information on the development of biomass-based technologies becomes available, these analyses can be modified to give a more representative process cost. The economic analysis of the pyrolysis-based process contains more error because adequate experimental data are not available. Fast pyrolysis is not as well understood as gasification, and the chemistry and yields which can be obtained on a consistent basis are uncertain. Further, data on reforming exists only for individual compounds found in pyrolysis oil; future experimental efforts will focus on reforming the actual oil.

The material and energy balance results from the ASPEN Plus™ simulation were used to determine the size and corresponding cost of major pieces of equipment for the gasification-based process. Costs were taken from the ChemCost software package and published literature and brought to January 1995 dollars using equipment cost escalation ratios from Chemical Engineering Magazine (March, 1995). Some costs, especially those related to gasification were taken from other studies (Double 1988, Dravo Engineering Companies 1987, Breault and Morgan 1992, Weyerhaeuser 1992)

Operating costs for the processes studied include feedstock costs, electricity to run the compressors (\$0.05/kWh), water for steam generation and cooling (\$330/m^3), and labor. The revenue from steam produced for export is taken as an operating cost credit. In the analysis of the pyrolysis-based process with the coproduct option, the revenue from selling the P/N fraction is also taken as a credit. To obtain a conservative result, the selling price of the adhesives coproduct was assumed to be 75% of the value of phenol.

The feedstock cost used in the analysis of the pyrolysis-based processes was the cost of the pyrolysis oil (Gregoire 1992). Economic analyses were conducted for two cases: first, the pyrolysis oil was assumed to be purchased, and thus includes a rate of return for the producer; second, the pyrolysis oil was assumed to be produced in-house and thus the cost reflects only that of production. In this make-versus-buy assessment, the production scenario yields the most profitable results. However, the alternative concept is more likely for two reasons. Once developed, a regionalized system where the pyrolysis oil is produced in several small units will probably involve multiple oil producers. Second, as more feasible coproduct options are developed, only a portion of the oil will be purchased and used for hydrogen production. Results using both pyrolysis oil selling price and production cost for the feedstock component of the operating costs are presented.

Economic Assumptions

The economic feasibility of producing hydrogen by steam reforming syngas from the BCL gasifier and oil from fast pyrolysis was studied using the DCFROR method. This method calculates the internal rate of return (IRR) that will be earned on the initial capital investment over the life of the project. Given this rate and a feedstock cost, the necessary selling price of the product can be calculated. Often, the IRR is specified as the minimum acceptable rate for an investor to finance a project; therefore, the perceived risk of the project can be incorporated into the IRR. Because the process of producing hydrogen from biomass currently carries higher risks than conventional hydrogen-generating processes, the IRR specified in this study was 15%, while the going rate for conventional processes is between 9% and 12%.

The economic analyses for this study were based on current dollars (inflation and escalation included), and performed using equity financing, assuming that the capital will not be borrowed. This assumption is probably valid for the smaller-scale plants, less so for the large plant. However, the higher IRR and discount rate of 15% make this project more attractive. The majority of the assumptions used in performing the economic analysis are shown in Table 6.

Table 6: Economic Assumptions

January, 1995 dollars	Inflation rate = 5%
Equity financing	Tax rate = 37%
90% on-line factor	20 year plant life
Two year construction period	50% plant capacity first year of production
Straight-line depreciation for ten years; first and last year at 50% of other years	30% of capital investment spent first year, 70% second year.

By-Product Credit: Steam

A by-product credit was taken for the steam generated in the process. A selling price of \$7.88/1000 kg (\$3.57/1000 lb) was assumed for 3,450 kPa (500 psig) steam. A price of \$5.18/1000 kg (\$2.35/1000 lb) was assumed for 690 kPa (100 psig) steam (Peters and Timmerhaus 1991) All steam produced contains 30°F superheat. The amount of steam produced in Scheme 1 of the gasification-based process is shown in Table 7. Schemes 2 and 3 are not expected to produce significantly different quantities of steam because roughly the same amount of heat will be available. Since the pyrolysis-based process was not simulated on ASPEN Plus™, the amount of steam produced in Scheme 1 was assumed to be the same as that produced in the gasification-based process. A better estimate will be used once experimental data are available. Because 80% less oil is reformed in the coproduct option, the amount of steam produced was calculated to be 80% of that produced when the full pyrolysis oil was reformed.

Table 7: By-Product Steam for Scheme 1 Gasification-Based Process

Source of Heat	Amount Produced, kg steam / kg dry biomass	Pressure, kPa (psig)
cooling gas between high and low temperature shift	0.32	3,450 (500)
syngas compressor interstage coolers	1.26	690 (100)
interstage coolers of compressor that supplies air to offgas combustor	0.12	690 (100)
offgas combustor flue gas	0.43	690 (100)
gas going to PSA	0.85	690 (100)

The assumption that the steam will be able to be sold is probably valid for the medium and large plants as they will most likely be located in more industrialized centers to take advantage of other infrastructure. However, it may be difficult to sell the steam produced by the small plant, as this size represents small refueling stations located near the demand for hydrogen.

Economic Analysis Results

The capital and operating costs for each of the scenarios studied are shown in Tables 8 and 9. These costs were calculated using a feedstock cost of \$16.50/T, a representative cost of waste biomass, for the small and medium size plants and \$46.30/T, the expected cost of biomass from a DFSS, for the large plant. Operating costs would increase significantly if the medium size plant obtained its biomass from a DFSS.

Table 8: Capital (MM$) and Operating Costs (MM$/year) for the Gasification-Based Process

	Scheme 1			Scheme 2			Scheme 3		
Plant size	sm	med	lg	sm	med	lg	sm	med	lg
Operating Costs	0.30	1.73	14.1	0.28	1.43	13.1	0.31	4.39	14.1
Fixed	0.15	0.27	0.33	0.16	0.27	0.33	0.16	0.27	0.33
Variable	0.16	1.60	5.33	0.13	1.30	4.32	0.16	1.60	5.32
Byproduct credit (steam)	-0.16	-1.62	-5.38	-0.16	-1.62	-5.38	-0.16	-1.62	-5.38
Feed	0.15	1.48	13.8	0.15	1.48	13.8	0.15	4.14	13.8
Capital Costs	6.08	34.5	90.4	5.05	29.3	80.0	6.02	34.0	89.1

Table 9: Capital (MM$) and Operating Costs (MM$/year) for the Pyrolysis-Based Process

	Scheme 1			Coproduct Option		
Plant size	sm	med	lg	sm	med	lg
Operating costs if oil is:						
produced in-house	0.46	3.31	18.16	0.48	3.49	18.76
purchased	1.02	8.87	36.56	1.04	9.05	37.18
Fixed	0.16	0.27	0.33	0.16	0.27	0.33
Variable	0.10	1.01	3.37	0.10	1.00	3.32
Byproduct credit (steam) *	-0.10	-0.97	-3.24	-0.08	-0.78	-2.59
Feed if oil is:						
produced in-house	0.30	3.00	17.7	0.30	3.00	17.70
purchased	0.86	8.56	36.1	0.86	8.56	36.12
Capital Costs**	3.07	20.2	58.7	2.89	18.2	52.6

* Revenue from adhesives byproduct is not taken as a credit here so that level comparisons can be made.

** Reforming operation only; pyrolysis capital costs are included in the cost of the feed.

The results of the DCFROR analysis are shown in Figures 3 through 9. A 37% tax rate and a 15% IRR were used in these analyses. With the market value of hydrogen between $5/GJ and $15/GJ, these figures show that hydrogen can be produced to compete with current hydrogen production methods on the large and medium scale for all processes studied. These figures give the biomass feedstock cost that can be paid within the current hydrogen market. The necessary hydrogen selling price is highly dependent upon the biomass feedstock cost, and unless very low-cost biomass can be obtained, some of the scenarios, particularly on the small scale, will not produce hydrogen at competitive prices. Many of the processes studied, however, yield competitive hydrogen prices at reasonable and even high biomass costs. For easy reference, a summary of these results is shown in Table 10. Hydrogen selling prices were calculated using biomass feedstock prices of $16.50/T for the small plant and $46.30/T for the large plant; since it is uncertain if nearly 300 T/day waste biomass at the lower price can be secured, both $16.50/T and $46.30/T were used to calculate the minimum selling price for the medium size plant. The results shown in this table are representative only of the situations for which biomass can be obtained at the listed prices. The actual biomass price for a given region and situation should be used when assessing the necessary hydrogen selling price from these processes. Figures 3 through 9 can be used when assessing specific situations.

Table 10: Necessary Hydrogen Selling Price for a 15% IRR After Taxes

	Plant size	Biomass cost ($/T)	Hydrogen selling price ($/GJ)
Gasification-based Scheme 1	small	16.50	23.20
	medium	16.50 / 46.30	13.10 / 16.20
	large	46.30	13.70
Gasification-based Scheme 2	small	16.50	25.10
	medium	16.50 / 46.30	14.20 / 18.20
	large	46.30	15.70
Gasification-based Scheme 3	small	16.50	24.30
	medium	16.50 / 46.30	13.70 / 17.00
	large	46.30	14.20
Pyrolysis-based Scheme 1 *	small	16.50	15.50
	medium	16.50 / 46.30	12.00 / 13.80
	large	46.30	13.10
Pyrolysis-based Coproduct option *	small	16.50	10.20
	medium	16.50 / 46.30	5.70 / 8.10
	large	46.30	7.10

* Pyrolysis oil is assumed to be purchased rather than produced in-house.

Figures 3, 4, and 5 show the necessary hydrogen selling price for the gasification-based process for each scheme as a function of the feedstock cost. In comparing Figures 4 and 5, it can be seen that the cost of producing less hydrogen in Schemes 2 and 3 is higher than the savings obtained by eliminating some unit operations in the reforming section of the process. Of the three process configurations studied, the most profitable is Scheme 1 (Figure 3). Of the two configurations with reduced reforming operations, Scheme 3 with the primary reformer and high temperature shift reactor is more economic than Scheme 2 with only the primary reformer. This is because the majority of the water gas shift reaction takes place in the high temperature shift reactor and only a fraction in the primary reformer. Scheme 3 is not as economic as Scheme 1 with all reforming unit operations because although capital costs are lower due to the absence of the low temperature shift reactor, the decreased amount of hydrogen that is made reduces the net income over the life of the plant. Figure 3 shows that for positive biomass feedstock costs, the necessary hydrogen selling price would have to be at least \$8.70/GJ and \$11.20/GJ for the large and medium size plants, respectively. Unless biomass at extremely low costs can be obtained, hydrogen produced from indirectly heated gasification on the small scale is not economically feasible. Figures 4 and 5 show similar results.

DCFROR results for the pyrolysis-based processes are shown in Figures 6 though 9. Figure 6 represents the case of reforming the entire pyrolysis oil (no coproducts) where the feedstock cost was assumed to be oil purchased from outside suppliers; Figure 7 assumes that the oil was produced in-house. Figures 8 and 9 show the necessary hydrogen selling price for the adhesives coproduct option for pyrolysis oil that is purchased and produced, respectively. As expected, the coproduct option is more economically feasible than reforming all of the pyrolysis oil to produce only hydrogen. Also expected is that the necessary hydrogen selling price is lower when pyrolysis oil is produced rather than purchased. However, this may not be feasible once a system to produce various chemicals and fuels from biomass pyrolysis oil is developed.

For positive feedstock prices, Figure 6 shows that hydrogen can be produced at economically competitive prices only for the large and medium size plants when the entire biomass pyrolysis oil is purchased and reformed. Hydrogen from the small plant is competitive only at the highest market values. If the oil can be produced in-house, Figure 7 shows that there is a wider range of feedstock costs for which hydrogen from reforming the entire pyrolysis oil can be economic, even at the small scale.

The economic position of the process to reform all of the pyrolysis oil versus reforming the gasification syngas depends upon the feedstock cost and plant size. For lower biomass costs, the gasification-based process is more economic than the pyrolysis-based process. If biomass can be obtained at cheaper than \$30/T for the large plant, the gasification-based process produces hydrogen at lower prices; the pyrolysis-based process produces hydrogen cheaper at biomass costs greater than \$30/T. This trade-off point occurs at \$-12/T and \$-170/T for the medium and small plant sizes, respectively. Since biomass costs are not expected to be lower than \$30/T, the pyrolysis-based process is more likely to be feasible. Again, it should be noted that the analysis of the pyrolysis-based process contains a higher degree of uncertainty than that of the gasification-based process. Therefore, the comparative position of these two processes may change as further experimental data are incorporated into the analysis. Hydrogen and an adhesives coproduct can be produced at economically competitive prices for all positive feedstock costs for the medium and small plants whether the oil is purchased (Figure 8) or produced (Figure 9). At positive feedstock costs, the hydrogen produced on the small scale can be sold for at least $9/GJ if the pyrolysis oil is purchased, and at least $3/GJ if the pyrolysis oil is produced in-house.

The most economic size for the processes studied depends upon the feedstock cost. If the medium size plant can be supplied with waste biomass at a cheaper price (i.e., $16.50/T) than the biomass supplied by a DFSS (expected to be $46.30/T), the necessary hydrogen selling price from the medium size plant is lower than that from the large plant. However, if the medium and large plants must both use biomass from a DFSS, the larger plant is more economically feasible. The medium size plant is more economical than the small plant if biomass at the same feedstock cost is used in each. Figures 3 through 9 also show that there is a larger economy of scale realized in going from the small to the medium size plant than in going from the medium to the large size plant.

Figures 10 through 12 show the cumulative cash flow for the three gasification-based plant sizes for Scheme 1 over a twenty year plant life. The corresponding curves for Schemes 2 and 3 are similar. Such figures for the pyrolysis-based processes were not generated because without more experimental data, the amount of useful information from such figures is limited. Figures 10 and 11 show the cash flow for the 27 and 272 T/day gasification-based plant using a biomass feedstock cost of $16.50/T, corresponding to the estimated cost of biomass waste. Figure 12 is the cash flow diagram for the 907 T/day plant using a DFSS cost of $46.30/T. Each cash flow diagram is based on a hydrogen selling price of $11/GJ ($12/MMBtu). The break-even point for the medium plant (6.3 years) is sooner than that for the large plant (7.2 years) because of the lower feedstock cost. If the medium plant were also using biomass at $46.30/T, the break-even point would be 9.5 years.

Conclusions

All processes studied in this analysis produce hydrogen at prices competitive with current market values. The coproduction of hydrogen and a phenolics-like adhesive from steam reforming biomass pyrolysis oil was the most economically feasible option studied. At reasonable biomass costs, reforming the entire pyrolysis oil to produce only hydrogen was more economic than reforming syngas from the BCL indirectly heated biomass gasifier. However, the difference in the necessary hydrogen selling price between these processes was small, and the results for the pyrolysis-based process are preliminary and are likely to change as more data become available. Nevertheless, the pyrolysis-based process has the advantage of added process flexibility. It can be designed as a regionalized system of pyrolysis units feeding one centralized reformer or as a combined operation. Additionally, the most economically feasible combination of coproducts can be used to increase the likelihood of commercialization. Such operations are expected to be similar to current petroleum refineries in that they would produce a slate of chemicals and fuels.

Of the three plant sizes studied, the 272 T/day plant is the most economic if waste biomass at a low price can be obtained. If biomass from a DFSS must be used, the 907 T/day plant is more economic. Hydrogen produced on the small scale in the gasification-based process and pyrolysis-based process without the coproduct option is not economically competitive with conventionally-produced hydrogen.

The break-even point for the gasification-based process is fairly long. However, this is partially due to the higher IRR that was specified in the analysis. As research continues into processes that utilize biomass and as uncertainties are addressed, the risk of investment in such projects will decrease. This will cause a decrease in the necessary hydrogen selling price and a shorter break-even point.

Future Work

As experimental data become available for reforming pyrolysis oil, it will be incorporated into the models developed for this analysis. An ASPEN Plus™ simulation will be developed for the reforming operation and integrated with the pyrolysis model currently available. In parallel with the development of a full pyrolysis-based process, other coproduct options will be explored. This work will be accomplished through the cooperation of researchers with expertise in market assessment, R&D, and engineering, and will incorporate work under progress at NREL.

The ASPEN Plus™ model of the reforming operation will be optimized to increase hydrogen production efficiency and reduce costs. One option that might help costs is the addition of a steam turbine to produce electricity from the excess heat in the reforming operation. Also, a quench operation will be tested to cool the feed to the PSA unit. Further sensitivity analyses will be performed on ASPEN Plus™ and within the economic spreadsheet model to ascertain other areas for improvement.

As biomass-based processes become better developed and the uncertainties associated with the cost of the biomass feedstock decrease, the assumptions made in this analysis will be revisited. Currently, the biomass feedstock cost is a result of the analysis, determined from the cost curves set between the current high and low market values of hydrogen.

A life cycle assessment will be conducted on these processes in order to determine their environmental impacts in terms of energy consumption and emissions to water and the air. This will include a comparative analysis of conventional hydrogen producing processes.

Pertinent Literature and References

Anand, M. (April, 1995). *Personal Correspondence.*

Bain, R. (January 14, 1992). *Material and Energy Balances for Methanol from Biomass Using Biomass Gasifiers*. Golden, Colorado: National Renewable Energy Laboratory.

Breault, R.; Morgan, D.; (1992). *Design and Economics of Electricity Production from and Indirectly Heated Biomass Gasifier*. Report TR4533-049-92. Columbus, OH: Battelle Columbus Laboratories.

Chornet, E.; Czernik, S.; Wang, D.; Mann, M. (1994). *Biomass to Hydrogen via Fast Pyrolysis and Reforming*. Proceedings of the 1994 DOE/NREL Hydrogen Program Review.

Chum, H.L.; Black, S.K. *Process for Fractionating Fast Pyrolysis Oils and Products Derived Therefrom*. U.S. Patent No. 4,942,269 (17 July 1990).

Double, J.M.; (1988) *Design, Evaluation and Costing of Biomass Gasifiers*. Doctoral Thesis.

Dravo Engineering Companies. (1987). Gasification Capital Cost Estimation. Obtained from Mark Paisley, Battelle Columbus Laboratories. August, 1994.

Gerhartz, W., ed. (1989). *Ullman's Encyclopedia of Industrial Chemistry*. Germany; Vols. A13, A17, A22.

Gregoire, C.E. (1992). *Technoeconomic Analysis of the Production of Biocrude from Wood*. Golden, CO. NREL Report TP-430-5435.

Moe, J. (March 1962). "Design of Water-Gas Shift Reactors." *Chemical Engineering Progress*; Vol. 58, [3], pp. 33–36.

Ogden, J.; Dennis, E.; Steinbugler, M.; Strohbehn, J.W. (January 18, 1995). *Hydrogen Energy Systems Studies*. Princeton University: Center for Energy and Environmental Studies, Figure 5b.

Peters, M.; Timmerhaus, K. (1991). *Plant Design and Economics for Chemical Engineers*. 4th edition. New York: McGraw-Hill.

Tindall, B.M.; King, D.L. (July 1994). "Designing Steam Reformers for Hydrogen Production." *Hydrocarbon Processing*; Vol. 73, [7], pp. 69–75.

Weenen, W.; Tielrooy, J. (February 1983). "Optimizing Hydrogen Plant Design." *Chemical Engineering Progress*; Vol. 79, [2], pp. 37–44.

Weyerhaeuser. (1992). Gasification Capital Cost Estimation. Obtained from Mark Paisley, Battelle

Columbus Laboratories. August, 1994.

Figure 1: The Battelle Indirectly Heated Gasification System

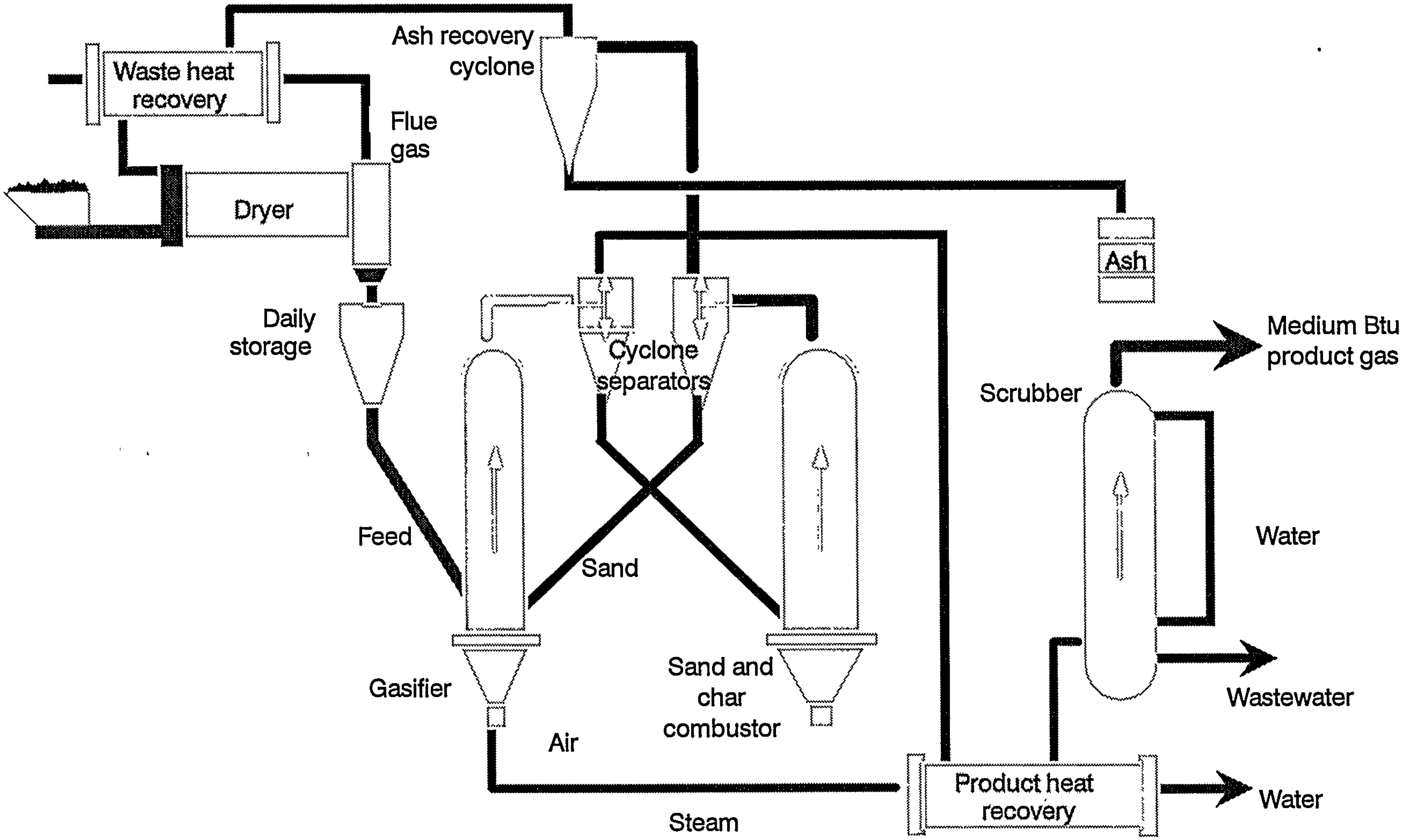


Figure 2: Reforming Process

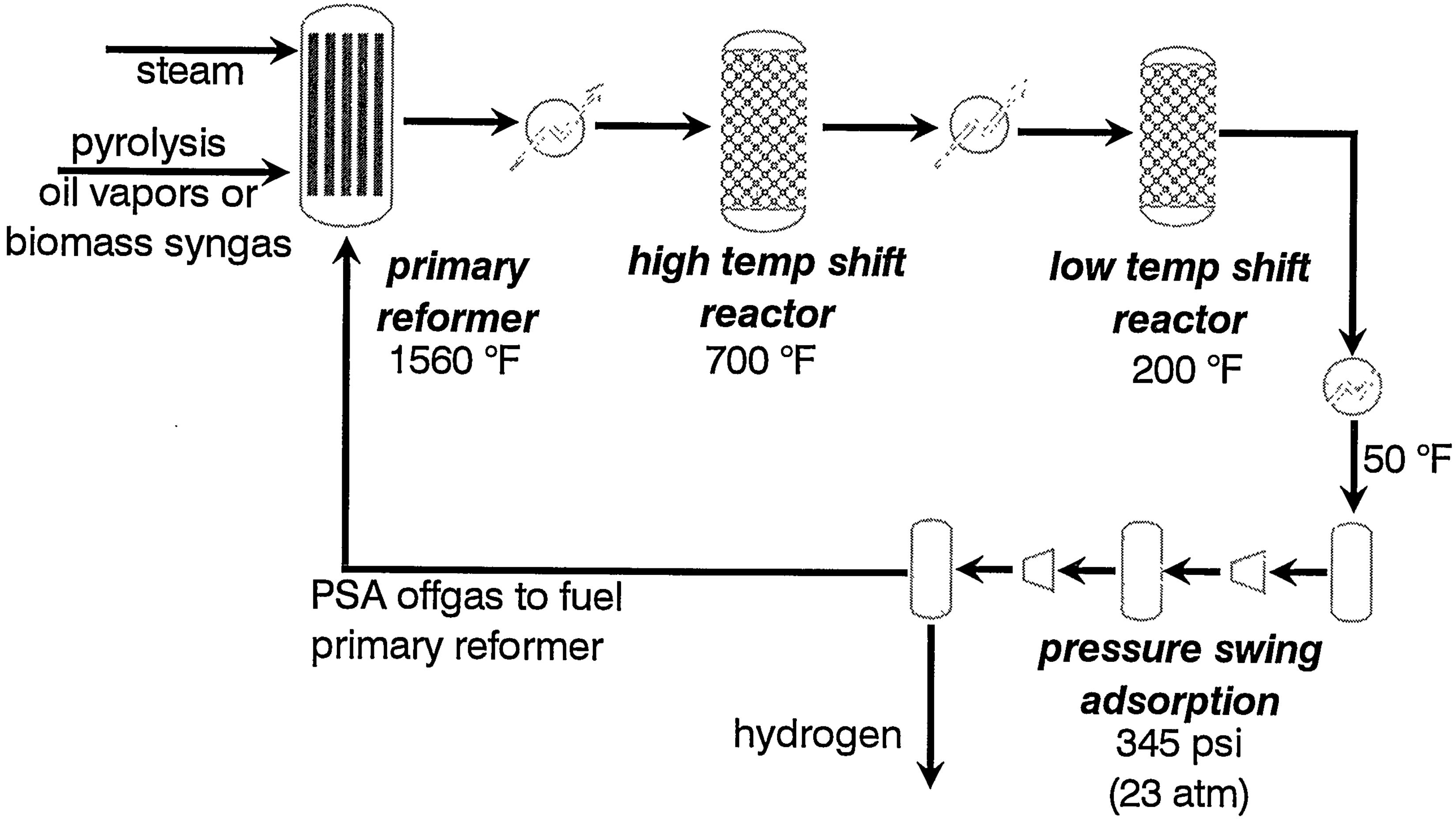


Figure 3: Selling Price of Hydrogen From Steam Reforming Biomass Syngas (Scheme 1), After Tax, 15% ROR

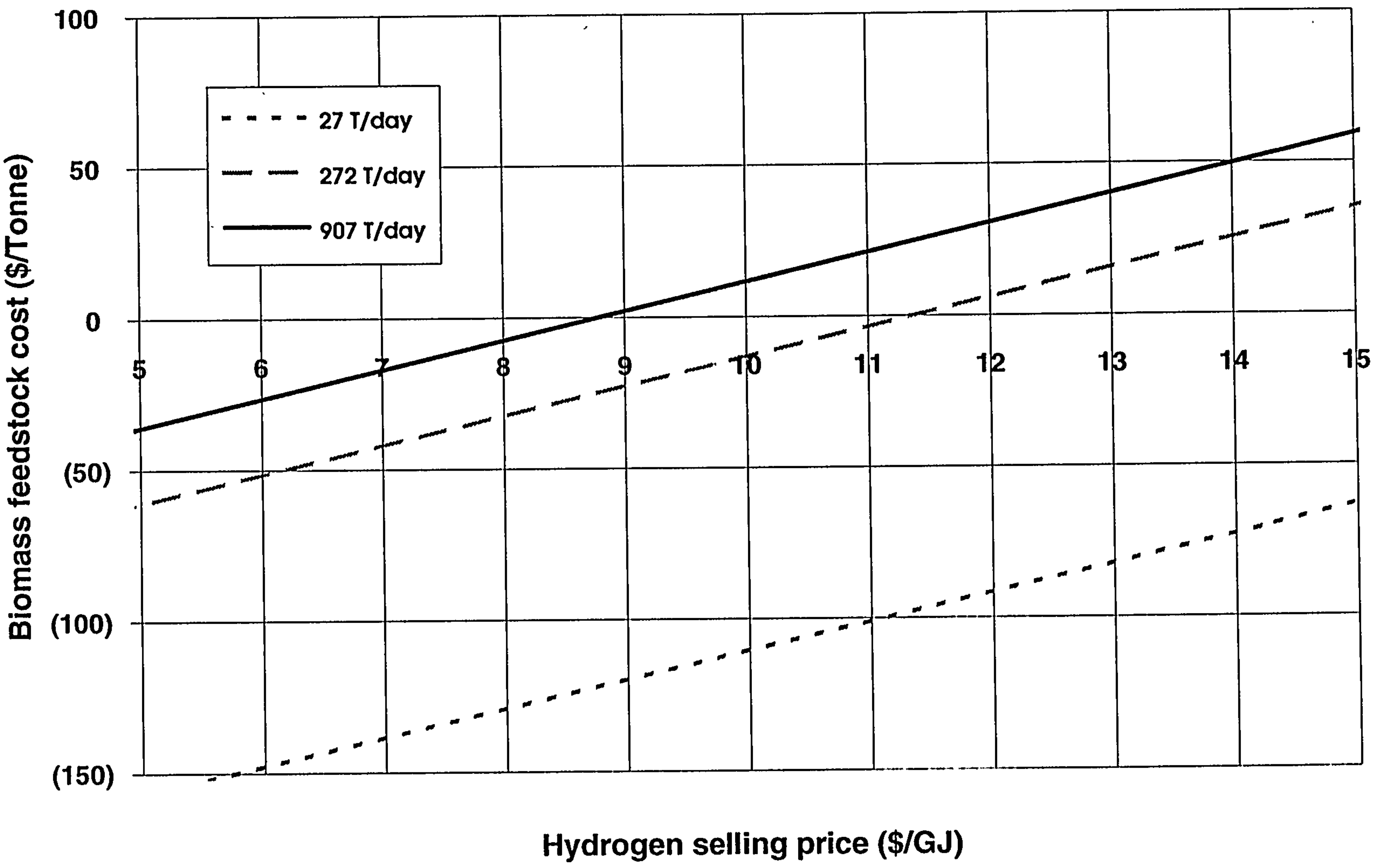


Figure 4: Selling Price of Hydrogen From Steam Reforming Biomass Syngas (Scheme 2), After Tax, 15% ROR

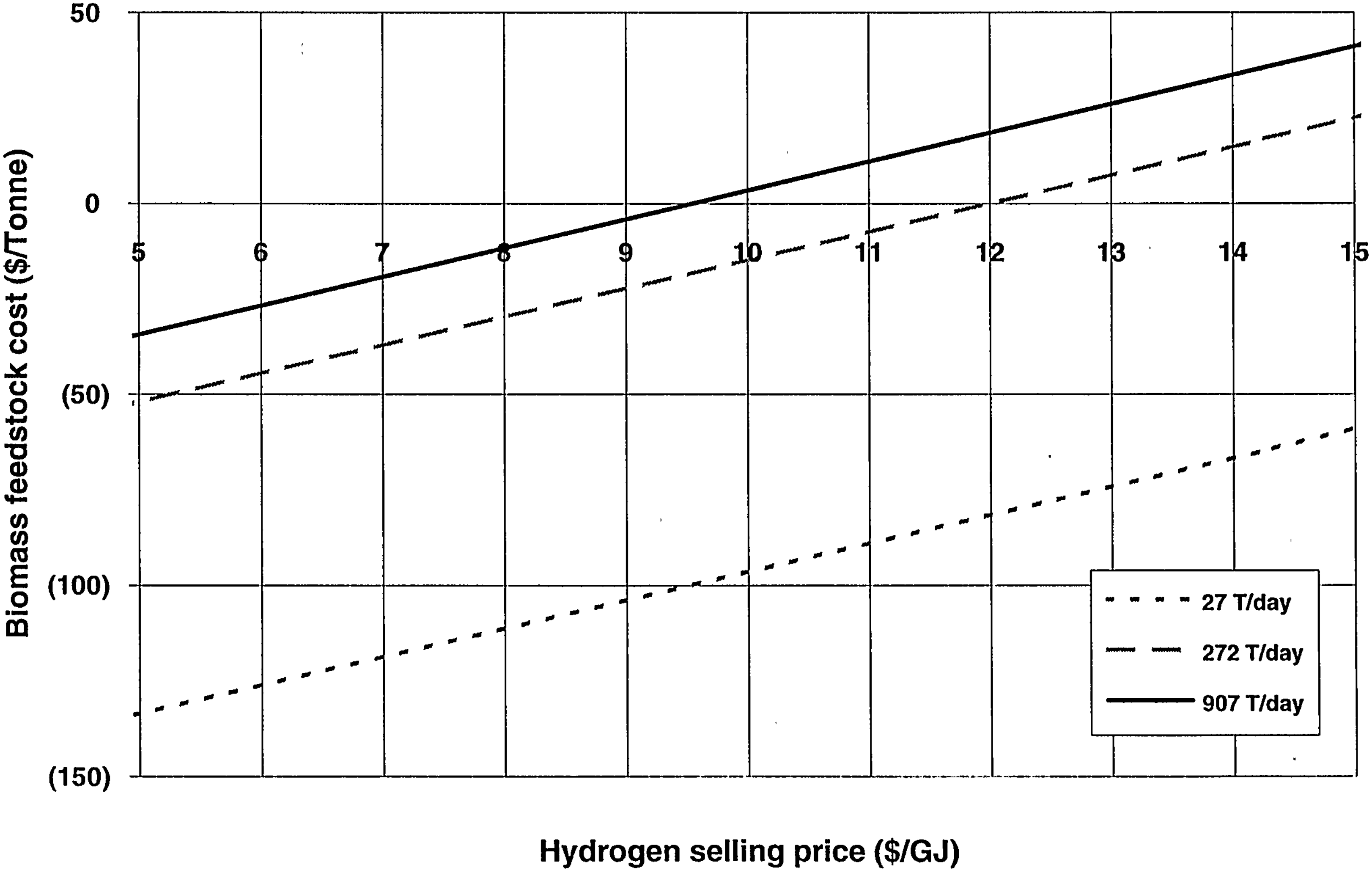


Figure 5: Selling Price of Hydrogen From Steam Reforming Biomass Syngas (Scheme 3), After Tax, 15% ROR

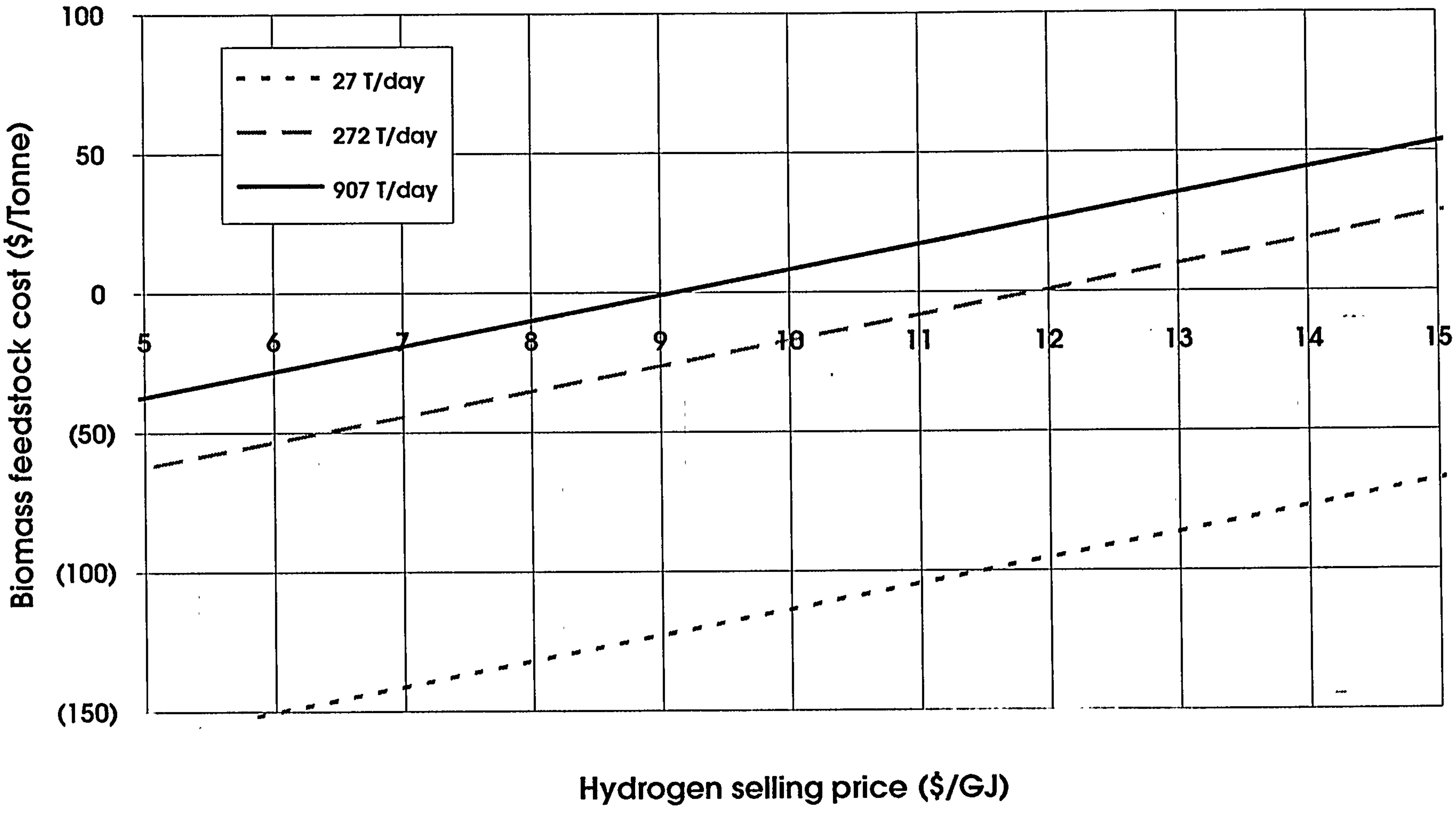
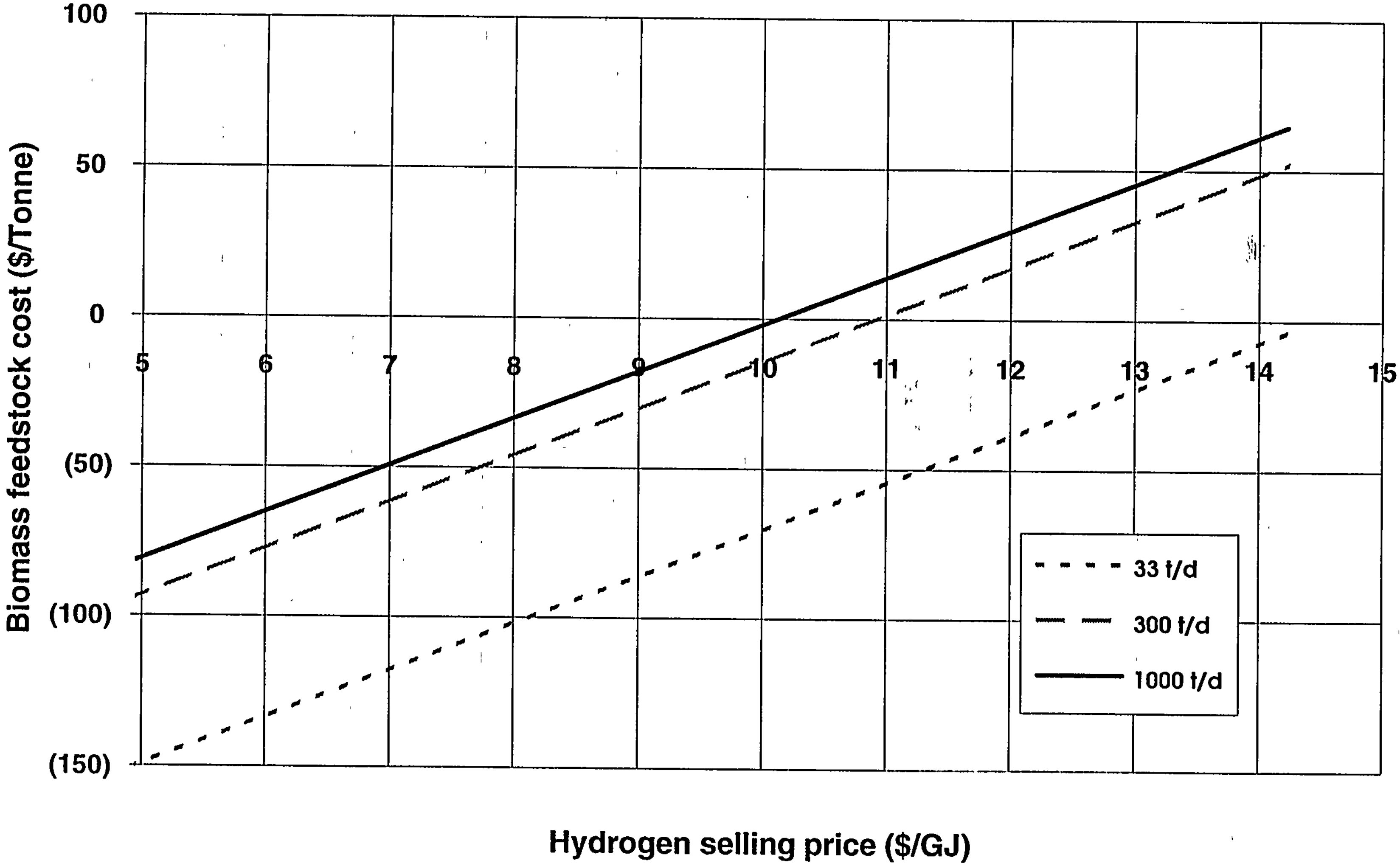
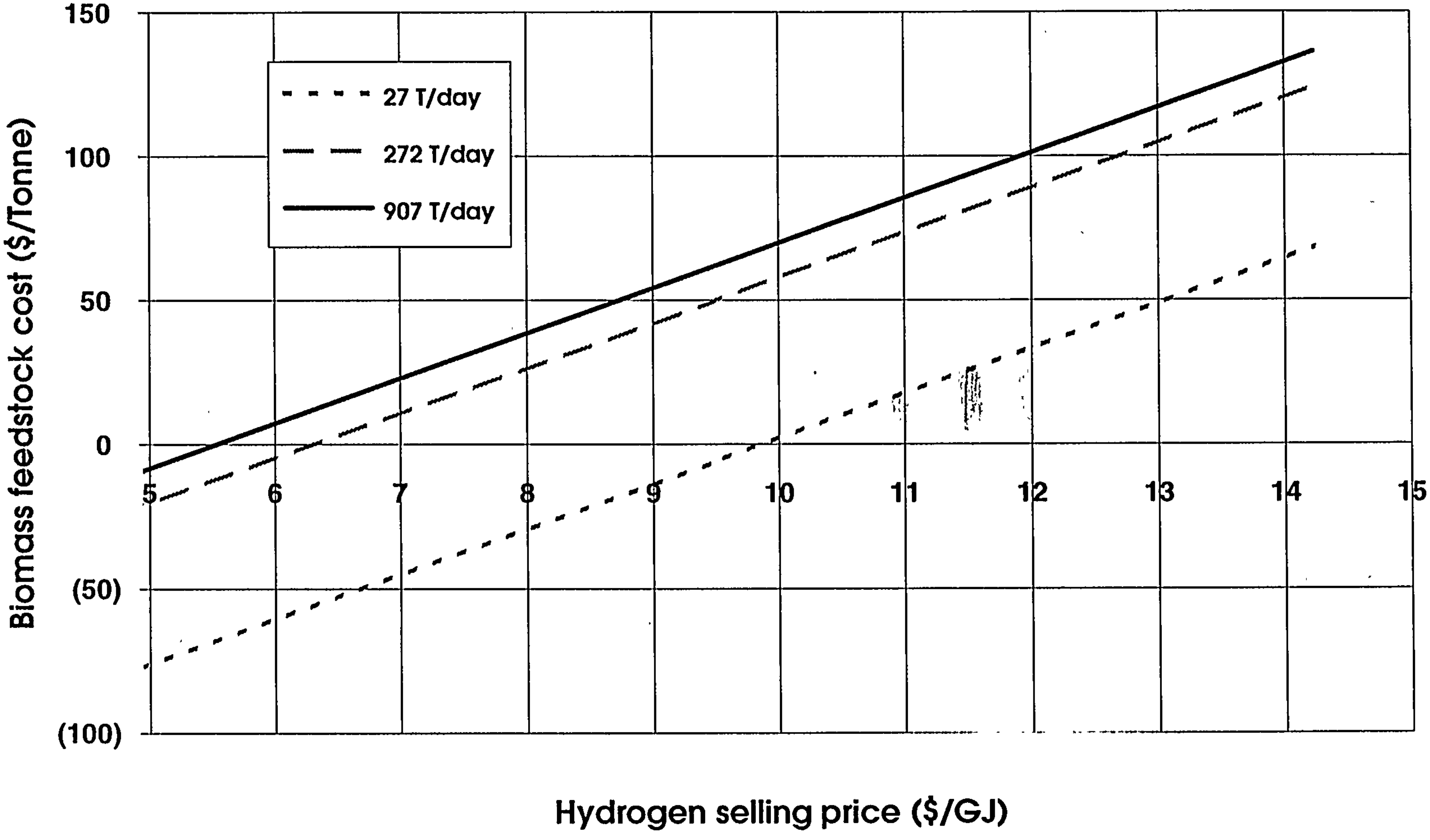


Figure 6: Selling Price of Hydrogen From Steam Reforming Entire Biomass Pyrolysis Oil, After Tax, 15% ROR



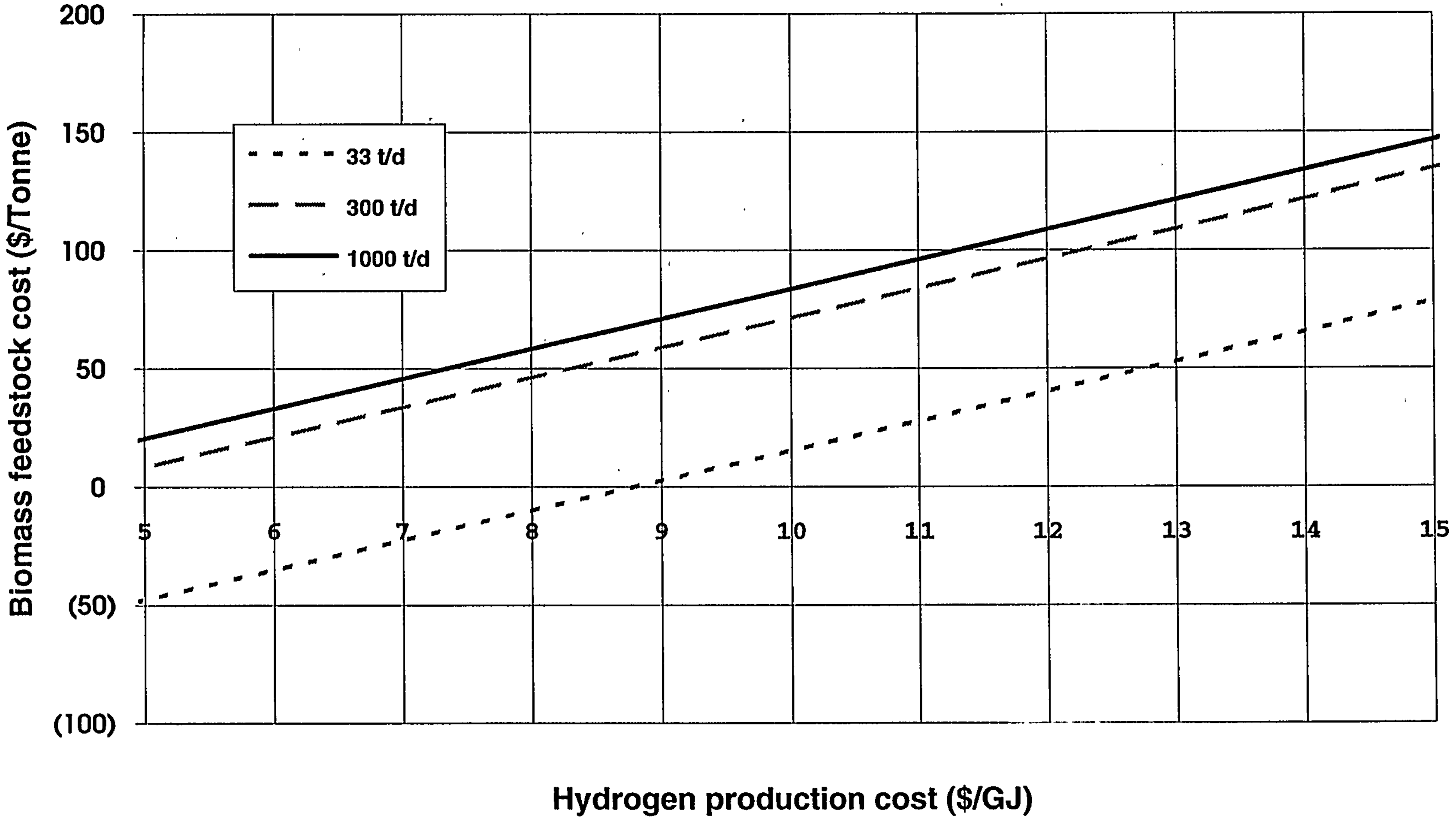
Feedstock is considered to be pyrolysis oil at selling price

Figure 7: Selling Price of Hydrogen From Steam Reforming Entire Biomass Pyrolysis Oil, After Tax, 15% ROR



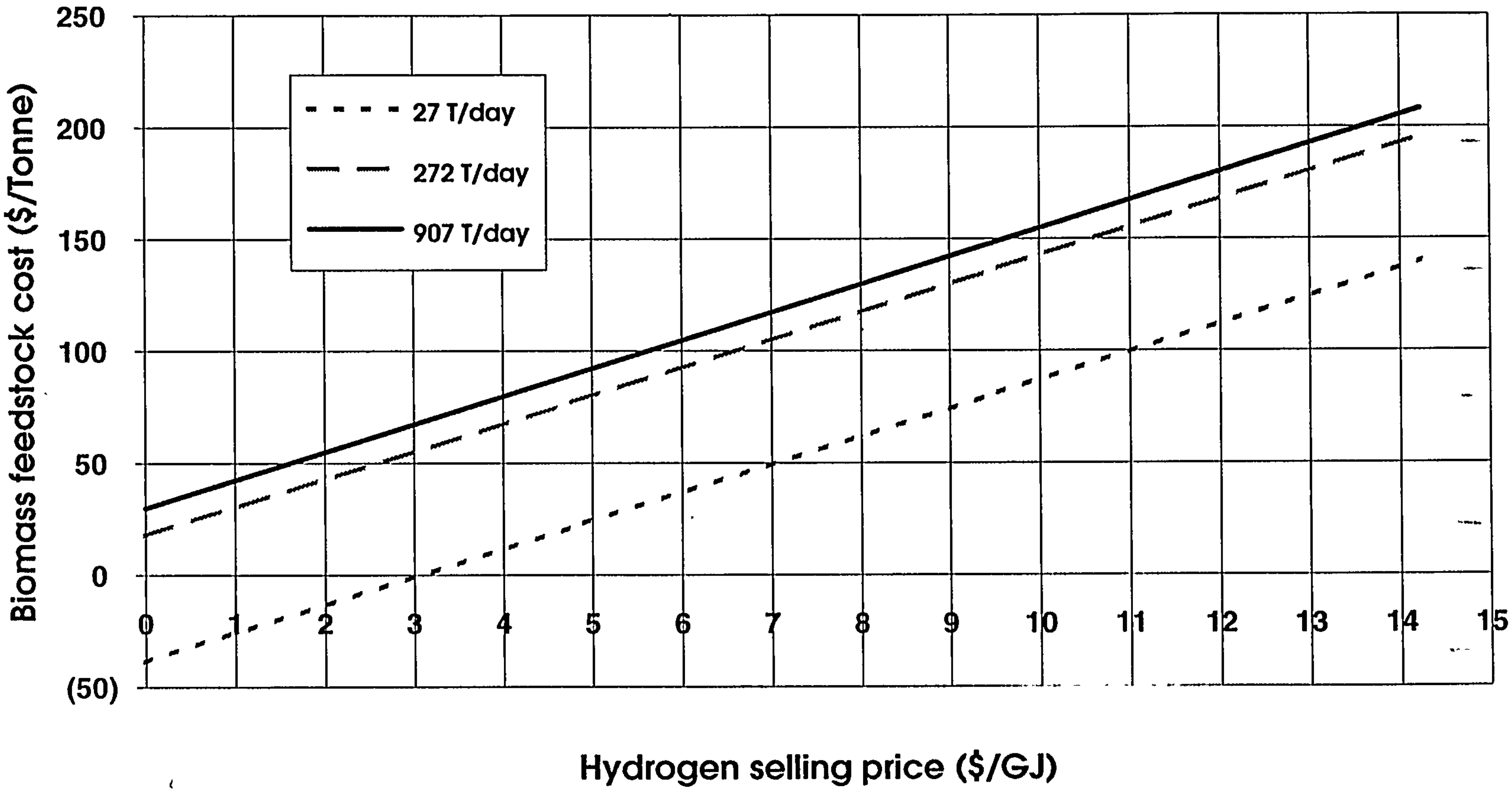
Feedstock is considered to be pyrolysis oil at production cost

Figure 8: Production Cost of Hydrogen From Steam Reforming Biomass Pyrolysis Oil and Selling P/N Fraction, After Tax, 15% ROR



Feedstock cost is considered to be pyrolysis oil at selling price

Figure 9: Selling Price of Hydrogen from Steam Reforming Biomass Pyrolysis Oil and Selling P/N Fraction, After Tax, 15% ROR



Feedstock is considered to be pyrolysis oil at production cost

Figure 10: Cumulative Cash Flow for a 27 T/day Biomass Gasification and Reforming Facility

Feedstock cost = $16.50/T

Hydrogen selling price = $12/GJ

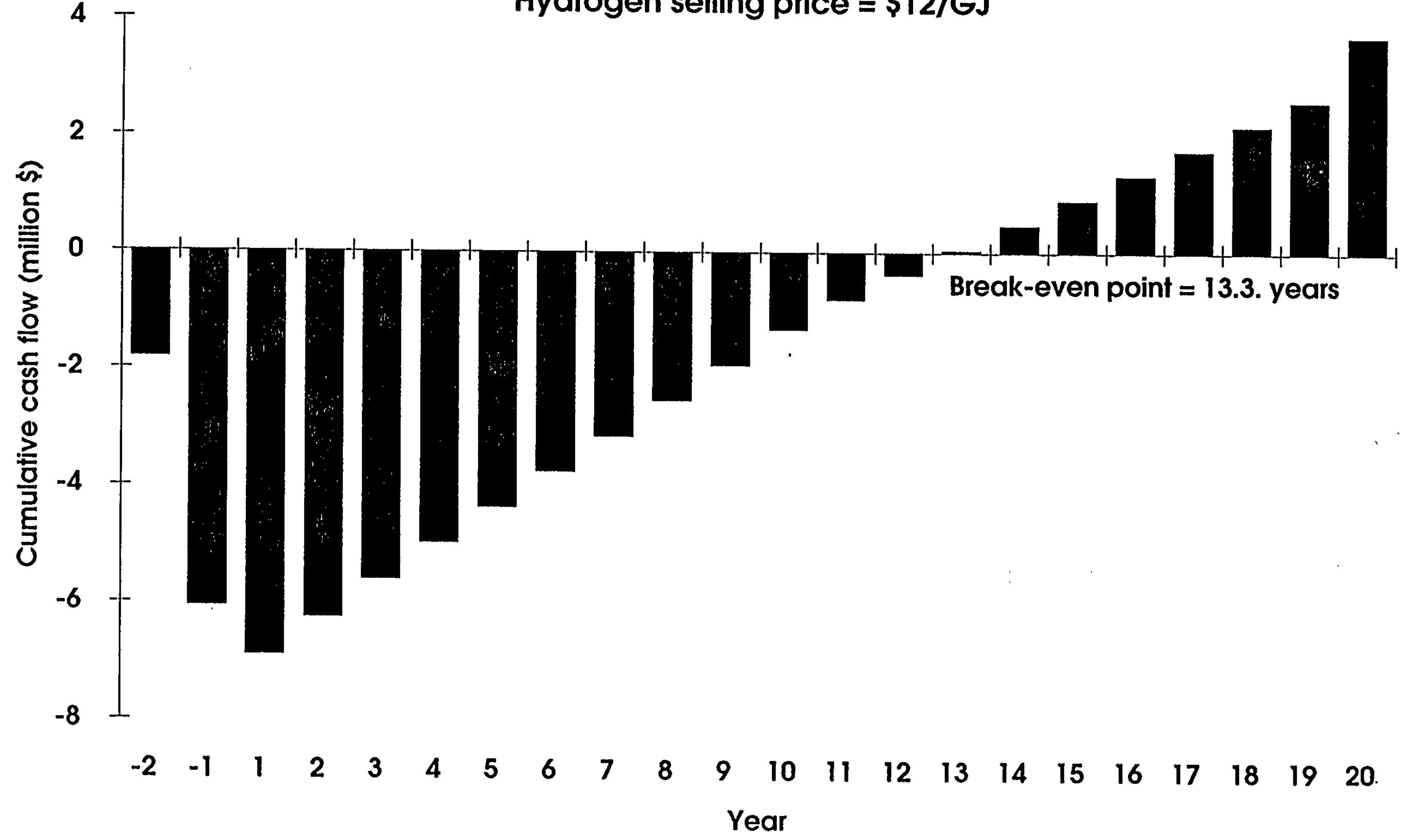
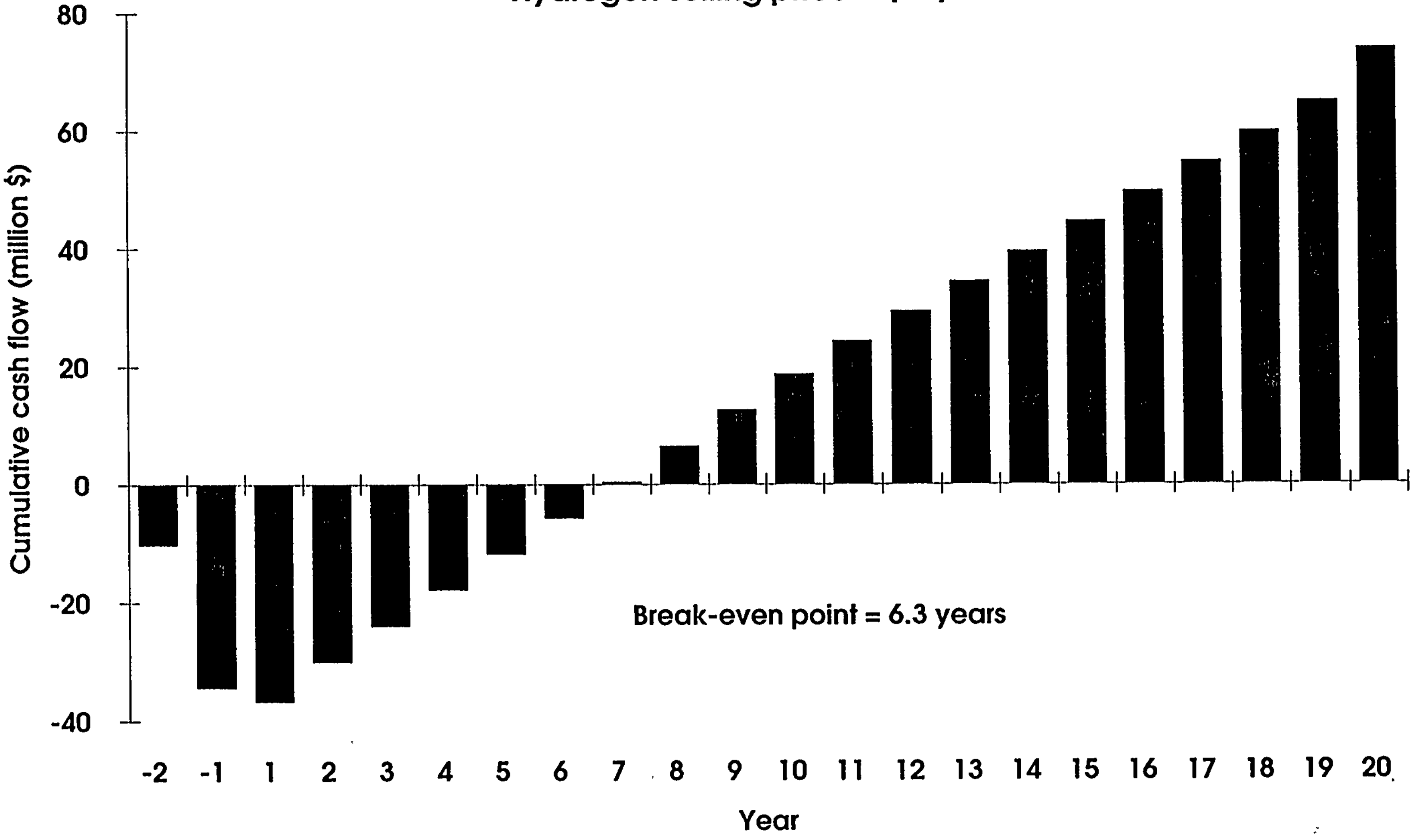


Figure 11: Cumulative Cash Flow for a 272 T/day Biomass Gasification and Reforming Facility

Feedstock cost = $16.50/T

Hydrogen selling price = $12/GJ

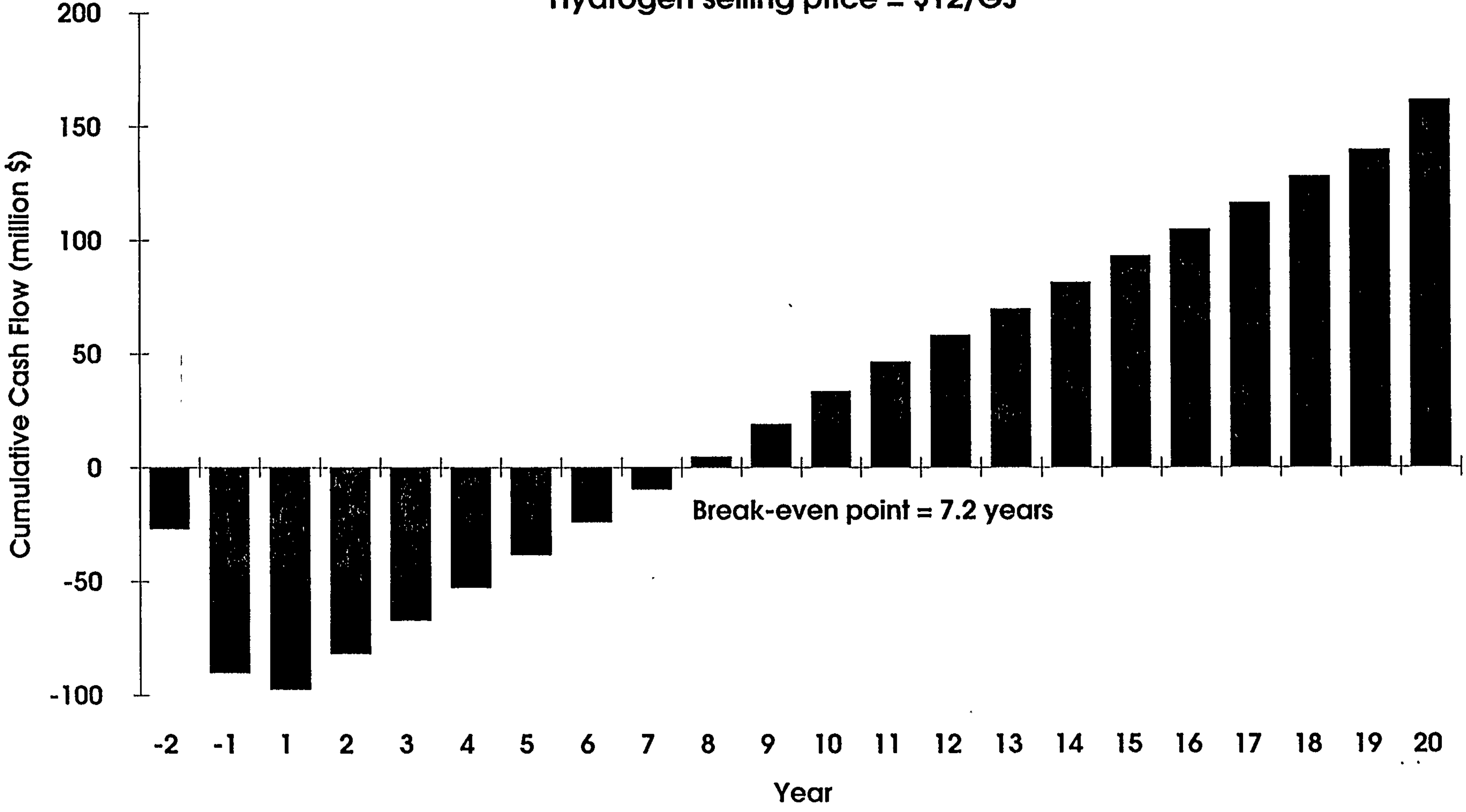


Break-even point = 6.3 years

Figure 12: Cumulative Cash Flow for a 907 T/day Biomass Gasification and Reforming Facility

Feedstock cost = $46/T

Hydrogen selling price = $12/GJ



HYBRID VEHICLE SYSTEM STUDIES AND OPTIMIZED HYDROGEN ENGINE DESIGN

J. Ray Smith and Salvador Aceves
Lawrence Livermore National Laboratory
Livermore, CA 94551

Abstract

We have done system studies of series hydrogen hybrid automobiles that approach the PNGV design goal of 34 km/liter (80 mpg), for 384 km (240 mi) and 608 km (380 mi) ranges. Our results indicate that such a vehicle appears feasible using an optimized hydrogen engine. We have evaluated the impact of various on-board storage options on fuel economy.

Experiments in an available engine at the Sandia CRF demonstrated NO_x emissions of 10 to 20 ppm at an equivalence ratio of 0.4, rising to about 500 ppm at 0.5 equivalence ratio using neat hydrogen. Hybrid simulation studies indicate that exhaust NO_x concentrations must be less than 180 ppm to meet the 0.2 g/mile ULEV or Federal Tier II emissions regulations.

LLNL has designed and fabricated a first generation optimized hydrogen engine head for use on an existing Onan engine. This head features 15:1 compression ratio, dual ignition, water cooling, two valves and open quiescent combustion chamber to minimize heat transfer losses. Initial testing shows promise of achieving an indicated efficiency of nearly 50% and emissions of less than 100 ppm NO_x. Hydrocarbons and CO are to be measured, but are expected to be very low since their only source is engine lubricating oil. A successful friction reduction program on the Onan engine should result in a brake thermal efficiency of about 42% compared to today's gasoline engines of 32%. Based on system studies requirements, the next generation engine will be about 2 liter displacement and is projected to achieve 46% brake thermal efficiency with outputs of 15 kW for cruise and 40 kW for hill climb.

Introduction

Two recent developments have increased the interest in high fuel economy and low emission vehicles. High fuel economy vehicles, with up to 34 km/l (80 mpg), are one of the goals of the Partnership for a New Generation of Vehicles (PNGV); and the California Air Resources Board (CARB) has mandated the sale of low and zero emission vehicles.

Series hybrid vehicles appear to be a good solution for obtaining high fuel economy, low emission vehicles (Burke 1992, Smith 1993, Ross and Wu 1995). Series hybrid vehicles operate with an engine in an on-off mode.* The engine is turned on when it is necessary to charge a buffer storage system (flywheel, ultracapacitor, battery). When the storage is full, the engine is turned off, and all the energy is provided by the storage system. Series hybrid vehicles cannot transfer mechanical energy between the engine and the wheels. All the energy out of the engine is first converted to electrical energy, which is then used or stored according to the vehicle demands.

Considering the importance of the storage system, it is not surprising that series hybrid vehicles are very sensitive to the turnaround efficiency, power capacity, and energy storage capacity of the storage system. If minimum values of these parameters are not achieved, series hybrid vehicles lose their advantage with respect to parallel hybrid and conventional vehicles. Recent flywheel (Post et al. 1993) and ultracapacitor (Burke 1995) developments indicate optimism in reaching target performance values, which would make series hybrid vehicles the best choice for high fuel economy, low emission vehicles.

Series hybrid vehicles have a high efficiency because the engine operates mostly at the conditions that result in maximum vehicle fuel economy, without idling. When additional power is required during long hill climbs, the engine can be switched to a higher power level, trading off some fuel economy for the capacity of climbing long hills at higher speed. Series hybrid vehicles have low emissions because engine operation is not linked to vehicle driving conditions, therefore avoiding high emissions during hard accelerations. The energy level in the energy storage system can also be monitored for predicting the time for engine startup. This prediction can be used for preheating the catalytic converter, if this is required to reduce emissions.

This paper presents system analysis and hydrogen engine development work directed to obtaining a vehicle that approaches the 34 km/l (80 mpg) PNGV goal, and has very low emissions. Some of the vehicle and engine characteristics have been described in previous papers (Smith 1993; Smith 1994; Aceves and Smith 1995). The system analysis section of this paper shows a comparison between the hydrogen series hybrid (considering all the possible ways that can be used to store the hydrogen in the vehicle) and other technologies currently being considered for obtaining high fuel economy and

*On-off mode operation in a conventional drivetrain automobile during coast and stopped periods has recently been brought to the European market by Volkswagen in its Ecomatic automobile (Volkswagen 1994).

low emissions. The engine development section of this paper gives a brief description of the engine characteristics, the expected engine performance, and the current status of the development work.

System Analysis

The system analysis presented in this paper uses HVEC, a vehicle evaluation code described in a previous publication (Aceves and Smith 1995). This code can be used to predict the fuel economy, range and performance of electric and series hybrid vehicles. In this paper, HVEC is used to compare series hybrid vehicles with several combinations of fuels (gasoline, natural gas, diesel, methanol, hydrogen) and primary power supplies (piston engines, turbines, fuel cells), to evaluate which of these vehicles are most likely to meet the PNGV goal of 34 km/l (80 mpg, combined EPA driving cycle, 55% urban, 45% highway).

The vehicle comparison presented in this paper considers that it is possible to build a gasoline series hybrid having a 1000 kg empty weight and a 384 km (240 mi) range. This vehicle is then used as the base case for the comparison. The weight of other vehicle configurations is calculated from the base case vehicle by replacing the engine and fuel storage with alternative components, and calculating the differences in weight between the replaced components. It is also assumed that the chassis weight has to be increased by 0.3 kg for each kg of power train weight increase, due to the need for providing the required structural support.

The comparison between the different series hybrid vehicles is carried out under equal performance requirements. All vehicles analyzed in this paper have equal time for 0-97 km/h (60 mph) acceleration (10 s), equal hill climbing capacity (6% infinitely long hill at 97 km/h, or 60 mph) and equal range [either 384 km (240 mi) or 608 km (380 mi)]. Requiring equal performance implies that power train components (engine, motor, transmission) have different power output for each vehicle, as the power required to keep a desired performance increases as the vehicle weight increases. This constant performance requirement guarantees that all vehicles are being compared on equal terms. Other vehicle parameters, also considered equal for all vehicle configurations, are listed in Table 1.

Figure 1 shows a schematic of the vehicle configuration. Flywheels are used for energy storage in all vehicles, due to their high energy and power densities, and high turnaround efficiency. A detailed flywheel model has been incorporated into HVEC, which describes the measured performance of a flywheel which is currently in the prototype stage (Post et al. 1993). The model predicts flywheel turnaround efficiency and bearing losses as a function of flywheel state of charge and power.

Figure 2 shows the main results of the simulation and comparison of the series hybrid vehicles considered in this analysis. The figure shows lines of constant fuel economy (combined cycle) as a function of vehicle test weight and engine brake thermal efficiency. These contours have been generated by HVEC for vehicles with the desired constant performance parameters listed above. Figure 2 also shows points and regions, which indicate where the different series hybrid vehicles fall within the weight-efficiency diagram, for both the 384 km (240 mi) and the 608 km (380 mi) ranges. For some vehicles, the difference in weight for the two ranges being considered is very small. In these cases, only a point is indicated in the figure. A summary of the weights, engine efficiencies, and fuel economies for the series hybrid vehicles is listed in Table 2. Table 3 shows the weights of the hydrogen storage systems for the two ranges. Each of the vehicles is briefly described in the next section.

Vehicle Descriptions

Gasoline hybrid

This is the base-case vehicle, and it is assumed to have an empty weight of 1000 kg (1136 kg test weight) for a 384 km (240 mi) range. Engine efficiency is assumed to be 32 %, based on the peak efficiency of a current 9.5:1 compression ratio production engine (Thomson et al. 1987).

Gasoline hybrid, Lean-burn engine

This vehicle is assumed to run with a lean-burn (0.7 equivalence ratio) gasoline engine, which is assumed to have a 35% efficiency. Emission control for NO_x in this engine may require the use of a lean burn catalyst, still in the development stage. This vehicle is heavier than the previous, because lean-burn engines have a lower power output per unit of displacement than stoichiometric engines. Hence to maintain the required performance the engine must be bigger and heavier which also adds slightly to the chassis weight as described above.

Diesel hybrid

The efficiency for the diesel engine is assumed to be 46%, based on a recent production truck engine (Tsujita et al. 1993). However, small diesel engine efficiencies can be substantially lower than this (Lawrence and Evans 1990). A region is shown in Fig. 2, which indicates the possible efficiency of current and future small diesel engines.

Compressed Natural Gas (CNG) hybrid

CNG engines can operate at a high (12:1) compression ratio, and therefore their efficiency can be higher than the efficiency of gasoline engines.

CNG hybrid, Lean-burn

CNG engines operating lean are assumed to have a 38% efficiency. This vehicle is slightly heavier than the previous, due to the extra weight of the lean engine.

Gas turbine hybrid

Gas turbines are expected to be lighter than any other engine. However, their efficiency is relatively low, due to the limit in maximum temperature that the turbine materials can withstand. A 32%

turbine efficiency is assumed here for automotive turbines. However, an area is indicated in Fig. 2, extending to a maximum efficiency of about 40%, which has been recently set as a PNGV goal (PNGV 1995), and may be possible in the future with high temperature turbines.

Hydrogen hybrid, Cryogenic liquid hydrogen storage

This vehicle operates with an optimized hydrogen engine, that is expected to have a 46% brake thermal efficiency (see the Engine Development section of this paper for a description). The engine operates at a very high compression ratio (15:1), very lean (0.4 equivalence ratio), and is therefore substantially heavier than a stoichiometric engine. The cryogenic liquid storage has a reasonable weight and volume, and has a proven record of safety (Peschka 1992).

Hydrogen hybrid, Iron-titanium hydride storage

Iron-titanium hydride is a very safe way to store hydrogen with a very low energy penalty for compressing or liquefying (Buchner 1977). The storage system also has a reasonable volume. The major drawback of hydride storage is the high system weight. The mileage penalty is 10 mpg for the nearly 400 kg vehicle weight increase over the liquid hydrogen hybrid.

Hydrogen hybrid, Magnesium hydride storage

Magnesium hydrides are lighter than iron-titanium hydrides. However, they require high temperature thermal energy for releasing the hydrogen. Exhaust gases emitted by the optimized hydrogen engine have a low temperature (~300°C). Therefore, it is necessary to burn some of the hydrogen fuel to desorb the hydrogen contained in the hydride. This reduces the engine-storage system efficiency to about 40 % (Handrock 1995).

Hydrogen hybrid, Pressure storage at 3600 psi

This system has a low weight, but a very high volume (about 300 liters for a 608 km range), which may rule out this form of storage for automobiles. The volume can be reduced by using higher pressure containers. However, cost and safety issues still have to be addressed for very high pressure tanks.

Hydrogen hybrid, Methanol and reformer

This vehicle is fueled by methanol, avoiding therefore many of the direct infrastructure problems associated with hydrogen. Methanol is reformed on board, and converted into hydrogen and carbon monoxide, which are then burned in the engine. The transformation of methanol does not introduce any energy losses if exhaust energy is used for the process [energy gains may even occur (Pettersson and Sjostrom 1991)]. An on-board reformer introduces a weight penalty. However, the system volume is acceptable (estimated at 120 liters, including the methanol tank).

Hydrogen-methane hybrid, Pressure storage at 3600 psi

This vehicle is fueled with a 50%-50% molar mixture of methane and hydrogen. The presence of hydrogen in the mixture allows the engine to operate very lean, while the presence of methane results in an acceptable volume for the pressure storage (150 liters for 608 km range). The efficiency of the engine is assumed to be slightly lower than the efficiency for the pure hydrogen engine, because the presence of higher hydrocarbons in the methane may limit the compression ratio to avoid engine knock.

Proton Exchange Membrane (PEM) fuel cell hybrid, Cryogenic liquid hydrogen storage

Fuel cell efficiency and weight are obtained from a recent publication (Allison 1993). This vehicle has the highest fuel economy of all vehicles being compared. A fuel cell region is also shown in Fig. 2 to indicate the possibility of future improvements.

System Analysis Summary

Figure 2 shows that the lines of constant fuel economy have a small slope, indicating that mass does not have a great effect on fuel economy (34 kg of weight reduction are necessary for a 1 mpg increase in fuel economy). This indicates that, in reaching the 34 km/l (80 mpg) PNGV goal, it is more important to achieve a high engine fuel economy than a low vehicle mass. Figure 2 also shows that turbines, CNG engines and gasoline engines are unlikely to achieve the PNGV goal in a vehicle with the characteristics considered in this paper. Diesels, hydrogen engines, and fuel cells remain as the three technologies that have the possibility of reaching the PNGV goal. However, these have other limitations that may restrict their access to the market. The main difficulty with diesel engines is meeting the emission requirements for NOx and particulate matter. Hydrogen vehicles can achieve very low emissions, but the need for a hydrogen infrastructure may limit their extended use. Hydrogen storage is also a problem. Fuel cells are currently bulky, heavy, and very expensive. Many of the existing fuel cells are fueled with hydrogen, and therefore have the same infrastructure and storage problems as hydrogen engine vehicles. Solving satisfactorily the problems associated with either one of these technologies will result in an efficient, low emission car that may reduce oil imports and urban pollution. At the present time, hydrogen engine vehicles appear to be the most likely to meet all the requirements, since the storage and infrastructure issues can be solved with current technology at a reasonable cost, as shown in this and in a recent publication (Berry et al. 1994).

Optimized Hydrogen Engine Development

Emissions

The major emissions from hydrogen-fueled engines are NO_x which consists of NO (nitric oxide) and NO_2 (nitrogen dioxide). These can be considerably higher than the NO_x emissions from conventional gasoline-fueled engines due to its higher adiabatic flame temperature. High NO_x emissions are the result of high combustion temperatures in the burned gases, which occur when engines are operated at or near stoichiometric fuel-air ratios. In stoichiometric spark-ignition engines, NO usually represents 98% or more of the NO_x, while in compression ignition engines (diesels) NO exceeds 90% only at high loads or high speeds. An excellent discussion of the detailed chemical kinetic mechanisms of the NO formation process can be found in the literature (Heywood 1988).

To reduce combustion temperatures, and hence NO_x, the fuel-air ratio is reduced, which dilutes the combustion products with air. It is also possible to achieve similar results by recirculating exhaust gases (EGR) to dilute the hot products (Ibid). However, as the equivalence ratio is decreased, flame speed decreases until unstable (incomplete or late) combustion precludes further leaning. In extreme cases the flame speed is so low that combustion is not completed before the exhaust valve opens. In some situations, turbulent gas motion mixes the flame front with products and the flame is quenched. This occurs at an equivalence ratio of about 0.65 when using hydrocarbon fuels. Fortunately, hydrogen has a unique property that allows it to be burned at significantly lower temperatures than any other fuel: its high flame speed. A comparison of the laminar flame speeds of hydrogen, gasoline methanol reformate, a hydrogen/CNG blend, and methane are shown in Fig. 3. Note that flame speeds comparable to the lower equivalence ratio limits for methane and gasoline (about 0.65) are in the region of 0.3 for hydrogen. The flame speed in an engine is much higher than the laminar flame speed because of turbulence. Turbulence and burned gas expansion act as multipliers on the laminar flame speed.

The extensive work of Homan (Homan 1978) on direct injection of hydrogen in a CFR (Cooperative Fuels Research) engine operated in both the spark-ignition and compression ignition modes indicates that late injection always results in one to two orders of magnitude more NO_x production than does lean, premixed, spark-ignited operation. Thus, it does not appear promising to consider diesel cycles when trying to minimize NO_x production. Homan measured 0.005 g of NO_x per kWh of work produced using a spark-ignited hydrogen air mixture at equivalence ratio 0.38 (Ibid). Das (Das 1990) measured the NO_x emissions from another hydrogen-fueled research engine as a function of equivalence ratio at compression ratios up to 11:1 and are consistent with the extensive measurements of Swain in an 8.5:1 CR engine (Swain et al. 1983). Figure 4 shows measurements made by this project on a Sandia CLR (Council for Lubricating Research) engine which are in agreement with Swain and Das.

Operation at premixed equivalence ratios that are too low will result in unburned hydrogen that can form hydrogen peroxide within the combustion chamber. Hydrogen peroxide emissions could act as a source of hydroxyl radicals to promote photochemical smog. Sinclair and Wallace (Sinclair and Wallace 1984) found that hydrogen peroxide levels rose as the equivalence ratio was reduced below 0.4. At low hydrogen peroxide levels, passage of the exhaust through a conventional tailpipe and muffler resulted in greatly reduced peroxide levels. They state that a high-surface-area exhaust system would easily decompose the hydrogen peroxide on the metal walls to negligible levels. Even so, hydrogen peroxide emissions will put a lower limit on useful equivalence ratio.

Hydrogen engines emit small quantities of hydrocarbons (HC) and carbon monoxide (CO) from the decomposition and partial oxidation of the lubricants left on the cylinder walls by piston rings and from the valve guides. The exact HC and CO levels produced are probably very dependent on the detailed engine design. However, it is possible to get what is probably an upper bound on these emissions from recent measurements made on a large two-stroke diesel engine that was run on hydrogen (Hedrick 1993). The average of the "11 Mode Emission Test" gave HC of 0.010 g/kWh and CO of 0.0176 g/kWh in the 9.05 liter displacement engine. These are probably upper bounds because this two-stroke diesel sweeps the piston rings across the intake ports, which is likely to cause more oil to be transported into the combustion chamber by the passage of intake air.

There is a considerable body of knowledge on how the design details of piston rings affects oil transport into the combustion chamber (McGeehan 1979). Experiments by Furuhama, Hiruma, and Enomoto (Furuhama et al. 1978) with a three-piece oil ring reduced HC by nearly a factor of two in a liquid-hydrogen-fueled premixed engine. These researchers also removed the chamfer from the upper piston rings, which reduced blowby by a factor of four. Thus, with attention to the design issues of lubricant contributions to hydrogen engine emissions and with the current knowledge of the emission causes, it should be possible to keep the HC and CO emissions extremely low.

It is interesting to note that the tests done (Hedrick 1993) determined a NO_x emission of 0.575 g/kWh for the diesel. This is more than 100 times the value measured by Homan in the premixed spark-ignition case. This again supports the conclusion that diesel operation of hydrogen engines is not likely to have tolerable NO_x emissions. However, there is the possibility of using very large amounts of EGR to reduce temperatures and NO_x production in diesels.

Thus the literature gives clear guidance that an optimized hydrogen engine that minimizes emissions should operate as a premixed homogeneous-charge, spark-ignition engine at an equivalence ratio of about 0.4, and that attention in its design should be given to limiting lubricant contributions to the emissions. Note that the low emissions achievable in this type of engine do not require a catalyst.

Efficiency

There are two primary reasons to optimize a hydrogen engine for maximum efficiency. First, on-board hydrogen storage is a difficult task for automotive applications and, second, the cost of hydrogen on an energy content basis will likely remain higher than gasoline for the next several decades. The automotive storage problem is discussed in some detail by Robinson and Handrock (Robinson and Handrock 1994). The cost of hydrogen depends not only on hydrogen production costs but also on the distribution and bulk storage systems used. These infrastructure issues are addressed (Berry et al. 1994).

The thermal efficiency as a function of compression ratio for a number of single-cylinder research engine experiments on hydrogen is shown in Fig. 5. Indicated efficiency is more appropriate to report for single-cylinder research engines (net work done on the piston), because the high friction of most research engines is not representative of modern multicylinder engines.

Included in Fig. 5 is a plot of:

$$\eta = 1 - [1/(R_c)^{\gamma-1}] \tag{1}$$

the Otto cycle indicated thermal efficiency for constant ratio of specific heats. R_c is the compression ratio and γ is the ratio of specific heats, taken here to be 1.3. The indicated efficiency data by King (King et al. 1958) is for the most part below the ideal indicated efficiency. A hint as to the possible cause for the rolloff in efficiency measured by King et al., is given by the work of Caris and Nelson (Caris and Nelson 1959), who achieved 44.5% indicated thermal efficiency at 17:1 compression ratio using highly leaded gasoline at an equivalence ratio of 0.93. Their experiment, like virtually all of the engine compression ratio variation experiments, reduced the clearance height (the distance between the top of the piston and the head) as the compression ratio was raised. Thus at low compression ratios the surface-area-to-volume ratio of the combustion chamber at Top Dead Center (TDC) is low, and at high compression ratios the surface to volume ratio is high. This can have a major effect on heat losses from the burned gas. Heywood states that the boundary layer during expansion is of the order of 2 to 3 mm (Heywood 1988) and that because it is cooler than the core gases, it contains the majority of the mass in the cylinder if the surface-to-volume ratio is high. This effect has been highlighted in a recent engine model that compared well with production engines of varying surface-to-volume ratios (Muranaka et al. 1987). Based on the dimensions supplied in King's work on a modified CFR engine, it is estimated that the clearance height at TDC was 8 mm at 12:1 compression ratio and only 4.6 mm at 20:1. Thus, at the higher compression ratios there is little or no unaffected (uniform high temperature) core gases — virtually all the mass is in the cooling boundary layer. This is supported by Fig. 6, where the difference between the ideal thermal efficiency calculated from Eq. (1) and the measured indicated thermal efficiency of King et al., Oehmichen (Oehmichen 1942), and Mathur (Mathur and Khajuria 1984) are plotted against the surface-to-volume ratio which has been estimated from the engine schematic and dimensions provided in their papers.

Thus heat transfer losses are likely to be the main reason for experiments to fall well short of the ideal efficiency. It is noted that "timing losses" also contribute to less than ideal performance since the heat addition is not at constant volume due to the finite time it takes for the charge to burn. However, as Muranaka et al. show this loss is small if the burn duration is less than 50 to 60 crank angle degrees. This is further supported in Fig. 6 by the comparison of King's 1200 rpm data with the 1800 rpm data, which shows slightly greater than 50% increase in losses. This is what would be expected because the time for heat transfer to take place is inversely proportional to engine speed, and the equivalence ratio for the lower-speed case is a bit larger than the 1800 rpm case. The effects of heat transfer losses (Muranaka et al. 1987) for stoichiometric gasoline engines can be reasonably well fit by:

$$Q_c/Q_f = 20\,(1400/N)^{0.5} \tag{2}$$

where Q_o/Q_f is the fraction of energy of the fuel lost in percent and N is engine rpm. This fit of the model output is for wide open throttle.

Thus an optimized engine should have a compact combustion chamber to minimize heat losses if it is to be successful. Using a conventional engine and merely raising the compression ratio by reducing the clearance height is not likely to give acceptable results. This implies a longer stroke engine, which raises issues about friction.

Care must also be exercised in the design of an optimized engine that friction does not reduce the output excessively. Since constant-speed, constant-load is the requirement for hybrid applications, there is an opportunity to reduce friction because intermittant high-speed operation is necessary only for hill climb. In addition, by matching the engine to its load (the electrical generator) accurately, only wide-open throttle operation is required. Thus pumping losses can be minimized, and the engine intake and exhaust system can be tuned for maximum volumetric efficiency. Such tuning could compensate for the nearly 12% loss in volumetric efficiency that occurs by operating at an equivalence ratio of 0.4 because of the volumetric displacement of air by hydrogen.

Engine friction rises rapidly with speed. A correlation of friction (in bars of pressure) for four-stroke engines in the range of 0.85 to 2 liter displacement was found by Barnes-Moss (Barnes-Moss 1975) as:

$$\text{fmep (bar)} = 0.97 + 0.15(N/1000) + 0.05(N/1000)^2 \qquad (3)$$

where fmep is friction mean effective pressure, and N is the rpm. This fit is in good agreement with data in the range of 1000 to 5000 rpm and was done for wide-open throttle. Thus there is a compromise that must be made in engine speed between friction rising with engine speed and heat losses dropping with increasing engine speed. Since the fraction of work lost to friction depends on the indicated mean effective pressure, it is not possible to predict analytically the optimum engine speed. However, it is likely that the ideal speed will be between 1500 and 3000 rpm. Therefore, optimized hydrogen engines probably will not be high-speed engines.

Although the points cited here about engine efficiency are encouraging for achieving brake thermal efficiencies in the mid-to-upper 40% range, low equivalence ratio and low speed will mean low power output for a given displacement. The displacement required for the projected need of about 40 kW (54 hp) for the hybrid vehicle application will probably require a 2.0 liter engine in a four-stroke version. A modern gasoline engine can produce 100 to 110 kW from a 2.0 liter displacement engine. The impact of turbocharging to raise specific output and indicated mean effective pressure needs to be considered. Alternatively, the problems of engine oil contributing to emissions in a two-stroke version may have to be addressed if the four-stroke engine is too large for integration into a low-aerodynamic-drag automobile. Combustion and engine models can guide our choices of the parameters for an optimized engine, but only experimental data can confirm our goals.

Engine Development Summary

From a review of the available experiments on hydrogen engines, the following conclusions are drawn:

- Low emissions can be achieved without a catalyst if a hydrogen engine is operated at an equivalence ratio between 0.3 and 0.5. The lower bound is controlled by rising hydrogen peroxide production, while the upper bound is controlled by NO_x production. In addition, the engine design should minimize lubricant contributions to the combustion chamber.

- High efficiency in an optimized hydrogen engine is likely to be achieved if:
  1. A compact chamber with low surface-to-volume ratio is used to minimize heat losses to the walls.
  2. Mechanical friction is minimized for the constant-speed/load conditions.
  3. High volumetric efficiency is achieved through intake and exhaust tuning techniques to maximize the indicated mean effective pressure and engine output relative to mechanical friction.

- Optimum engine speed cannot be accurately predicted but will be relatively low.

- Specific power output will be relatively low and may require either turbocharging or consideration of two-stroke operation.

Current Engine Development Status

We have designed and fabricated a cylinder head for an existing Sandia Onan engine. This engine was originally a small, single cylinder diesel. The new head draws upon our understanding of the literature implications on NO_x emissions and efficiency. It also incorporates many of the suggestions by Professor Mike Swain to minimize oil intrusion into the combustion chamber. The design includes dual ignition from spark plugs located to minimize the flame travel distance for low cyclic variation at very low equivalence ratios. This will compensate for the low flame speed of lean operation. The design uses a low turbulence right circular cylinder shaped combustion chamber to minimize heat loss. This choice of chamber shape appears to be the best based on the recent work of the Lund Institute (Johansson and Olsson 1995) where ten chamber shapes were compared at 12:1 compression ratio. Using CNG at an equivalence ratio of about 0.6, they achieved 49% indicated efficiency. The Onan design uses 14.8:1 compression ratio to achieve high efficiency, but has higher surface to volume ratio than the Lund Institute experiments. To date, as shown on Fig. 5, Sandia researchers have measured 42 to 46% indicated efficiency on the Onan experiments. The authors remain hopeful that higher volumetric efficiency and higher engine speeds will result in higher efficiencies. The surface to volume ratio in the Onan experiment is limited by the engine stroke which will be changed in the next generation engine for improved efficiency.

Acknowledgments

This work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under Contract No. W-7405-ENG-48.

References

Aceves, S.M., and J.R. Smith, 1995, "A Hybrid Vehicle Evaluation Code and Its Application to Vehicle Design," SAE paper #950491,

Allison Gas Turbine Division, GM Corp., 1993, "Research and Development of Proton Exchange Membrane (PEM) Fuel Cell system for Transportation Applications, Initial Conceptual Design Report," report EDR 16/94, prepared for the Office of Transportation Technologies, Department of Energy.

Berry, G.D., A.D. Pasternak, G.D. Rambach, J.R. Smith and R.N. Schock, 1994, "Hydrogen as a Future Transportation Fuel," Lawrence Livermore National Laboratory report no. UCRL-JC-117945.

Barnes-Moss, H.W., 1975, "A Designer's Viewpoint," Passenger Car Engines Conference Proceedings, Institution of Mechanical Engineers, London, pp. 133-147.

Buchner, H., 1977, "The Hydrogen/Hydride Energy Concept," in Andresen and Maeland, editors: "Hydride for Energy Storage," Pergamon Press.

Burke, A.F., 1992, "Hybrid/Electric Vehicle Design Options and Evaluations," SAE paper 920447.

Burke, A.F., 1995, "The Potential of Electrochemical Capacitors for Electric and Hybrid Vehicle Applications," Proceedings of the Workshop Basic Research Needs for Vehicles of the Future," New Orleans, LA

Caris D.F., and E.E. Nelson, 1959, "A New Look at High Compression Engines," *Society of Automotive Engineers Transactions*, Vol. 67, pp. 112-124.

Das, L.M., 1990, "Hydrogen Engines: A View of the Past and a Look into the Future," *International Journal of Hydrogen Energy*, Vol. 15, No. 6, pp. 425-443.

Furuhama, S., M. Hiruma and Y. Enomoto, 1978, "Development of a Liquid Hydrogen Car," *International Journal of Hydrogen Energy*, Vol. 3, pp 61-81.

Handrock, J., 1995, personal communication, Sandia/California, Livermore, CA.

Hedrick, J.C., 1993, "Advanced Hydrogen Utilization Technology Demonstration," Southwest Research, Inc., Final Report, Project No. 03-5080.

Heywood, J.B., 1988, *Internal Combustion Engine Fundamentals*, McGraw-Hill, New York, Ch 11.

Heywood, J.B., *Internal Combustion Engine Fundamentals*, p. 697.

Homan, H.S., "An Experimental Study of Reciprocating Internal Combustion Engines Operated on Hydrogen," PhD thesis, Cornell University, January 1978, p. 69.

Johansson, B., and K. Olsson, 1995, "Combustion chambers for National Gas SI Engines Part I: Fluid Flow and Combustion," SAE paper 950469.

King, R.O., S.V. Hayes, A.B. Allan, R.W.P. Anderson, and E.J. Walker, "The Hydrogen Engine: Combustion Knock and the Related Flame Velocity," *Transactions of the Engineering Institute of Canada*, Vol. 2, No. 4, December 1958.

Lawrence, R.J, and R.W. Evans, 1990, "The Ford 1.8L Four Cylinder Turbocharged Diesel Engine for Passenger Car Application," SAE paper 901716.

Mathur, H.B., and P.R. Khajuria, 1984, "Performance and Emission Characteristics of Hydrogen Fueled Spark Ignition Engine," International Journal of Hydrogen Energy, Vol. 9, pp. 729-735.

McGeehan, J.A., 1979, "A Survey of the Mechanical Design Factors Affecting Engine Oil Consumption," *Society of Automotive Engineers Transactions*, Vol. 88, SAE paper 790864.

Muranaka, S., Y. Takagi and T. Ishida, 1987, "Factors Limiting the Improvement in Thermal Efficiency of S. I. Engine at Higher Compression Ratio," *Society of Automotive Engineers Transactions*, SAE paper No. 870548.

Oemichen, M., 1942, "Hydrogen as an Engine Fuel," Engine Laboratory of the Technische Hochschule, Dresden, Germany, VDI-Verlag GmbH, Berlin NW, V.D.I. Paper No. 68.

Peschka, W., 1992, "Liquid Hydrogen: Fuel of the Future," Springer-Verlag, New York.

Pettersson, L. and K. Sjostrom, 1991, "Decomposed Methanol as a Fuel - A Review," Combustion Science and Technology, Vol. 80, pp 265-303.

PNGV, 1995, "Inventions Needed for PNGV," U.S. Department of Commerce, Washington, DC.

Post, R.F., T.K. Fowler, and S.F. Post, March 1993, "High Efficiency Electromechanical Battery," *Proceedings of the IEEE*, Vol. 81, No. 3.

Robinson S.L., and J.L. Handrock, February 1994, "Hydrogen Storage for Vehicular Applications: Technology Status and Key Development Areas," Sandia National Laboratories White Paper, Livermore, CA.

Ross, M., and W. Wu, 1995, "Fuel Economy Analysis for a Hybrid Concept Car Based on a Buffered

Fuel-Engine Operating at a Optimal Point," SAE paper 950958.

Sinclair L.A., and J.S. Wallace, 1984, "Lean Limit Emissions of Hydrogen-Fueled Engines," *International Journal of Hydrogen Energy*, Vol. 9, No. ½, 00. pp. 123-128.

Smith, J.R., 1993, "The Hydrogen Hybrid Option," Proceedings of the Workshop on Advanced Components for Electric and Hybrid Electric Vehicles, Gaithersburg, MD, NIST special publication 860.

Smith, J.R., "Optimized Hydrogen Piston Engines," SAE's Convergence'94, Detroit, MI, October 18, 1994, Lawrence Livermore National Laboratory Report No. UCRL-JC-116894..

Swain, M.R., R.R. Adt, Jr., and J.M. Pappas, May 1983, *Experimental Hydrogen-Fueled Automotive Engine Design Data-Base Project,* Vol. 1, DOE Contract No. E(04-3)-1212, p. 20.

Thomson, M.W., A.R. Frelund, M. Pallas, and K.D. Miller, 1987, "General Motors 2.3L Quad 4 Engine," SAE paper 870353.

Tsujita, M., S. Niino, T. Ishizuka, A. Kakinai, and A. Sato, "Advanced Fuel Economy in Hino New PIIC Turbocharged and Charge-Cooled Heavy Duty Diesel Engine," SAE paper 930272.

Volkswagen, 1994, "Green VW," Vehicle News, Number 211, November/December, pp. 196-199.

Table 1. Parameters common to all vehicle configurations being analyzed.

Frontal area, m^2	2.04
Aerodynamic drag coefficient	0.24
Coefficient of rolling friction	0.007
Transmission efficiency (single speed transmission)	0.95
Flywheel energy storage capacity, kWh	1.0
Flywheel maximum power output, kW	100.0
Generator efficiency	0.95
Accessory load, W	1000

Table 2. Engine efficiencies, weights and combined cycle (55% urban, 45% highway) fuel economies for the vehicles being compared in the paper. All vehicles have the same performance parameters. Two vehicle ranges are considered: 384 km (240 mi) and 608 km (380 mi). Overall test weights assume a 136 kg pay load which is added to the empty weight.

Vehicle description	Engine efficiency, %	Test weight, kg		Fuel economy km/l (mpg)	
		384 km	608 km	384 km	608 km
Gasoline hybrid, stoichiometric engine	32	1136	1146	25(58)	25(58)
Gasoline hybrid, lean-burn engine	35	1174	1183	27(63)	27(63)
Diesel hybrid	46	1148	1158	35(83)	35(83)
CNG hybrid, stoichiometric engine	35	1137	1152	27(64)	27(64)
CNG hybrid, lean-burn engine	38	1174	1188	29(69)	29(69)
Gas turbine hybrid	34	1105	1115	26(62)	26(62)
Hydrogen hybrid, cryogenic liquid storage	46	1218	1247	34(81)	34(80)
Hydrogen hybrid, Fe-Ti hydride storage	46	1479	1643	31(74)	30(70)
Hydrogen hybrid Mg hydride storage	40[1]	1409	1514	28(66)	27(63)
Hydrogen hybrid, 3600 psi pressure storage	46	1239	1262	34(80)	34(79)
Hydrogen hybrid, methanol and reformer	46	1283	1302	34(79)	33(78)

Hydrogen-methane hybrid 3600 psi pressure storage	45	1226	1242	34(79)	33978)
PEM fuel cell hybrid, cryogenic liquid H_2 storage	47[2]	1171	1192	36(85)	36(84)

---

[1] This value takes into account the amount of hydrogen that is necessary to burn to extract the hydrogen from the storage.

[2] Fuel cells do not require a generator, therefore, "engine efficiency" for a fuel cell is given as the fuel cell efficiency divided by the generator efficiency (95%), to allow a direct comparison with engine efficiencies.

Table 3. Empty weights for hydrogen storage systems, for the two ranges being considered.

Cryogenic liquid	25	39
FE - Ti hydride	202	321
Mg Hydride	153	232
3600 psi	35	47
Methanol and reformer	46	48
Hydrogen - methane 3600 psi	21	28

Figure Captions

1. Hybrid car schematic
2. A comparison of series hybrid automobiles with equal acceleration, hill climb and range. Open symbols are for 240 mile range, filled symbols are for 380 mile range.
3. Comparison of the laminar flame speed of hydrogen (data compiled by Marinov, LLNL) with that of methane, gasoline (Heywood 1988), methanol reformate and a hydrogen/CNG blend.
4. Based on recent Sandia experiments in a CLR research engine, NOx decreases dramatically as a hydrogen engine is leaned below 0.5 equivalence ratio.
5. Thermal efficiency of various hydrogen-fueled research engines compared with ideal indicated efficiency.
6. Efficiency loss (ideal minus indicated) versus estimated surface-to-volume ratio in King et al., Oehmichen and Mathur experiments on a hydrogen engines. Preliminary and predicted data for the Onan experiment are also shown.

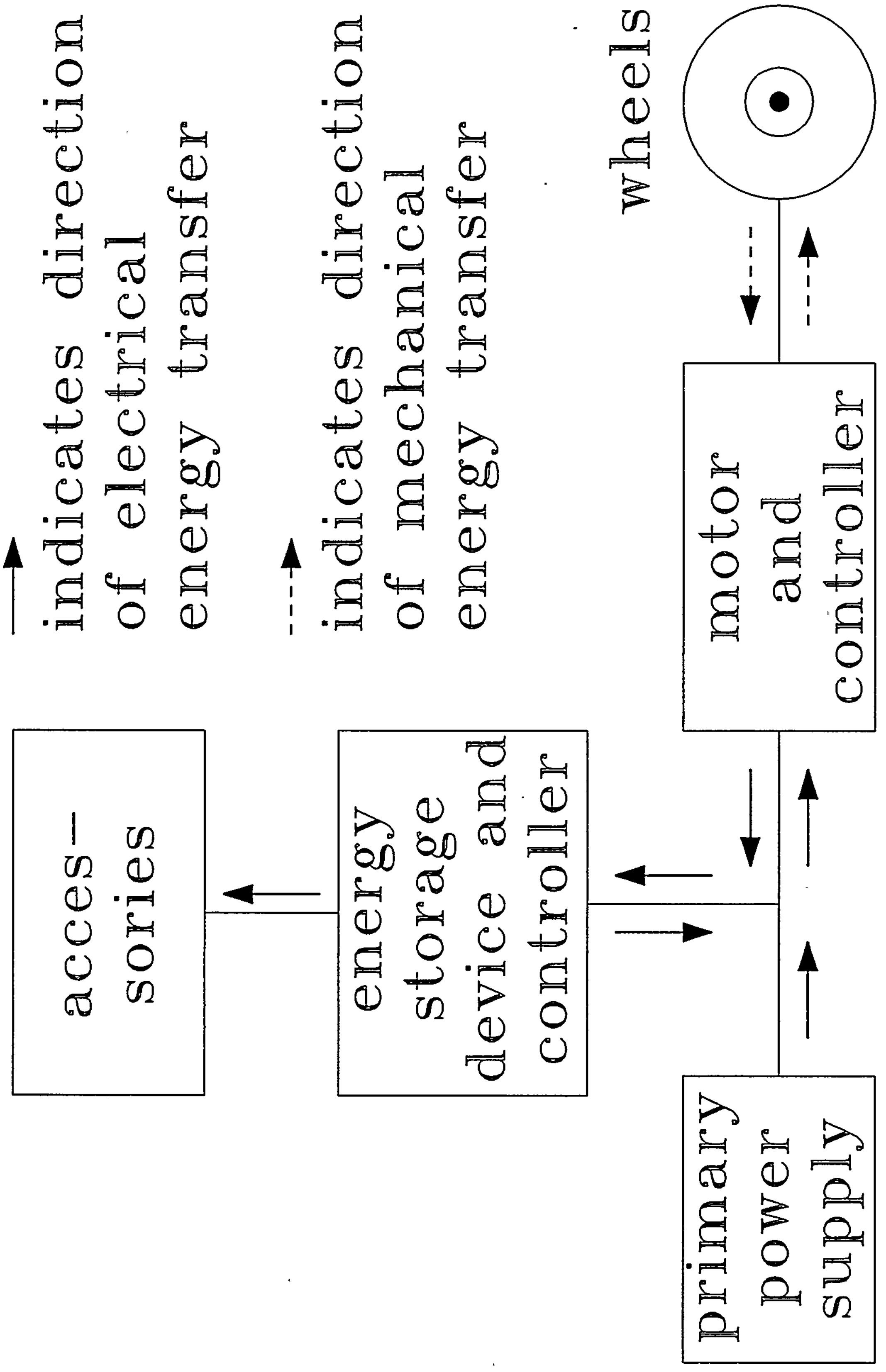

indicates direction of electrical energy transfer
indicates direction of mechanical energy transfer
wheels
motor and controller
acces–sories
energy storage device and controller
primary power supply

Figure 1

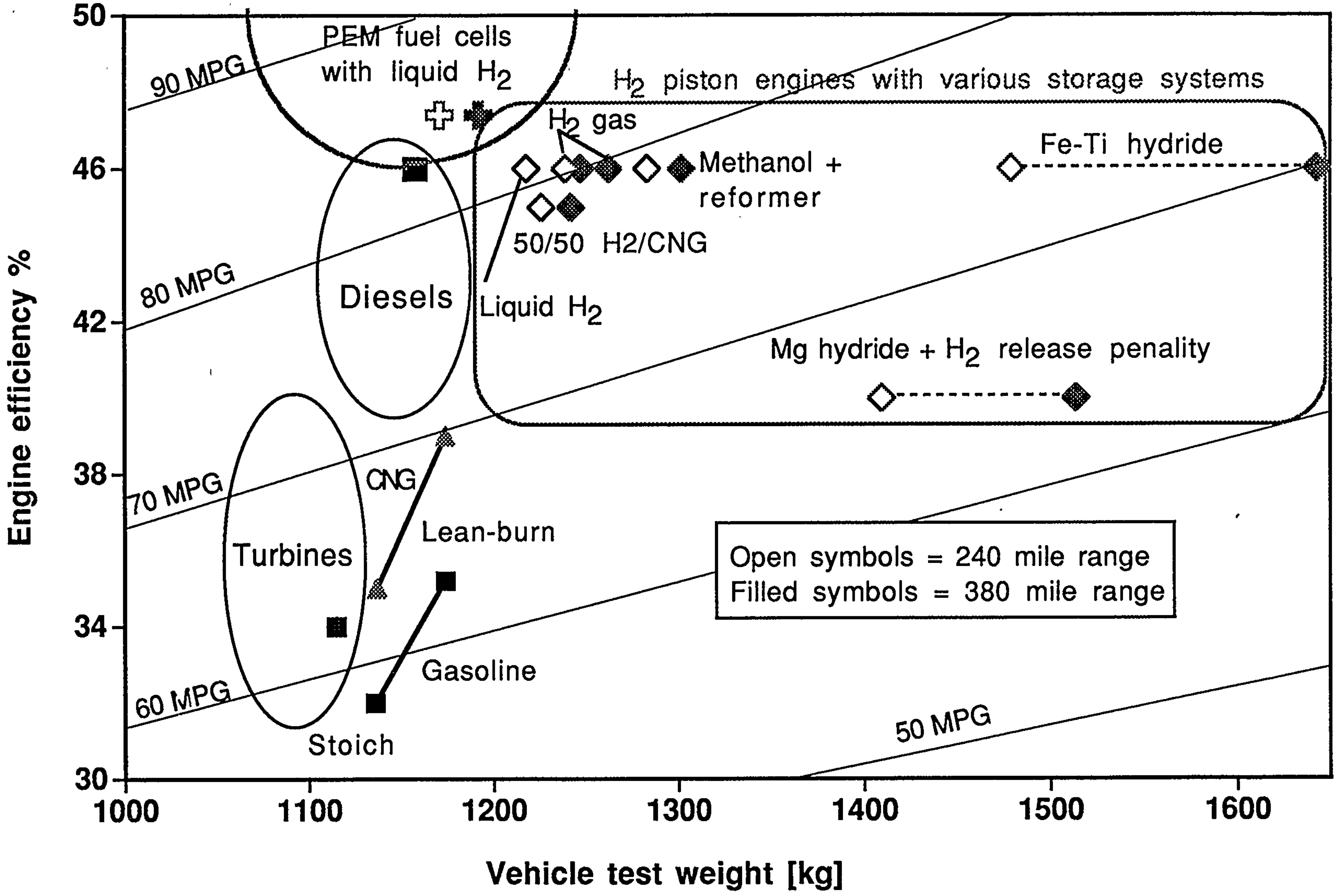

PEM fuel cells
with liquid H_2
H_2 piston engines with various storage systems
H_2 gas
Methanol +
reformer
Fe-Ti hydride
50/50 H2/CNG
Liquid H_2
Mg hydride + H_2 release penality
Diesels
Turbines
CNG
Lean-burn
Gasoline
Stoich
Open symbols = 240 mile range
Filled symbols = 380 mile range
90 MPG
80 MPG
70 MPG
60 MPG
50 MPG
Engine efficiency %
50
46
42
38
34
30
Vehicle test weight [kg]
1000
1100
1200
1300
1400
1500
1600

Figure 2

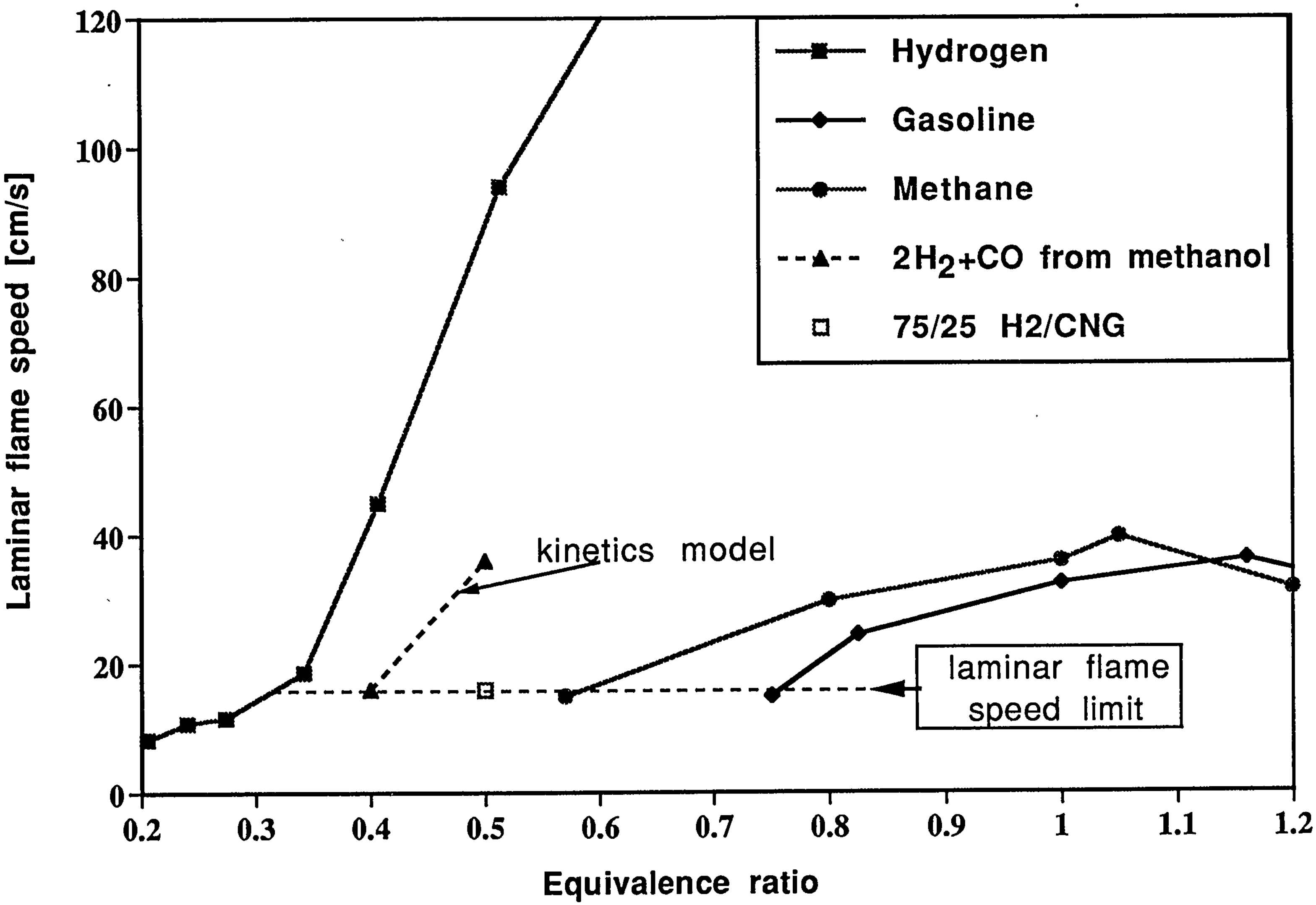

Hydrogen
Gasoline
Methane
$2H_2$+CO from methanol
75/25 H2/CNG
kinetics model
laminar flame speed limit
Laminar flame speed [cm/s]
120
100
80
60
40
20
0
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2
Equivalence ratio

Figure 3

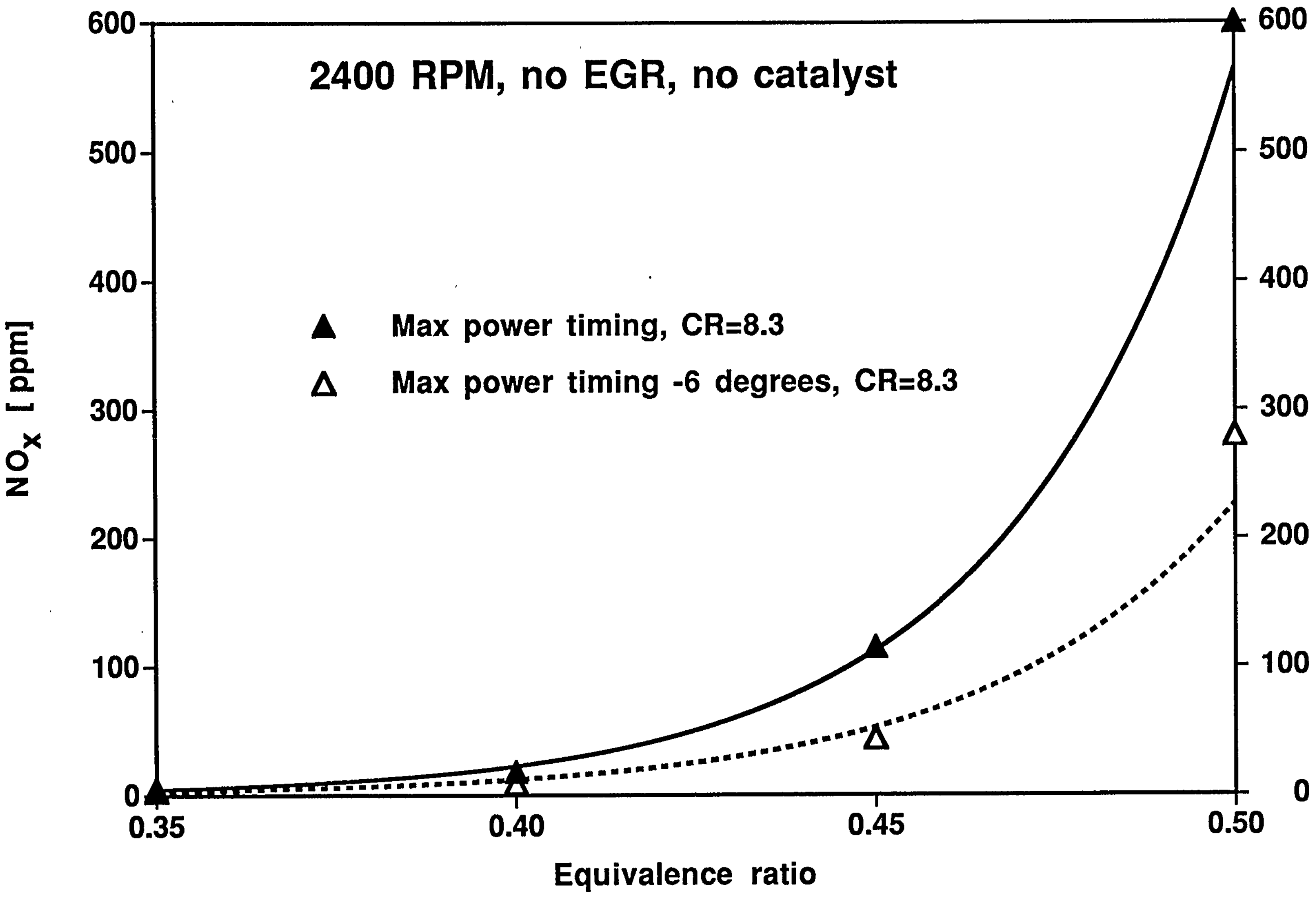

2400 RPM, no EGR, no catalyst
▲ Max power timing, CR=8.3
△ Max power timing -6 degrees, CR=8.3
NO$_x$ [ppm]
600
500
400
300
200
100
0
0.35
0.40
0.45
0.50
Equivalence ratio

Figure 4

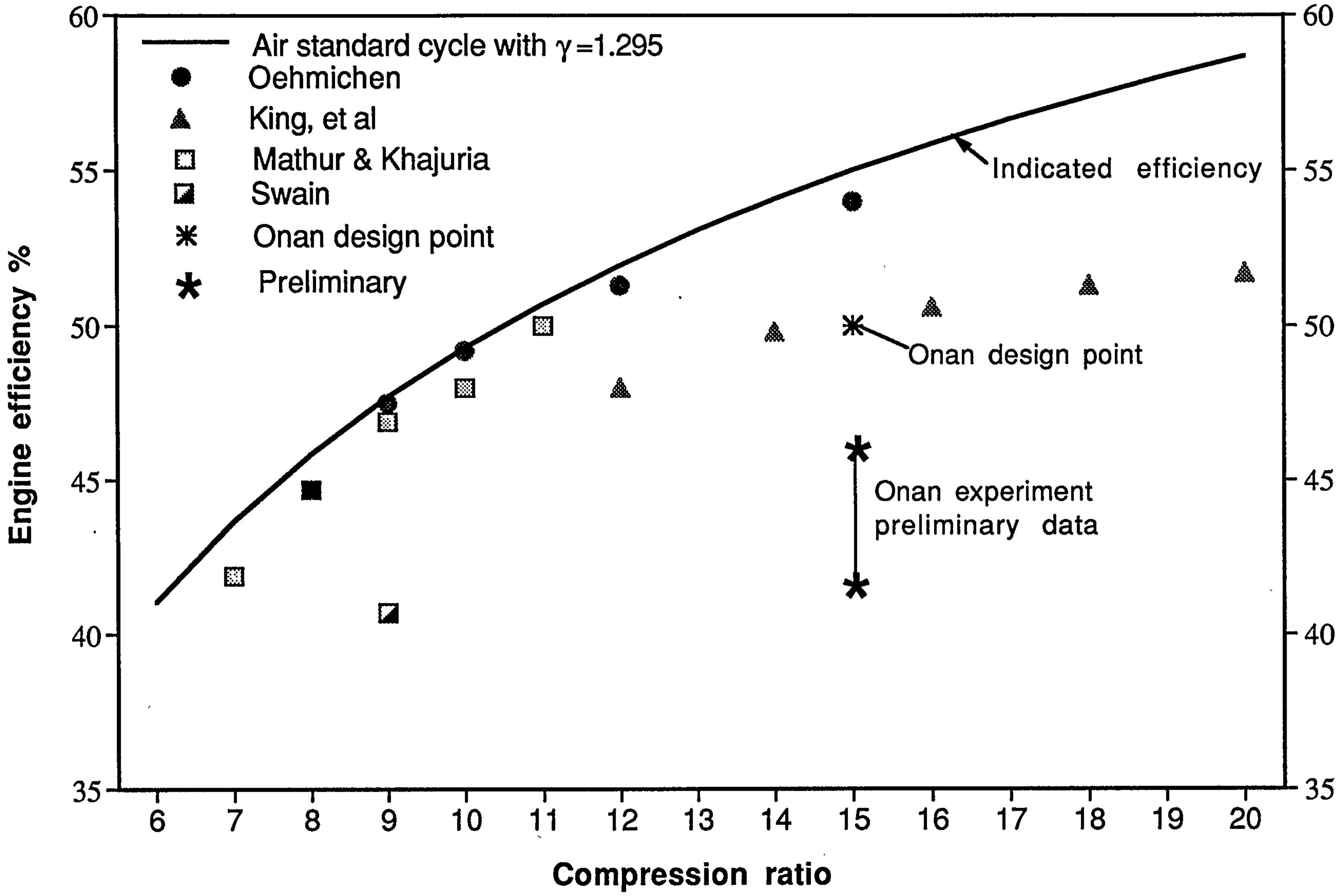

Air standard cycle with γ=1.295
Oehmichen
King, et al
Mathur & Khajuria
Swain
Onan design point
Preliminary
Indicated efficiency
Onan design point
Onan experiment preliminary data
Engine efficiency %
60
55
50
45
40
35
Compression ratio
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20

Figure 5

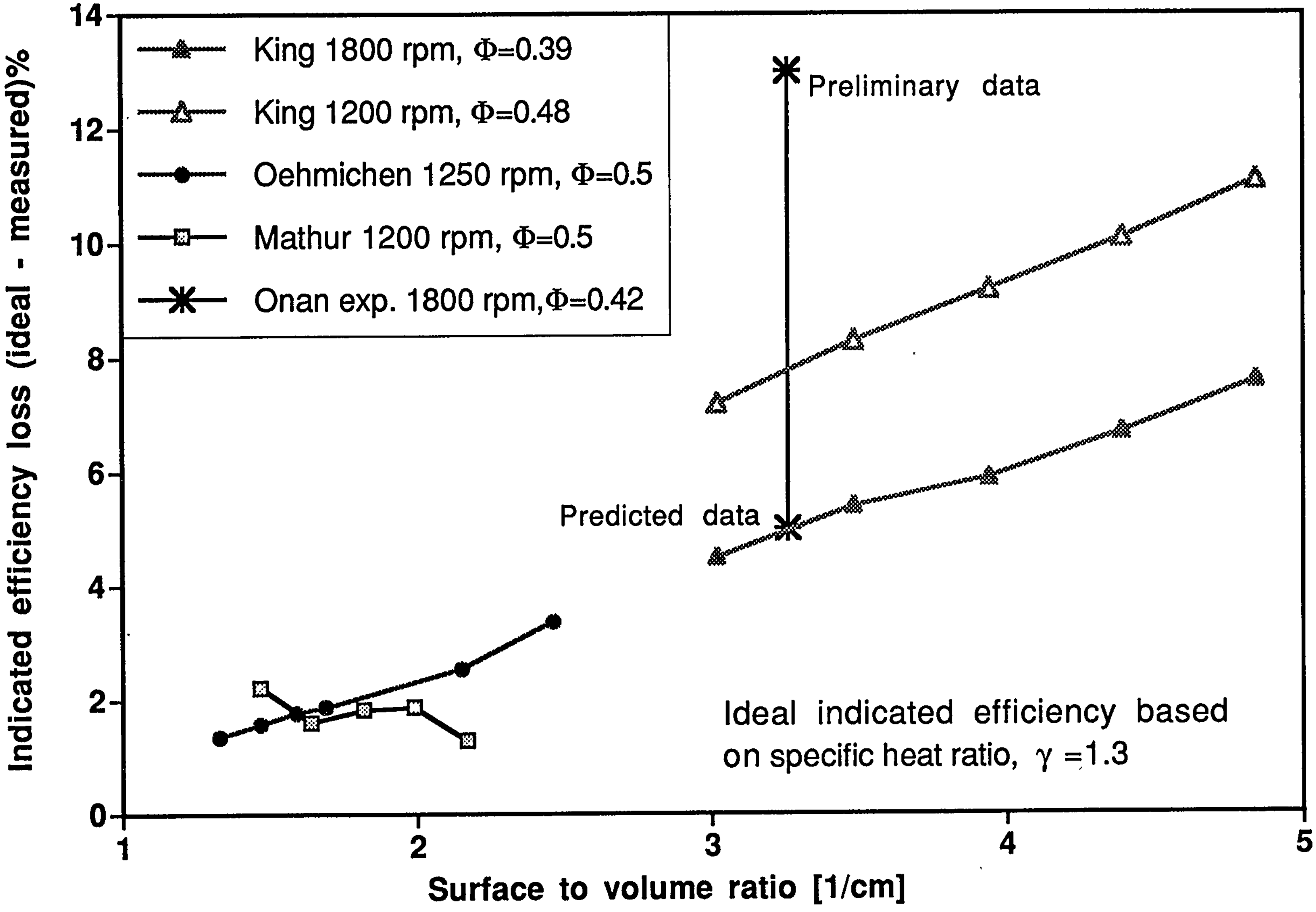

King 1800 rpm, Φ=0.39
King 1200 rpm, Φ=0.48
Oehmichen 1250 rpm, Φ=0.5
Mathur 1200 rpm, Φ=0.5
Onan exp. 1800 rpm,Φ=0.42
Preliminary data
Predicted data
Ideal indicated efficiency based on specific heat ratio, γ =1.3
Indicated efficiency loss (ideal - measured)%
Surface to volume ratio [1/cm]
0
2
4
6
8
10
12
14
1
2
3
4
5

Figure 6

HYDROGEN HYBRID VEHICLE ENGINE DEVELOPMENT: EXPERIMENTAL PROGRAM

Peter Van Blarigan
Sandia National Laboratory
Livermore, Ca 94550

Abstract

A hydrogen fueled engine is being developed specifically for the auxiliary power unit (APU) in a series type hybrid vehicle. Hydrogen is different from other internal combustion (IC) engine fuels, and hybrid vehicle IC engine requirements are different from those of other IC vehicle engines. Together these differences will allow a new engine design based on first principles that will maximize thermal efficiency while minimizing principal emissions.

The experimental program is proceeding in four steps:

1. Demonstration of the emissions and the *indicated* thermal efficiency capability of a standard CLR research engine modified for higher compression ratios and hydrogen fueled operation.

2. Design and test a new combustion chamber geometry for an existing single cylinder research engine, in an attempt to improve on the baseline *indicated* thermal efficiency of the CLR engine.

3. Design and build, in conjunction with an industrial collaborator, a new full scale research engine designed to maximize *brake* thermal efficiency. Include a full complement of combustion diagnostics.

4. Incorporate all of the knowledge thus obtained in the design and fabrication, by an

industrial collaborator, of the hydrogen fueled engine for the hybrid vehicle power train illustrator.

Results of the CLR baseline engine testing are presented, as well as preliminary data from the new combustion chamber engine. The CLR data confirm the low NOx produced by lean operation. The preliminary *indicated* thermal efficiency data from the new combustion chamber design engine show an improvement relative to the CLR engine. Comparison with previous high compression engine results shows reasonable agreement.

Introduction

Hydrogen fueled hybrid vehicle IC engines are unique and offer high thermal efficiency potential while at the same time minimizing emissions.

Hydrogen is different from other IC engine fuels. First, the low flammability limit of hydrogen/air mixtures allows operation at very lean conditions. Second, the high laminar flame speed of hydrogen produces rapid reaction rates without excessive forced turbulence. Third, hydrogen has a high effective octane which permits the utilization of high compression ratios (CRs). Finally, carbon-based emissions can come only from other sources (lubricants) and can thus be very low.

Hybrid vehicle IC engine requirements are different from those of other IC vehicle engines. First, the engine is required to run throughout a small dynamic range, not even being required to idle. Second, the majority of operating time is at one power and speed condition, with only occasional excursions to higher power output. Finally, the power output is low, perhaps one third of a modern conventional vehicle engine.

When hydrogen and hybrid vehicle characteristics are combined, the potential exists to design a new engine that is both high in thermal efficiency and low in emissions. For high thermal efficiency, lean (low equivalence ratio) operation, low turbulence combined with high reaction rates and high compression ratios are virtues attributable to hydrogen. For low emissions, the lack of fuel generated carbon emissions and the low NO_x levels associated with low equivalence ratios are major contributors.

The design approach for an IC engine that takes advantage of these attributes has been presented earlier by J. Ray Smith (1994). The balance of this paper will lay out the experimental program and present results to date.

This work represents a key element in the overall multi-laboratory effort to develop hydrogen fueled power plants as suitable alternatives for the transportation sector. This is a three year program with the level of support averaging approximately 2 full time equivalents (FTEs). The level of support is planned to change throughout the program depending on requirements.

Experimental Program

The largest part of an IC engine design program is by necessity experimental in nature. This program has been configured in four parts, each part building on the information gleaned from its predecessor.

Part 1. Baseline Performance

The first step in improving an IC engine is to assess the performance of a representative existing engine. Verification of the low NO_x emissions possible with lean operation is important, as is assessment of the *indicated* thermal efficiency characteristics as a function of compression ratio, speed and equivalence ratio. A Sandia CLR engine was chosen as the baseline engine. The engine was configured to operate at compression ratios of 8.25, 11.1 and 13.7. Testing occurred in July 1994, and the results are now presented.

CLR ENGINE SPECIFICATIONS

Displacement = 42.53 cubic inches
Stroke = 3.75 inches
Bore = 3.80 inches
Speeds: 1200, 1800, 2400 RPM
Equivalence ratios: .35, .40, .45, .50
Compression ratios: 8.25, 11.1, 13.7
Volumetric efficiency: 100%
Hydrogen/air premixed
Unthrottled

Figure 1 shows the geometry of the CLR engine combustion chamber. The piston is shown in the top dead center (TDC) position in the 13.7 CR configuration. The boss which projects from the piston top up into the valve/spark plug volume is what produces the 13.7 CR. When no boss is present, the CR is 8.25, while a smaller boss than that shown produced the 11.1 CR. A pressure transducer (not shown) is also included.

Figure 2 portrays the *indicated* thermal efficiency of the CLR engine at a speed of 1200 RPM as a function of compression ratio and equivalence ratio.

The *indicated* thermal efficiency for the CLR engine is determined by calculating the net work performed by the pressure on the piston during the full 720 degree cycle and dividing this by the lower heating value energy (LHV) available in the fuel consumed. Thus work performed during the gas exchange part of the cycle is also included.

Figure 3 displays the efficiency performance at 1800 RPM, while figure 4 presents all efficiency data at an equivalence ratio of 0.35.

Generally, this data show the improvement in indicated thermal efficiency expected as compression ratio is increased. The data also show a trend towards higher indicated thermal efficiency as engine speed is increased.

Figure 5 displays the NO_x emissions at 1200 RPM as a function of CR and equivalence ratio. Performance at other speeds is similar. The data confirm that low NO_x generation is indeed possible by operation at low but usable equivalence ratios, with CR a secondary effect.

The final CLR data is shown in figure 6, which shows ignition timing required for maximum torque as a function of equivalence ratio at the three compression ratios tested.

One consequence of the CLR test series was a tendency to ignite the hydrogen/air mixture in the inlet manifold at 2400 RPM and 13.7 CR. Thus data there is only available at an equivalence ratio of 0.35.

Part 2. New Design Combustion Chamber

Based on the results of the baseline CLR data and a literature survey, J. Ray Smith of Lawrence Livermore National Laboratory, in collaboration with Mike Swain of the University of Miami, proposed a new cylinder head design to increase indicated thermal efficiency. They theorized that less heat loss at TDC conditions would help. The CLR combustion chamber geometry generates high gas turbulence from piston motion due to the squish zones and the piston boss used to increase the compression ratio. Several changes to improve this situation were included in the new design, namely:

1. Create a quiescent combustion chamber to minimize heat transfer as a result of less destruction of the gaseous boundary layer at the combustion chamber surfaces. The resultant geometry is a flat cylinder head/flat piston crown with no squish zone.

2. Provide inlet flow that does not swirl, again in an attempt to retain the gaseous boundary layer as an insulator.

3. Utilize two spark plugs, each located equidistant from the wall and the cylinder centerline, to produce reasonable reaction rates in this now quiescent chamber.

Figure 7 is a cross-sectional view of the new geometry combustion chamber. Clearly portrayed are the two spark plugs and the flatness of the cylinder head and piston crown. This new head was machined out of aluminum bar stock by Lawrence Livermore National Laboratory for application to an Onan research engine at Sandia with the following characteristics:

ONAN ENGINE SPECIFICATIONS

Displacement = 30.07 cubic inches
Stroke = 3.625 inches
Bore = 3.25 inches
Speeds: 1200, 1500, 1800 RPM
Equivalence ratios 0.35 - 0.5
Compression ratio 14.8:1
Volumetric efficiency: 84 - 106%
Hydrogen / air premixed
Dual spark plugs
Unthrottled

Operation at higher speeds, higher equivalence ratios and both higher and lower compression ratios is planned. Presented here are data from specific conditions that while not complete are felt to be accurate.

Figure 8. presents Onan data at 1200 RPM, as well as one point at 1500 RPM and one point at 1800 RPM, compared with data at similar conditions. It is obvious to the most casual observer that an improvement has been realized, more than could be credited to the slightly higher compression ratio. The ignition timing necessary to produce these results is shown in figure 9. Clearly shown is the improvement in reaction rate achieved in the new configuration, as well as the slower burn times at lower equivalence ratios.

It should be reinforced that *indicated* thermal efficiency as presented so far has been determined by integrating the PdV product over the full 720 degree cycle of a four stroke cycle engine, and dividing this by the lower heating value (LHV) of the hydrogen consumed. If comparison with data from other researchers is to be made, it is important to measure *indicated* efficiency by consistent methods. Two alternate methods are found in the literature.

The first alternate is to integrate the PdV product only during the power cycle (360 degrees), thus eliminating the negative work required for gas exchange. This is particularly valuable for part-throttle comparison with unthrottled (our case) operation.

The difference between these two methods can be seen in figure 13. This Onan engine data show two closed loops, the small inlet/exhaust cycle loop at the bottom and the larger, slanted power cycle loop. The power cycle (360 degree) integration is represented by the area contained within the power cycle loop, while the full cycle (720 degree) integration subtracts the area within the small bottom inlet/exhaust cycle loop from the power cycle loop.

The second technique involves measuring the shaft power **output** (brake power) and then measuring the shaft power **input** required to drive the engine with the spark shut off. The indicated power is then calculated by adding these two powers.

For the shaft power method to be valid, the power to motor the engine when it is not firing must be defined as equal to the losses in converting pressure to shaft power when the engine is firing. The validity of this assumption was investigated by Kerley and Thurston (1962). Their results, run at 1800 RPM in a single cylinder engine of 41.38 cubic inch displacement, show that the shaft power (torque) method predicted efficiencies 3 points higher (i.e., 41% vs 38%) than the 360 degree integration method at a compression ratio of 12:1.

Figure 10 elucidates a similar comparison for the Onan engine based on the data shown in figure 13. For the conditions shown, it can be seen that the torque method produced higher *indicated* thermal efficiencies that the PdV integration techniques. In fact, it can also be noted that engine operation temperature affects the results, as evidenced by the different values recorded at two different water inlet temperatures. It is also reasonable to assume that the discrepancy is a function of the particular engine employed.

While the integration method, if carefully done, should produce valid results, comparison with other high compression ratio results necessitates the torque method since most of the work is older and uses this technique.

Figure 11 depicts the Onan *indicated* thermal efficiency measured by both full cycle integration and torque for a warmed up engine. When this Onan torque method is compared with well documented work by other authors, figure 12 results.

The comparison cannot be made at identical conditions due to the scarcity of data at high compression ratios. Shown with the data is an ideal cycle (adiabatic with constant volume combustion) calculation for Octene in which real gas properties, both before and after combustion, are employed (Edson and Taylor (1964)). It can be seen that, given the possible variation of the torque method, the Onan data is consistent with the performance reported here. All authors are included in the bibliography.

Part 3. Full scale brake output engine

The above discussion regarding *indicated* thermal efficiency is necessitated by the utilization of single cylinder research engines for combustion optimization. Since the Onan results appear to be in the same range as other similar engines, the next phase in developing a high efficiency engine is to measure *brake* output of a full scale engine. Certainly operation at low equivalence ratios will increase the fraction of produced mechanical work that is consumed generating shaft power. Thus recording *brake* output is crucial in developing this concept.

Towards this end we (all collaborators) intend to develop a full scale engine in conjunction with an industrial partner. To date the following organizations have expressed interest in working with us:

Mercury Marine
Perkins Technology
Southwest Research Institute
Batten Corporation
Roush Industries

This full scale engine will still be a research engine in the sense that combustion chamber parameters will be adjustable. It will also, however, employ state of the art component design to minimize mechanical losses and judge success by *brake* thermal efficiency results.

Summary

The combination of hydrogen as a fuel and a series type hybrid vehicle application allow for a new engine design that will maximize *brake* thermal efficiency while meeting stringent new emissions requirements. Towards this end an experimental development program has been initiated to culminate in the delivery of a prototype engine for application in a hybrid vehicle drive train illustrator.

Part 1 of this four part development program has been completed, consisting of the demonstration of the *indicated* thermal efficiency and NOx emissions characteristics of a single cylinder CLR research engine. NOx performance at low equivalence ratios was excellent as expected, with *indicated* thermal efficiency in the range of 34 - 39%.

Part 2 involves the improvement of *indicated* thermal efficiency relative to the CLR engine of part 1. Preliminary data indicate an improvement of 4 points at 1200 RPM (41% vs 37%), with the remaining operating space to be mapped out shortly. Part 2 has also noted, due to the capability to measure *indicated* thermal efficiency in various ways, that it is difficult to benchmark with older *indicated* thermal efficiency data.

Part 4 involves designing and testing a full scale *brake* output research engine. This phase is just beginning, yet the importance of developing this engine as a function of *brake* thermal efficiency cannot be overstated. Discussions with industrial partners, one of whom will design and fabricate this engine, have begun.

Acknowledgments

The CLR engine testing and data collection was done by Bob Green of Sandia National Laboratory and J. Ray Smith of Lawrence Livermore National Laboratory. Their permission for me to present their results is appreciated.

References

1. Bolt, Jay A. and Holkeboer, David H., "Lean Fuel/Air Mixtures for High-Compression Spark-Ignited Engines", presented at SAE summer meeting 1961, pp. 195-202.

2. Caris, D.F. and Nelson, E.E., "A New Look at High Compression Engines", *SAE Transactions*, volume 67, pp. 112-124, 1959.

3. Edson, Murray H. and Taylor, C. Fayette, "The Limits of Engine Performance - Comparison of Actual and Theoretical Cycles", *SAE Progress in Technology,* volume 7: pp. 65-81, 1964.

4. Kerley, R.V. and Thurston, K.W., "The Indicated Performance of Otto-Cycle Engines", *SAE Transactions,* volume 70, pp. 5-37, 1962.

5. King, R.O., Hayes, S.V., Allan, A.B., Anderson, R.W.P. and Walker, E.J., "The Hydrogen Engine : Combustion Knock and the Related Flame Velocity", *The Engineering Institute of Canada Transactions,* volume 2, number 4, pp. 143-148, December 1958.

6. Smith, J.R., "Optimized Hydrogen Piston Engines", presented at *SAE Convergence '94*, Detroit, MI, October 18, 1994.

List of Figures

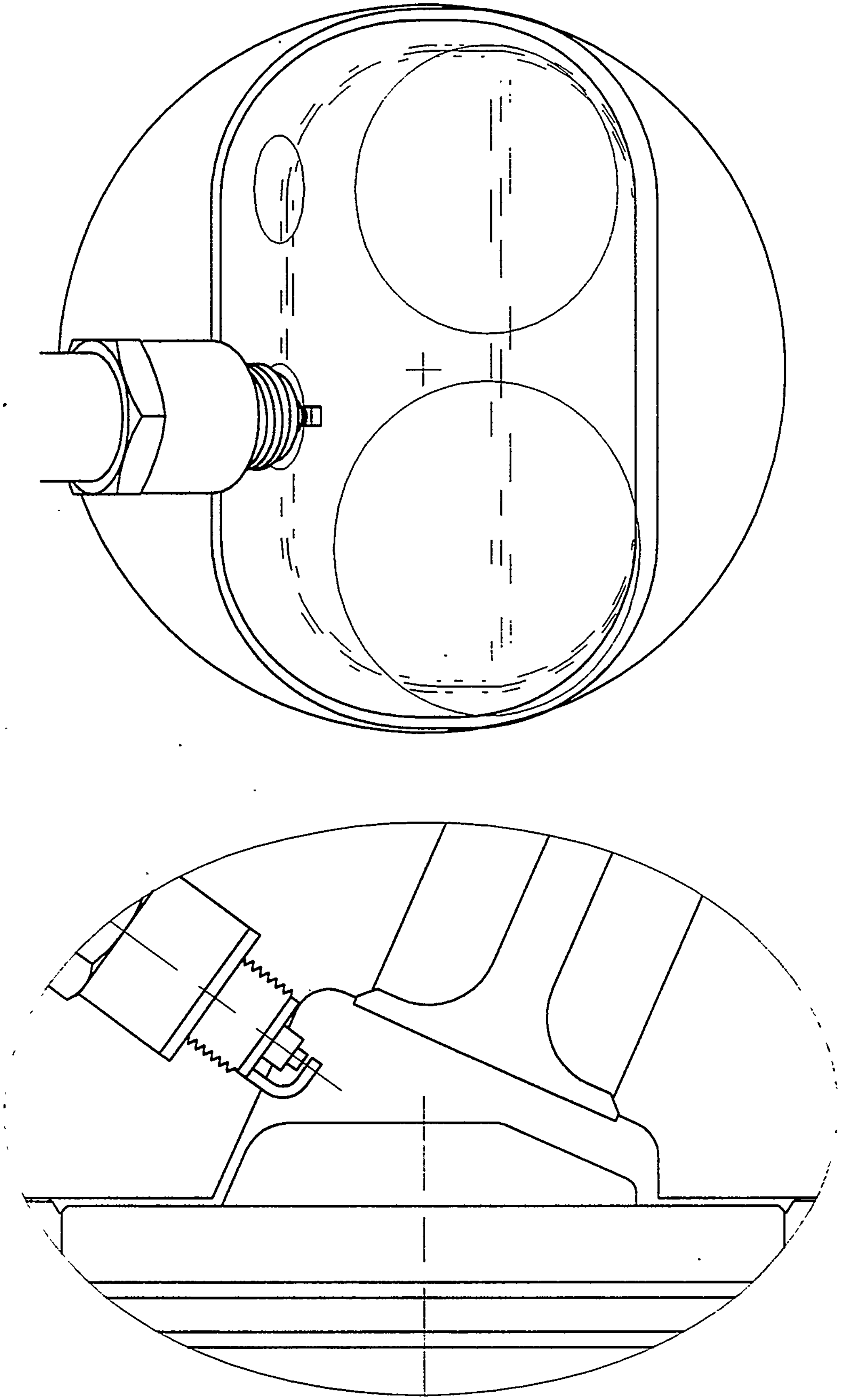


Figure 1. CLR engine geometry

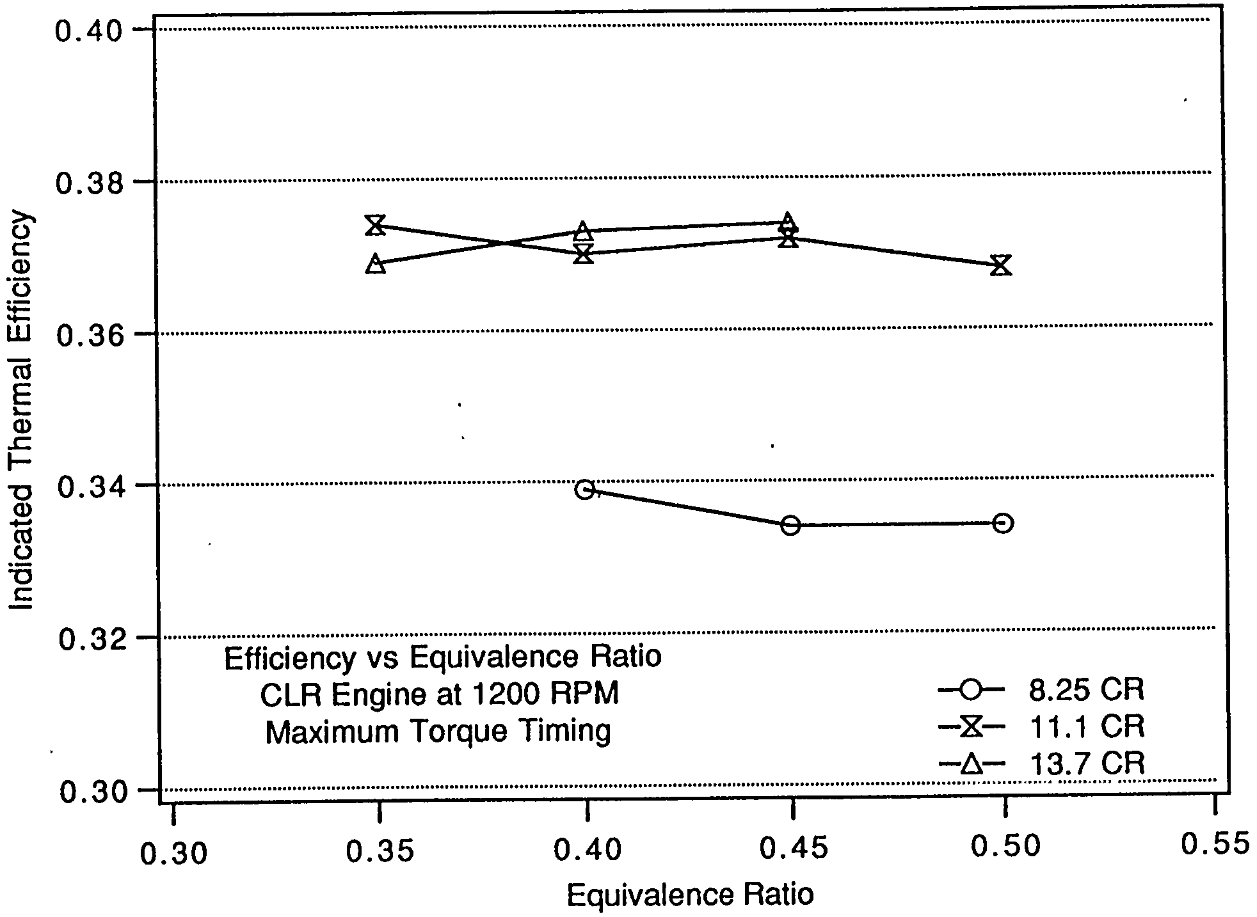


Figure 2. CLR 1200 RPM data

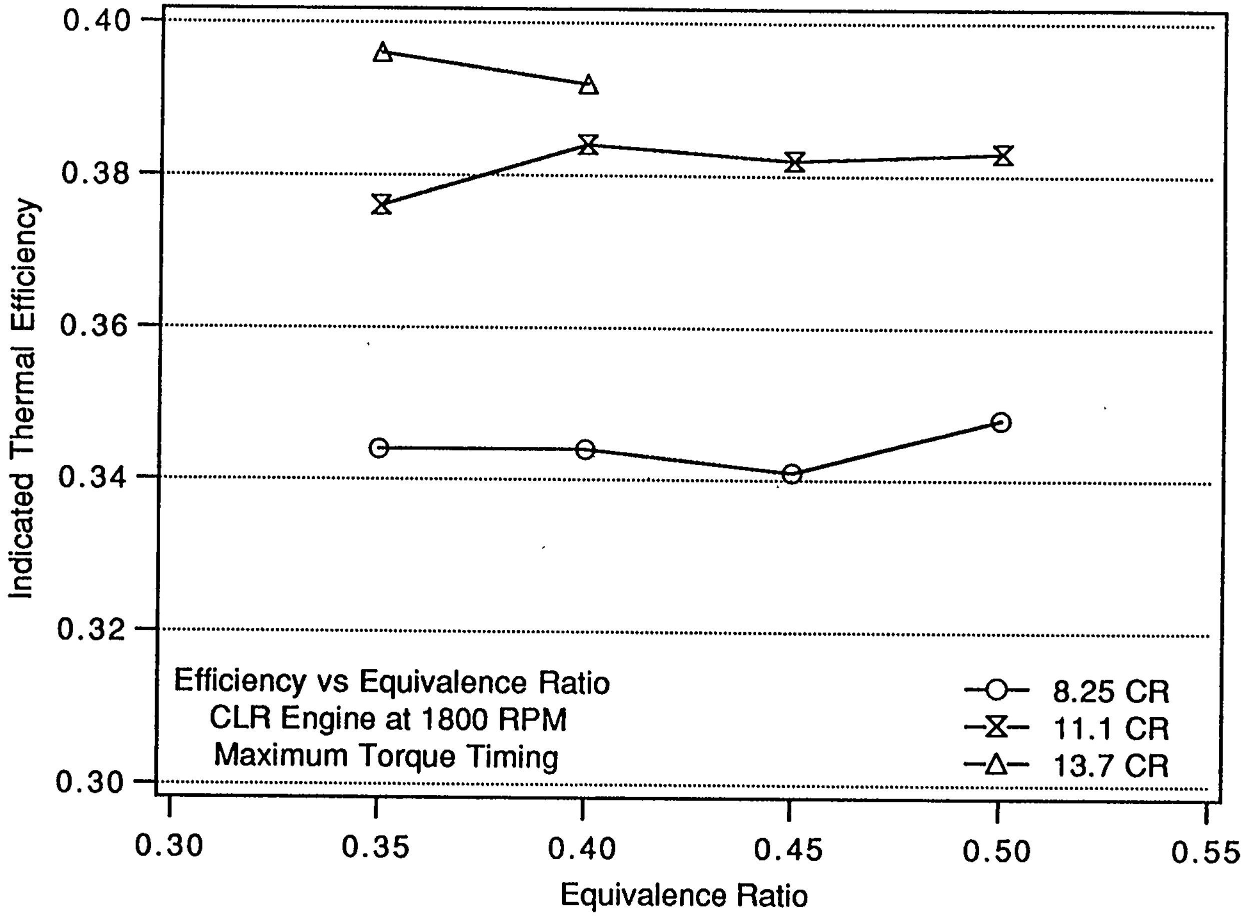


Figure 3. CLR 1800 RPM data

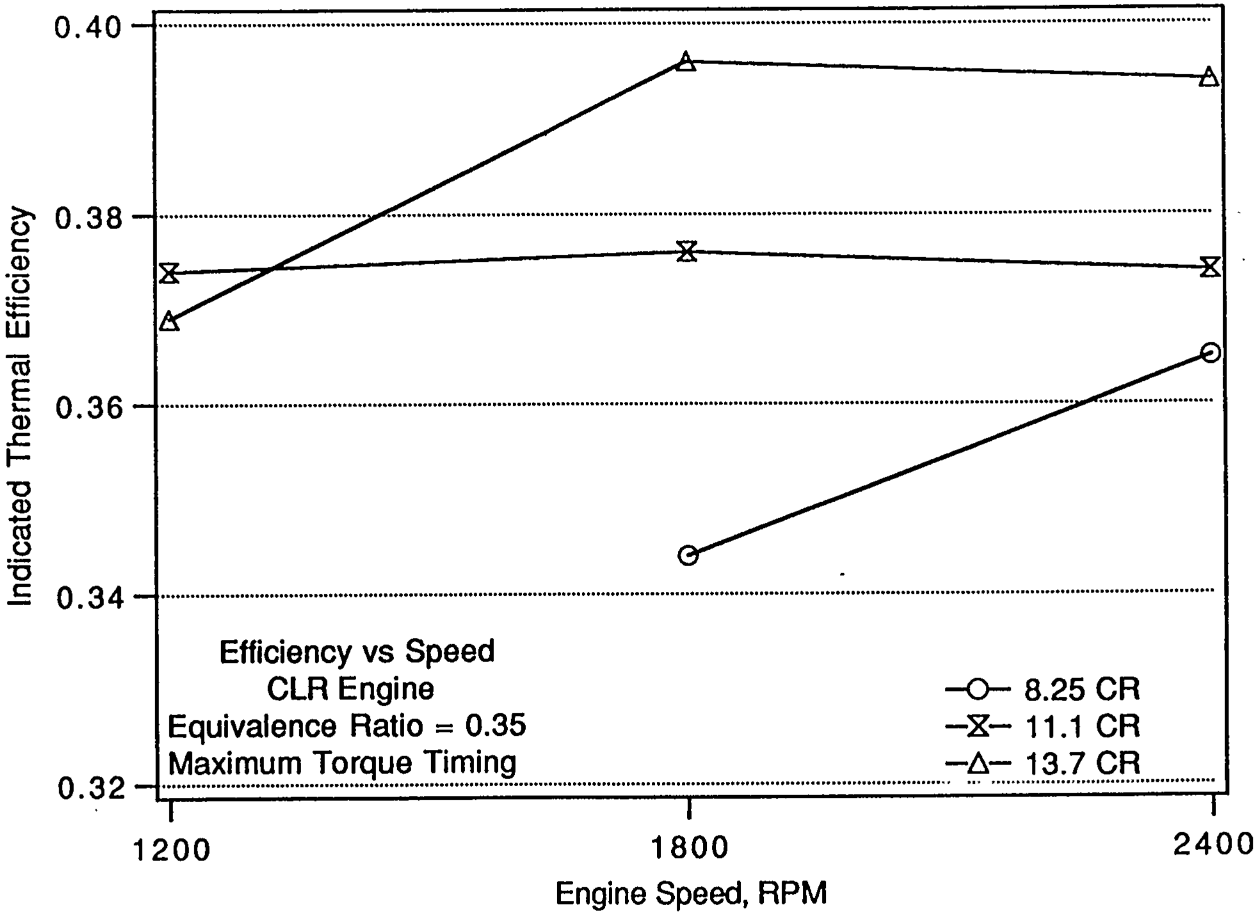


Figure 4. CLR 0.35 equivalence ratio data

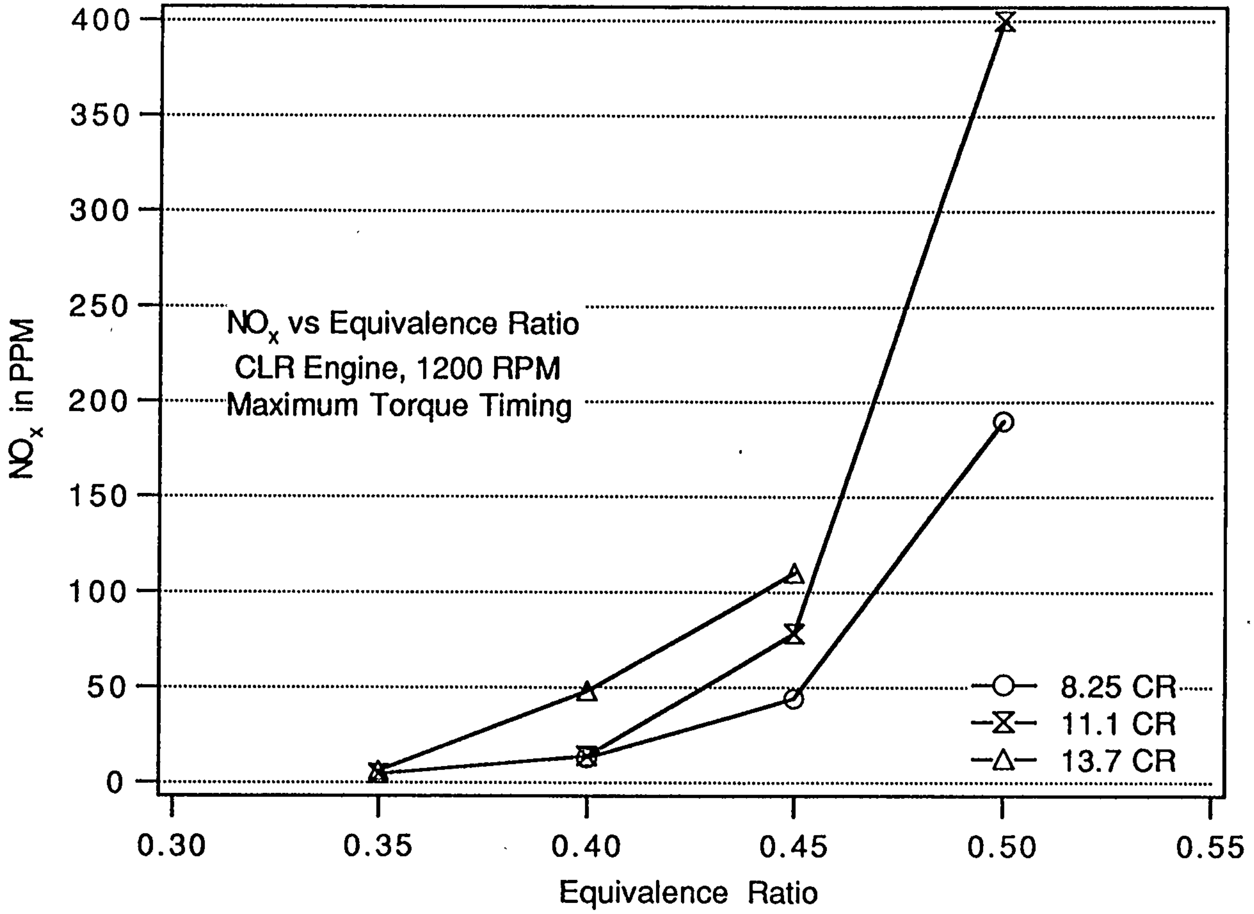


Figure 5. CLR 1200 RPM NOx data

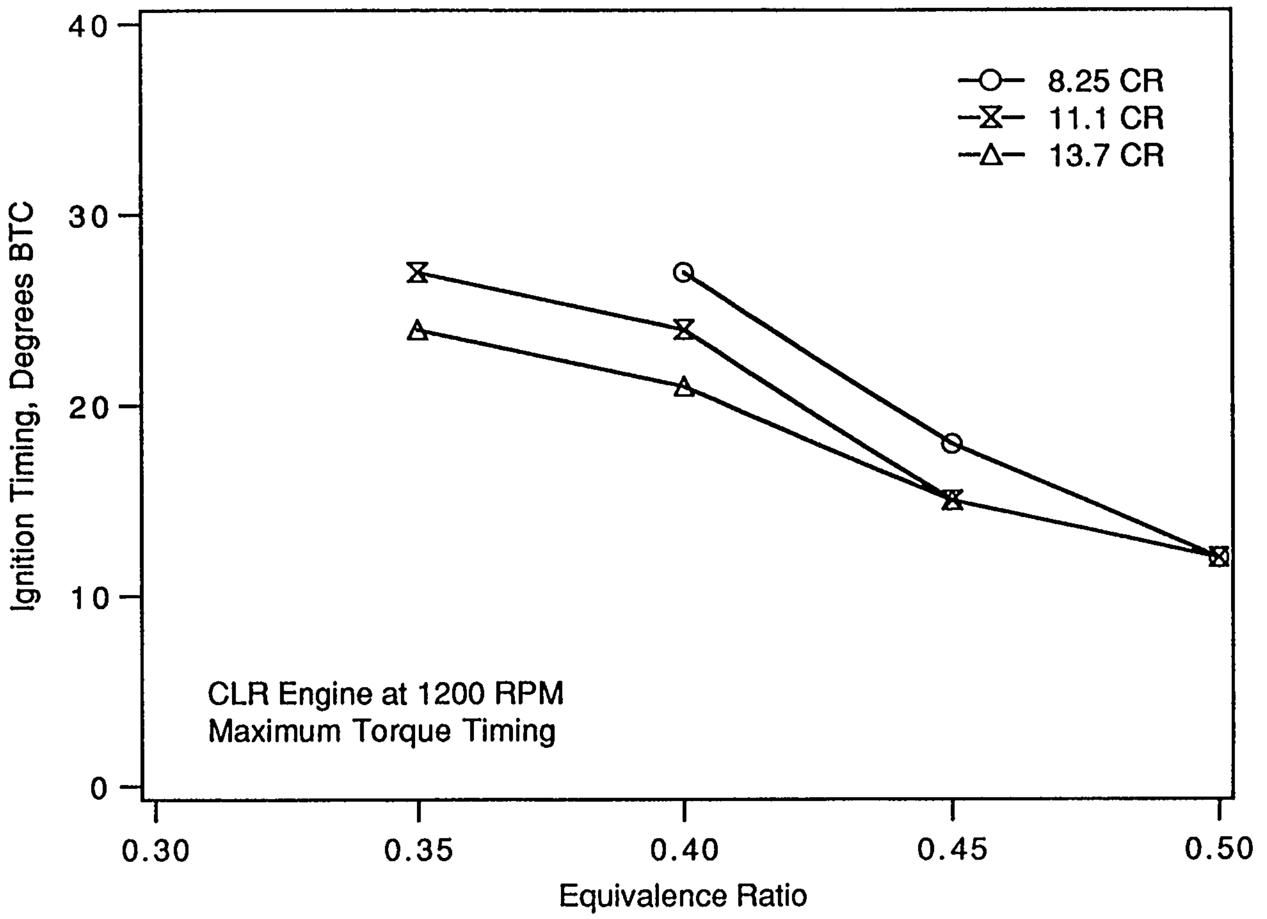


Figure 6. CLR 1200 RPM ignition timing

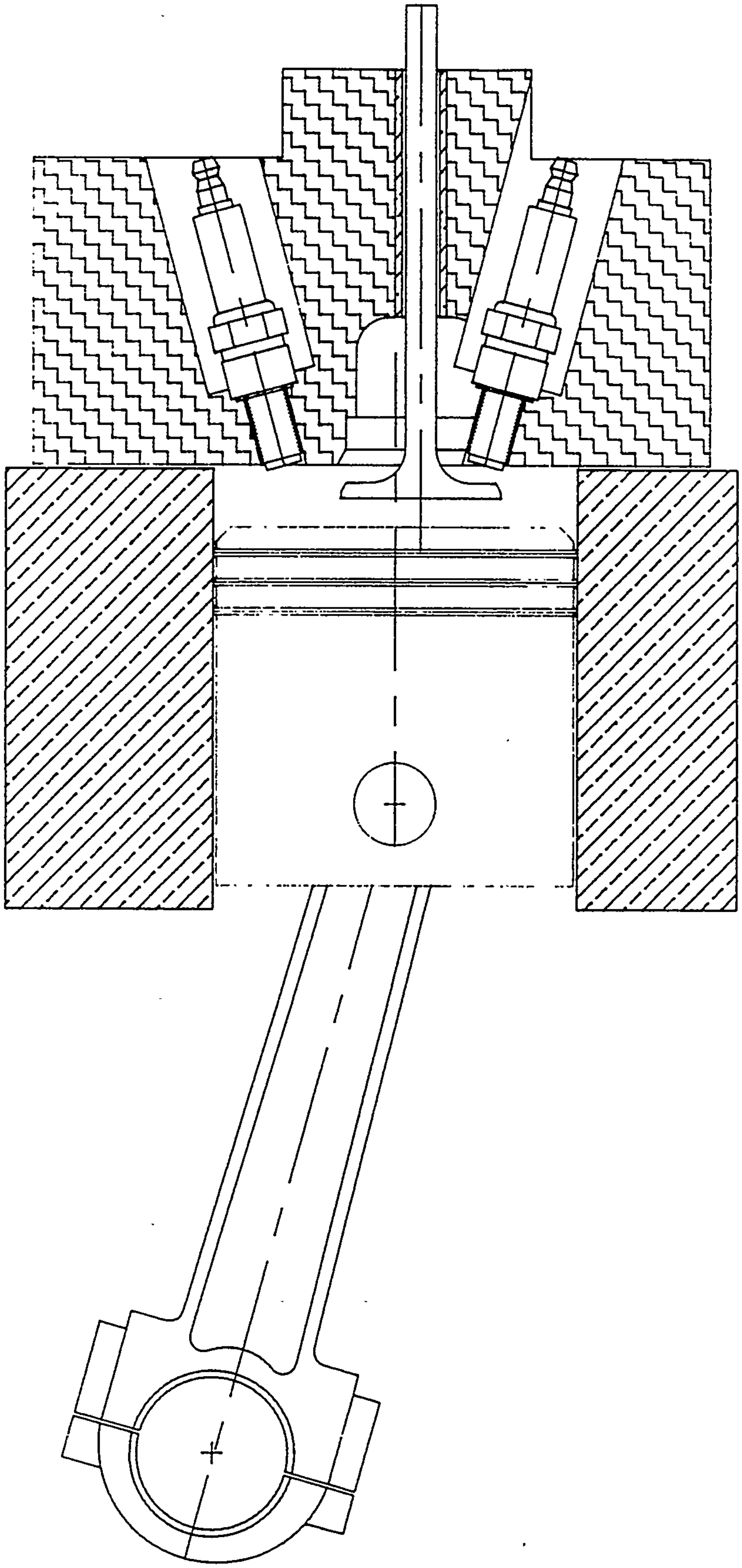


Figure 7. Onan engine geometry

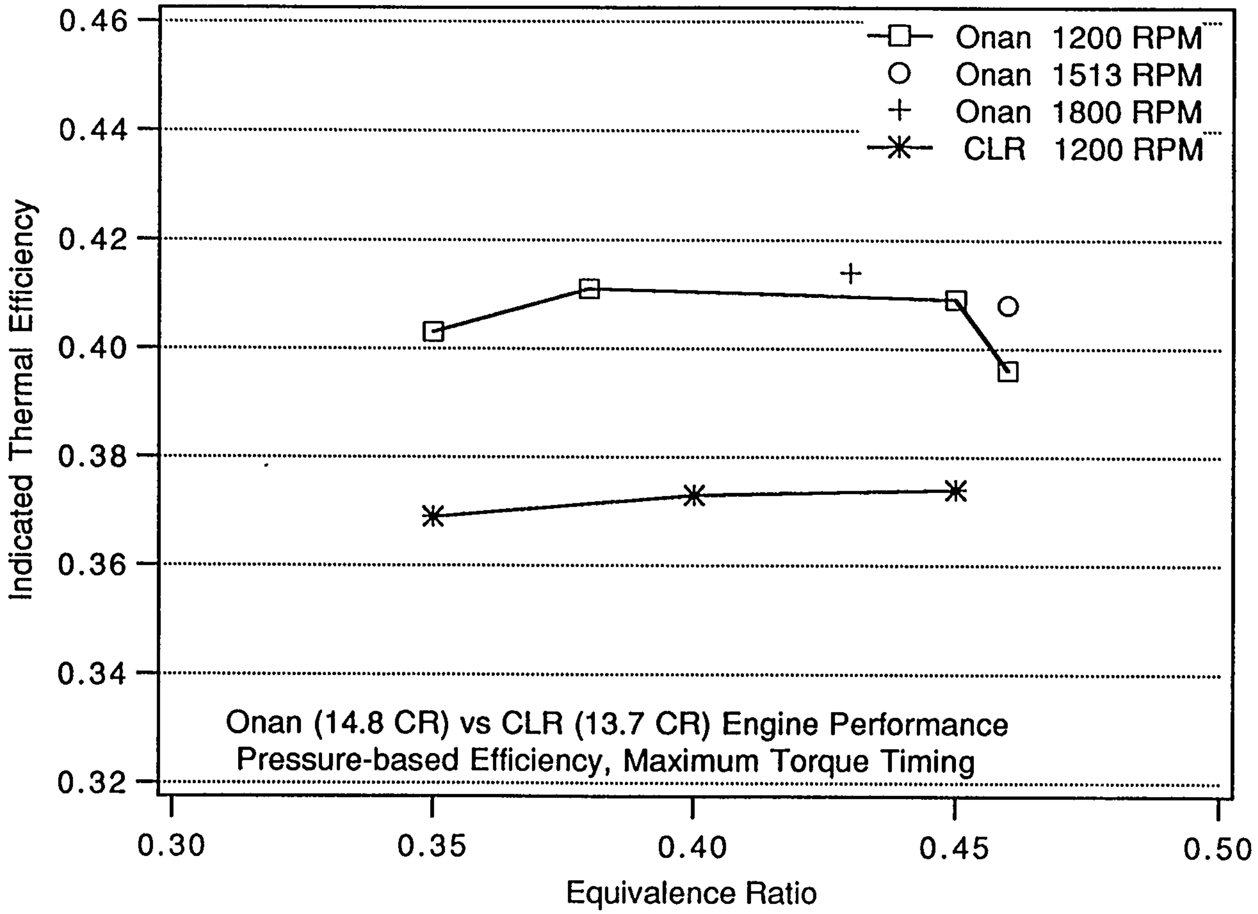


Figure 8. Onan efficiency data

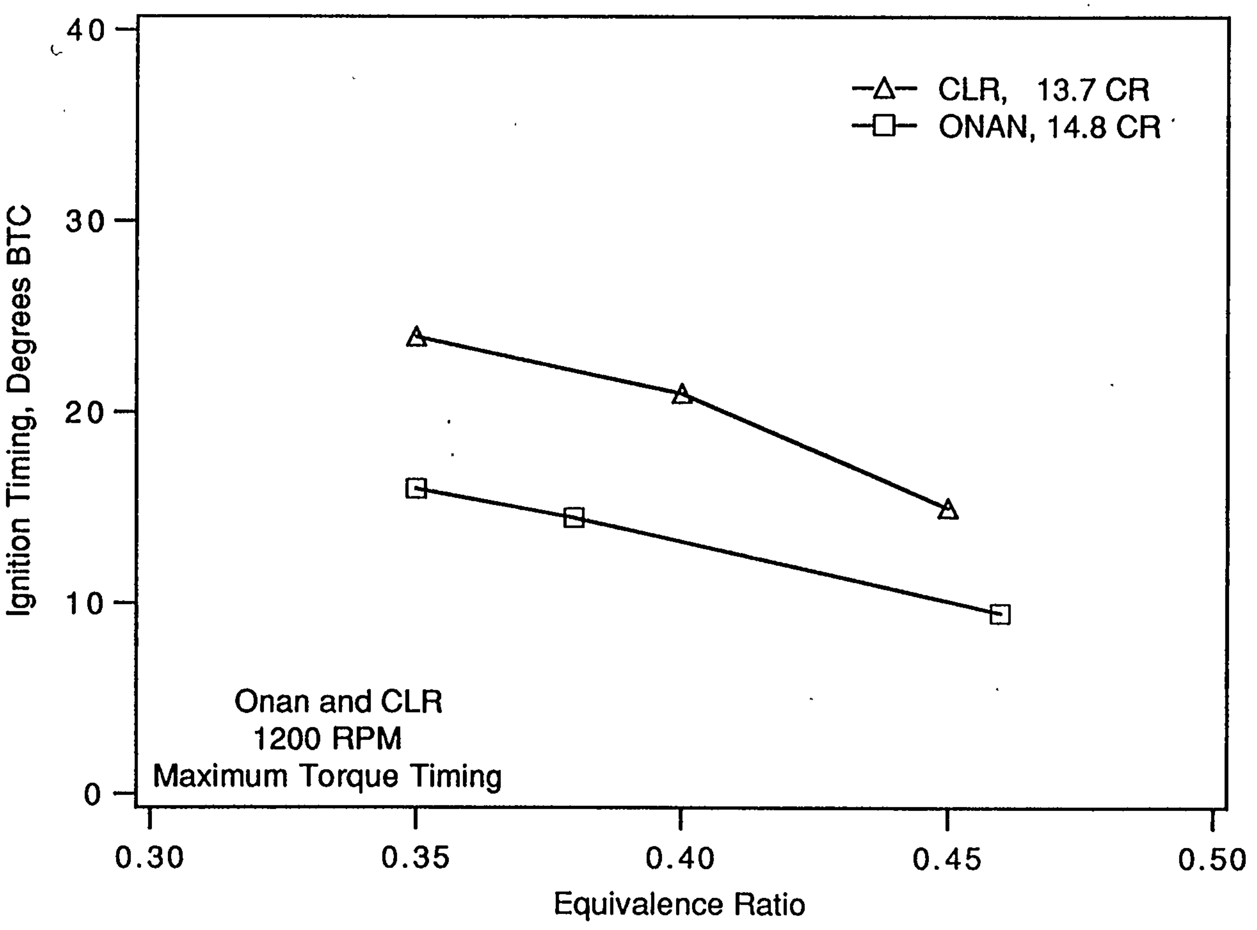


Figure 9. Onan ignition timing

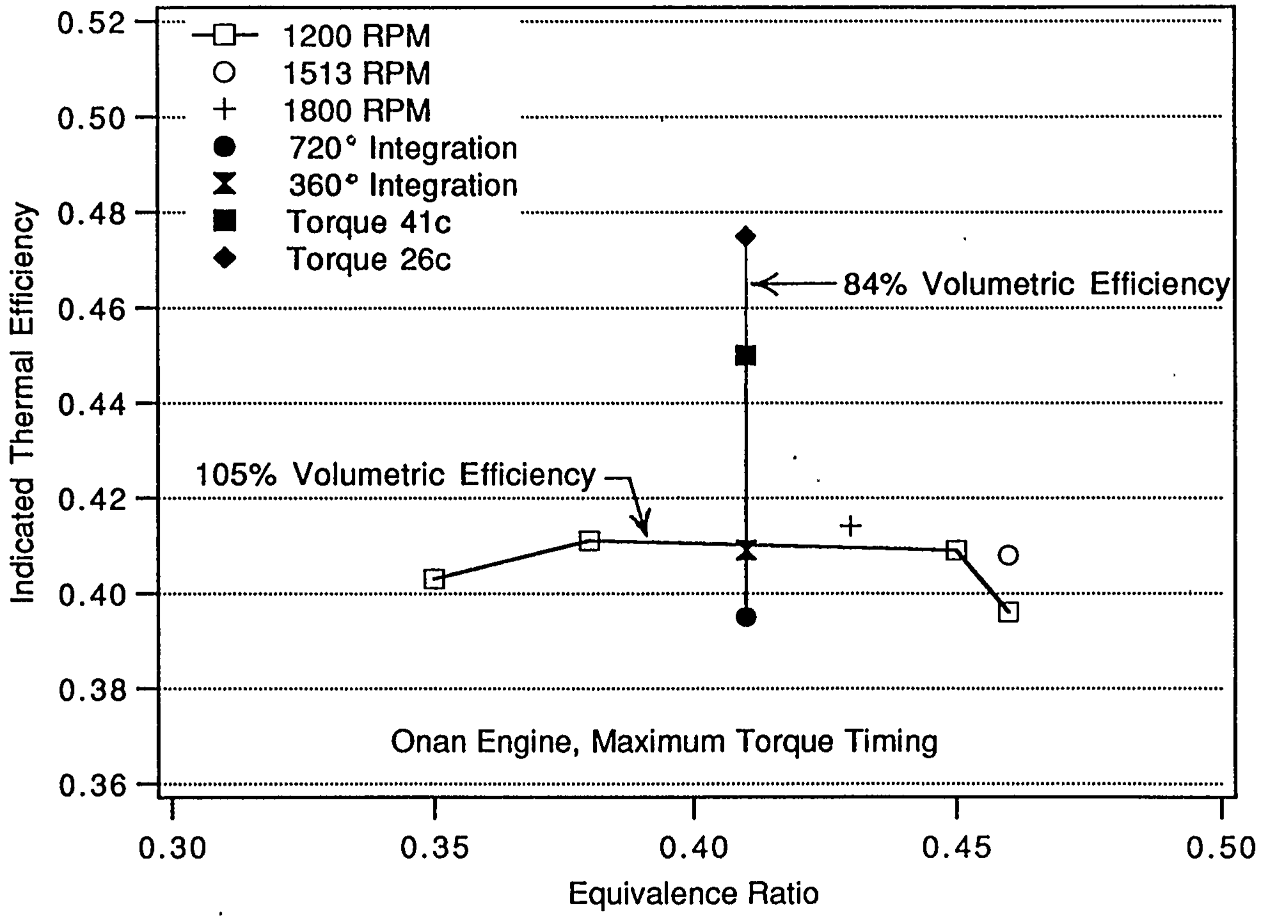


Figure 10. Onan indicated efficiency sensitivity

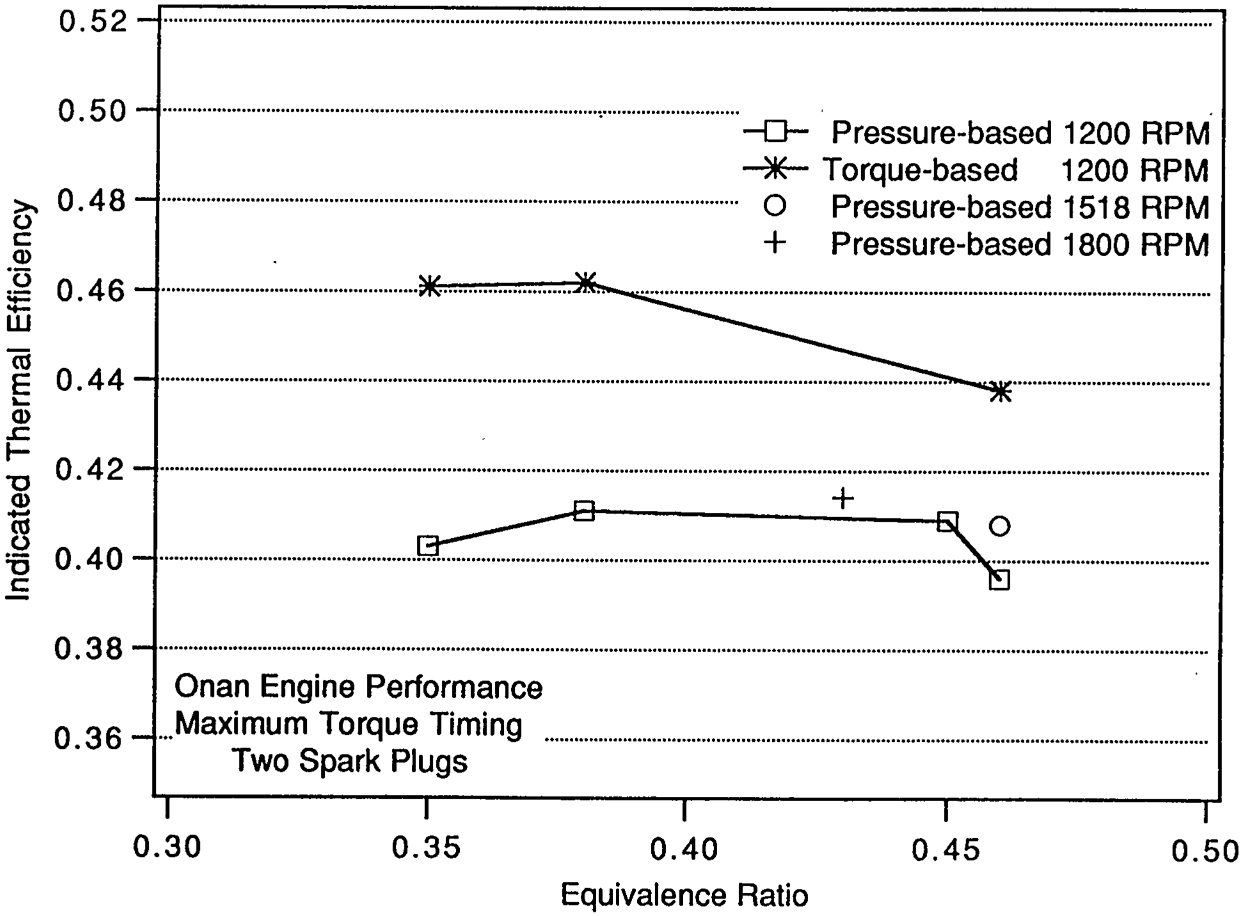
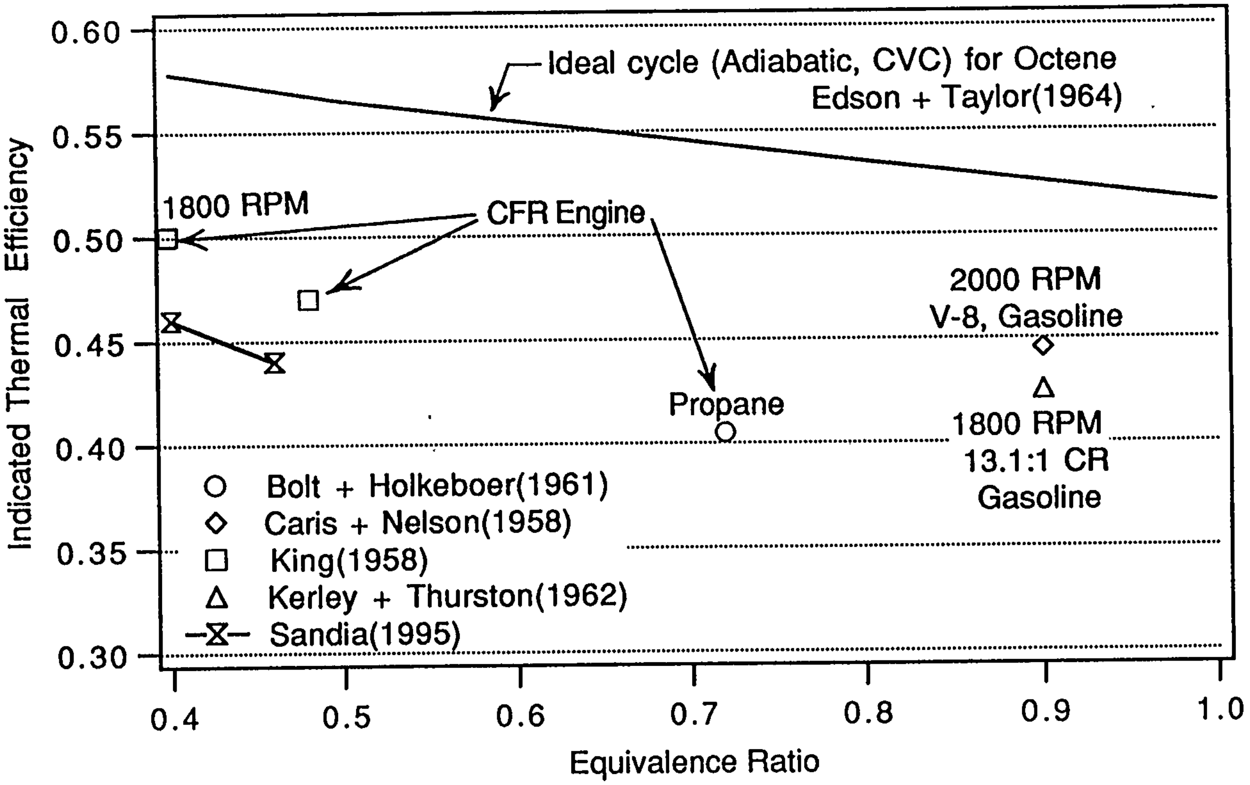


Figure 11. Onan indicated efficiency range



Unless otherwise noted: Speed = 1200 RPM, fuel = hydrogen
CR = 18.8:1, single cylinder engine, efficiency from torque

Figure 12. Other data comparison.

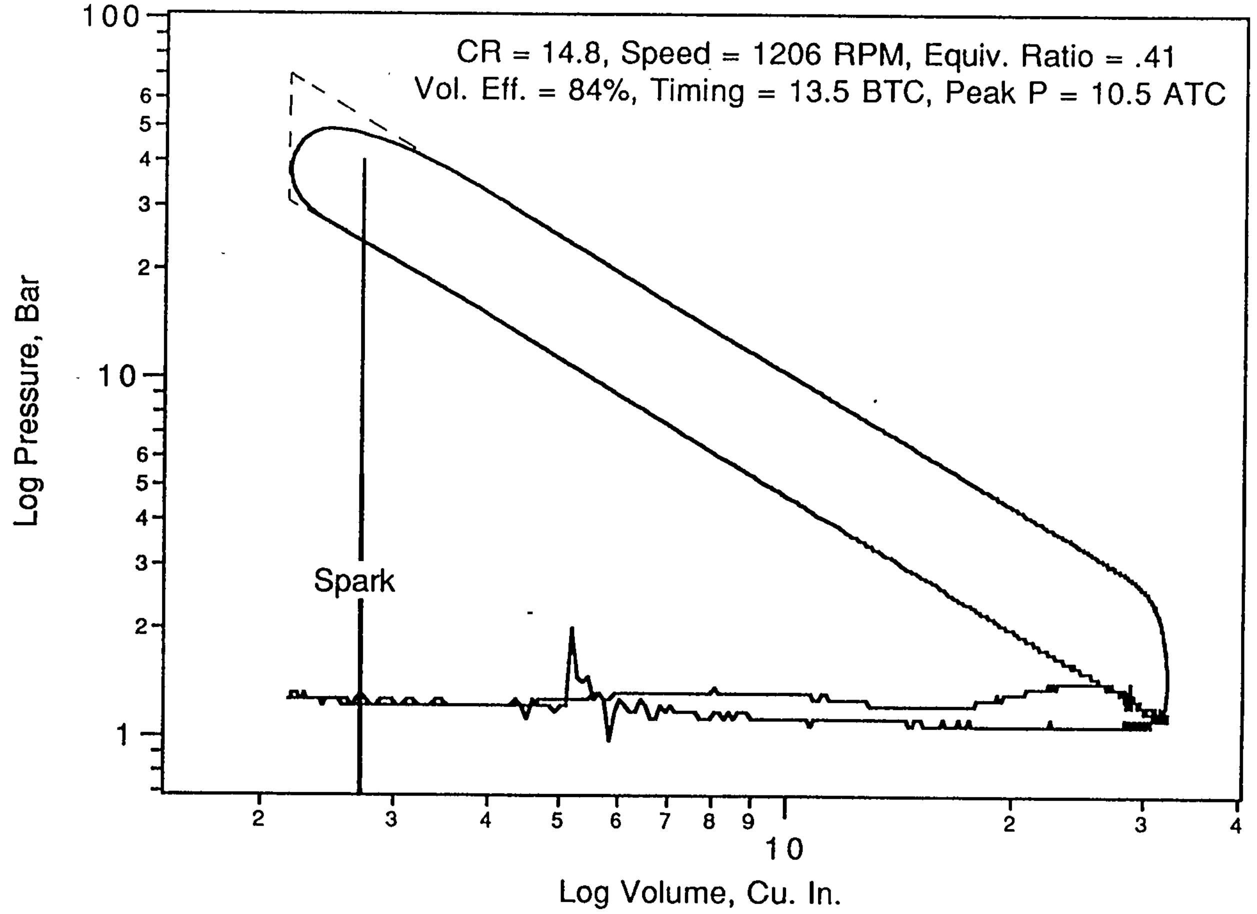


Figure 13. Onan engine log P vs log V

HYDROGEN PROGRAM COMBUSTION RESEARCH: THREE DIMENSIONAL COMPUTATIONAL MODELING

Norman L. Johnson, Anthony A. Amsden, and T. Daniel Butler
Los Alamos National Laboratory
Los Alamos, NM 87545

Abstract

In the past year we have significantly increased our computational modeling capability by the addition of a vertical valve model in KIVA-3, a reactive flow code used internationally for engine design. In this report the implementation and application of the valve model is described. The model is shown to reproduce the experimentally verified intake flow problem examined by Hessel. Furthermore, the sensitivity and performance of the model is examined for the geometry and conditions of the hydrogen-fueled Onan engine in development at Sandia National Laboratory. Overall the valve model is shown to have comparable accuracy as the general flow simulation capability in KIVA-3, which has been well validated by past comparisons to experiments. In the exploratory simulations of the Onan engine, the standard use of the single kinetic reaction for hydrogen oxidation was found to be inadequate for modeling the hydrogen combustion because of its inability to describe both the observed laminar flame speed and the absence of autoignition in the Onan engine. We propose a temporary solution that inhibits the autoignition without sacrificing the ability to model spark ignition. In the absence of experimental data on the Onan engine, a computational investigation was undertaken to evaluate the importance of modeling the intake flow on the combustion and NOx emissions. A simulation that began with the compression of a quiescent hydrogen-air mixture was compared to a simulation of the full induction process with resolved opening and closing of the intake valve. Although minor differences were observed in the cylinder-averaged pressure, temperature, bulk-flow kinetic energy and turbulent kinetic energy, large differences where observed in the hydrogen combustion rate and NOx emissions. We conclude that the flow state at combustion is highly heterogeneous and sensitive to the details of the bulk and turbulent flow and that an accurate simulation of the Onan engine must include the modeling of the air-fuel induction.

Introduction

Rapid utilization of hydrogen for stationary power plants and combustion engines for hybrid vehicles requires the development of computational tools to aid in the design of new engines by industry and government laboratories. Our goals are to develop the required computational tools, to validate them by comparison to experimental data, and to demonstrate the utility of the computational approach in a research program to design such internal combustion engines and then to collaborate with industry and government laboratories in their applications of the computer models. Los Alamos has developed a family of computer models that have gained wide acceptance in the automotive industry, as well as the gas turbine, stationary combustion and aerospace industries, primarily for hydrocarbon fuels. Our approach is to refine, modify and utilize computer models embodied in the KIVA-3 and KIVA-F90 computer codes as applied to combustion of both pure hydrogen as a fuel and mixtures of hydrogen and hydrocarbon gases. The work supports collaboration in the DOE Hydrogen Program by developing the knowledge to (1) enable industry to build a stationary hydrogen fueled internal combustion engine to power an electric generator system, and (2) to build an advanced internal combustion engine fueled by hydrogen to meet zero emission requirements. Because of the wide use of the KIVA family of codes in the automotive, diesel and aerospace industries, the capability to use hydrogen fuel in the KIVA family of codes can be quickly utilized by industry.

Los Alamos National Laboratory (LANL) will use the chemistry submodels under development at Lawrence Livermore National Laboratory (LLNL). The hydrogen combustion simulation capability can then be benchmarked with experiments performed by Sandia National Laboratory (SNL) and LLNL and then be used to aid in the support of the development of the optimized test engine and demonstration engine, currently under development by SNL and LLNL.

Earlier investigations, prior to the work described in this report, focused on the hydrodynamics and combustion of a hydrogen jet (Amsden, et al., 1994; Johnson, et al., 1995). From a comparison of detailed experiments performed by SNL, we observed that the KIVA simulations of methane injection modeled accurately the penetration and pressure history, with and without combustion. By contrast, the modeling of the combustion of hydrogen was unsatisfactory using either a single Arrhenius kinetic equation or a 22-reaction model. In particular the simulations prematurely autoignited and required that the combustion be delayed to the experimentally observed value. After the examination of hydrogen injection and combustion, simulations were made of the spark ignited CLR engine being operated at SNL. Preliminary results led us to suspect that simulations without detailed information about the bulk flow and turbulent levels at the onset of spark ignited combustion were deficient. In order to properly simulate the intake flow, the flow through an opening and closing valve was required. We then undertook the implementation of a valve model in KIVA-3.

This report summarizes the new vertical valve capability that has been implemented into

KIVA-3, its validation and its application to the spark-ignited, hydrogen-fueled Onan engine being operated by SNL.

Details of the SNL Onan engine can be found in the report by Van Blarigan (1995). The Onan engine is a converted diesel engine with a modified head containing two valves and two spark plugs. Table 1 summarizes the engine specifications. The design of the Onan engine is based on the arguments put forth in the report by Smith and Aceves (1995). The engine design is such that the bulk flow and turbulence are minimized in order to reduce the heat transfer losses, thereby increasing the operating efficiency. The engine operates at low fuel equivalency ratios (0.4–0.5) to reduce the combustion temperature and thereby significantly reduces the NOx emissions. Because of the symmetry of the engine design, the flow and combustion is symmetric through a plane passing through the two valves.

Table 1 Modified Onan Engine Specifications

Bore	**82.55 mm**
Stroke	**92.08 mm**
Displacement	**493.0 cm^3**
Geometric compression ratio	**14.82**
Rings	**4**
Valve pocket volume	**3.60 cm^3**
Spark plug volume	**1.30 cm^3**
Volume above rings	**0.27 cm^3**
Volume of depressed gasket	**7.52 cm^3**
Squish volume	**35.65 cm^3**

Implementation of the Valve Model in KIVA

The KIVA family of codes, developed at LANL, is a mature, three-dimensional, computational fluid dynamics software for chemically reactive, transient flows with fuel sprays (Amsden et al., 1989). The code features sophisticated sub-models, which simulate the complex flow, thermodynamic and chemical processes accompanying combustion. These models include for applications to combustion engines: turbulence, spray atomization, fuel penetration and vaporization, auto-ignition and combustion. The chemical combustion model can describe complex equilibrium and kinetic reactions, giving it the capability of modeling soot in the presence of carbon and NOx production. The KIVA-3 version (Amsden, 1993) enables complex geometries to be modeled, typical of combustion engines with moving pistons and inlet and exhaust ports. KIVA-3 runs on generic workstations and on supercomputers. A new version of KIVA, KIVA-F90, is written in FORTRAN-90 and will execute on massively parallel machines. For the current application, KIVA-3 is used to model the SNL experiments.

Once the need for a valve model in KIVA was established, the examination of available valve models were considered. It was decided that a valve model that had comparable accuracy as the other fluid flow models in KIVA was desirable, because the experience with the performance of valve models is limited in the engine modeling community. An implementation of the desired valve model was developed in a research version of KIVA-3 by Hessel (1993). This modified version of KIVA-3 was obtained by LANL, and the valve capability was moved to the most recent version of KIVA-3 and made compatible with all existing features. Details of the model can be found in the Ph. D. thesis by Hessel; the highlights of the model as implemented at LANL are summarized below.

The valve model uses an existing capability, the SNAPPER model (Amsden, 1993), in KIVA-3 for modeling pistons in complicated geometries. The SNAPPER model moves the solid surface of the piston (or valve) until the mesh above the piston is reduced in height to a specified value. The squished cells next to the piston are removed from the computational mesh, and their state quantities are added to the expanded cells now above the piston. When the piston is withdrawn, the process is reversed. Consequently, the shape of the piston or valve is resolved to arbitrary degree as determined by the mesh resolution. The implementation, as with the piston model, requires a special mesh generation capability in which the shape of the valve during its entire movement history is included in the fluid portion of the mesh. As a consequence of this restriction on the mesh, parallel with the valve implementation in KIVA-3, the mesh generation capability for valves was also implemented in the companion mesh generator for KIVA-3. In both implementations, additional capabilities and simplification of input were made over the original Hessel implementation. These include, for example, the ability to have an arbitrary number of valves with independent movement histories and automatic reporting of the flow through each valve. Furthermore, some errors in the original implementation were found and corrected. Finally a more efficient sorting routine, which is required after the SNAPPER operates, is used and significantly reduces the execution times.

Because the valve model makes no approximations for the flow through the valve opening, the accuracy of the valve model is comparable to the accuracy of the standard flow solution in the code and dependent upon the mesh resolution in the region of the valve. This is a significant advantage of the model because the accuracy of the valve flow need not be independently validated but can rely on prior comparisons of the performance of KIVA on other flow problems (e.g., Amsden et al., 1992).

To validate the valve model, the intake flow problem examined by Hessel was simulated using the original mesh of 122,000 cells, as shown in Fig. 1. Hessel achieved satisfactory comparisons between the KIVA-3 results and the detailed experimental data for the same flow. The final simulation using the new implementation of the valve model duplicated the results obtained by Hessel to within expected differences associated with the correction of the errors. Due to the improved sorting routine and the elimination of certain errors that had reduced the time step, the simulation time for the new implementation was reduced by about 50%. Based on this comparison, we are confident that the valve model in the current version of KIVA-3 accurately reproduces Hessel's original implementation.

Three-Dimensional Modeling of SNL ONAN Engine

Mesh generation

The development of a three-dimensional mesh for a complex geometry is a significant undertaking. The mesh used to model the modified Onan engine resulted from progressive refinements over a period of several months. The final mesh is shown in Fig. 2. The mesh is generated with a preprocessor that has been written specifically for KIVA-3 without the need for additional modifications. The mesh is generated with 41 pseudo-blocks, resulting in 5 logically hexahedral blocks of mesh with 37,722 cells in the full mesh. As stated in the last section, the setup of the mesh requires the shape of the valves along their path to be included in the initial mesh, as illustrated in Fig. 2. Because the current geometry of the modified Onan engine has a plane of symmetry through the two valves, for the computational results presented here only half of the engine is simulated. The only major simplifications made in the computational mesh were square cross-section of the intake and exhaust manifolds and their reduced length. To reduce the effect of the simplification, the flow area of the simulated and actual manifolds are identical. Because the pressure boundary conditions at the intake and exhaust manifolds were expected to be modified in order to obtain agreement with the breathing performance of the engine, the simplification of the length and cross-section of the manifolds is not considered to be significant. Other simplifications are the omission of the volume associated with the spark plugs (3.5% of the minimum cylinder volume) and the volume above the piston rings (0.7% of the minimum volume). The valve shapes and seating were modeled accurately to within the resolution of the mesh. Other boundary conditions are specified in Table 2.

Table 2. Initial and boundary conditions

Cylinder wall temperature	373 K
Piston temperature	430 K
Head temperature	373 K
Intake valve temperature	373 K
Exhaust valve temperature	585 & 800 K
Exhaust gas temperature	585 & 800 K
Engine speed	1200 & 2400 RPM
Exhaust pressure boundary	0.949 - 1.0 atm
Intake pressure boundary	0.949-1.2 atm
Intake manifold composition	0.4 - 0.41 fuel equivalence ratio in air
Exhaust manifold composition	combustion products of the intake gas
Initial cylinder composition	same as exhaust manifold

Further validation of the valve model

Various validation checks were made to assess the accuracy of the valve model within KIVA-3. For overall flow accuracy, the duplication of the results of the intake flow problem by Hessel summarized in the last section is the primary validation in the absence of detailed experimental data on the Onan engine. Because KIVA-3 has been validated for ported engines (e.g., Amsden et al., 1992), we are confident in the accuracy of the valve model as long as the behavior of the valve flow exhibits no anomalous behavior, because the valve model introduces no new physical or numerical models.

To check for anomalous behavior, the flow through the valve during opening and closing were examined. A simulation was done with the geometry described in the previous section at an RPM of 300, in order to make the primary resistance to flow the valve opening. The velocities in the intake valve gap were measured as a function of time and plotted against the pressure drop across the intake valve at a given time (see Fig. 3). At steady state the velocity through the valve gap should be proportional to the pressure drop across the gap. As can be seen in Fig. 3, most of the points reflect an approximately linear relationship between the velocity and the pressure drop, with the breadth in the plot attributable to unsteady state conditions and the changes in flow area. The only points that lie outside this band of data are when the valve first opens and all the flow is though one cell. This anomalous behavior is attributed to the absence of the law of the wall boundary layer approximation being applied between solid surfaces that have only one cell between them. This treatment allows for a larger flow for a given pressure drop than at other times, and hence, the cause of the outlying points at these times in Fig. 3. Because the mass flow through the valve during these times is small compared to the total mass flow, the effect of this anomaly is considered small. We are investigating alternative treatments that would alleviate this effect. As a result of this analysis we conclude that the valve model within KIVA-3 has been properly implemented and has comparable accuracy to the rest of the code.

The sensitivity of the shape of the valve has on the flow was examined by comparing the flow past an approximate valve shape to the experimental valve shape, as shown in Fig. 4 for identical driving conditions and mesh resolution. The peak velocity during maximum valve opening was observed to be 41% higher (17.3 m/s versus 12.3 m/s) in the resolved shape than in the approximate valve shape. Because turbulence generation is most sensitive to large gradients in velocity and because combustion is sensitive to turbulence levels, we would expect these two geometries to exhibit different combustion and emission behavior. This observed difference in velocity is a significant indication that care must be taken in resolving the geometric details in the neighborhood of the valves.

Exploratory Simulations of the SNL Onan Engine

In the absence of experimental data on the Onan engine for comparison to the KIVA simulation results, a variety of simulations were done to evaluate the performance and sensitivity of the model. The different operating conditions are listed in Table 2. Simulations were initialized at just before intake valve opening (–20 CA BTDC) and carried though the intake cycle, the closing of the intake valve and the compression of the gas, and then stopped just before spark ignition. The state of the calculation was stored at this time so that the simulation could be continued with a variety of spark ignition times and changes in the reactive kinetic models.

The kinetics of hydrogen oxidation were modeled by a single forward kinetic equation, with an Arrhenius temperature dependence. Zeldovich kinetics for the slow NOx production is also included. The effect of turbulence on the combustion rate was included by using a mixing controlled combustion model (a slight variation of the model proposed by Magnussen and Hjertager, 1977) in which the reaction rate is proportional to the ratio of the turbulent kinetic energy divided by the rate of dissipation of turbulence. The inclusion of the mixing controlled model is essential because the flame speed of the hydrogen combustion can be many times the laminar flame speed in the presence of typical turbulent intensities found in engines (Meier et al., 1994), and increases of factors of 25 times the laminar flame speed are observed for propane (Abdel-Gayed and Bradley, 1977). In turn, flame speed is related to combustion temperature and thereby is reflected in NOx emission levels. The present mixing controlled combustion model is applied routinely to hydrocarbon combustion, but has not been applied to hydrogen combustion. Until the model is validated, results using the mixing turbulent combustion model should only be used to examine trends in the simulations. Before reporting detailed simulation results, the following summarizes the early exploratory simulations of the Onan engine.

All the simulations ran without difficulty or unexpected termination. Execution times were about two hours on a Cray YMP to reach the time of spark ignition, or about 360 degrees of crank angle. Combustion simulations from –20 CA to 20 CA required about a hour of computational time. All aspects of the simulations associated with the fluid dynamics were reasonable, and we expect them to be predictive of the Onan engine performance.

The only area of difficulty arose in the simulation of combustion of hydrogen. The primary difficulty that was encountered was the autoignition of the hydrogen during compression, when parameters in the single step oxidation kinetics were used which reproduce the laminar flame speed (Westbrook, 1994). Preliminary experimental results (Van Blarigan, 1995) indicate that for these operating conditions, autoignition does not occur. This deficiency of the hydrogen kinetics was also observed in the KIVA simulations of hydrogen injection and combustion (Johnson et al., 1995) by the absence of an autoignition delay. Our solution to the difficulty is similar: enforce that the hydrogen kinetics reproduce the observed behavior by preventing the hydrogen reaction from proceeding until the cell temperature has exceeded 1000 K. This approach does not require a modification of KIVA, because a cut-off temperature, typically 800 K, is commonly used in which the kinetics will not be calculated if the cell temperature is below this value. The consequence of this approach is to inhibit the reaction as compression of the fuel mixture occurs and enable the reaction at and behind the combustion front, typically at temperatures over 2000 K. We consider this to be a temporary solution until better kinetics are available from the work being done at LLNL. In the absence of the higher cutoff temperature, the hydrogen fuel would autoignite when it reached 800 K, typically about −10 degrees BTDC for an intake manifold pressure of 1.2 atm, independent of the time of spark ignition.

Importance of Modeling Fuel-Air Induction on Combustion and Emissions

In the absence of experimental data to benchmark the performance of KIVA-3 for the Onan engine, we undertook a computational study to evaluate the importance of including the induction of air-fuel into the cylinder prior to combustion. We made two simulations, one with no induction into the cylinder and another with flow through the intake valve and the subsequent generation of bulk flow and turbulence, and then compared the effects on combustion and time histories of flow energies. The simulation with intake flow was accomplished as described in the previous section. The simulation without induction was begun just after intake valve closing and the composition was set to be identical to the simulation with induction at the same crank angle. The bulk flow was specified to be quiescent, and the turbulence kinetic energy per mass was taken to be ten percent of the kinetic energy per mass as obtained from the maximum piston velocity. These are typical starting conditions for a quiescent engine when more detailed information is not known.

Figures 5 and 6 show the cylinder-averaged pressure and temperature during the compression, combustion, and expansion part of the cycle, up until the opening of the exhaust valve at 500 CA (the simulation without induction was only run to 390 CA because after this time the two simulations are similar). Up until the time of combustion these curves are identical for both runs. After combustion at 13.5 CA BTDC (346.5 CA in the simulation), there is significant divergence in the two simulations, a difference of 35 bars in pressure and 400 K in temperature. A plot of the hydrogen mass in the cylinder as a function of crank angle in Fig. 7 shows a further difference in the two simulations: the observed flame speed is about 3.5 times smaller in the non-inducted simulation. The differences in the combustion behavior have a significant impact on the production of NOx emissions. In Fig. 8 the NOx production is 14 times higher in the fast burning combustion, due to the higher temperatures.

The large difference in the combustion and NOx emissions in the two simulations illustrate the importance of modeling the bulk flow and turbulence levels accurately. In Figs. 9 and 10 are plotted the total kinetic energy of the bulk flow and the turbulent kinetic energy as modeled by the k-ε turbulence model. These curves show a significant difference in the initial kinetic energy levels of the two simulations. As the initial high kinetic energy level dissipates in the induction run and as the piston adds kinetic energy during compression, the averaged kinetic energy for both the bulk flow and turbulence are within 10–20 percent of each other just after ignition (350 CA). If the averaged kinetic energy values represented the values near the combustion front, this would result in a comparable increase in the reaction rate, not the factor of 350 percent observed. This is strong evidence that the flow is nonhomogeneous and sensitive to the details of the flow history.

Conclusions and Future Work

A significant extension of the KIVA-3 reactive simulation code was accomplished by the addition of a vertical valve model, which works in concert with all other capabilities of the code. The valve model was validated by comparisons to a experimentally-verified intake flow for a four valve engine. Further test simulations were made to assure that the model has comparable accuracy as the rest of the flow model used in the code and to ascertain the sensitivities of the model, such as the details of the valve-seat geometry. A computational mesh was created of the SNL Onan engine, with an accurate description of the intake and exhaust valves. In the absence of experimental data on the performance of the engine, we focused on observed trends in the simulations. The model of the Onan engine was used to investigate the induction process of fresh air and the subsequent compression and combustion of hydrogen with NOx formation. A major conclusion of the investigation is that the use of a single kinetic reaction for hydrogen oxidation is unable to describe both the observed laminar flame speed and the lack of autoignition in the Onan engine. We also observed that the combustion and emissions are sensitive to the initial flow field at the beginning of combustion. NOx emissions were observed to vary by a factor of 14 with typical choices for the initial conditions of the simulation. We conclude that any modeling of the Onan engine must include the effects of the intake flow on the bulk flow and turbulence levels during combustion.

The KIVA-3 simulations are now at the ideal stage of development to begin the validation process as the experimental data becomes available from SNL. The observed sensitivity of hydrogen combustion on turbulence and bulk flow highlights the need for improved kinetics and then for validation of the kinetics in conjunction with the mixing controlled models. In addition, as experimental data for the Onan engine is available, the simulation conditions can be improved to better model the experiments. For example, the constant pressure boundary conditions can be replaced by time-varying pressure boundary conditions as determined from the experiments. The pressure history and the mass of charge in the engine can then be compared to the experimental results to further validate the performance of the valve model in KIVA-3. Finally, comparison of NOx formation and engine efficiencies will be made. Once the simulations are validated, an analysis of the operation of the engine will be undertaken to better understand the experimental observations of the effect of combustion chamber geometry, turbulence levels, flame speed, and heat transfer on NOx formation and efficiency. The simulations can also be used to suggest modifications to the Onan engine to improve the performance and reproducibility of the engine. For example, the trends in the present report suggest that a reduction in the turbulence levels of the engine through the introduction of shrouds on the valves may improve the NOx emissions of the engine. This is an ideal application of using computer simulations to improve the success of expensive modifications of an experiment.

References

Amsden, A. A., O'Rourke, P. J., Butler, T. D., Meintjes K., and Fansler, T. D. 1992. "Comparisons of Computed and Measured Three-Dimensional Velocity Fields in a Motored Two-Stroke Engine," SAE Paper 920418.

Amsden, A. A. 1993. "KIVA-3: A KIVA Program with Block-Structured Mesh for Complex Geometries," Los Alamos National Laboratory report LA-12503-MS.

Amsden, A. A., Butler, T. D., and O'Rourke, P. J. 1989. "KIVA-II: A Computer Program for Chemically Reactive Flows with Sprays," Los Alamos National Laboratory report LA-11560-MS.

Abdel-Gayed, R. G., and Bradley, D. 1977. "Dependence of Turbulent Burning Velocity on Turbulent Reynolds Number and Ratio of Laminar Burning Velocity to RMS Turbulent Velocity," Sixteenth Symposium on Combustion, The Combustion Institute, pp. 1725.

Hessel, R. P. 1993. "Numerical Simulation of Valved Intake Port and In-Cylinder Flows Using KIVA-3," Ph.D. Thesis, University of Wisconsin, Madison, Prof. C. J. Rutland advisor.

Johnson, N. L., Amsden, A. A., Naber, J. D., and Siebers, D. L. 1995. "Three-Dimensional Computer Modeling of Hydrogen Injection and Combustion," Transaction paper for the '95 High Performance Computing Conference, edited by Adrian Tentner, pp. 61–69. Published by the Society for Computer Simulation.

Magnussen, B. F., and Hjertager, B. H. 1977. Sixteenth Symposium on Combustion, The Combustion Institute, pp. 719–729.

Meier, F., Köhler, J., Stolz, W., Bloss, W. H., and Al-Garni, M. 1994. "Cycle-Resolved Hydrogen Flame Speed Measurements with High Speed Schlieren in a Hydrogen Direct Injection SI Engine," SAE Fuels and Lubricants Meeting and Expositions, #942036.

Smith, J. R., Aceves, S. April 1995. "Hybrid Vehicles Studies and Optimized Engine Design," Lawrence Livermore National Laboratory, Proceedings of the 1995 DOE/NREL Hydrogen Program Review.

Van Blarigan, P. April 1995. "Hydrogen Hybrid Vehicle Engine Development: Experimental Program," Sandia National Laboratory, Proceedings of the 1995 DOE/NREL Hydrogen Program Review.

Westbrook, C. K. September 1994. Hydrogen Program Progress Report as submitted to Neil Rossmeissl.

Westbrook, C. K. April 1995. "Chemical Kinetics of Hydrogen," Lawrence Livermore National Laboratory, Proceedings of the 1995 DOE/NREL Hydrogen Program Review.

Figure Captions

Figure 1. The mesh for the intake flow problem through two valves as examined by Hessel. The two separate valve manifold combine into one large manifold. The two exhaust ports are not modeled.

Figure 2. The mesh for the Onan engine showing the entire perspective view at the top and a cut through the symmetry plane at the bottom. In the lower figure, the inlet valve is on the right, shown at its full open position, and the exhaust valve is on the left, shown closed.

Figure 3. The velocity in the intake valve gap as a function of the pressure drop across the valve.

Figure 4. The velocity vector field when the intake valve is fully open for the Onan engine. The square valve representation is on the left. The peak velocity is 41 percent higher in the more refined valve model on the right.

Figure 5. Pressure histories averaged over the cylinder after intake valve closing.

Figure 6. Temperature histories averaged over the cylinder after intake valve closing.

Figure 7. H_2 mass in the cylinder during combustion.

Figure 8. NO_x production in the cylinder during combustion.

Figure 9. Total bulk-flow kinetic energy averaged over the cylinder.

Figure 10. Total turbulent kinetic energy averaged over the cylinder.

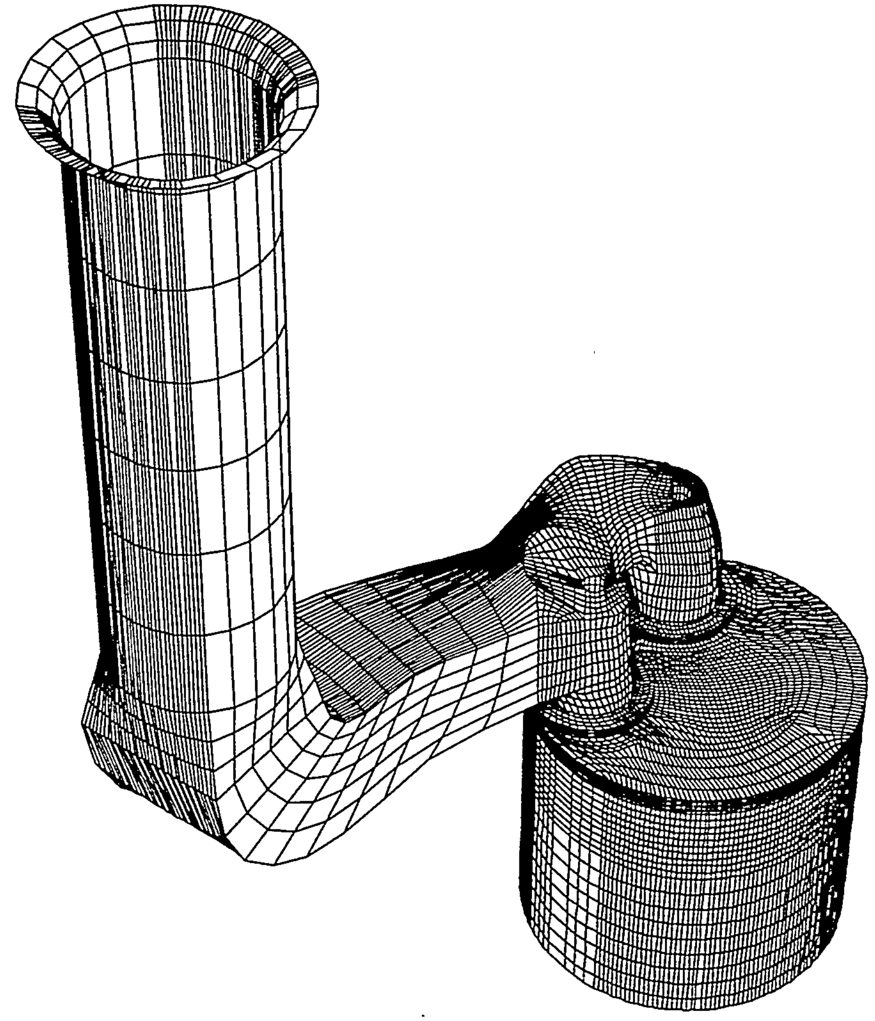


Figure 1. The mesh for the intake flow problem through two valves as examined by Hessel. The two separate valve manifold combine into one large manifold. The two exhaust ports are not modeled.

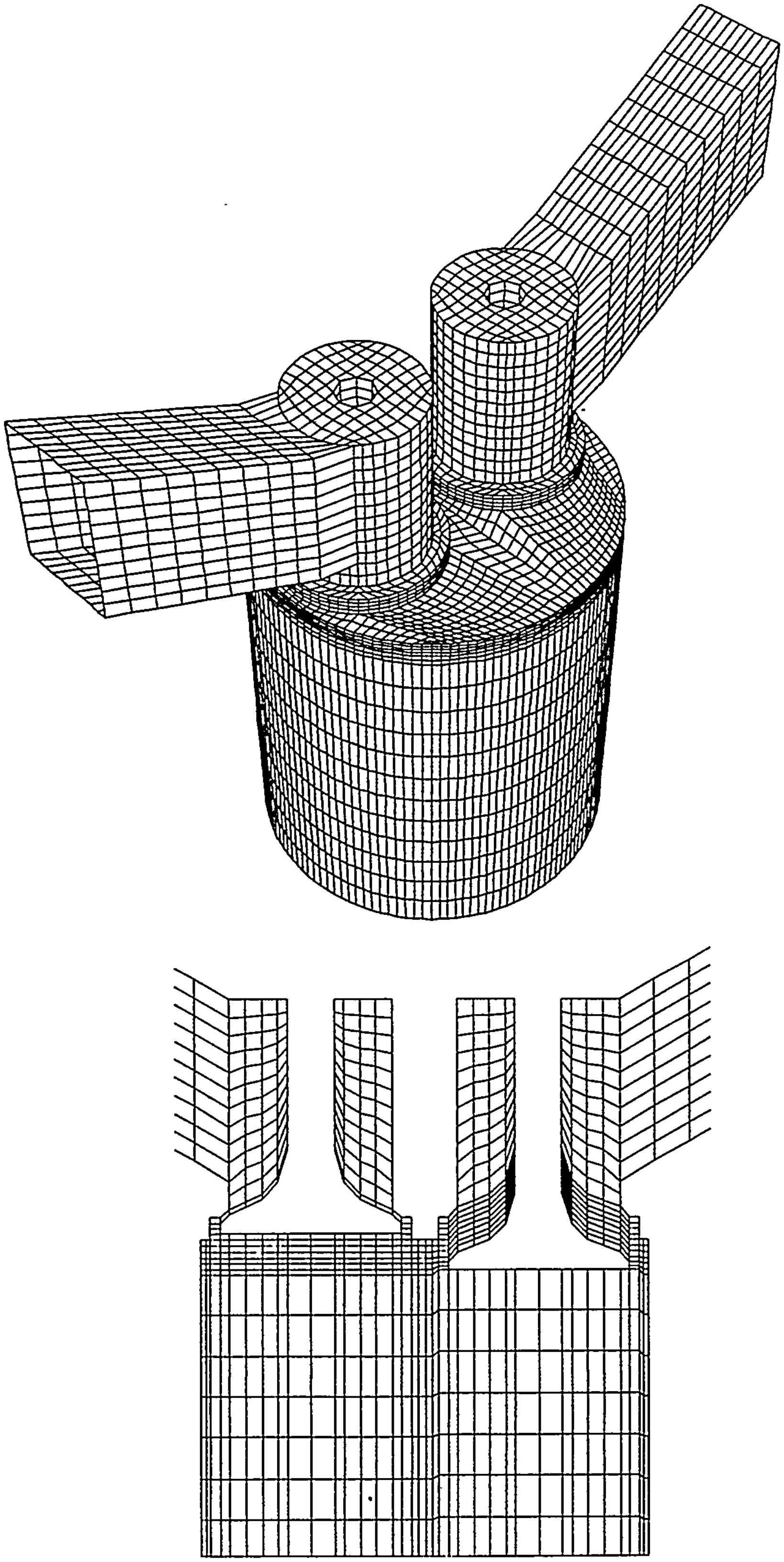


Figure 2. The mesh for the Onan engine showing the entire perspective view at the top and a cut through the symmetry plane at the bottom. In the lower figure, the inlet valve is on the right, shown at its full open position, and the exhaust valve is on the left, shown closed .

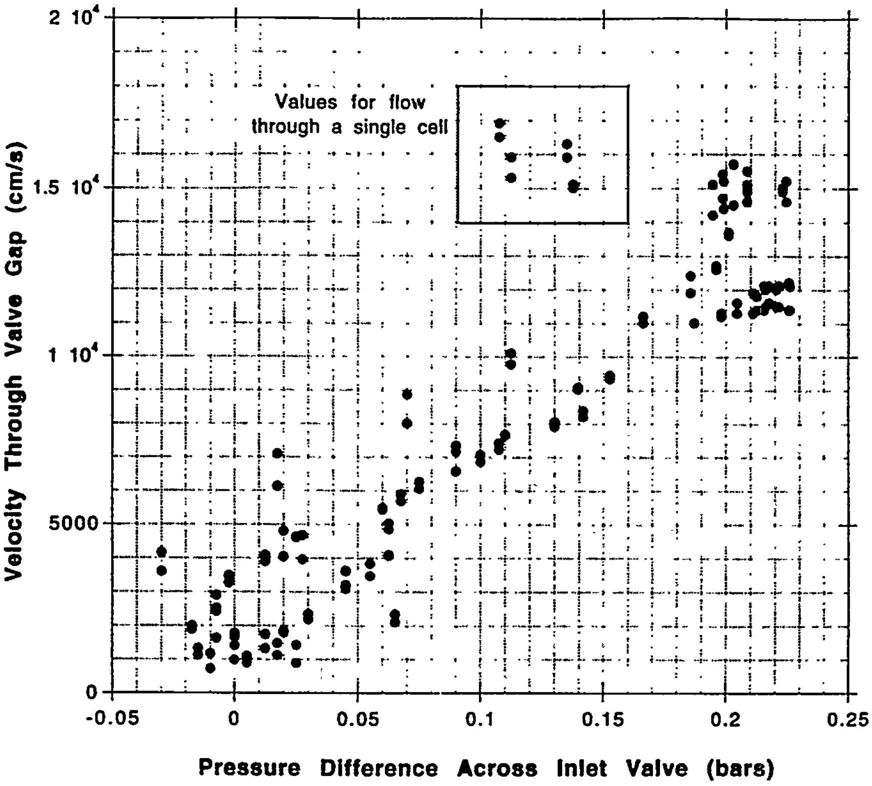


Figure 3. The velocity in the intake valve gap as a function of the pressure drop across the valve.

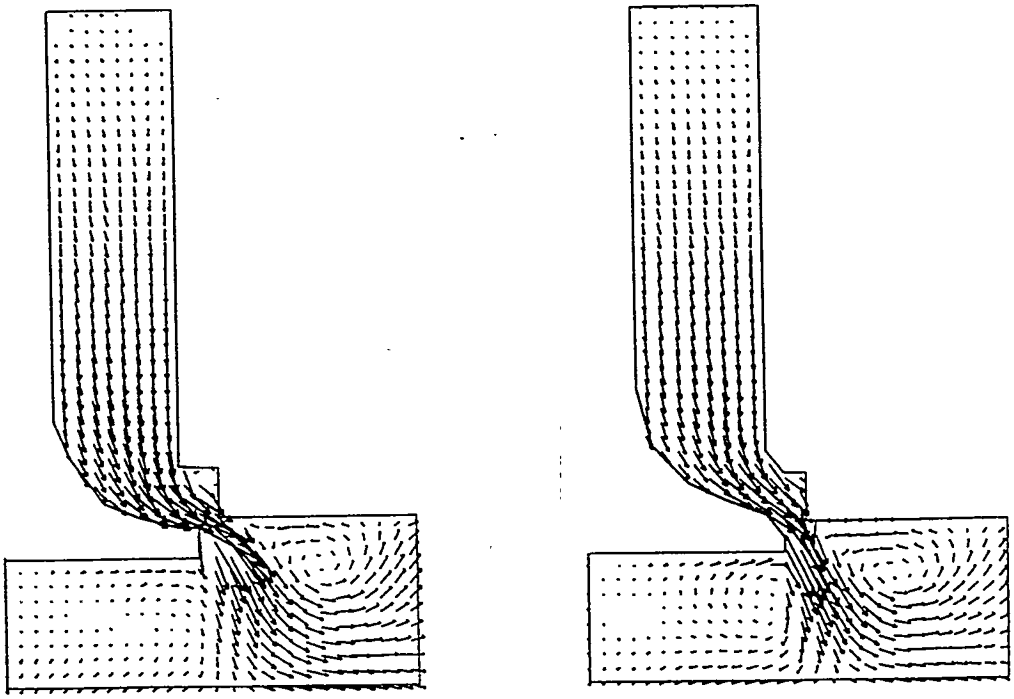


Figure 4. The velocity vector field when the intake valve is fully open for the Onan engine. The square valve representation is on the left. The peak velocity is 41 percent higher in the more refined valve model on the right.

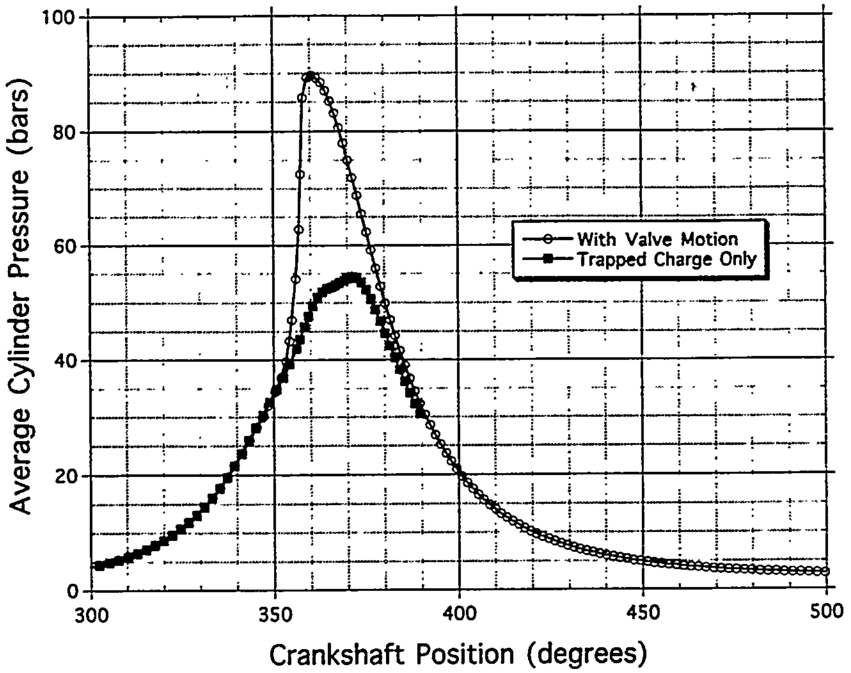


Figure 5. Pressure histories averaged over the cylinder after intake valve closing.

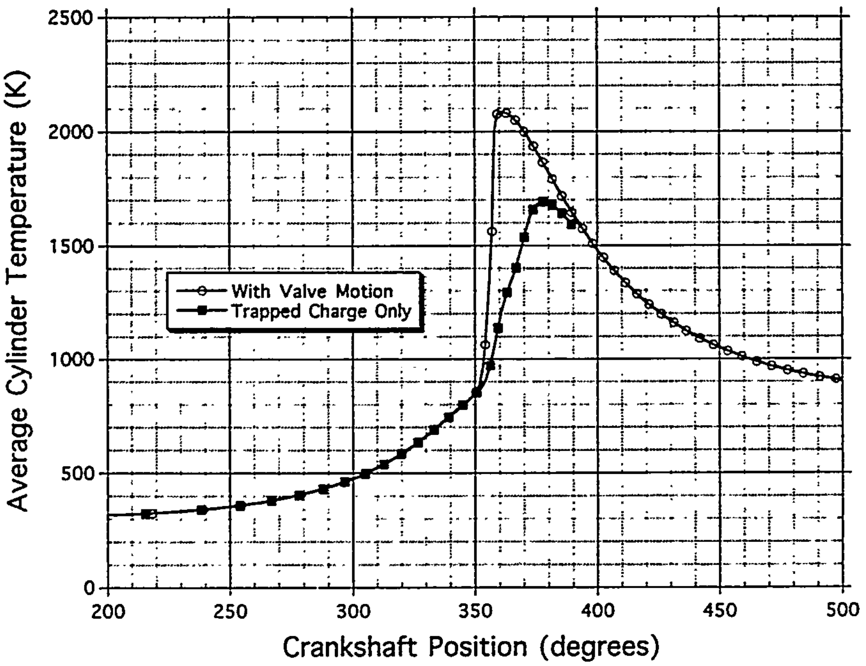


Figure 6. Temperature histories averaged over the cylinder after intake valve closing.

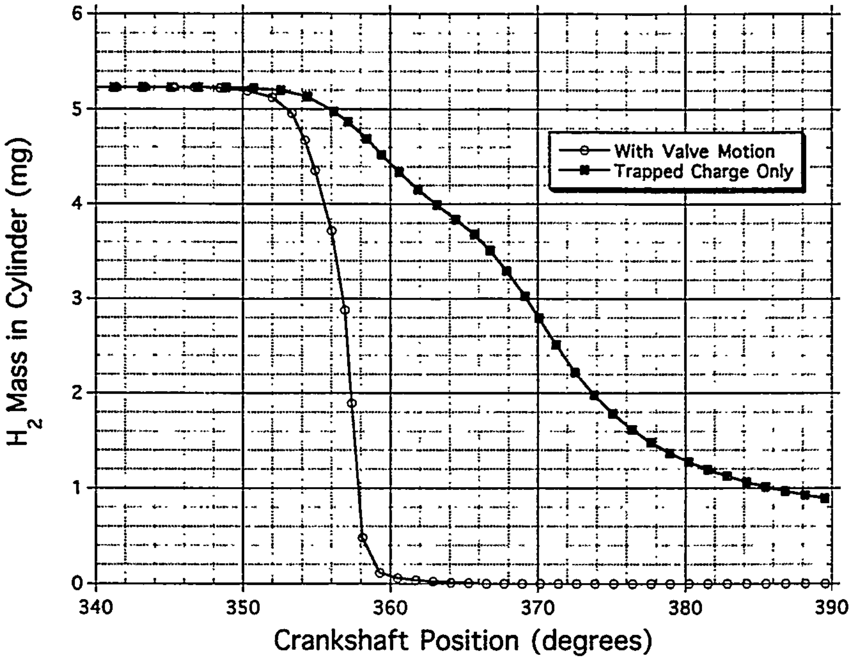


Figure 7. H_2 mass in the cylinder during combustion.

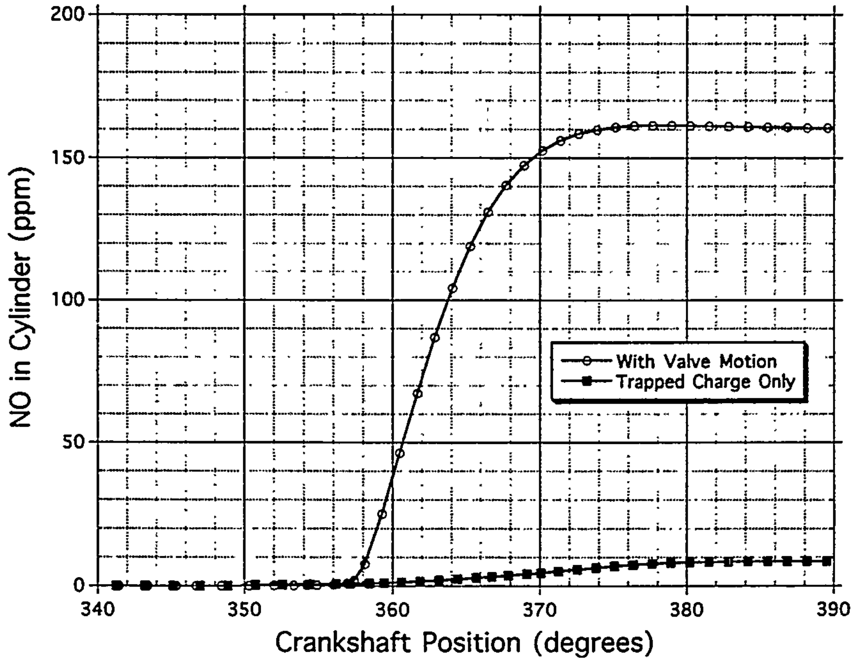


Figure 8. NO_x production in the cylinder during combustion.

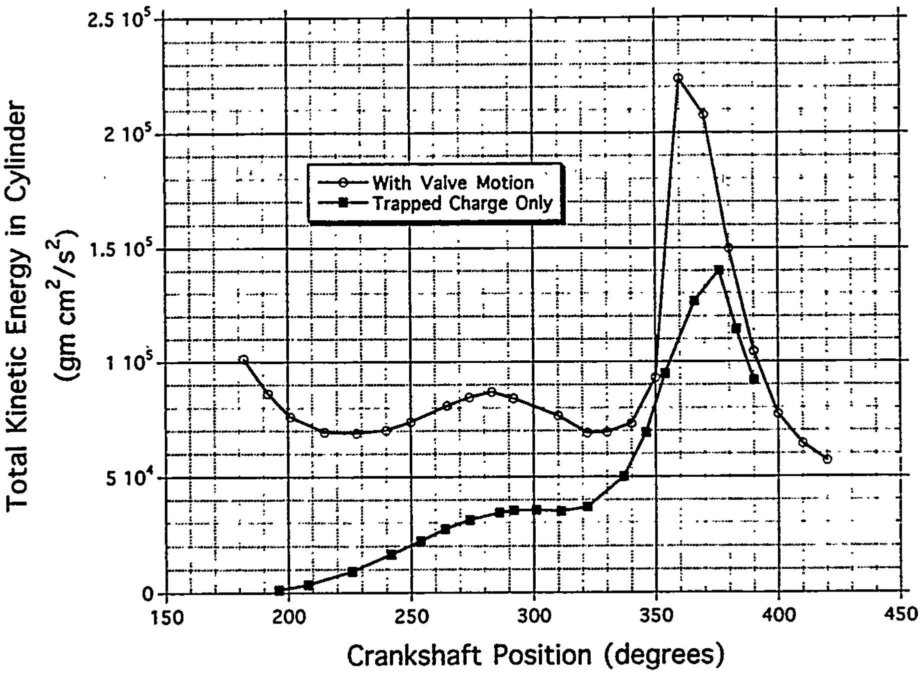


Figure 9. Total bulk-flow kinetic energy averaged over the cylinder.

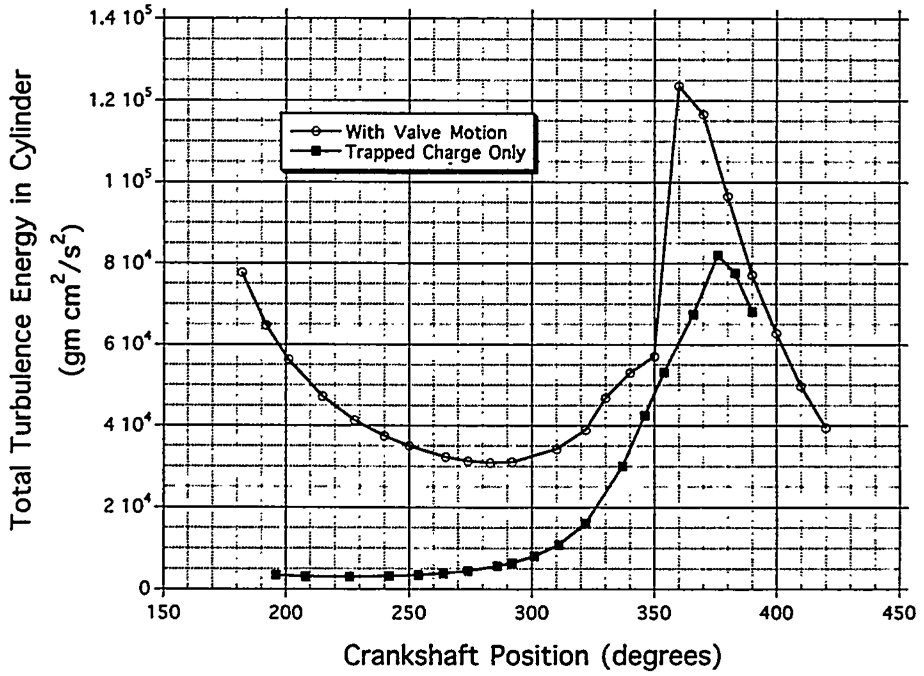


Figure 10. Total turbulent kinetic energy averaged over the cylinder.

CHEMICAL KINETIC MODELING OF H_2 APPLICATIONS

Nick M. Marinov
Charles K. Westbrook
Lawrence D. Cloutman
William J. Pitz
Lawrence Livermore National Laboratory
Livermore, CA 94550

Abstract

Work being carried out at LLNL has concentrated on studies of the role of chemical kinetics in a variety of problems related to hydrogen combustion in practical combustion systems, with an emphasis on vehicle propulsion. Use of hydrogen offers significant advantages over fossil fuels, and computer modeling provides advantages when used in concert with experimental studies. Many numerical "experiments" can be carried out quickly and efficiently, reducing the cost and time of system development, and many new and speculative concepts can be screened to identify those with sufficient promise to pursue experimentally. This project uses chemical kinetic and fluid dynamic computational modeling to examine the combustion characteristics of systems burning hydrogen, either as the only fuel or mixed with natural gas. Oxidation kinetics are combined with pollutant formation kinetics, including formation of oxides of nitrogen but also including air toxics in natural gas combustion. We have refined many of the elementary kinetic reaction steps in the detailed reaction mechanism for hydrogen oxidation. To extend the model to pressures characteristic of internal combustion engines, it was necessary to apply theoretical pressure falloff formalisms for several key steps in the reaction mechanism. We have continued development of simplified reaction mechanisms for hydrogen oxidation, we have implemented those mechanisms into multidimensional computational fluid dynamics models, and we have used models of chemistry and fluid dynamics to address selected application problems. At the present time, we are using computed high pressure flame and auto-ignition data to further refine the simplified kinetics models that are then to be used in multidimensional fluid mechanics models. Detailed kinetics studies have investigated hydrogen

flames and ignition of hydrogen behind shock waves, intended to refine the detailed reactions mechanisms. Numerical studies of hydrogen oxidation under extremely fuel-lean conditions have been coupled to thermal (i.e., Zeldovich mechanism) theories of production of oxides of nitrogen (No_x). Studies being initiated include examinations of preignition or knock in hydrogen-fueled internal combustion engines development of simplified kinetic ignition submodels to predict knock and extensions of global kinetics models for hydrogen oxidation to elevated pressures. We have also continued to use kinetic modeling techniques to examine the combustion properties of mixtures of hydrogen with gaseous hydrocarbon fuels, especially natural gas.

Introduction

The public concern for improved urban air quality, finite fossil fuel resources, and global warming trends support the need for a clean burning alternative fuel. Hydrogen is an attractive alternative fuel, because it does not produce CO_2 greenhouse gas, offers the potential of reduced NO_x pollutant emissions, can enhance fuel economy when used in hydrocarbon mixtures and is virtually limitless in supply.

Hydrogen as a fuel is unique because of its simple oxidation kinetics, very fast mass diffusivity and low molecular weight. Interestingly, all chemical reactions that consume molecular hydrogen in the H_2 - O_2 system produce atomic hydrogen which is an extremely reactive and diffusive species. The hydrogen atom is the most important radical needed for flame propagation and ignition in virtually all combustion systems.

In this report, the reaction kinetics for hydrogen combustion which is suitable for treating flame propagation, flame composition measurements and ignition delay times. A detailed reaction mechanism was developed and validated against laminar flame speeds for a wide range of hydrogen - air stoichiometries, flame structure measurements of a low pressure rich H_2 / O_2 / Ar laminar flame and shock tube ignition delay times near the second explosion limit. In addition, a one-step global rate expression for the single step reaction $H_2 + 1/2\ O_2 = H_2O$ was developed and validated against laminar flame speed data.

Program Goals

There are two major approaches to combustion modeling in practical systems. In the first approach, the physical geometry of the combustion system is simplified to deal with a zero or one-dimensional formulation. This makes it possible then to deal in great detail with selected subprocesses, including the detailed chemical kinetics of fuel oxidation, NO_x production and pollutant emission. On the other hand, it is also possible to simplify the detailed chemical and physical process submodels and deal in detail with the multidimensional fluid mechanics. Both approaches have been used extensively in the past to study combustion in practical systems, including particularly internal combustion engines. In the present program, both approaches are being pursued, using current models for complex chemical kinetics and multidimensional fluid mechanics. Additionally, we have begun to combine both features together and carry out model analyses on a scale that was not possible previously.

With both of these approaches in mind, the work to be done at LLNL will provide kinetic and fluid mechanical models that will both advance our current capabilities and will also address specific applications problems. In the area of simplified fluid mechanics modeling, we will examine a number of problems associated with hydrogen oxidation. We will also develop and apply simplified kinetic submodels for use within complex fluid mechanics models.

Kinetics Studies

The detailed kinetic models are being developed to calculate the laminar flame speed of hydrogen-air mixtures. Flame speed is a major factor in determining the burn rate in an engine. Also the detailed models allow the prediction of the autoignition characteristics of the H2-air mixture which determines whether a mixture will autoignite and produce knock in an engine. The detailed kinetic models are also being used to develop simplified kinetic models for hydrogen and hydrocarbon/hydrogen mixture. It is recognized that such simplified submechanisms are needed to deal with real chemistry and real fluid mechanics.

Detailed reaction mechanism

The detailed reaction mechanism used in this study is given in Table 1. The reverse rate constants are calculated from the forward rate constants through the equilibrium rate constants derived from the CHEMKIN thermochemical database [11]. The chemical kinetic reaction rates used for the H_2 - O_2 chain branching/propagating submechanism (reactions 1- 4) are well known and are considered to be accurate to within a factor of 1.5 for the 300K-2500K temperature range. The H_2 - O_2 dissociation/recombination reactions have been critically reviewed by Dixon-Lewis [5] and, Tsang and Hampson [6]. Reactions 5, 6, and 8 are accurate to within a factor of 2, and reaction 7 is accurate to a factor of 10. Greater uncertainty in the kinetics exists for those reactions which form or consume HO_2 radicals and H_2 - O_2. A detailed review of the chemical kinetics literature was performed to critically evaluate these reactions.

Table 1: H_2 / O_2 / N_2 / Ar Reaction Mechanism

Units are cm^3 - mole - sec - kcal - K

$k = A\,T^n \exp(-E_a/RT)$

No.	Reaction	DH°_{298K}	A_{fwd}	n_{fwd}	$E_{a,fwd}$	Reference
1.	$O + OH = O_2 + H$	-16.77	2.02E+14	-0.40	0.0	Masten et al. [1]
2.	$OH + H_2 = H + H_2O$	-15.01	2.14E+08	1.52	3.449	Michael et al. [2]
3.	$OH + OH = O + H_2O$	-16.88	3.57E+04	2.40	-2.112	Wooldridge et al. [3]
4.	$O + H_2 = OH + H$	1.85	5.06E+04	2.67	6.290	Sutherland et al. [4]
5a.	$H + H + M = H_2 + M^{a,b}$	-104.2	1.00E+18	-1.00	0.000	Dixon-Lewis [5]
5b.	$H + H + H_2 = H_2 + H_2$	-104.2	9.27E+16	-0.60	0.000	Dixon-Lewis [5]
5c.	$H + H + H_2O = H_2 + H_2O$	-104.2	6.00E+19	-1.25	0.000	Dixon-Lewis [5]
6.	$O + O + M = O_2 + M$	-119.1	1.89E+13	0.00	-1.788	Tsang et al. [6]
7.	$O + H + M = OH + M$	-102.3	4.71E+18	-1.00	0.000	Tsang et al. [6]
8.	$H + OH + M = H_2O + M$	-119.2	2.21E+22	-1.25	0.000	Tsang et al. [6]
9a.	$H + O_2 + M = HO_2 + M^c$	-49.6	$k_o = 1.05E+19\ T^{-1.257}$			Compiled Fit [d,e]
			$k_o = 4.517E+13$			Cobos et al. [7]
9b.	$H + O_2 + H_2 = HO_2 + H_2$	-49.6	$k_o = 1.52E+19\ T^{-1.133}$			Compiled Fit [d,f]
			$k_o = 4.517E+13$			Cobos et al. [7]
9c.	$H + O_2 + N_2 = HO_2 + N_2$	-49.6	$k_o = 2.031E+20\ T^{-1.590}$			Compiled Fit [d,f]
			$k_o = 4.517E+13$			Cobos et al. [7]
9d.	$H + O_2 + H_2O = HO_2 + H_2O$	-49.6	$k_o = 2.10E+23\ T^{-2.437}$			Compiled Fit [d]
			$k_o = 4.517E+13$			Cobos et al. [7]
10.	$HO_2 + H = H_2 + O_2$	-54.6	8.45E+11	0.65	1.241	Compiled Fit [d]
11.	$HO_2 + H = OH + OH$	-35.97	1.50E+14	0.00	1.000	Warnatz [8]
12.	$HO_2 + H = O + H_2O$	-52.85	3.01E+13	0.00	1.721	Baulch et al. [9]
13.	$HO_2 + O = OH + O_2$	-51.73	3.25E+13	0.00	0.000	Baulch et al. [9]
14.	$HO_2 + OH = H_2O + O_2$	-69.61	2.89E+13	0.00	-0.497	Baulch et al. [9]
15.	$HO_2 + HO_2 = H_2O_2 + O_2$	-37.53	k = 4.20E+14exp(-11.98/RT) + 1.30E+11exp(+1.629/RT)			Hippler et al. [10]
16.	$OH + OH + M = H_2O_2 + M^g$	-51.14	$k_o = 1.24E+14\ T^{-0.37}$			Compiled Fit [d]
			$k_o = 3.041E+30T^{-4.63}\exp(-2.049/RT)$			
	Troe Parameters / a=0.47 T***=100. T*=2000. T**=1.E+15 /					
17.	$H_2O_2 + H = H_2O + OH$	-68.05	3.07E+13	0.00	4.217	Baulch et al. [9]
18.	$H_2O_2 + H = HO_2 + H_2$	-17.07	1.98E+06	2.00	2.435	Compiled Fit [d]
19.	$H_2O_2 + O = OH + HO_2$	-15.20	9.55E+06	2.00	3.970	Tsang et al. [6]
20.	$H_2O_2 + OH = H_2O + HO_2$	-32.08	2.40E+00	4.042	-2.162	Compiled Fit [d]

a) $[M] = \hat{A}\, e_i\, [c_i]$ where e_i represents the chaperon efficiency and $[c_i]$ represents the concentration of the i^{th} species. b) $e_{H2} = 0.0$; $e_{H2O} = 0.0$ and all other species have efficiencies equal to unity.

c) $e_{H2} = 0.0$; $e_{H2O} = 0.0$; $e_{N2} = 0.0$ and all other species have efficiencies equal to unity.

d) See text for description of the reaction rate expression fit. e) See Figure 1 f) See Figure 2

g) Troe fall - off reaction form: $F_{cent} = (1 - a) \exp(-T/T^{***}) + a \exp(-T/T^{*}) + \exp(-T^{**}/T)$

In figures 1 and 2, the $H + O_2 + M = HO_2 + M$ (M = any third body) reaction was evaluated over the 300K - 2500K temperature range. The $H + O_2 + M = HO_2 + M$ (M = Ar) reaction was primarily fit to the measurements of Wong and Davis [12], Carleton et al. [13], Hsu et al. [14], Pirraglia et al. [15], Gay and Pratt [16], and Pamidimukkala and Skinner [17]. The $H + O_2 + H_2 = HO_2 + H_2$ reaction was fitted to the data of Nielsen et al. [18] and Kochubei and Moin [19]. The $H + O_2 + N_2$

$= HO_2 + N_2$ reaction was fitted primarily to the studies of Hsu et al. [14], Slack [20] and Peeters et al. [21]. These resulting fits are within the uncertainty factor of three prescribed to the Baulch recommended rates involving these reactions for the 300K - 2000K temperature range [9]. The kinetic rate applied to the $H + O_2 + H_2O = HO_2 + H_2O$ reaction was derived from using the fitted rate of reaction 9a and then using the Hsu et al. [14] relation of $k_{H2O} / k_{He} = 23.9\ (T / 300)^{-1.18}$ (assuming $M = He = Ar$) for the 298K - 635K temperature range. Discrepancies in the literature values for third body efficiencies of H_2O at temperatures greater than 1000K makes the kinetic rate for reaction 9d suspect to error. However, the fitted kinetic rate for this reaction agrees, to within a factor of two, with the Baulch recommendation in the 1000K - 2000K temperature range.

The kinetic rate for $H + HO_2 = H_2 + O_2$ was fitted to the low temperature measurements of Keyser [22], intermediate temperature measurements of Baldwin and Walker [23], and to the reverse rate of this reaction at high temperatures as determined by Koike [24]. The $OH + OH (+M) = H_2O_2 (+M)$ reaction was fitted by using a complex set of rate parameters in the Troe fall-off formulation [25]. This complex fit was validated against the experimental measurements of Zellner et al. [26], Troe [27,28], Brouwer et al. [29] and Basevich et al. [30]. The $H_2O_2 + H = HO_2 + H_2$ reaction was fitted to a T^2 expression (analogous to the H-atom abstraction reaction $H_2O_2 + O = OH + HO_2$) by using the data of Albers et al. [31], and Baldwin and Walker [23]. The $H_2O_2 + OH = H_2O + HO_2$ reaction was primarily fitted to the measurements of Hippler and Troe [32], Baldwin et al. [33,34], Kurylo et al. [35], and Keyser [36].

Laminar Flames and Shock Tube Ignition

Reaction Kinetics of H_2 - Air Laminar Flame Speeds

Recent experimental data [37 - 44] for the laminar flame speed (S_L) of atmospheric H_2 / Air mixtures have been compiled and are shown in figures 3 and 4. In figure 3, a ~70cm/sec variation in S_L around F (H_2 fuel to air equivalence ratio) of 1.4 is exhibited, while in figure 4, considerable scatter by as much as ~60cm/sec in S_L is found for lean hydrogen mixtures. The observed discrepancies in the H_2 / Air laminar flame speeds is due to aerodynamic flame strain (or stretch). Aerodynamic flame strain is caused by preferential mass and thermal diffusion, and flow divergence [45,46]. Experimental data uncorrected for these effects represent a strain dependent flame speed and *not* the true (strain-free) laminar flame speed (S_L). This study has modeled the flame strain corrected experimental data for H_2 / Air laminar flame speeds at one atmosphere. A one-dimensional, premixed, laminar flame code (PREMIX) [47] was used to perform the computations with the detailed $H_2 / O_2 / N_2 / Ar$ mechanism and transport [48]. All calculations were performed using multi-component mass transport and thermal diffusion.

Numerical calculations show good agreement with the experimental laminar flame speed data for the full range of hydrogen-air stoichiometries (figure 3). A laminar flame speed maximum of 300 cm/sec at an equivalence ratio of 1.6 and atmospheric pressure was calculated, also in agreement with the measured data. In addition, computations performed at equivalence ratios of 0.30, 1.0 and 4.0

predict flame speed values of 5.9 cm/sec, 210 cm/sec, and 144 cm/sec, all of which are good.

A sensitivity analysis of the important chemical reactions which influence the mass burning rate (or the laminar flame speed) was performed at equivalence ratios of 0.6, 1.0 and 1.4. The results are shown in figure 5. The normalized sensitivity coefficient was calculated through the expression,

$$(A_i / m_L) (\Delta m_L / \Delta A_i) \qquad (1)$$

where A_i is the pre-exponential factor of the i^{th} reaction rate expression and m_L is mass burning rate (where $m_L = r_u S_L$, r_u is the unburned gas density). The results show that the dominant reactions promoting flame propagation are the chain reactions $OH + H_2 = H_2O + H$, $O + OH = O_2 + H$ and $O + H_2 = OH + H$, and the HO_2 consumption reaction $HO_2 + H = OH + OH$. The dominant reaction retarding flame propagation is $HO_2 + H = H_2 + O_2$.

As the H_2 / Air stoichiometry goes from rich to lean, the laminar flame speed becomes more sensitive to $OH + O = O_2 + H$ and reactions involving the HO_2 radical. The forward reaction in $H + O_2 = OH + O$ is endothermic and therefore its chemical kinetic rate is especially sensitive to temperature changes as hydrogen mixtures become leaner. The HO_2 radical, primarily produced by $H + O_2 + M = HO_2 + M$ (M = any third body), competes with the $H + O_2 = O + OH$ reaction for the H-atom. At ultra-lean conditions (F less than 0.5), reactions involving the HO_2 radical become very important. For example, the $H + O_2 + M = HO_2 + M$ reaction competes with $H + O_2 = OH + O$ for H-atom thereby strongly influencing the OH radical pool for the main H_2 consumption reaction $OH + H_2 = H_2O + H$, and/or the $H + HO_2 = OH + OH$ reaction can convert an unreactive HO_2 radical to a reactive OH thereby promoting the chain propagating reaction $OH + H_2 = H_2O + H$. As indicated in figure 5, the highest sensitivity coefficient calculated was for the $OH + H_2 = H_2O + H$ reaction at F = 0.6 and this reaction is most important for flame propagation at lean conditions.

Global kinetics

While detailed reaction mechanisms provide insight into flame structure and reactivity of gas mixtures, there is a great need for one-step global kinetics for use in complex fluid mechanics codes that utilize two- to three-dimensional geometry. The computational effort of using detailed kinetics in such models is not practical. Therefore, a one-step overall reaction was developed and validated against laminar flame speed data. The global reaction study made use of the HCT code [49] for the laminar flame speed computations. The global reaction rate parameters were varied in order to obtain good agreement between computed and experimentally observed flame speeds. The global rate expression for hydrogen-air laminar flame speeds was determined to be

$$k_{global} = 1.8x10^{13} \exp(-17614K / T) [H_2]^{1.0}[O_2]^{0.5} \qquad (2)$$

for the single step reaction $H_2 + 1/2\ O_2 = H_2O$.

Figures 3 and 4 shows the comparison of the experimentally measured laminar flame speeds with the computed ones using the global reaction model. The predicted flame speed well represented the experimental data for only the 0.55 - 1.1 equivalence ratio range. Predictions by the global reaction model were considered poor outside this equivalence ratio range. The poor prediction is attributed to chemical and thermal structure changes in the flame as the stoichiometry varies which could not be properly accounted for in the global reaction model.

Reaction Kinetics of a Low Pressure Rich Hydrogen-Oxygen-Argon Flame

While comparison with laminar flame speed data is a valuable test of a detailed reaction mechanism, a more demanding validation method is to compare experimental flame structure data with numerical computations. The structure of a low pressure rich H_2 /O_2 /Ar laminar flame investigated by Vandooren and Bian [50] was used to validate the chemical kinetic model. These experimental measurements were performed at a pressure of 35.5 torr (0.047 atm) which differed from the laminar flame speed measurements performed at 1 atmosphere. This large difference in pressure allowed the two body reactions in the detailed mechanism to be tested at these conditions.

The experimental data were obtained using a premixed, flat flame burner. The composition of the incoming reactants was 39.7% H_2, 10.3% O_2 and 50% Ar (equivalence ratio of 1.91) and had an in flow velocity of 131 cm/sec. Flame structure measurements were performed by molecular beam sampling with a mass spectrometer. Measurement errors of the stable compounds (H_2, O_2, H_2O) were estimated to be ~2% and for radicals (OH, O-atom, H-atom) ~10%. Computations were performed using the PREMIX code with the measured temperature profile as given in the reference [50].

Figure 6 shows the comparison of the experimental mole fraction profiles of the stable species with the computed ones. The predicted molecular hydrogen profile agreed very well with the measured profile. About 40% of the initial hydrogen was predicted to remain in the burnt gases, in good agreement with the experimental results. as supported by the model prediction. The predicted profile for the molecular oxygen mole fraction agreed well with the data. However, there exists some discrepancy between the model and the experimental data for O_2 in the preheating zone of the flame close to the burner. The experimental and computed maximum concentrations of water were identical and both profiles exhibited the same gradient of H_2O formation. If the experimental profile for water was shifted by approximately 0.5 mm towards the burner surface, better agreement would result. Reaction flux analysis was applied to this flame and determined that H_2 was destroyed a factor of two faster by reaction 2 than reaction 4. The O_2 was primarily removed by reaction 1 with secondary reactions 9a and 9b playing a minor role. Water was formed exclusively from reaction 2.

Figure 7 shows the comparison of the experimental mole fraction profiles of the radical species with the computed ones. For all three radical species, the model predictions are somewhat higher than the measured values. The computed profile for the hydroxyl radicals exhibited the same profile behavior as the experimental measurements, however the detailed kinetic model overestimated the hydroxyl concentration by a factor of 1.75 - 2.0 at the peak OH level and in the post-flame zone. The location of the predicted maximum for the O-atom corresponds well with experimental data. The model overpredicted the O-atom concentration by a factor of 1.7 - 2.0 in the flame and post-flame zones. The model overpredicted the H-atom concentration by ~60% at the peak H-atom level and predicted to within a factor of two the H-atom concentration in the post-flame zone. Model predictions for the radical species were worse in the preheat zone of the flame with the H-atom overpredicted by a factor of five. The HO_2 concentration was not measured in this flame but the model predicted a peak HO_2 mole fraction of 7.5E-6 at ~0.05mm downstream from the burner surface. Reaction flux analysis was applied to this flame and determined that the OH radical was primarily produced by reactions 1 and 4 and destroyed by reaction 2, while in the preheat zone OH was also formed by reaction 11. The O-atom was produced by reaction 1 and destroyed by reaction 4. The H-atom was produced a factor of two faster by reaction 2 than reaction 4, while H-atom was removed by reaction 1. The HO_2 radical was formed a factor of two faster by reaction 9b than reaction 9a, while reaction 11 consumed HO_2 a factor of three faster than reaction 10.

The predicted stable species profiles agreed very well with the measured profiles. However, the H. O, and OH radical concentration was overpredicted by approximately a factor of two. This study did not consider wall destruction of the free radicals within the sample probe which could explain the discrepancy between the numerically predicted and experimentally measured free radical concentration.

Reaction Kinetics of Shock Tube Ignition Delay Times

It is essential to validate the chemical kinetic model at pressures above one atmosphere because the gases in the combustion chamber of an internal combustion engine are at elevated pressures which affect the reaction rate. The shock tube experimental data of Slack [20] were used to test the present $H_2/O_2/N_2/Ar$ mechanism for ignition delay near the second explosion limit. Stoichiometric hydrogen-air mixtures were heated by reflected shock waves at 2 atmospheres and for the 980K - 1176K reflected shock temperature range. Numerical simulations were performed with the SENKIN code [51] assuming that the gas dynamics behaves in an adiabatic constant volume process.

In figure 8, the ignition delay data of Slack are compared to the numerical computations. For temperatures below ~1025K, the experimental ignition delay times become significantly longer as the experimental conditions approach the second explosion limit (classically defined as $2\ k_{rev,1} /\ k_{9a,b,c,d} = [M]$). The detailed chemical model predicted the same behavior. For temperatures above ~1100K, the ignition delay time is shorter and is predicted correctly by the model.

A sensitivity analysis of the important chemical reactions which influence the ignition delay time was conducted at temperatures of 1000K and 1111K. The results are shown in Table 2. In the sensitivity analysis, the pre-exponential factor, A, for each reaction was perturbed upward by a factor of 2 while maintaining the same equilibrium rate constant. The ignition delay was then computed at the same experimental conditions as the baseline case. The sensitivity coefficient values shown in Table 2 are represented by the expression:

$$\ln\left(t_{ign}(\text{perturbed}) / t_{ign}(\text{baseline})\right) \qquad (3)$$

Table 2: Sensitivity Analysis of Computed Ignition Delay Times

		$\ln(t_{ign}(\text{perturbed}) / t_{ign}(\text{baseline}))$	
No.	Reaction	1000K	1111K
9b.	$H + O_2 + H_2 = HO_2 + H_2$	3.03	0.18
9c.	$H + O_2 + N_2 = HO_2 + N_2$	3.03	0.18
1.	O + OH = O2 + H	-1.67	-0.61
9a.	$H + O_2 + M = HO_2 + M$	0.48	0.04
11.	$HO_2 + H = OH + OH$	-0.13	-0.02
4.	$O + H_2 = OH + H$	-0.09	-0.08
10.	$HO_2 + H = H_2 + O_2$	0.08	-0.02
8.	$H_2O_2 + H = HO_2 + H_2$	-0.03	0.00
2.	$OH + H_2 = H + H_2O$	-0.02	-0.02
12.	$HO_2 + H = O + $ H2O	-0.02	-0.01
13.	$HO_2 + O = O_2 + OH$	0.01	0.00

A positive coefficient denotes an increase in the ignition delay time and a negative coefficient denotes a decrease in ignition delay. An inspection of Table 2 shows that the chain branching reaction 1 and the chain terminating reactions 9a, 9b and 9c [52] are, as expected, of greatest importance. An increase of a factor of two in the chemical kinetic rate of reactions 9b and 9c resulted in a factor of ~20 increase to the ignition delay time at 1000K. The uncertainty factor associated with these reactions is a factor of three for the 300K - 2000K temperature range [9]. The perturbed change in the kinetic rate for $H+O_2+M = HO_2+M(M = N_2,H_2)$ is well within the uncertainty factor established for this reaction and demonstrates the need for further kinetic rate studies involving this important chain terminating process. The $O + OH = O_2 + H$ reaction showed a factor of ~5 decrease in the ignition delay time at 1000K and its kinetic rate is relatively well-known. For temperatures at 1111K, reaction 1 exhibited the highest sensitivity to the ignition delay time with reactions 9b and 9c showing a minor influence at this higher temperature.

Although the ignition delay time is very sensitive to reactions 1, 9a, 9b, and 9c, this study also examined the sensitivity of the ignition delay times to other reaction rates. Chain reactions such as $O + H_2 = OH + H$ and $H + HO_2 = OH + OH$ reduce ignition delay by producing reactive radicals OH and H. The $H + HO_2 = H_2 + O_2$ reaction is chain terminating at 1000K as it consumes a reactive H-atom plus an unreactive HO_2 radical to make stable products. However, at 1111K, the reverse rate of this reaction begins to become important as the reactants H_2 and O_2 produce H and HO_2 radicals at these very short residence times.

Fluid Mechanics Models

We are studying a variety of applications in which the chemical kinetics must be simplified in order to consider the computational needs of the fluid mechanics model. Simulations of hydrogen combustion in automotive engines, industrial burners, and other practical systems often require full three-dimensional modeling treatments, although some types of devices may possess enough symmetry to permit two-dimensional treatment. In either case, the computational needs of the fluid dynamics portion of the model alone are considerable, and it is not yet possible in most cases to also include a full chemical kinetic submodel, even for hydrogen oxidation. In such models, it is possible to develop and use a single or global reaction submodel that provides a reasonably accurate description of the overall rate of heat release. We have developed such submodels in the past for a range of hydrocarbon fuels [54] which have then been incorporated into large-scale combustion models [55], and we are repeating that process for hydrogen. The global reaction rate parameters must be properly evaluated in order to reproduce the stoichiometric laminar burning velocity as well as its variation with equivalence ratio, pressure, and unburned fuel/air temperature.

Since the detailed chemical kinetic reaction mechanism for hydrogen is quite simple, consisting of only eight chemical species (H, H_2, O, O_2, OH, H_2O, HO_2 and H_2O_2), there are some applications for which a full CFD and detailed chemical kinetic treatment may be feasible. For example, if an axisymmetric burner model requiring only two spatial dimensions were combined with a kinetic model that perhaps omitted the minor species HO_2 and H_2O_2, selected model calculations could be carried out in order to determine quantities of interest. As models are converted to use massively parallel computers or clusters of workstations, this type of calculation will gradually become more realistic.

The COYOTE two-dimensional fluid dynamics program [56] has been used as a testbed for a new chemistry package developed from the HCT program [49]. HCT is a one-dimensional Lagrangian fluid dynamics program with a sophisticated chemistry package capable of simulating reactive flows with chemical mechanisms of arbitrary levels of complexity. We modified HCT by removing the fluid mechanics and wrote a short subprogram to interface the resulting chemistry package to COYOTE. This combined program gives us a new capability to simulate two-dimensional, in-cylinder combustion with detailed kinetics.

We have begun testing of the combined program with a detailed kinetics mechanism for hydrogen oxidation. The first problem we solved was a one-dimensional planar laminar flame. The pressure is one atmosphere, the initial temperature is 298 K, and the mixture is stoichiometric. The test kinetics mechanism includes 9 species and 17 reactions. A number of numerical difficulties peculiar to hydrogen occurred. Due to the high flame speed, which is driven by high reaction rates, the time step had to be reduced by over two orders of magnitude compared with those used by global mechanisms for typical hydrocarbon fuels. For reasons not yet completely understood, hydrogen flames seem to require significantly more spatial resolution than hydrocarbons. Furthermore, the numerical solution exhibited significant levels of acoustic waves that are negligible for hydrocarbons. In spite of these difficulties, the predicted flame speed of 208 cm/s is in excellent agreement with experiments.

We have begun a two-dimensional simulation of a hydrogen flame in a constant-volume combustion vessel using the detailed kinetics mechanism from the one-dimensional flame. This solution has not yet been completed.

Summary

Detailed and global chemical kinetics for hydrogen-air mixtures have been validated against data derived from flame propagation, flame structure and shock tube ignition delay time studies. The chemical kinetic mechanism for the detailed reaction model was critically reviewed and well-simulated the experimental measurements. A global rate expression validated against hydrogen-air laminar flame speeds was developed for the single step reaction $H_2 + 1/2\ O_2 = H_2O$.

A two-dimensional fluid dynamics program with detailed chemical kinetics has been developed and tested on a 1-D laminar flame. A 2-dimensional, constant volume combustion problem for hydrogen is the process of being solved.

Acknowledgments

This work is supported by the U. S. Department of Energy, Office of Utility Technology, and was carried out under the auspices of the U. S. Department of Energy by the Lawrence Livermore National Laboratory under contract No. W-7405-ENG-48.

References

1. Masten, D.A.; Hanson, R.K.; and Bowman, C.T.: J. Phys. Chem., 94, 7119, 1990.
2. Michael, J.V.: Prog. Energy Comb. Sci., 18, 327, 1992.
3. Wooldridge, M.S.; Hanson, R.K., and Bowman, C.T.: Int. J. Chem. Kin.,26, 389, 1994.
4. Sutherland, J.W.; Patterson, P.M.; and Klemm, R.B.: J. Phys. Chem.,94 ,2471 ,1990.
5. Dixon-Lewis, G.: Archivum Combustionis, 4, 279, 1984.
6. Tsang, W.; and Hampson,R.F.: J. Phys. Chem. Ref. Data, 15, 1095, 1986.
7. Cobos,C.J.; Hippler, H.; and Troe, J.: J. Phys. Chem., 89, 342, 1985.
8. Warnatz, J.: *In Combustion Chemistry*; (Gardiner, W.C., Ed.); Chapter 5,Springer-Verlag, 1984.
9. Baulch, D.L.; Cobos, C.J.; Cox,R.A.; Esser, C.; Frank, P.; Just, Th.; Kerr, J.A.; Pilling, M.J.; Troe, J.; Walker, R.W.; and Warnatz, J.: J. Phys. Chem. Ref. Data, 21, 411, 1992.
10. Hippler, H.; Troe, J. ; and Willner, J.: J. Chem. Phys., 93, 1755, 1990.
11. Kee, R.J.; Rupley, F.M.; and Miller, J.A.: Sandia National Laboratory, Albuquerque, N.M., SAND87-8215B, 1987.
12. Wong, W.; and Davis, D.D.: Int. J. Chem. Kin., 6, 401, 1974.
13. Carleton, K.L.; Kessler, W.J.; and Marinelli, W.J.: J. Phys. Chem., 93, 1018, 1989.
14. Hsu, K.J.; Anderson, S.M.; Durant, J.L.; and Kaufman, F.: J. Phys. Chem., 93, 282, 1989.
15. Pirraglia, A.N.; Michael, J.V.; Sutherland, J.W.; and Klemm, R.B.; J. Phys. Chem., 93, 282, 1989.
16. Gay, A.; and Pratt, N.H.: *Proceedings of Eighth (international) Shock Tube Symposium*, Chapman and Hall, London, 39, 1971.
17. Pamidimukkala, K.M.; and Skinner, G.B.: *Thirteenth (International) Symposium of Shock Tubes and Waves*, SUNY Press: Albany, N.Y., 585, 1981.
18. Nielsen, O.J.; Sillesen, A.; Luther, K.; and Troe, J.: J. Phys. Chem., 86, 2929, 1982.
19. Kochubei, V.F.; and Moin, F.B.: Ukr. Khim. Zh., 39, 888, 1973.
20. Slack, M.W.: Comb. Flame, 28, 241, 1977.
21. Peeters, J.; and Mahnen, G.: Fourteenth Symposium (International) on Combustion, 133, The Combustion Institute, 1973.
22. Keyser, L.F.: J. Phys. Chem. , 90, 2994, 1986.
23. Baldwin, R.R.; and Walker, R.W.: Seventeenth Symposium (International) on Combustion, 525, The Combustion Institute, 1979.
24. Koike, T.: Bull. Chem. Soc. Jpn., 62, 2480, 1989.
25. Gilbert, R.G.; Luther, K.; and Troe, J.: Ber. Bunsenges. Phys. Chem., 87, 169, 1983.
26. Zellner, R.; Ewig, F.; Paschke, R.; and Wagner, H.: J. Phys. Chem., 92, 4184, 1988.
27. Troe, J.: Ber. Bunsenges. Phys. Chem., 73, 946, 1969.
28. Troe, J.: J. Chem. Soc. Faraday Trans., 90, 2303, 1994.
29. Brouwer, L.; Cobos, C.J.; Troe, J.; Dubai, H.R.; and Crim, L.L.: J. Chem. Phys., 86, 6171, 1987.
30. Basevich, V. Y.; Kogarko, S.M.; and Berezin, O.Y.: Izv. Akad. Nauk SSR, 9, 1986, 1979.
31. Albers, E.A.; Hoyerman, H.; Wagner, H.G.; and Wolfrum, J.: *Thirteenth Symposium (International) on Combustion*, 81, The Combustion Institute, 1971.
32. Hippler, J.; and Troe, J.: Chem. Phys. Lett., 192, 333, 1992.
33. Baldwin, R.R.; and Mayor, L.: Trans. Faraday Soc., 57, 1578, 1960.

34. Baldwin, R.R.; and Bratten, D.: *Eighth Symposium (International) on Combustion*, 110, The Combustion Institute, 1962.
35. Kurylo, M.; Murphy, J.; Haller, G.; and Curnett, K.: Int. J. Chem. Kin., 14, 1149, 1982.
36. Keyser, L.: J. Phys. Chem., 84, 1659, 1980.
37. Koroll, G.W.; Kumar, R.K.; and Bowles, E.M.: Comb. Flame, 94, 330, 1993.
38. Vagelopoulos, C.; Egolfopoulos, F.N.; and Law, C.K.: *Twenty-Fifth Symposium (International) on Combustion,* The Combustion Institute, 1994.
39. Berman, M.: Sandia National Laboratory, Albuquerque, N.M., SAND84-0689, 1984.
40. Takahashi, F.; Mizomoto, M.; and Ikai, S.: Alternative Energy Sources III (T. Nejat Veziroglu, Ed.), 447, Vol. 5 Nuclear Energy / Synthetic Fuels, 1983.
41. Wu, C.K.; and Law, C.K.: *Twentieth Symposium (International) on Combustion*, 1941, The Combustion Institute, 1984.
42. Dowdy, D.R.; Smith, D.B.; Taylor, S.C.; and Williams, A.: *Twenty-Third Symposium (International) on Combustion*, 325, The Combustion Institute, 1990.
43. Egolfopoulos, F.N.; and Law, C.K.: *Twenty-Third Symposium (International) on Combustion*, 333, The Combustion Institute, 1990.
44. Iijima, T.; and Takeno, T.: Comb. Flame, 65, 35, 1986.
45. Matalon, M.; and Matkowsky, B.J.: J. Fluid. Mech., 124, 239, 1982.
46. Law, C.K.: *Twenty-Second Symposium (International) on Combustion*, 1381, The Combustion Institute, 1988.
47. Kee, R.J.; Grcar, J.F.; Smooke, M.D.; and Miller, J.A.: Sandia National Laboratory, Albuquerque, N.M., SAND85-8240, 1985.
48. Kee, R.J.: Dixon-Lewis, G.; Warnatz, J.; Coltrin, M.E.; and Miller, J.A.: Sandia National Laboratory, Albuquerque, N.M., SAND86-8246, 1986.
49. Lund, C.M.: Lawrence Livermore National Laboratory Report UCRL- 52504, 1978.
50. Vandooren, J.; and Bian, J.: *Twenty-Third Symposium (International) on Combustion*, 341, The Combustion Institute, 1990.
51. Lutz, A.E.; Kee, R.J.; and Miller, J.A.: Sandia National Laboratory, Albuquerque, N.M.; SAND87-8248, 1988.
52. The HO_2 radical produced from reaction 9 exhibits very low reactivity and, therefore, reaction 9 behaves more as a chain terminating reaction than a chain propagating reaction.
53. Clyne, M.A.A.; and Thrush, B.A.: Proc. R. Soc. London, Ser. A, A275, 559, 1963.
54. Westbrook, C. K., and F. L. Dryer. 1981. "Simplified Reaction Mechanisms for the Oxidation of Hydrocarbon Fuels in Flames." Combustion Science and Technology, 27:31-43.
55. Amsden, A. A. 1993. "KIVA-3: A KIVA Program with Block-Structured Mesh for Complex Geometries." Los Alamos National Laboratory report LA-12503-MS.
56. Cloutman, L. D. 1990. COYOTE: A Computer Program for 2-D Reactive Flow Simulations, Lawrence Livermore National Laboratory report UCRL -ID-103611. Livermore, CA.

Figure Captions

FIGURE 1. An Arrhenius plot for $H + O_2 + M = HO_2 + M$ reaction, M = Ar. Data from references [12 - 17] were used to generate the curve fit.

FIGURE 2. Arrhenius plots for $H + O_2 + H_2 = HO_2 + H_2$ and $H + O_2 + N_2 = HO_2 + N_2$. Data from references [18,19] were used to generate the curve fit to $H + O_2 + H_2 = HO_2 + H_2$. Data from references [14,20,21] were used to generate the curve fit to $H + O_2 + N_2 = HO_2 + N_2$.

FIGURE 3. Hydrogen -air laminar flame speeds at 1 atmosphere and $T_u = 298K$ as a function of equivalence ratio. Equivalence ratio range is 0.15 to 6.0. Comparison between experimental data [37 - 44] (symbols) and computations (detailed model - solid line, global reaction model - dashed line).

FIGURE 4. Hydrogen -air laminar flame speeds at 1 atmosphere and $T_u = 298K$ as a function of equivalence ratio. Equivalence ratio range is 0.15 to 0.80. Comparison between experimental data [37 - 44] (symbols) and computations (detailed model - solid line, global reaction model - dashed line).

FIGURE 5. Sensitivity Analysis of hydrogen - air laminar flame speeds at 1 atmosphere and $T_u = 298K$. Normalized first order sensitivity coefficients given by (A_i / m_L) $(D m_L / D A_i)$ where A_i is the pre-exponential factor to the rate constant of the i-th reaction and m_L is mass burning rate $(m_L = r_u S_L)$.

FIGURE 6. Rich Hydrogen-Oxygen-Argon Flame [50] of the inlet composition 39.7% H_2, 10.3% O_2, and 50.0% Ar (F = 1.91 equivalence ratio), operating pressure 35.5 torr and initial velocity of 131 cm/sec. Comparison between computations (lines) and experimental data for H_2, O_2 and H_2O (symbols).

FIGURE 7. Rich Hydrogen-Oxygen-Argon Flame [50] of the inlet composition 39.7% H_2, 10.3% O_2, and 50.0% Ar (F = 1.91 equivalence ratio), operating pressure 35.5 torr and initial velocity of 131 cm/sec. Comparison between computations (lines) and experimental data for OH, O-atom and H-atom (symbols).

FIGURE 8. Ignition delay times of stoichiometric hydrogen - air at 2 atmospheres. Comparison between experimental data [20] (circles) and computations (lines).

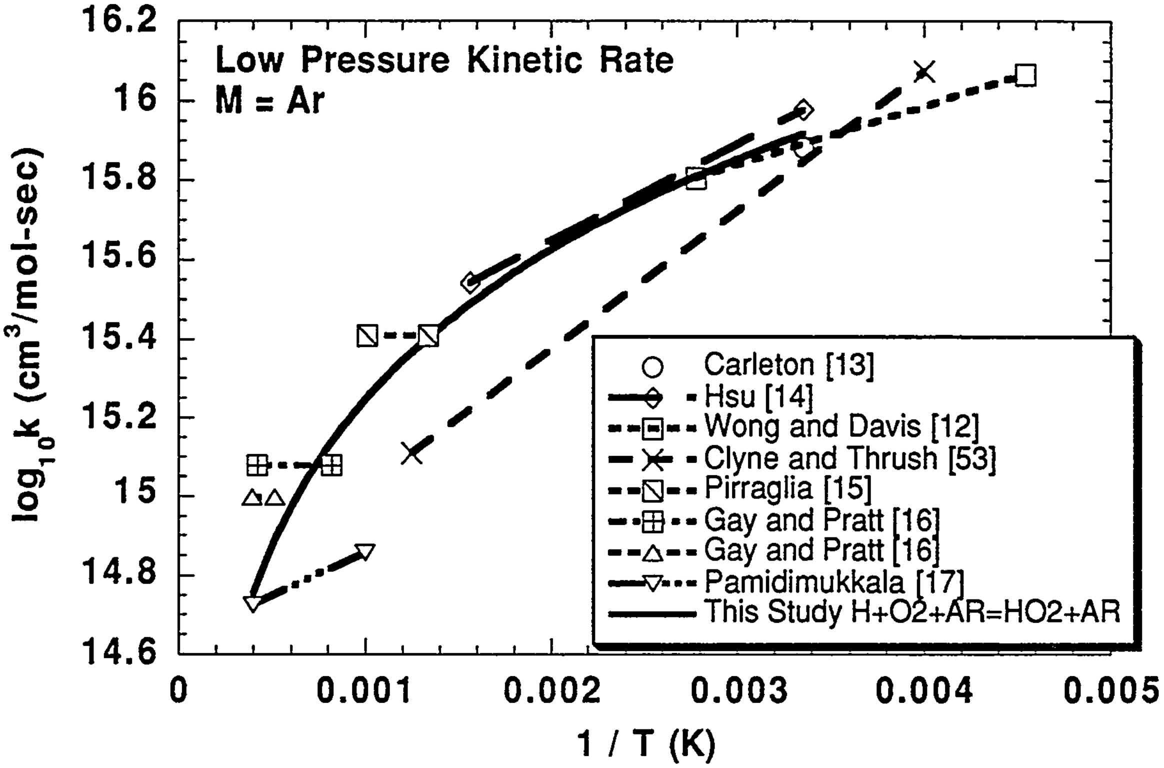
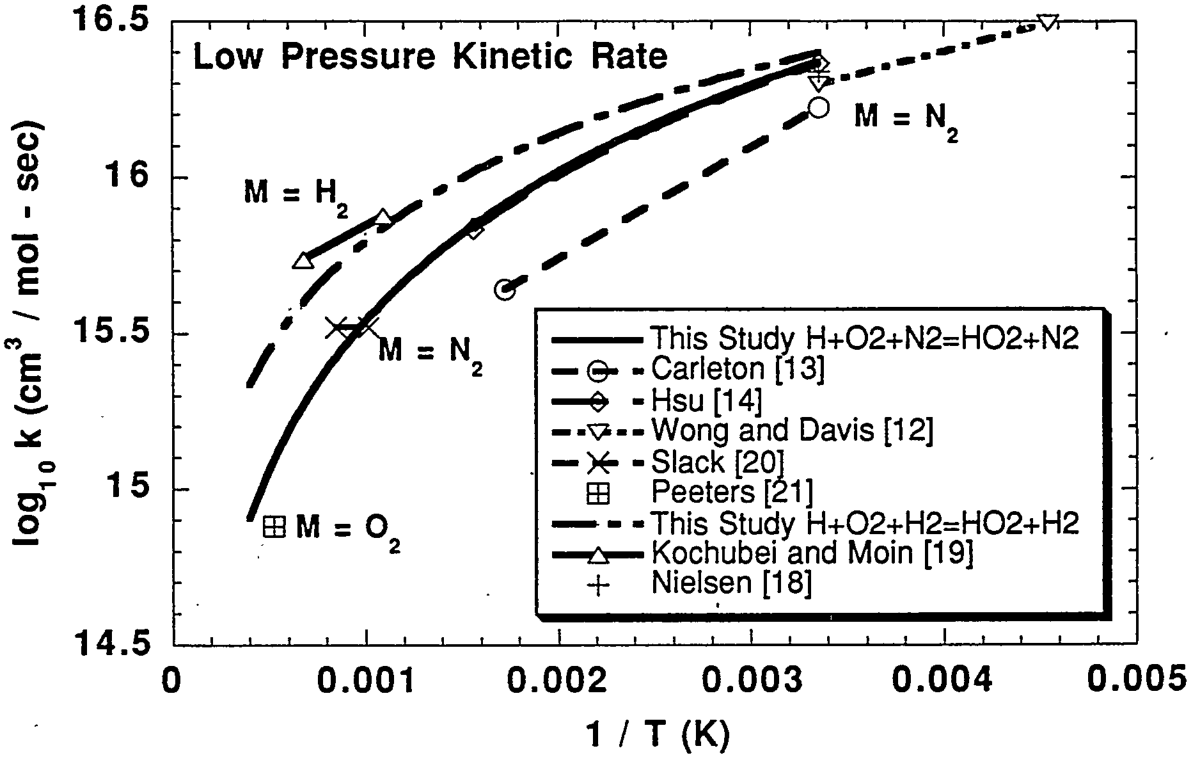
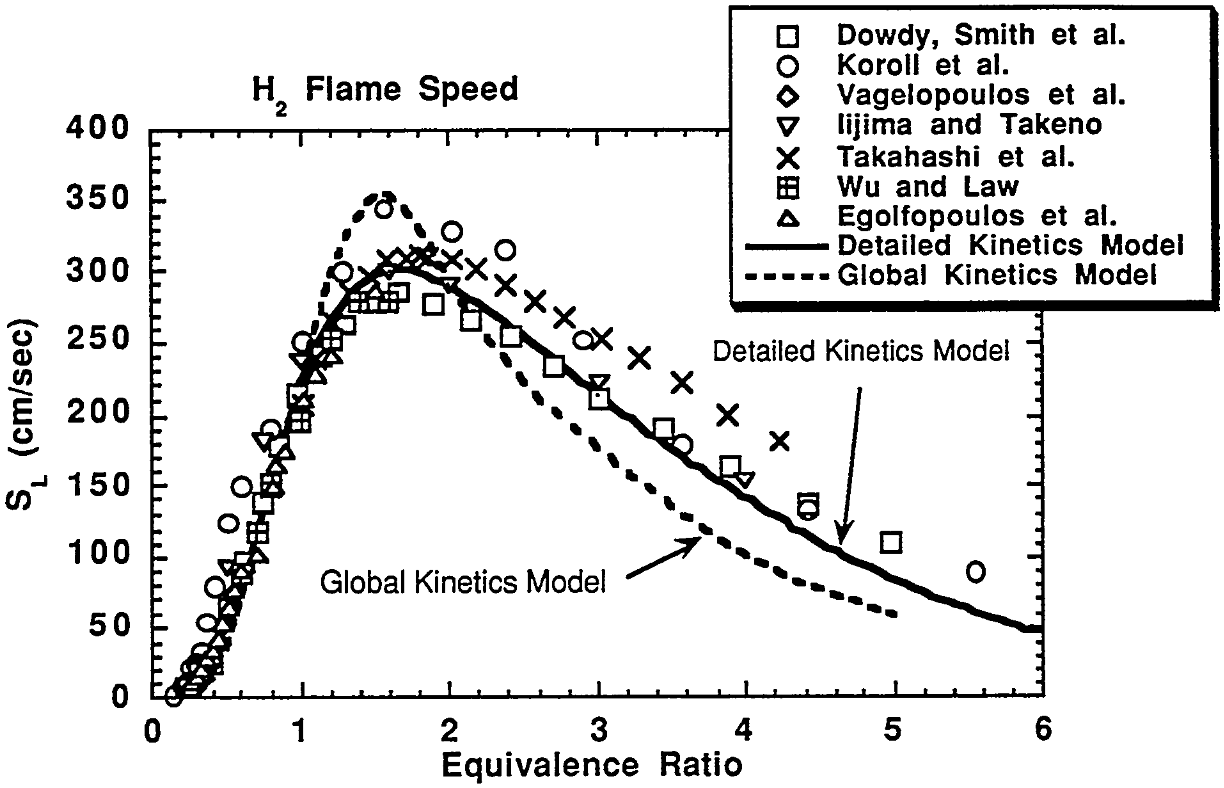

Low Pressure Kinetic Rate
M = Ar
log10k (cm3/mol-sec)
16.2
16
15.8
15.6
15.4
15.2
15
14.8
14.6
0
0.001
0.002
0.003
0.004
0.005
1 / T (K)
Carleton [13]
Hsu [14]
Wong and Davis [12]
Clyne and Thrush [53]
Pirraglia [15]
Gay and Pratt [16]
Gay and Pratt [16]
Pamidimukkala [17]
This Study H+O2+AR=HO2+AR

Fig. 1



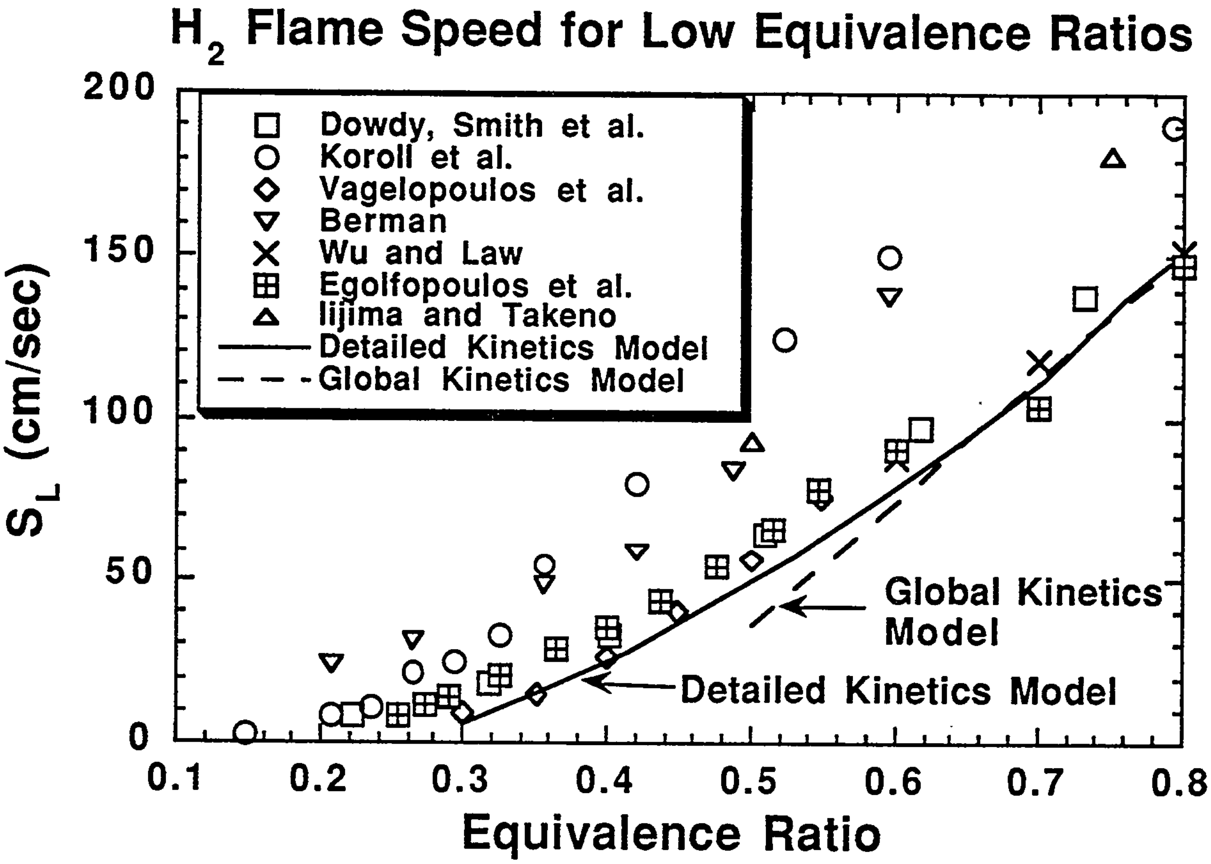
Low Pressure Kinetic Rate
M = H2
M = N2
M = N2
M = O2
This Study H+O2+N2=HO2+N2
Carleton [13]
Hsu [14]
Wong and Davis [12]
Slack [20]
Peeters [21]
This Study H+O2+H2=HO2+H2
Kochubei and Moin [19]
Nielsen [18]
16.5
16
15.5
15
14.5
0
0.001
0.002
0.003
0.004
0.005
log10 k (cm3 / mol - sec)
1 / T (K)

Fig. 2



H_2 Flame Speed
S_L (cm/sec)
400
350
300
250
200
150
100
50
0
0
1
2
3
4
5
6
Equivalence Ratio
Dowdy, Smith et al.
Koroll et al.
Vagelopoulos et al.
Iijima and Takeno
Takahashi et al.
Wu and Law
Egolfopoulos et al.
Detailed Kinetics Model
Global Kinetics Model
Detailed Kinetics Model
Global Kinetics Model

Fig. 3



H_2 Flame Speed for Low Equivalence Ratios
□ Dowdy, Smith et al.
○ Koroll et al.
◇ Vagelopoulos et al.
▽ Berman
✕ Wu and Law
⊞ Egolfopoulos et al.
△ Iijima and Takeno
Detailed Kinetics Model
Global Kinetics Model
Global Kinetics Model
Detailed Kinetics Model
S_L (cm/sec)
200
150
100
50
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
Equivalence Ratio

Fig. 4

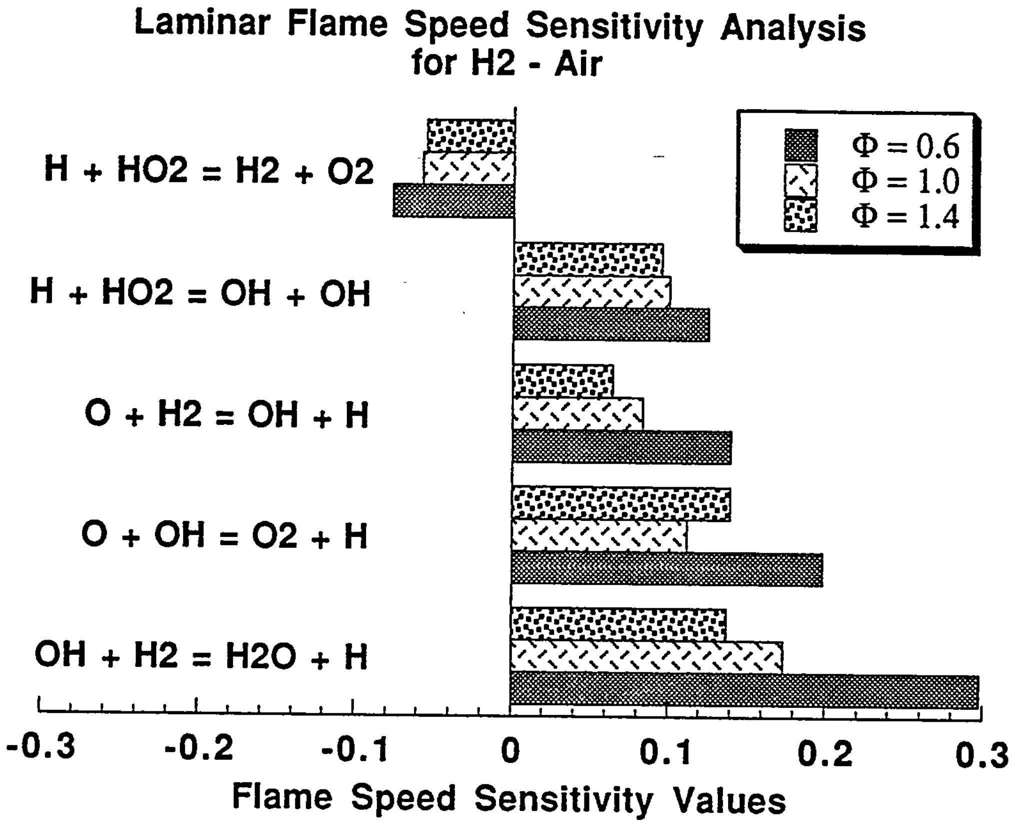
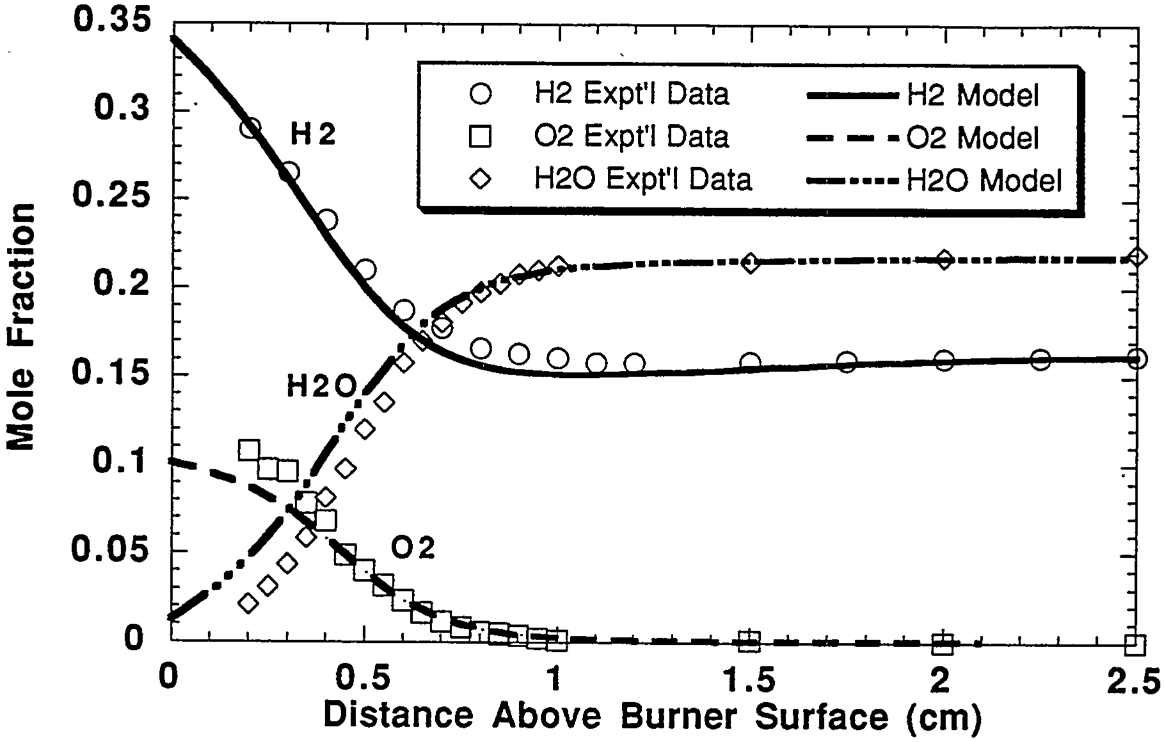

Laminar Flame Speed Sensitivity Analysis
for H2 - Air
H + HO2 = H2 + O2
H + HO2 = OH + OH
O + H2 = OH + H
O + OH = O2 + H
OH + H2 = H2O + H
Φ = 0.6
Φ = 1.0
Φ = 1.4
-0.3
-0.2
-0.1
0
0.1
0.2
0.3
Flame Speed Sensitivity Values

Fig. 5



0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
Mole Fraction
0
0.5
1
1.5
2
2.5
Distance Above Burner Surface (cm)
H2
H2O
O2
○ H2 Expt'l Data
□ O2 Expt'l Data
◇ H2O Expt'l Data
H2 Model
O2 Model
H2O Model

Fig. 6

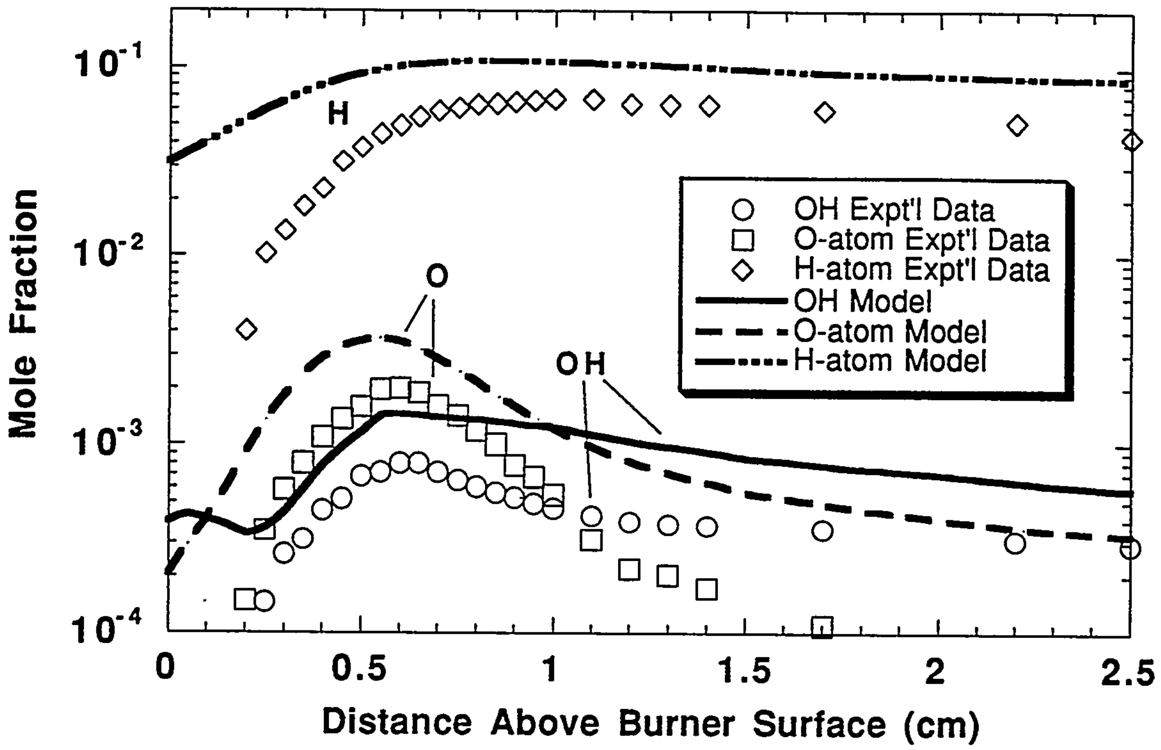
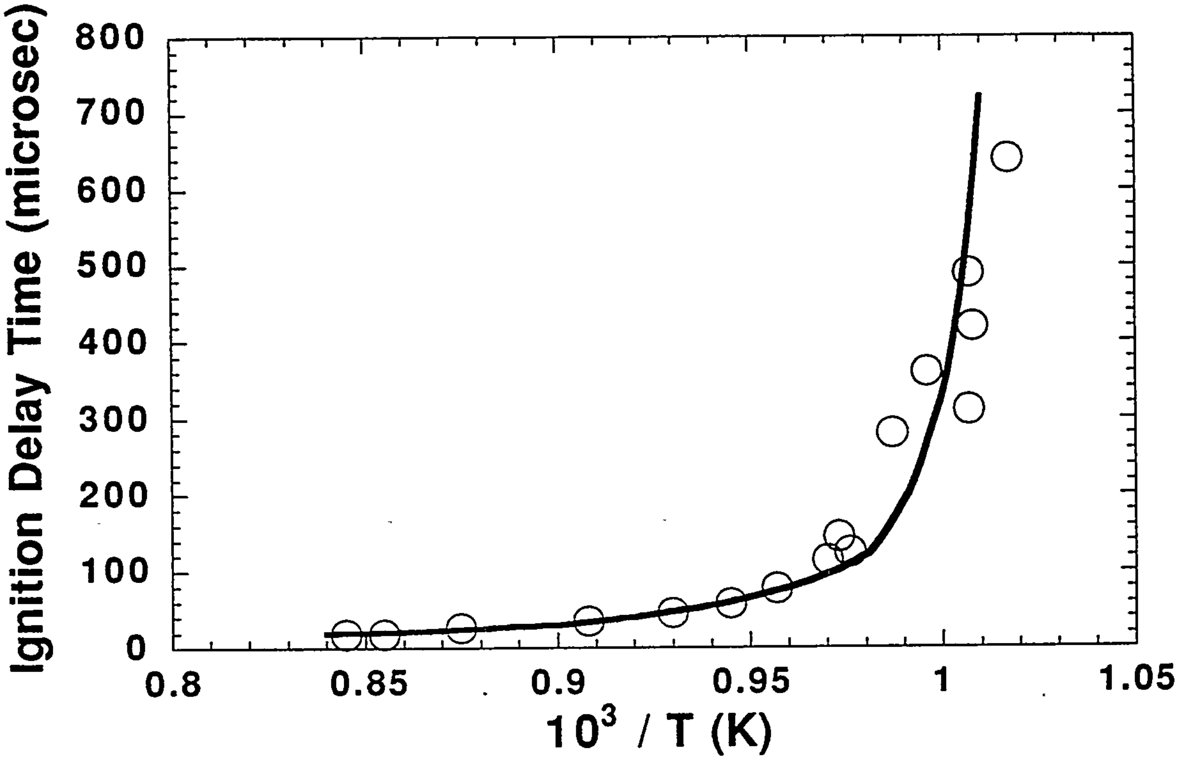

10^-1
10^-2
10^-3
10^-4
Mole Fraction
0
0.5
1
1.5
2
2.5
Distance Above Burner Surface (cm)
H
O
OH
○ OH Expt'l Data
□ O-atom Expt'l Data
◇ H-atom Expt'l Data
OH Model
O-atom Model
H-atom Model

Fig. 7



Ignition Delay Time (microsec)
800
700
600
500
400
300
200
100
0
0.8
0.85
0.9
0.95
1
1.05
10^3 / T (K)

Fig. 8

HYDROGEN FUEL DISPENSING STATION FOR TRANSPORTATION VEHICLES

Suman P. N. Singh and Andrea A. Richmond
Chemical Technology Division
Oak Ridge National Laboratory*
Oak Ridge, Tennessee 37831-6495

Abstract

A technical and economic assessment is being conducted of a hydrogen fuel dispensing station to develop an understanding of the infrastructure requirements for supplying hydrogen fuel for mobile applications. The study includes a process design of a conceptual small-scale, stand-alone, grassroots fuel dispensing facility (similar to the present-day gasoline stations) producing hydrogen by steam reforming of natural gas. Other hydrogen production processes (such as partial oxidation of hydrocarbons and water electrolysis) were reviewed to determine their suitability for manufacturing the hydrogen. The study includes an assessment of the environmental and other regulatory permitting requirements likely to be imposed on a hydrogen fuel dispensing station for transportation vehicles.

The assessment concludes that a dispensing station designed to produce 0.75 million standard cubic feet of fuel grade (99.99%+ purity) hydrogen will meet the fuel needs of 300 light-duty vehicles per day. Preliminary economics place the total capital investment (in 1994 U.S. dollars) for the dispensing station at $ 4.5 million and the annual operating costs at around $ 1 million. A discounted cash-flow analysis indicates that the fuel hydrogen product price (excluding taxes) to range between $1.37 to $2.31 per pound of hydrogen, depending upon the natural gas price, the plant financing scenario, and the rate of return on equity capital.

A report on the assessment is due in June 1995. This paper presents a summary of the current status of the assessment.

---

*Managed by Martin Marietta Energy Systems, Inc., under contract DE-AC05-84OR21400 with the U.S. Department of Energy.

Introduction

The transportation sector is a major consumer of fossil-derived fuels. For example, in 1993, in the United States (U.S.), this sector was responsible for 27 percent of the energy consumed and 66 percent of the petroleum used in the country (Patil and Zegers 1994, Gross 1994). The transportation sector is also a major contributor to the total U.S. emissions and is responsible for the increasing level of petroleum imports to the country. In the future, unless an alternate fuel significantly penetrates the transportation market, petroleum imports are expected to increase significantly to meet the transportation sector needs. These imports will have a major impact on the national well-being by being a drain on the national wealth and a national security concern. To staunch this drain on the national wealth, to decrease our dependence on imported fuels, and to decrease the environmental insult due to the continued use of petroleum-derived fuels, hydrogen is being evaluated as a desirable replacement for fossil-derived fuels.

Hydrogen as a fuel for transportation applications has several desirable attributes. Hydrogen can be converted to energy either thermally (for example, in an internal combustion engine) or chemically (for example, in a fuel cell). Unlike fossil-derived fuels (such as gasoline) hydrogen, when converted, produces water and no toxic, noxious, or hazardous emissions such as carbon and nitrogen oxides, particulates, aldehydes, and other non-methane hydrocarbons (NMHCs). Because hydrogen is very light and a gas at ambient conditions, any accidental open release will result in the hydrogen rapidly diffusing into the atmosphere and, unlike petroleum-derived fuels, will not result in any soil or water pollution. Hydrogen potentially has a very much larger and globally widely distributed resource base than petroleum. For example, hydrogen can be readily manufactured from water, fossil fuels, biomass, or other hydrocarbon resources. Hydrogen as a fuel has three times the energy content of gasoline, on an equivalent mass basis. When used as a fuel in fuel cell powered vehicles, it can provide 2 to 3 times the energy conversion efficiency of conventional gasoline-fueled, internal combustion engine powered vehicles because fuel cells being electrochemical conversion devices are not limited by the Carnot heat cycle. Hydrogen fuel cell vehicles operate quietly and produce no emissions other than water. They are environmentally benign and can be considered to be true "zero emission vehicles" unlike electric powered vehicles which are, in reality, "transferred emission vehicles".

One of the obstacles to the increased use of hydrogen in transportation is the lack of the supply infrastructure needed to make fuel hydrogen readily available to the public, similar to the present-day ready availability of motor fuels such as gasoline. To help surmount this obstacle, Oak Ridge National Laboratory (ORNL) was tasked by the U. S. Department of Energy to conduct an evaluation of a hydrogen fuel dispensing station for light-duty vehicles. The objective of this work is to perform technical and economic assessments to develop the infrastructure requirements to facilitate the introduction of hydrogen as an environmentally-desirable replacement for present day petroleum-derived transportation fuels. The work includes the development of design requirements for a conceptual hydrogen fuel dispensing facility similar to the present-day gasoline dispensing stations. This facility will be designed as a stand-alone plant to produce hydrogen from natural gas using conventional steam reforming and water gas shift processes. Other hydrogen production processes (such as partial oxidation of hydrocarbons and water electrolysis) would be reviewed to determine their suitability for manufacturing the hydrogen for the stand-alone dispensing station. The study will also include an assessment of the environmental permitting and other regulatory requirements likely to be imposed on building and operating a hydrogen dispensing station for fueling light-duty transportation vehicles.

This paper provides a summary of the current status of the assessment and preliminary results. A draft report (Singh and Richmond 1995) on the assessment is due to be issued in June 1995. This report will contain a review of the fuel hydrogen production technologies, an economic assessment for a conceptual, small-scale, stand-alone, grassroots hydrogen fuel dispensing station, and an assessment of the environmental and permitting requirements for the hydrogen fuel dispensing station.

Technology Assessment

Hydrogen can be produced by numerous methods from a wide range of resources such as fossil fuels, water, biomass, and other organic raw materials. Industrial hydrogen production processes include steam reforming (of natural gas and light hydrocarbons), partial oxidation (of heavy oils and tars), electrolysis (of water), gasification (of coal and biomass), and plasma conversion of natural gas or other hydrocarbons. Of all these processes, steam reforming of natural gas is the most widely used process because it is considered to be the most economic route for hydrogen production (Bochow 1995, Khurana 1994, Tindall and King 1994, McKetta and Cunningham 1987, and Baird 1983). Large quantities of hydrogen are produced as an intermediate stream for captive use in petroleum refineries and petrochemical plants for product upgrading operations. However, very little is sold as merchant or commodity hydrogen. Because of economics, most non-captive hydrogen for commodity sales is produced by the steam-reforming of a hydrocarbon (usually natural gas).

The hydrogen fuel dispensing station was designed as a grassroots facility with on-site production of hydrogen from natural gas. Steam reforming of natural gas was chosen as the conversion process because of economics and the ready availability of natural gas in the U. S. The process design of the production facility was performed using the ASPEN PLUS™ process simulator. The production plant was sized to produce 0.75 million standard cubic feet per day (MMscfd) of fuel grade (99.99%+ purity) hydrogen from 0.34 MMscfd of pipeline quality natural gas. The dispensing station was designed to produce and deliver gaseous fuel hydrogen at 3700 psia delivery pressure at the dispensing pumps to service an average of 300 light-duty vehicles per day.

The design premises for the dispensing station are summarized in Table 1. these premises were developed based on the following:

- The vehicle fuel requirements were developed to meet Goal 3 given in the ***Partnership for a New Generation of Vehicles (PNGV) Program Plan*** (U.S. Department of Commerce 1994).
- The light-duty vehicles would likely be powered by a proton exchange membrane (PEM) fuel cell stack requiring high purity (99.99%+) hydrogen as fuel.

- The fuel hydrogen would be stored on the vehicle in appropriate gas cylinders as high pressure (3600 psia) gas.
- The dispensing station would be staffed around the clock by trained operators.

Table 1. Basic Premises for Designing the Stand-alone, Small-scale, Grassroots Hydrogen Fuel Dispensing Station

Given below are the basic premises used for designing the small-scale, stand-alone hydrogen fuel dispensing station with on-site hydrogen production:

- Station capacity = 300 light-duty vehicles per day.
- Vehicle hydrogen requirements = 5 kg (11 lbs) for 640 km (400 mi) range at 38 km/L (90 mi/gal) of gasoline equivalent.
- Fueling station design capacity = 1800 kg/day (3970 lbs/day) or 21×10^3 std. m^3/day (0.75 MMscfd) (at 60°F and 14.7 psia) of hydrogen.
- Fueling station designed to produce and dispense 99.99%+ pure hydrogen gas at 3700 psia.
- The hydrogen is to be produced by steam-methane reforming from pipeline quality natural gas.
- Number of fueling bays at the station = 4.
- Average fueling time per vehicle = 15 minutes.
- The fueling facility will be capable of dispensing fuel 24 hours per day.
- Fueling station staffing level = 3 operators per shift or 13 operators total for the facility. This staffing level does not include the administrative and maintenance staff that may be required for the facility.
- All cost estimates are to be in 1994 U. S. dollars.

Further details of the process design of the dispensing station are given in Singh and Richmond (1995). A block flow diagram of the dispensing station is shown in Figure 1 and Figure 2 is an artist's view of the conceptual stand-alone, small-scale, grassroots hydrogen fuel dispensing station.

Economic Assessment

An economic assessment was conducted of the conceptual hydrogen fuel dispensing station to estimate the price of the hydrogen produced at the facility and to evaluate the station's profitability under different financing scenarios. Briefly, the economic assessment consisted of developing the total capital investment for the facility, the estimated annual operating costs, and performing a discounted cash flow economic analysis under different financing scenarios to build the facility. The financing scenarios examined included 100 percent equity capital, 70 percent equity and 30 percent debt capital, 50 percent equity and 50 percent debt capital, and 30 percent equity and 70 percent debt capital. All costs in the economic assessment were developed in terms of 1994 U. S. dollars.

The estimated plant capital investment is given in Table 2. The capital investment was developed using plant costs obtained from various sources including King (1995) and Ogden, Dennis, and Strohbehn (1994). The estimated annual operating costs for the dispensing station are given in Table 3. Data to develop the annual operating costs were obtained from various sources such as King (1995) and Brown (1995). The economic analysis was performed using an ORNL-developed discounted cash flow analysis computer program called "PRP" (Salmon 1983). Briefly, this program determines the product price from a production plant given the economic parameters associated with building and operating the plant. The PRP program was used to determine the product or selling price for the hydrogen from the dispensing station given the capital investment, estimated annual operating costs, financing scenarios, and other cost accounting parameters such as taxation rates and depreciation schedules. The results of the economic analysis are summarized in Table 4 and are plotted in Figure 3 for different natural gas feed prices. From Table 4 and Figure 3, it can be seen for example, that the product price of the hydrogen for, say, $ 2.00 per thousand standard cubic feet (Mscf) of natural gas and for 100 percent equity financing, ranges between $ 1.47 and $ 2.04 per pound of fuel hydrogen, for a rate of return on equity capital ranging between 10 and 20 percent. The hydrogen product price shown is exclusive of taxes that may be imposed on the hydrogen fuel.

Sensitivity studies are being conducted to determine the impact on the fuel hydrogen price of changes in several economic parameters such as changes in the plant capital investment and the annual operating costs. The results of these sensitivity studies will be available in the technology assessment report by Singh and Richmond (1995).

Environmental Assessment

The environmental assessment consisted of determining the environmental and regulatory permitting requirements likely to be imposed on the conceptual small-scale, stand-alone, grassroots hydrogen fuel dispensing station. These regulatory and permitting requirements were developed assuming that the dispensing station was to be located in an industrial area in the Los Angeles Basin in southern California. The above assumption was made for the following reasons:

- Hydrogen fuels for transportation are most likely to be first introduced in the Los Angeles Basin in the U. S. as this area of the country has a chronic air pollution problem and has taken the lead in the introduction of alternate, clean-burning transportation fuels.

- The environmental permitting regulations for siting industrial plants are most stringent in this location. If a production facility is designed to meet these strict regulations, then such a facility will readily be able to meet the permitting regulations in other parts of the country.

Table 2. Estimated Plant Capital Investment for Hydrogen Fuel Dispensing Station with On-Site Hydrogen Production Using Steam Methane Reforming

		$ (1994)
●	Installed cost for 0.75 MMscfd H_2 production plant	2,900,000
●	Installed cost for 6-h GH_2 production storage tank	120,000
●	Installed cost for GH_2 product compressor	150,000
	SUBTOTAL installed cost of modular plant equipment	3,170,000
●	Installed cost of buildings and structures (5%)	160,000
●	Installed cost of interconnecting electricals, piping, instrumentation and controls between modules	150,000
●	Installed cost of dispensing bays	100,000
●	Land costs (1 acre @ $ 20,000/acre)	20,000
	SUBTOTAL direct plant costs	3,600,000
●	Allowance for permitting and other regulatory costs	150,000
●	Allowance for other indirect plant construction costs	200,000
	SUBTOTAL installed plant cost	3,950,000
●	Contingency (at approximately 10% installed plant cost)	350,000
	SUBTOTAL fixed capital investment	4,300,000
●	Working capital (@ approximately 5% of fixed capital investment)	200,000
	TOTAL plant capital investment	4,500,000

Table 3. Estimated Annual Operating Costs for Hydrogen Fuel Dispensing Station with On-Site Hydrogen Production Using Steam Methane Reforming

	$ (1994)
• Direct labor–13 operators @ $50,000/person-year	650,000
• Supervision and maintenance labor @ 25% of direct labor	163,000
• Supplies and chemicals	30,000
• Insurance @ 1% of depreciable capital cost	36,000
• Power @ 6 ¢/kWh	15,000
• Water @ $2/1,000 gallons	5,000
• Waste disposal	5,000
TOTAL annual operating costs	904,000

Table 4. Summary of Economic Analysis for Hydrogen Fuel Dispensing Station

		Hydrogen Product Price, $/lb.			
		Debt[b] /Equity Ratio, Percent			
Natural Gas Price $/Mscf[a]	Return on Equity %	0/100	30/70	50/50	70/30
	10	1.47	1.43	1.40	1.37
	12	1.57	1.50	1.46	1.41
2.00	15	1.74	1.63	1.55	1.48
	20	2.04	1.85	1.72	1.60
	10	1.56	1.56	1.48	1.46
	12	1.66	1.59	1.54	1.50
3.00	15	1.82	1.71	1.64	1.57
	20	2.13	1.94	1.81	1.69
	10	1.64	1.60	1.57	1.54
	12	1.75	1.68	1.63	1.59
4.00	15	1.91	1.80	1.73	1.66
	20	2.22	2.03	1.90	1.77
	10	1.73	1.69	1.66	1.63
	12	1.83	1.77	1.72	1.68
5.00	15	2.00	1.89	1.82	1.74
	20	2.31	2.11	1.99	1.86

[a] Mscf = thousand standard cubic feet.

[b] Interest rate on debt = 9%

The likely effluents from the conceptual hydrogen fuel dispensing facility evaluated in this assessment will consist of the following:

- Combustion flue gases from the steam-reformer heater. An analysis of the flue gas from the hydrogen production plant at the dispensing station is given in Table 5. The principal components present are nitrogen, water vapor, and carbon dioxide. The flue gas contains no noxious components [other than up to 20 parts per million (ppm) of nitrogen oxides].

- Blowdown water from the water treatment operations and domestic sewage from the dispensing station. This wastewater should contain no hazardous or toxic components and could be discharged to, for example, a municipal wastewater treatment facility for treatment and disposal.
- Solid wastes consisting principally of domestic trash and debris (e.g., waste paper, cardboard, plastics, and glass). The solid wastes should normally not contain any hazardous or toxic compounds requiring special disposal. These wastes could be sent to the local solid waste disposal facility for destruction and/or disposal. Spent catalysts which are periodically removed from the production plant are expected to be returned to the catalyst manufacturer for recycling.

The innocuous nature of the dispensing station effluents and wastes suggests that the station should not have to obtain any special permits other than those required for conducting normal manufacturing and distribution operations. Nonetheless, the dispensing station will likely have to comply with several federal and/or state environmental regulations and local permitting ordinances. The likely permits, regulations, and ordinances that the dispensing station will have to comply with are listed in Table 6. Because the dispensing station is basically a small chemical production plant, the equipment used at the station will have to be designed to comply with accepted industrial codes. A list of these potential codes is given in Table 7. Tables 6 and 7 present the potential regulatory requirements for the dispensing station; the actual codes, permits, and regulations will be decided when the conceptual plant moves into the detail design phase.

California has published a handbook entitled 1994 California Permit Handbook (Holanda 1994) which is an excellent guide to the permitting process involved in siting a production plant in the state. This handbook (or an update) would need to be consulted when the conceptual hydrogen fuel dispensing station moves into reality.

Conclusions

Some of the conclusions from the assessment are as follows:

- Fuel hydrogen likely will be produced from natural gas in the near-term as a transition fuel until the commercial production of hydrogen using solar energy can be demonstrated.
- Hydrogen production from natural gas by steam-methane reforming is an accepted commercial process in the petrochemical industry and dispensing station sized facilities can be built.
- Dispensing facilities producing fuel-grade (99.99%+ purity) hydrogen are feasible however, no such stations have been built to demonstrate and validate this conclusion.

Table 5. **Flue Gas Analysis from the Hydrogen Production Plant at the Conceptual Dispensing Station.**

Components	Molecular Weight	Flow Rate (moles per day)	Composition (mole percent)
CH_4	16.04	—	—
C_2H_6	30.07	—	—
C_3H_8	44.10	—	—
H_2	2.016	—	—
CO	28.01	—	—
CO_2	44.01	919.06	16.41
N_2	28.02	3,360.58	60.01
O_2	32.0	81.04	1.45
Ar	39.94	38.21	0.68
Mercaptans	48.11	—	—
H_2O	18.02	1,201.21	21.45
NO_x	46.02	0.11	0.002
Totals	—	5,600.21	100.00
Steam mol. weight	—	28.64	28.64
Vol. flow rate MMscfd	—	2.13	—
Mass flow rate, (lb/d)	—	160390	—
Temperature, °F Pressure, psia	—	180 20	—

Table 6. Summary of Federal, State, and Local Regulations and Permits for Hydrogen Fuel Dispensing Station.

- <u>Federal Regulations</u>

  - Energy [Title 10 Code of Federal Regulations (CFR)]
    - Department of Energy (Chapters II, III, and X)
  - Commerce and Foreign Trade [Title 15 (CFR)]
    - Department of Commerce (Chapters II, VIII, IX, and XI)
  - Commercial Practices [Title 16 (CFR)]
    - Federal Trade Commission (Chapter I)
    - Consumer Product Safety Commission (Chapter II)
  - Conservation of Power and Water Resources [Title 18 (CFR)]
    - Federal Energy Regulatory Commission (Chapter I)
  - Employees' Benefits [Title 20 (CFR)]
    - Department of Labor (Chapters I. IV-VII)
    - Department of Health and Human Services (Chapter III)
  - Highways [Title 23 (CFR)]
    - Department of Transportation (Chapters I-III)
  - Internal Revenue [Title 26 (CFR)]
    - Department of the Treasury (Chapter I)
  - Labor [Title 29 (CFR)]
    - Department of Labor (Chapters I, II, IV, V, IX, XIV, and XXV)
    - Occupational Safety and Health Administration (Chapter XVII)
    - Occupational Safety and Health Review Commission (Chapter XX)
  - Protection of Environment [Title 40 (CFR)]
    - Environmental Protection Agency (Chapter I)
    - Council on Environmental Quality (Chapter V)
  - Public Health [Title 42 (CFR)]
    - Public Health Service (Chapter I)
  - Emergency Management and Assistance [Title 44 (CFR)]
    - Federal Emergency Management Agency (Chapter I)
    - Departments of Commerce and Transportation (Chapter IV)
  - Transportation [Title 49 (CFR)]
    - Department of Transportation (Chapters I, III, and V)
    - Interstate Commerce Commission (Chapter X)

- State Regulations (e.g., for California)
  - Title 4 Business Regulations
  - Title 5 Environmental Review Process
  - Title 8 Industrial Relations
  - Title 22 Social Security
  - Title 23 Waters

- Regional Permits (e.g., for California)[a]
  - Public Utilities Commission Permit
  - Development Permit
  - Industrial Works Department Permit
  - Public Works Department Permit
    - Conditional Use Permit
    - Building Inspection Permit
    - Land Development Approvals
  - Hazardous Materials Risk Management: A Prevention Plan (HMPP)
  - Hazardous Waste Generation Permit
  - Air Permits/Air Toxics Regulations
  - Wastewater Discharge Permit
  - Solid Wastes Disposal Permit
  - General Construction Permit
  - Site Occupancy Permit

---

[a] Source: Koner, H.C., W. D. Gaukett, and J. Abbott, November 29–December 2, 1992. Pages 336-339 in "Licensing and permitting considerations for fuel cell project," *Fuel Cell Programs and abstracts 1992 Fuel Cell Seminar*; Tucson, Arizona.

Table 7. Potential Codes for the Equipment Design and Construction of the Hydrogen Fuel Dispensing Station.*

- American Gas Association (AGA): Report No. IS 100-1.
- American Society of Mechanical Engineers (ASME): Boiler and Pressure Vessel Code, Section VIII.
- American Society of Heating, Refrigerating, and Air-Conditioning Engineers (ASHRAE): ASHRAE/IES 90.1-1089.
- American National Standards Institute (ANSI) Codes: A4.3, B31.3, B31.5, B93.5, B93.9, D56, D1018, Z48.1
- American Society for Testing and Materials (ASTM) Standards: A193, B57.1, B849, D1018, E136, E162, F113, F1129, F1459, Z11.7.
- American Petroleum Institute (API): Standards 620 and 750, Bulletins 6FA, 6FB, and Publications 910 and 2009.
- Chemical Manufactures Association (CMA) Guides: 018026, 018030, 057003, 024041, 047024, 047023, 024010,022002, 022008.
- Compressed Gas Association (CGA) Codes: B96, C4, C6-8, C10, C14-16, C341, E1, E6, G5.3, G5.4, P1, P8, P12, P19, S1.1-S1.3, S3, S4, S7, TB9, V1, V6, V7, V9.
- Fluid Controls Institute (FCI): 68.1, 69.1, 70.1, 70.2, 73.1, 79.1, 81.1, 85.1, 87.1, 87.2, 89.1.
- Gas Processors Association (GPA) Standards: 2140, 2261, 2265, 2337, 3132, 8173, 8182.
- Instrumentation Society of America (ISA): Recommended Procedures (RP) 7.1, 12.6, 12.13, and Standards 51, 12.13, 20.
- National Fire Protection Association (NFPA) Codes: 30, 30A, 50, 50A, 50B, 51, 51B, 53, 54, 70, 90A, 497A, 497M.

- A steam-methane reforming hydrogen fuel dispensing station demonstration facility needs to be built and operated to demonstrate the commercial viability of producing hydrogen fuel for vehicles thereby increasing the public acceptability of environmentally superior hydrogen as a transportation fuel.
- Preliminary cost estimates (in 1994 U. S. dollars) place the total capital investment for the stand-alone dispensing station at $ 4.5 million and the annual operating costs around $1 million.

Acknowledgements

The authors express their gratitude to the U.S. Department of Energy/Energy Efficiency and Renewable Energy Office for sponsoring this project and to the innumerable people in the growing hydrogen community for providing insightful discussions on the future of hydrogen as a transportation fuel. Included in this, of necessity incomplete, list are Barry Bhatt, Carl Buchow, Ranji George, Tom Halvorsen, Paul Howard, Scott Hynek, Vinay Khurana, Dave King, Alan Lloyd, Bob Moore, Dave Nahmias, Joan Ogden, Venki Raman, Glenn Rambach, Rajat Sen, Ray Smith, Doug Wheeler, and many more. The authors are also grateful to their colleagues at ORNL for their assistance and to Nancy Smith and Ralph Sharpe for their alacrity in the preparation of this paper.

References

Baird, H. A. 1983. "Hydrogen Energy: An Engineer's Perspective." *Int. J. Hydrogen Energy*, **8**:867-870.

Bochow, C. 1995. Howe-Baker Engineers, Inc., Tyler, Texas, personal communication with S. P. N. Singh, Oak Ridge National Laboratory, Oak Ridge, Tennessee, February 17, 1995.

Brown, A. 1995. Knoxville Utilities Board, Knoxville, Tennessee, personal communication with S. P. N. Singh, Oak Ridge National Laboratory, Oak Ridge, Tennessee, March 21, 1995.

Gross, T. J. 1994. "Office of Transportation Technologies - Moving the Nation with Advanced Transportation." Handout given at the Annual Automotive Technology Development Contractors' Coordination Meeting, Dearborn, Michigan, October 24, 1994.

Holanda, V. 1994. *1994 California Permit Handbook*, Trade and Commerce Agency, Office of Permit Assistance, Sacramento, California.

Khurana, V. J. 1994. Kinetics Technology International Corporation, San Dimas, California, personal communication with S. P. N. Singh, Oak Ridge National Laboratory, Oak Ridge, Tennessee, December 16, 1994.

King, D. L. 1995. Howe-Baker Engineers, Inc., Tyler, Texas, personal communication with S. P. N. Singh, Oak Ridge National Laboratory, Oak Ridge, Tennessee, February 9, 1995.

McKetta, J. J. and W. A. Cunningham, eds. 1987. "Hydrogen" in *Encyclopedia of Chemical Processing and Design*, New York: Marcel Dekker, Inc.

Ogden J. M., E. Dennis, and J. W. Strohbehn. 1994. "A Technical and Economic Assessment of the Role of Natural Gas in a Transition to Hydrogen Transportation Fuel," paper presented at the 10th World Hydrogen Energy Conference, Cocoa Beach, Florida, June 20-24, 1994.

Patil, P. and P. Zegers. 1994. "Fuel cell road traction: an option for a clean global society." *J. Power Sources*, **49**:169-184.

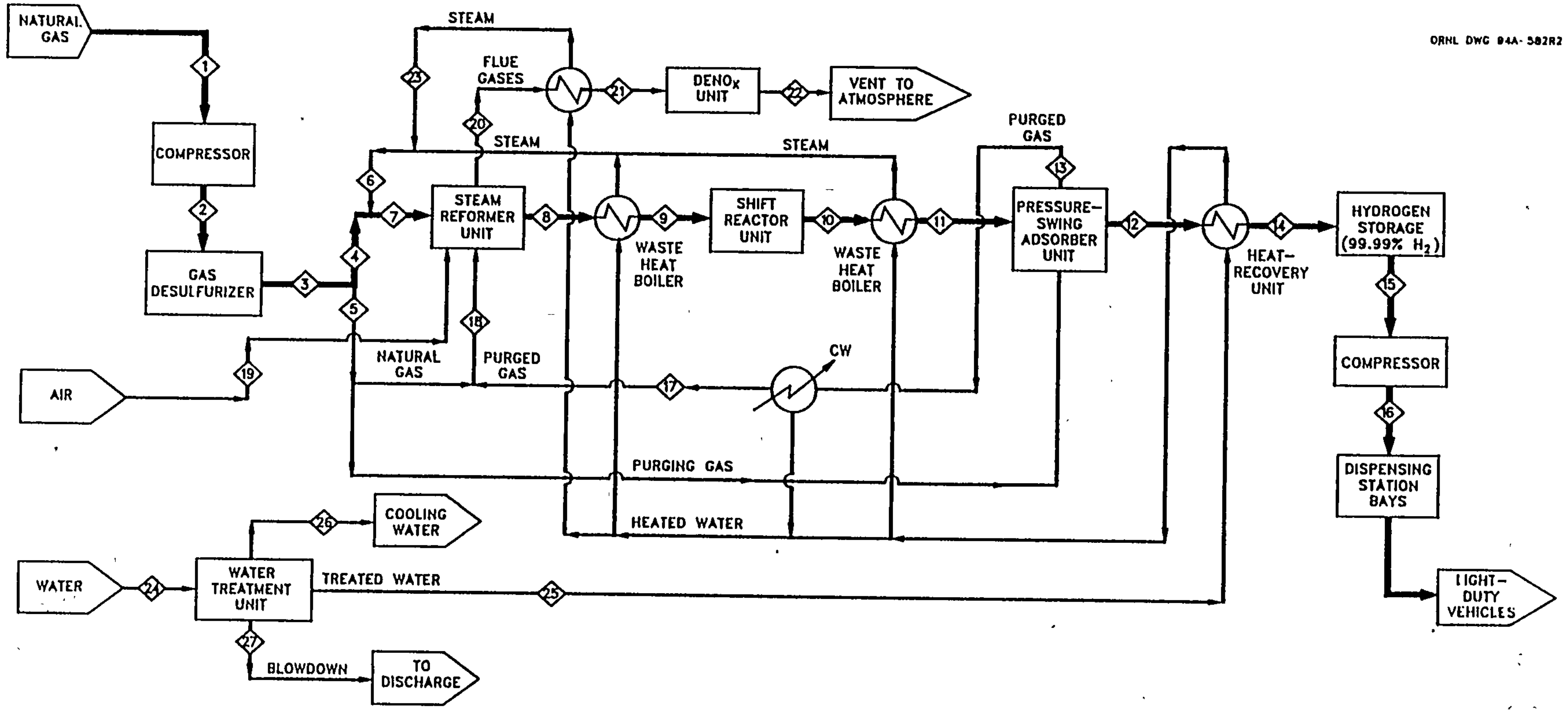
Salmon, R. 1983. *PRP-4: An Updated Version of the Discounted Cash Flow Program PRP*, **ORNL-5723**, Oak Ridge National Laboratory, Oak Ridge, Tennessee, May 1983.

Singh, S. P. N. and A. A. Richmond. 1995. *Hydrogen Fuel Dispensing Station for Transportation Vehicles*, **ORNL/TM-12982**, Oak Ridge National Laboratory, Oak Ridge, Tennessee, (in preparation).

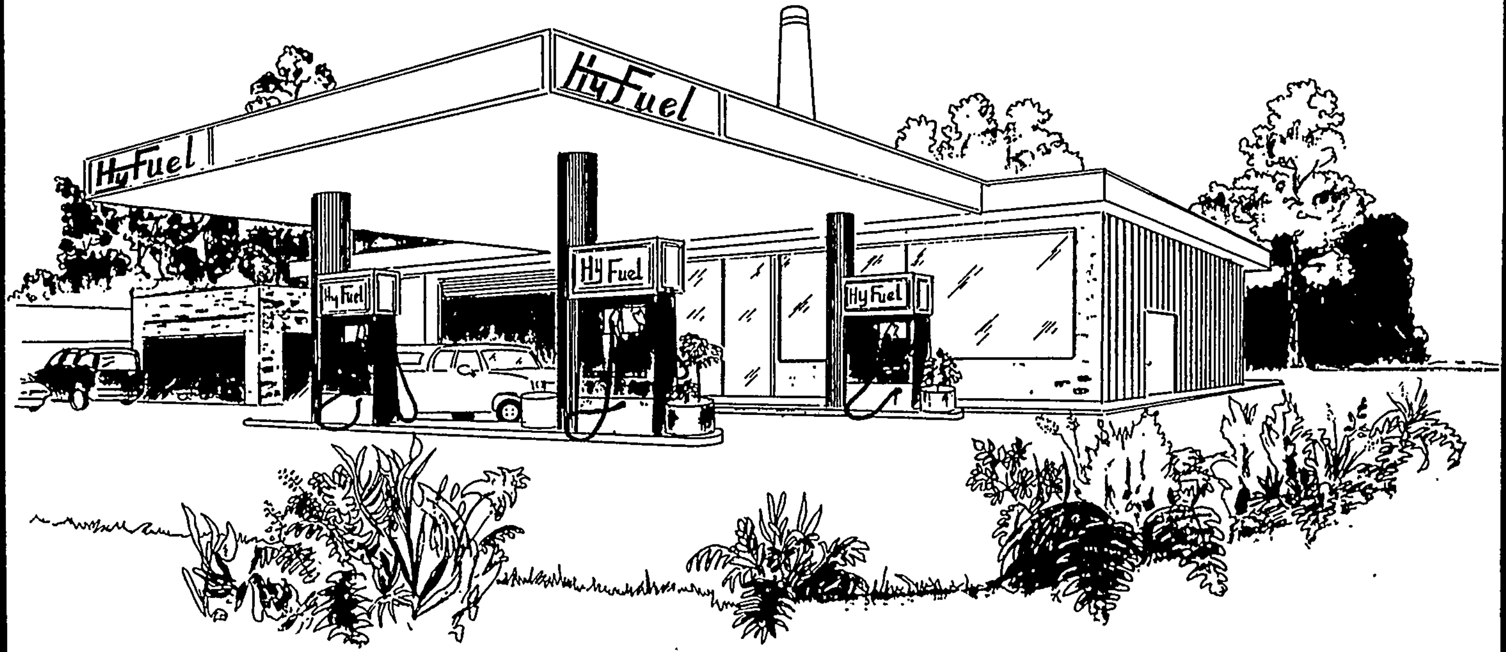
Tindall, B. M. and D. L. King. 1994. "Designing steam reformers for hydrogen production," *Hydrocarbon Proc.*, July 1994.

U.S. Department of Commerce. 1994. *Partnership for a New Generation of Vehicles (PNGV) Program Plan*, Washington, D. C.

Figures



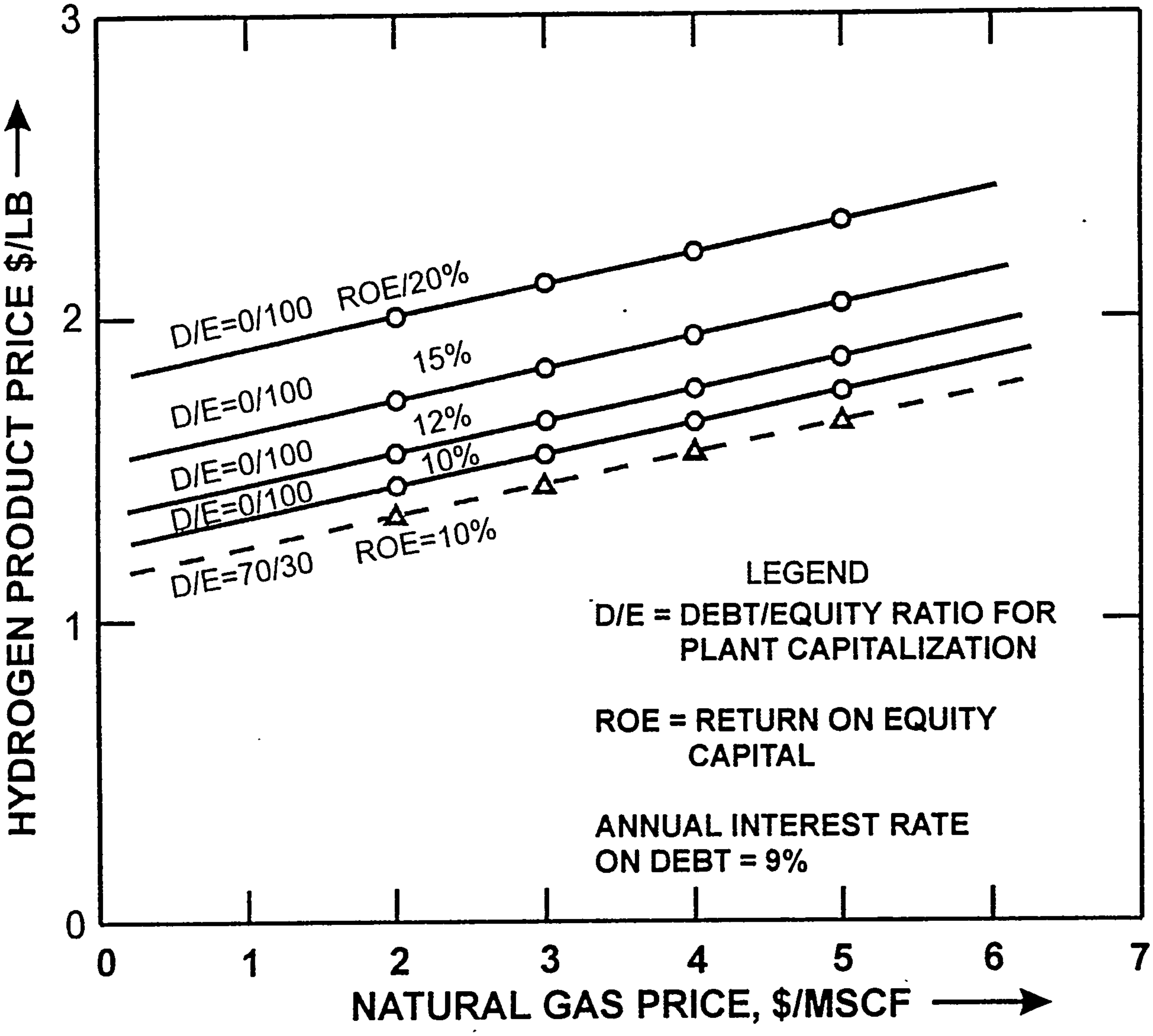
BLOCK FLOW DIAGRAM FOR DISPENSING STATION WITH ON-SITE HYDROGEN GENERATION USING CONVENTIONAL TECHNOLOGY



ARTIST'S VIEW OF CONCEPTUAL
HYDROGEN FUEL DISPENSING STATION

ORNL DWG 95C-274

HYDROGEN PRODUCT PRICE FROM CONCEPTUAL DISPENSING STATION



HYDROGEN VEHICLE FUELING STATION

David E. Daney, Fred J. Edeskuty, Mark A. Daugherty, F. Coyne Prenger, and
Dallas D. Hill
Los Alamos National Laboratory
Los Alamos, NM 87545

Abstract

Hydrogen fueling stations are an essential element in the practical application of hydrogen as a vehicle fuel, and a number of issues such as safety, efficiency, design, and operating procedures can only be accurately addressed by a practical demonstration. Regardless of whether the vehicle is powered by an internal combustion engine or fuel cell, or whether the vehicle has a liquid or gaseous fuel tank, the fueling station is a critical technology which is the link between the local storage facility and the vehicle. Because most merchant hydrogen delivered in the US today (and in the near future) is in liquid form due to the overall economics of production and delivery, we believe a practical refueling station should be designed to receive liquid. Systems studies confirm this assumption for stations fueling up to about 300 vehicles. Our fueling station, aimed at refueling fleet vehicles, will receive hydrogen as a liquid and dispense it as either liquid, high pressure gas, or low pressure gas. Thus, it can refuel any of the three types of tanks proposed for hydrogen-powered vehicles -- liquid, gaseous, or hydride.

The paper discusses the fueling station design. Results of a numerical model of liquid hydrogen vehicle tank filling, with emphasis on no vent filling, are presented to illustrate the usefulness of the model as a design tool. Results of our vehicle performance model illustrate our thesis that it is too early to judge what the preferred method of on-board vehicle fuel storage will be in practice -- thus our decision to accommodate all three methods.

Project Rationale

We believe it is now time to have a practical validation of hydrogen fueling and safety. In this way we can determine what the real issues and problems are, and we gain the kind of practical knowledge useful for technology transfer. A fundamental assumption guiding the LANL program is that hydrogen should be delivered to the station in liquid form because of near term economics which result from the very favorable weight and volume advantages that accrue from liquid transport. This view is confirmed by our conversations with US. industry, which delivered 92 percent of non-pipeline Merchant hydrogen as liquid in 1993 (Heydorn 1994) and by systems studies which favor LH2 supplied fueling stations for capacities up to about 300 vehicles/day (Ogden 1995). Because it is unclear what the practical preferred method of onboard storage will be, or whether there will be just one method, we are designing our fueling station to deliver hydrogen as either a liquid, high pressure gas, or low pressure gas. Thus it can accommodate vehicles with liquid, high pressure gas, or hydride storage. Figure 1. illustrates the LANL fueling station concept.

Approach

Our approach is to investigate H2 fueling station technology and safety through a practical demonstration. Thus, we plan to build a fueling station and test it to discover problems, investigate operating parameters, and demonstrate safety. Of particular importance is safety which encompasses both technical risk and public perception. The system design and testing proposed here is vital in demonstrating the possibility of safe operation with hydrogen fuel, and equally important, in convincing the public of this possibility. Industrial interaction is a key component of our approach. Several industrial partners have expressed interest in participating in the demonstration: Air Products, Minnesota Valley Engineering (MVE) , and PRAXAIR. Air Products (a major US supplier of liquid hydrogen together with PRAXAIR) is willing to sponsor free consulting on hydrogen safety, system design, and infrastructure development, and is willing to send their experts to LANL at their expense. MVE will provide free consulting on fuel tank design, and possibly provide a liquid hydrogen fuel tank. PRAXAIR has offered to sponsor consulting on safety and system design.

In FY95 LANL will develop a conceptual design of the fueling station to serve as the basis for modeling liquid and gaseous transfer, safety analysis, and identification and pricing of major components. A hydrogen transfer model is being developed as a design tool. Based on the results of the transfer model, a detailed design of the fueling station will begin in FY95. A complementary model of vehicle fuel efficiency as a function of the on-board storage method (liquid, compressed gas, or hydride) is being developed to specify design parameters for the H2 delivery system.

Key Results

Fueling Station Design

Figure 2 shows the schematic design of the LANL fueling station which will receive H2 as a liquid and dispense it as either liquid, high pressure gas or low pressure gas. Near the center of the schematic is the LH2 dewar which receives liquid from a commercial LH2 tanker truck. We anticipate that this dewar will be a leased Customer Service Station, as it is known in the trade.

For LH2 refueling the transfer is assisted by a centrifugal pump. From the pump the LH2 flows to the vacuum insulated valve box which controls the filling by sequencing solenoid valves. Prior to the start of liquid transfer, the connecting lines are vacuum purged and automatically checked for leaks by the pressure rise technique. A control line sequences the vehicle tank valves and shuts off the vehicle ignition interlock. All valve sequencing is done automatically by a microprocessor controller. Under normal transfer conditions there will be no venting from the vehicle tank once the lines are cooled down. To prevent venting to the atmosphere of any gas generated in line cooldown, a gas holder, compressor, and gas storage cylinders are provided. This collected gas is used to maintain the dewar pressure and supply gaseous hydrogen for GH2 refueling.

For GH2 refueling, high pressure hydrogen gas is generated by a high pressure piston pump in combination with a heat exchanger -- a pump-vaporizer unit. To reduce the size of the pump-vaporizer required, high pressure gas storage cylinders are provided. These are interconnected for cascade type discharge which maximizes their effective storage capacity. As with liquid discharge, valve sequencing is automatic, and there is a vehicle ignition interlock to prevent the vehicle from starting while refueling.

LH2 Transfer Model

As a design tool, we have modified a computer code developed by one of us (DED) and co-workers at NIST (Louie 1985) which simulates both vented and non-vented transfer between the fueling station tank and the vehicle tank. It is a thermodynamic model which uses actual hydrogen properties. It is developed from the differential mass and energy balances applied to both the fueling station tank and vehicle tank, and both single-phase and two-phase conditions are considered in the vehicle tank. Either pump-assisted or pressure induced H2 transfer can be analyzed. The program accepts a wide range of input variables, including heat leaks, tank temperatures, and piping and equipment specifications.

We are using the model to investigate the effects on transfer time of the vehicle tank initial condition, supply tank subcooling and pressure, transfer pipe size and configuration, and transfer pump power. Figure 3, which shows the rise in vehicle tank pressure during a no-vent transfer, illustrates the detail inherent in the model. Figure 4, which gives the transfer time as a function of supply tank subcooling and initial pressure difference, illustrates the importance of subcooling. Close to 0.9 K of subcooling is required, and more is desirable. For the 1/2-inch line in these simulations, rapid (below 5 minutes) transfer is feasible with good subcooling. Figure 5 shows that use of a centrifugal transfer pump can further reduce the transfer time as well as extend the supply tank operating range. For vented transfer, of course, no subcooling is required in the supply tank. Figure 6, which shows transfer time as a function of transfer pipe size, illustrates how the model aids in the design of individual components. A 5/8-inch diameter transfer line size appears to be a good compromise between fast transfer times and easily handled flexible lines with low thermal mass.

Vehicle Performance Model

The three standard options for the storage of hydrogen fuel on passenger vehicles are compressed gas, metal hydride and cryogenic liquid storage. The fueling station we are developing at Los Alamos will have the capability of fueling any of these on-board storage systems. In order to better understand the advantages and disadvantages of different types of on-board storage we have developed a model which can predict the effect of the type of on-board hydrogen storage system on vehicle performance. The model can be applied to hydrogen fueled internal combustion or fuel cell powered vehicles. Different driving cycles can be used to determine vehicle performance under urban or highway driving conditions. The Environmental Protection Agency urban dynamometer driving schedule is used to represent typical urban driving conditions. The impact of auxiliary power requirements for heating or air conditioning can also be included.

The model estimates the performance of the hydrogen vehicle as a function of storage system weight and vehicle range. More fuel is required to carry a heavy storage system than a light storage system over a given driving profile. The penalty for a heavy storage system is more severe for internal combustion engines due to their lower efficiency. The components of the drive train must also be increased in size to provide the same performance with a heavier fuel storage system. This effect can be more important than the additional fuel consumed. It means a larger engine and transmission for the internal combustion option or a larger fuel cell, drive and motor for the fuel cell option. As these systems are enlarged they weigh more, which means that an iterative solution is required to determine the final drive component sizes and vehicle fuel efficiency. The model allows one to estimate these effects which can assist in the overall evaluation of the tradeoffs involved in the design of the on-board fuel storage system.

Preliminary results given in Figure 7 indicate that for a fuel cell powered vehicle with a range of 350 miles, fuel consumption relative to a liquid hydrogen storage system is increased by 5 percent for a compressed gas storage system and 35 percent for an FeTi hydride storage system. Figure 8 shows the maximum required fuel cell output power is increased by 7 percent with a compressed gas storage system and 39 percent for a hydride system. These preliminary results do not include the extra weight of the larger drive components.

Definition of Success

The long term goal of the project is to have a practical and safe demonstration of hydrogen vehicle fueling. For FY95 our goals are:

- Complete the preliminary design of the H2 fueling station,
- Complete the LH2 transfer model,
- Complete the vehicle performance model,
- Start the detailed design.

Proposed Future Work

The LANL fueling station can serve as a test bed for safety testing and evaluation of vehicle tank designs. Plans for FY96 call for completion of the detailed design, construction of the fueling the station, and successful practical demonstration of H2 fueling. Funding is needed for this stage of the project. Beyond that, it would we are interested in safety testing and evaluation of H2 tank designs, and of course, a H2 vehicle demonstration. Upon completion, the fueling station would serve as a testbed for vehicle tank evaluation for both performance and safety.

Technology Transfer

As discussed above, several industrial partners (Air Products, Minnesota Valley Engineering and PRAXAIR) have expressed interest in participating in the demonstration, and interaction with industry on safety and technology issues is ongoing. Both the design of the fueling station and the results of the study will be available to US industry.

Summary

We believe that the time is now ripe for a practical demonstration of hydrogen fueling. LANL's design concept for the H2 fueling station provides for dispensing hydrogen as a liquid, high pressure gas or low pressure gas. Thus, it can refuel any of the three types of tanks proposed for hydrogen-powered vehicles -- liquid, gaseous, or hydride. The station will be supplied with LH2, because for the near term, this is the most economical and technically feasible method. We have developed the modeling tools necessary for the detailed design of the station, and are now ready to begin that design. The goal of our project is to build and demonstrate the H2 fueling station as soon as possible.

References

Heydorn, B. 1994. *Hydrogen*, Chemical Economics Handbook. Menlo Park, CA: SRI International.

Louie, B., N.J. Kemp, and D.E. Daney. 1985. *Cryogenic Propellant Scavenging,* NBS Technical Report NBSIR 85-3023. Boulder, CO: National Bureau of Standards.

Ogden, J.M., E. Dennis, M. Steinbugler, J.W. Strohbehn. 1995. *Hydrogen Energy Systems Studies*, Technical Report. Princeton, NJ: Center for Enviromental Studies, Princeton University.

Figure Captions

Figure 1. Conceptual schematic of fueling station.

Figure 2. Detailed schematic of fueling station.

Figure 3. Typical vehicle tank pressure history during LH2 transfer.

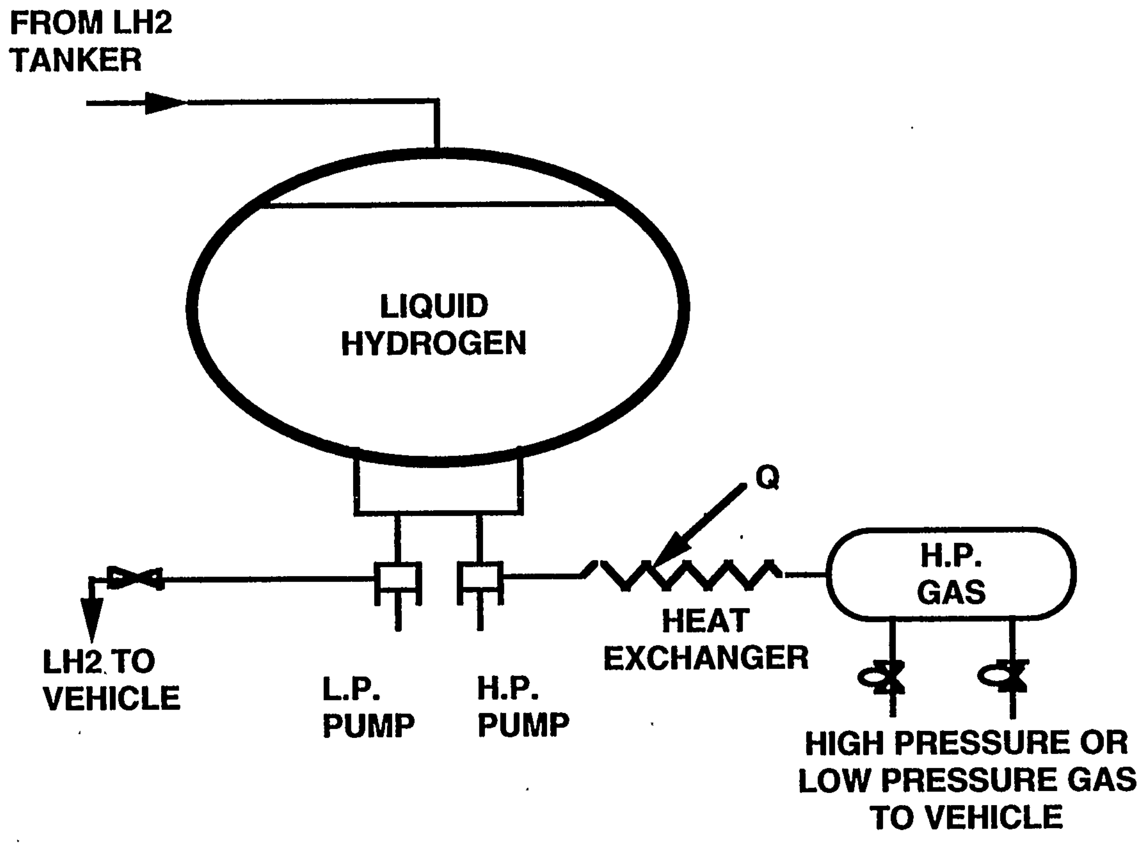
Figure 4. Effect of supply tank subcooling on LH2 transfer time .

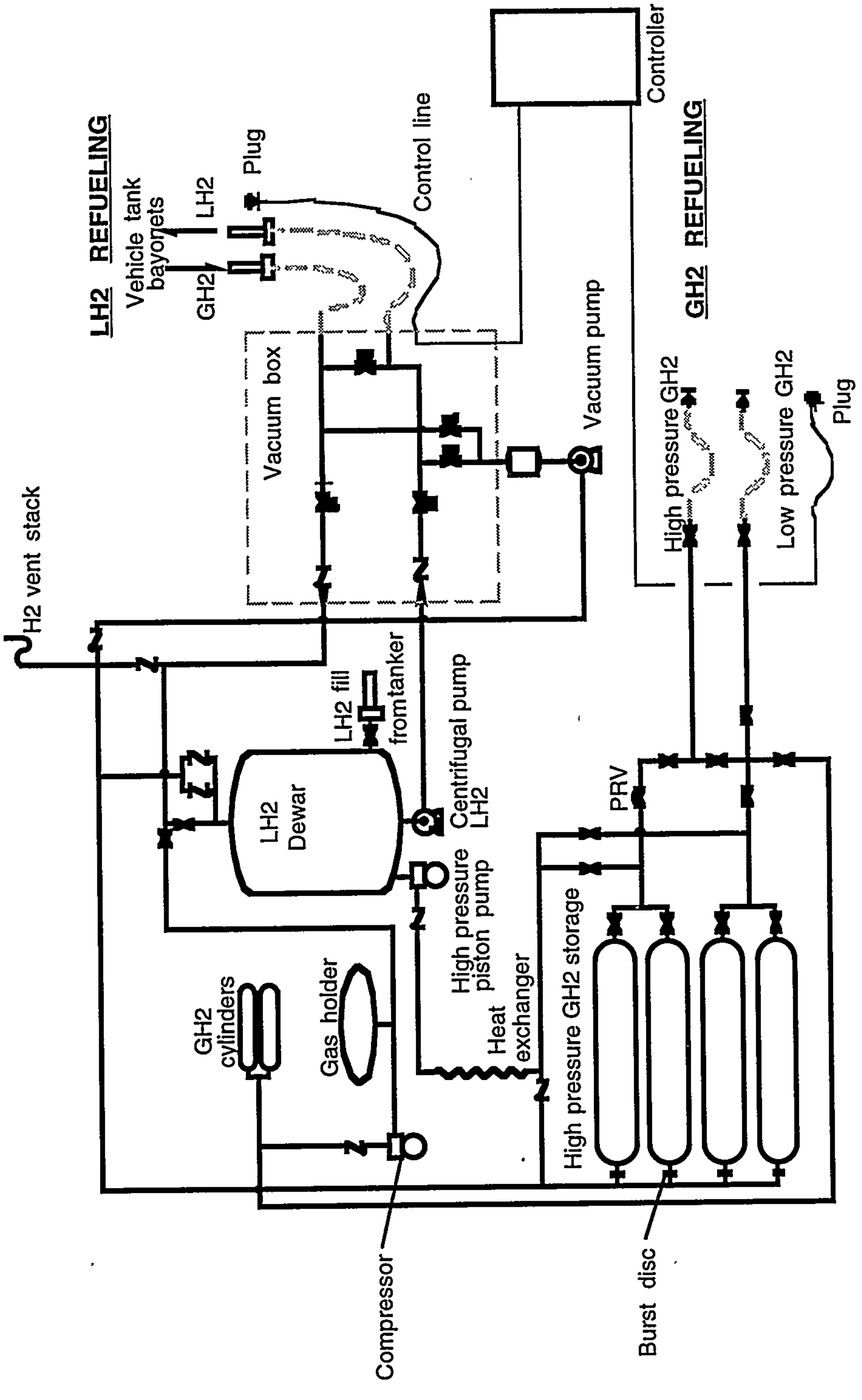
Figure 5. Effect of transfer pump power on LH2 transfer time .

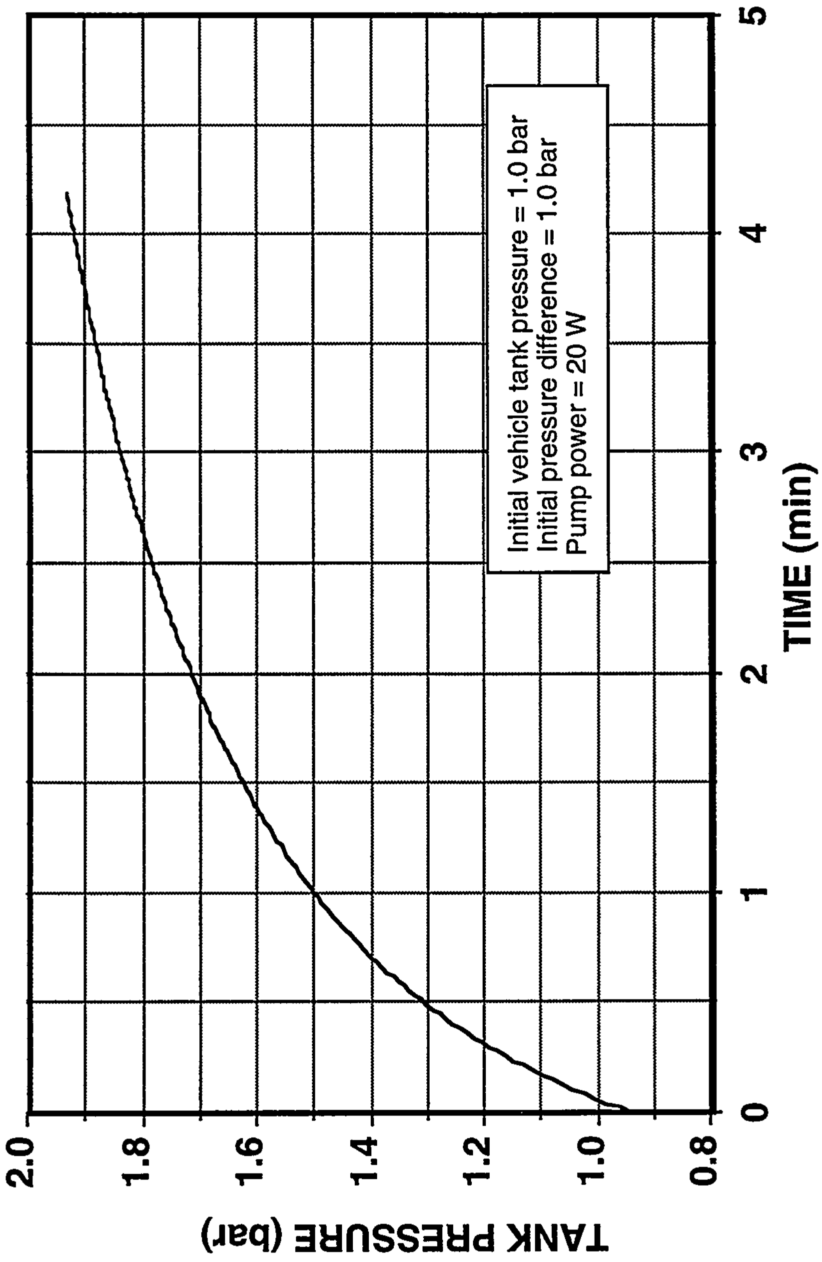
Figure 6. Dependence of LH2 transfer time on pipe diameter.

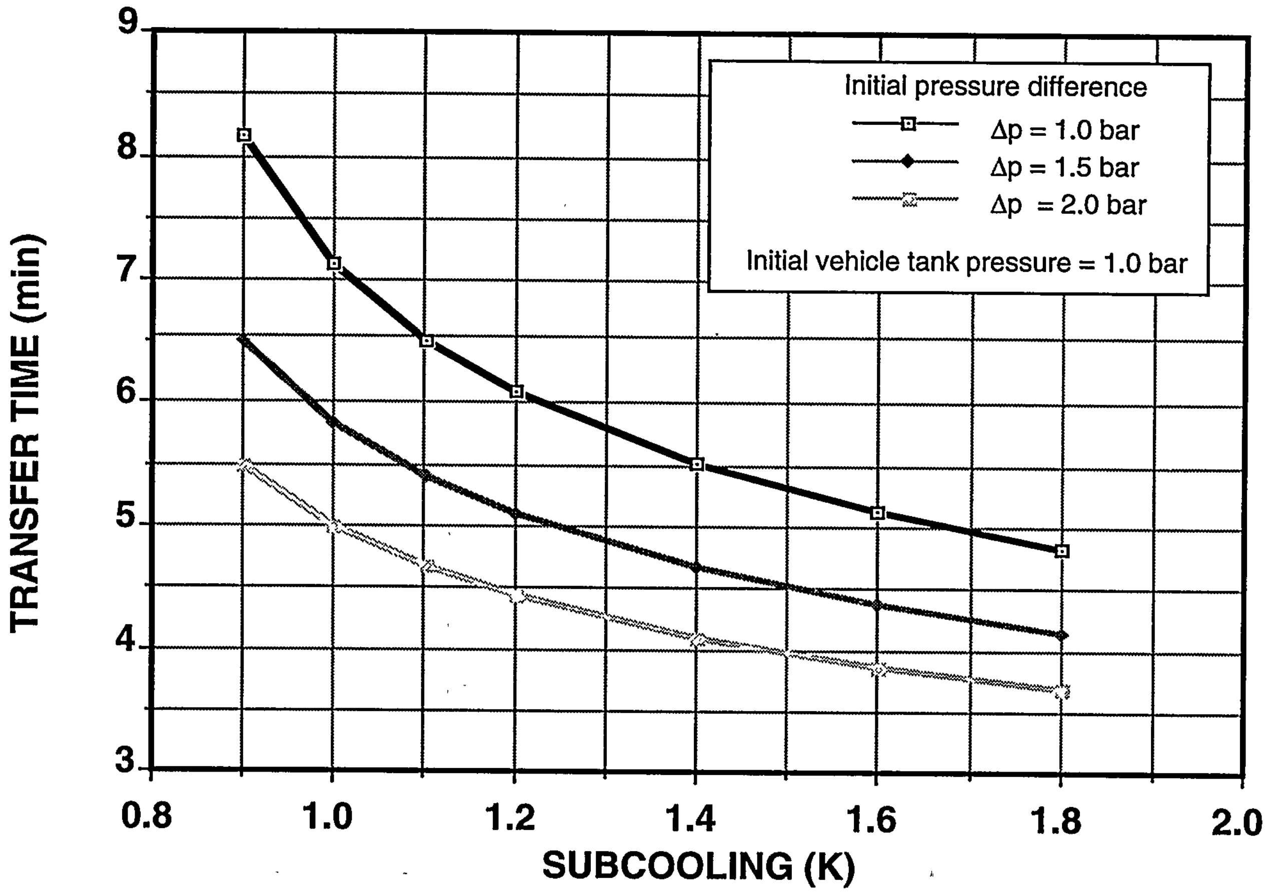
Figure 7. Effect of vehicle storage system type on fuel consumption.

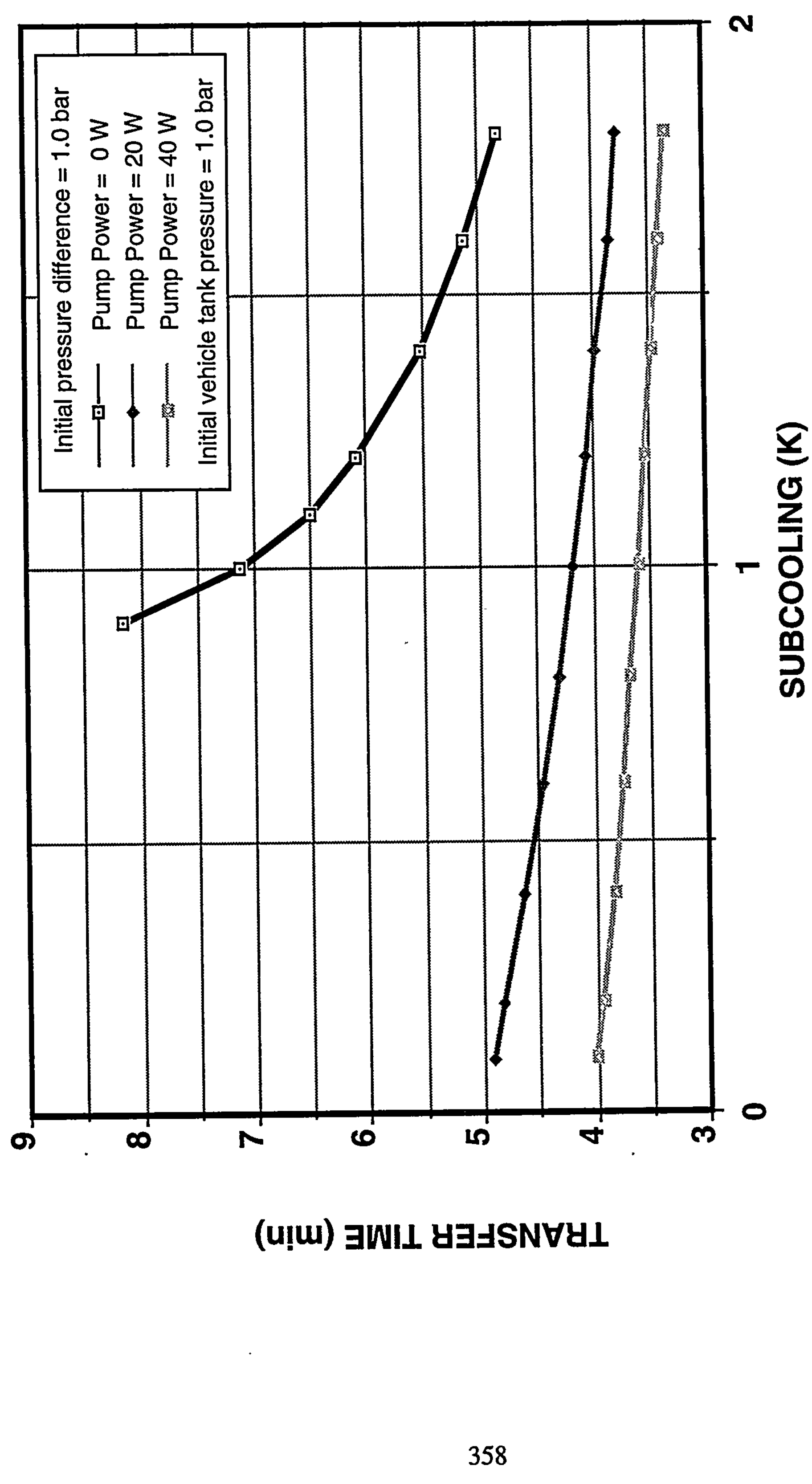
Figure 8. Effect of vehicle storage system type on maximum power required.

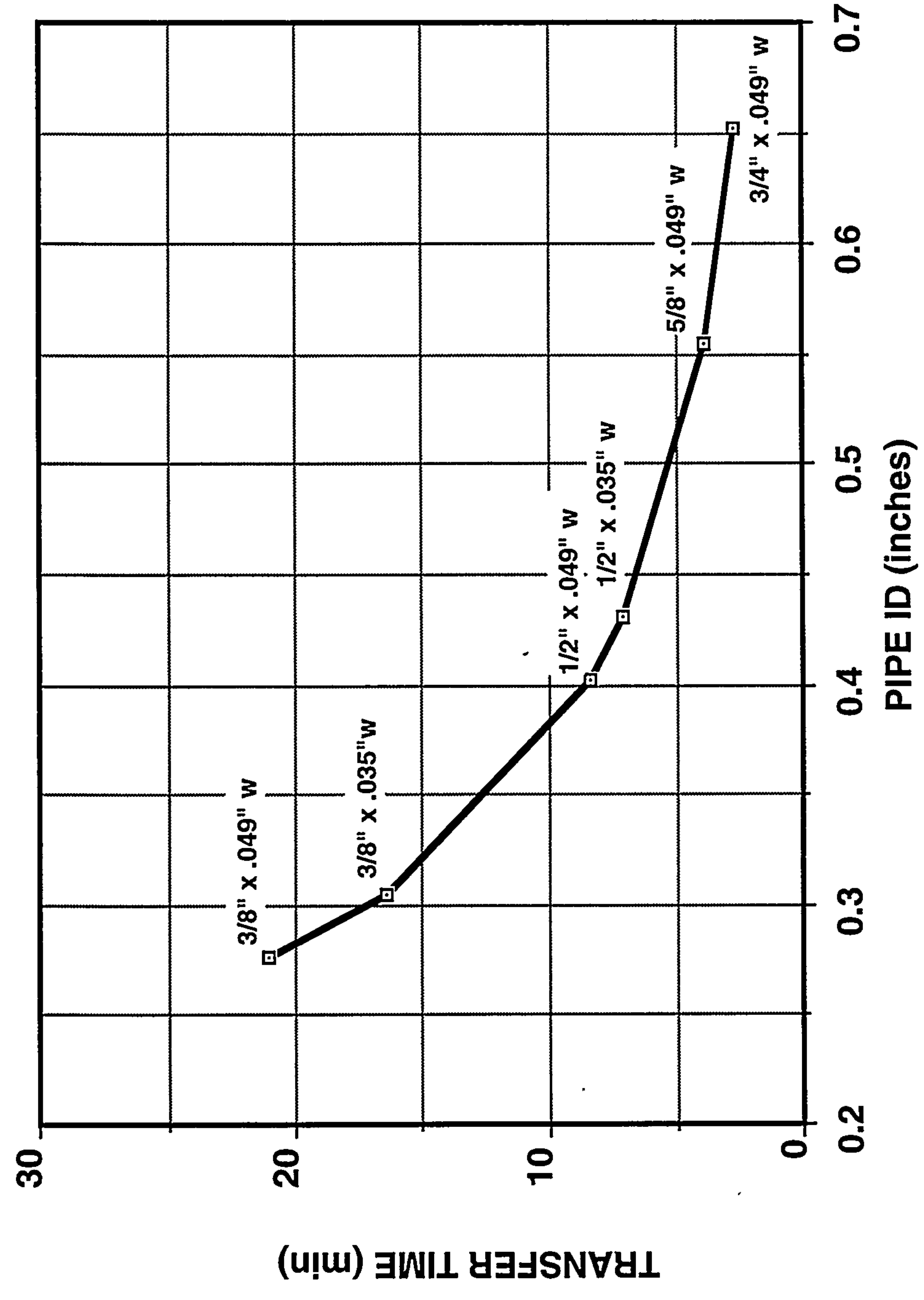

FROM LH2
TANKER
LIQUID
HYDROGEN
Q
H.P.
GAS
LH2 TO
VEHICLE
L.P.
PUMP
H.P.
PUMP
HEAT
EXCHANGER
HIGH PRESSURE OR
LOW PRESSURE GAS
TO VEHICLE

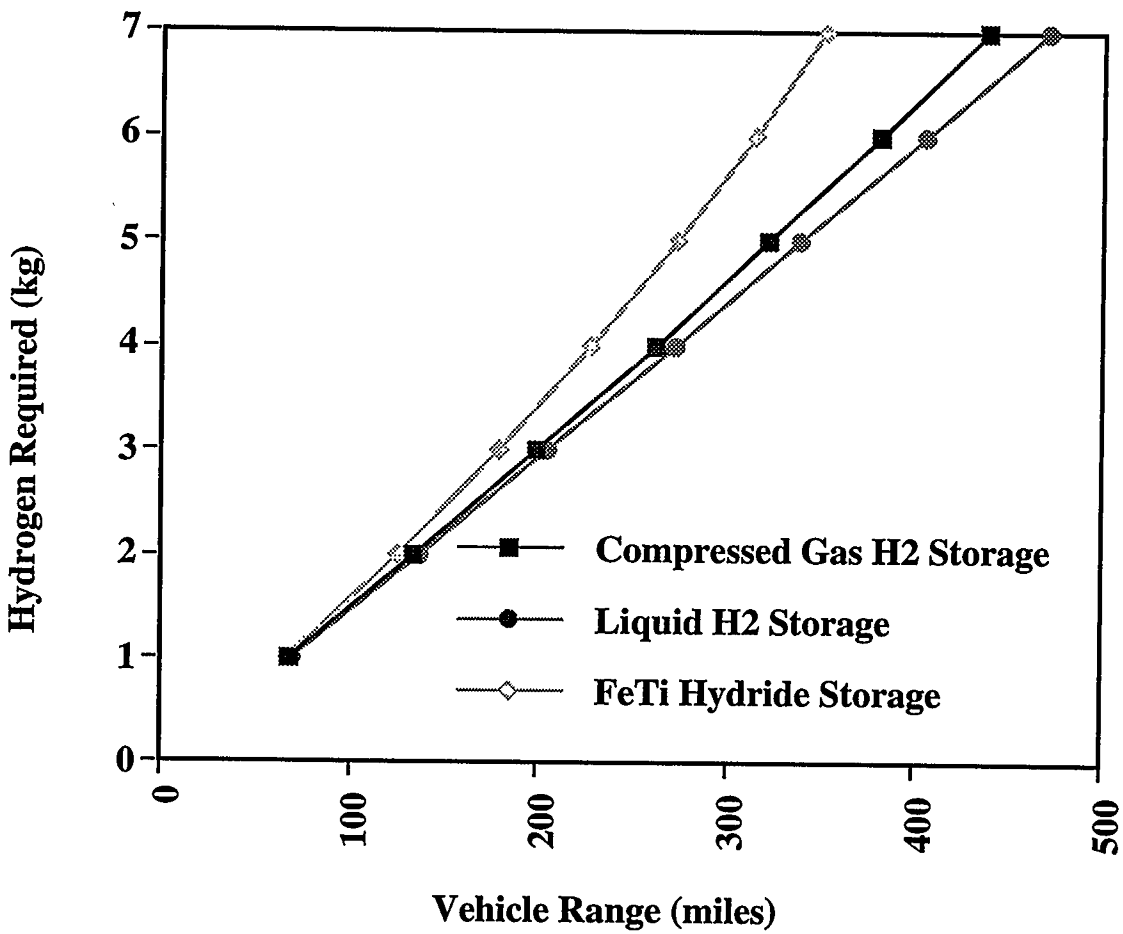

LH2 REFUELING
Vehicle tank bayonets
GH2
LH2
Plug
Control line
Controller
Vacuum box
Vacuum pump
GH2 REFUELING
High pressure GH2
Low pressure GH2
Plug
H2 vent stack
LH2 fill from tanker
Centrifugal pump LH2
LH2 Dewar
High pressure piston pump
PRV
Heat exchanger
High pressure GH2 storage
GH2 cylinders
Gas holder
Compressor
Burst disc

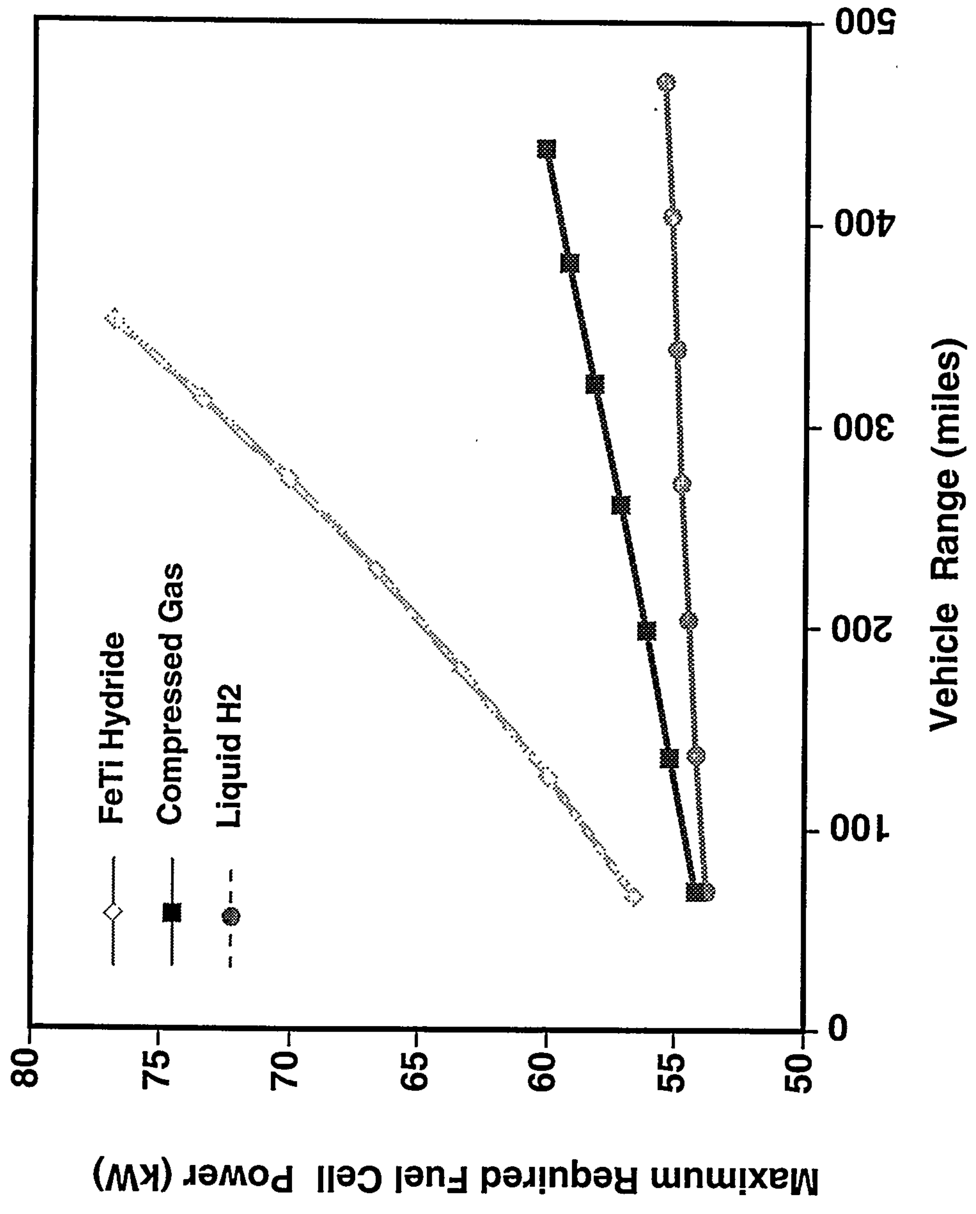

TANK PRESSURE (bar)
2.0
1.8
1.6
1.4
1.2
1.0
0.8
TIME (min)
0
1
2
3
4
5
Initial vehicle tank pressure = 1.0 bar
Initial pressure difference = 1.0 bar
Pump power = 20 W


Initial pressure difference
Δp = 1.0 bar
Δp = 1.5 bar
Δp = 2.0 bar
Initial vehicle tank pressure = 1.0 bar
TRANSFER TIME (min)
9
8
7
6
5
4
3
0.8
1.0
1.2
1.4
1.6
1.8
2.0
SUBCOOLING (K)


Initial pressure difference = 1.0 bar
Pump Power = 0 W
Pump Power = 20 W
Pump Power = 40 W
Initial vehicle tank pressure = 1.0 bar
TRANSFER TIME (min)
9
8
7
6
5
4
3
0
1
2
SUBCOOLING (K)


TRANSFER TIME (min)
0
10
20
30
PIPE ID (inches)
0.2
0.3
0.4
0.5
0.6
0.7
3/8" x .049" w
3/8" x .035"w
1/2" x .049" w
1/2" x .035" w
5/8" x .049" w
3/4" x .049" w


Hydrogen Required (kg)
0
1
2
3
4
5
6
7
Vehicle Range (miles)
0
100
200
300
400
500
Compressed Gas H2 Storage
Liquid H2 Storage
FeTi Hydride Storage


Maximum Required Fuel Cell Power (kW)
50
55
60
65
70
75
80
0
100
200
300
400
500
Vehicle Range (miles)
FeTi Hydride
Compressed Gas
Liquid H2

DEVELOPMENT OF A FIBER-OPTIC SENSOR FOR HYDROGEN LEAK DETECTION

David K. Benson
C. Edwin Tracy
National Renewable Energy Laboratory
Golden, CO 80401

Abstract

The real and perceived risks of hydrogen fuel use, particularly in passenger vehicles, will require extensive safety precautions including hydrogen leak detection. Conventional hydrogen gas sensors require electrical wiring and may be too expensive for deployment in multiple locations within a vehicle. In this recently initiated project, we are attempting to develop a reversible, thin-film, chemochromic sensor that can be applied to the end of a polymer optical fiber. The presence of hydrogen gas causes the film to become darker. A light beam transmitted from a central instrument in the vehicle along the sensor fibers will be reflected from the ends of the fiber back to individual light detectors. A decrease in the reflected light signal will indicate the presence and concentration of hydrogen in the vicinity of the fiber sensor.

The typical thin film sensor consists of a layer of transparent, amorphous tungsten oxide covered by a very thin reflective layer of palladium. When the sensor is exposed to hydrogen, a portion of the hydrogen is dissociated, diffuses through the palladium and reacts with the tungsten oxide to form a blue insertion compound, H_xWO_3. When the hydrogen gas is no longer present, the hydrogen will diffuse out of the H_xWO_3 and oxidize at the palladium/air interface, restoring the tungsten oxide film and the light signal to normal.

The principle of this detection scheme has already been demonstrated by scientists in Japan. However, the design of the sensor has not been optimized for speed of response nor tested for its hydrogen selectivity in the presence of hydrocarbon gases. The challenge of this project is to modify the basic sensor design to achieve the required rapid response and assure sufficient selectivity to avoid

false readings.

Background

Widespread use of hydrogen as a portable fuel will require appropriate use of leak detection for safety assurance. In an automobile, for example, hydrogen leak sensors may be needed in several locations and the cost and complexity of conventional hydrogen leak sensors may be too great for the cost-sensitive automobile market.

The most commonly used hydrogen gas sensor is a sintered tin-oxide, semiconductor whose resistance changes when it is exposed to a reducing gas at high temperature (typically 400 C). In large quantities, their cost is more than $20 each. These sensors require electrical wiring for their integral heaters and resistance readouts and the cost of this wiring to several sensor locations in a hydrogen-fueled automobile would also be significant. Any electrical fault at a sensor location could cause ignition of a hydrogen leak (see Table 1, McCarty 1981). Also, these semiconductor sensors are not very selective; other reducing gases such as carbon monoxide, gasoline vapors, methane, etc. which may be commonly present in the transportation environment, can cause a false signal.

Table 1. Hydrogen Hazards (in Perspective)

	Hydrogen	Gasoline
Limits of flammability in air (vol. %)	4-75	1-7.6
Limits of detonability in air (vol. %)	18.3-59	1.1-3.3
Energy of explosion* (Kg TNT/m^3 of gaseous fuel)	2.02	44.22

*Theoretical maximum at STP

In 1984, Kentaro Ito at Shinshu University took a well-known phenomenon called the hydrogen chemochromic effect in tungsten oxide films (Shaver 1967) and proposed its use in a fiber-optic hydrogen sensor (Ito 1984). This approach appears to be free of many of the problems associated with the use of conventional sensors: it does not require electrical wiring to the sensor location; it is inherently low-cost; and it is much more selective for hydrogen. Over the last ten years this sensor concept has been investigated further (Ito 1992, Oh 1993 and Ito 1993) but no attempt has been reported to develop a practical detector based upon the phenomenon.

While the concept of optical detection of hydrogen gas with the chemochromic effect in tungsten oxide has been demonstrated in the laboratory, there still remain important uncertainties of a practical nature. Will the response speed of the sensor be adequate? Is its selectivity suitable in the presence of other reducing gases? Can the sensor be made to be sufficiently reliable and durable? And, can this sensor scheme be successfully integrated into a fiber-optic leak detection system.

This paper describes a new project at NREL that is intended to optimize the operation of a chemochromic tungsten oxide hydrogen sensor and to test a bench-scale, fiber-optic hydrogen leak detector system based upon this optimized sensor. The project takes advantage of ten years of materials research on tungsten oxide films at NREL where they have been studied extensively for their use in electro-optically active, electrochromic window coatings under the DOE Office of Building Energy Research Advanced Windows Program (Benson 1993).

The Chemochromic Hydrogen Sensor

Atomic hydrogen reacts reversibly with tungsten oxide at room temperature to form a topotactic insertion compound H_xWO_3 with x varying up to about 0.4; above this concentration, the hydrogen changes the crystal structure and makes the reaction less reversible. The WO_3 is transparent, but the H_xWO_3 absorbs light strongly across the visible and near-infrared portions of the spectrum with a peak at about 1.3 eV (950 nm). If a layer of WO_3 coated with a thin film of palladium is exposed to hydrogen, a portion of the hydrogen will be dissociated, diffuse through the palladium and react with the WO_3. Figure 1 (Ito 1984) shows how the optical absorption of such a WO_3/Pd stack changes with exposure to different concentrations of hydrogen. In air, the reaction is reversible because the hydrogen can diffuse out of the H_xWO_3 to the air/Pd interface where it is oxidized.

Such a coating stack on the end of an optical fiber can provide remote optical detection of hydrogen gas. A light beam can be propagated along the fiber, reflect off the Pd film and return to a detector (Fig. 2). In the presence of hydrogen gas, the H_xWO_3 absorbs part of the light and decreases the detector signal. This change in detector signal can be correlated with the concentration of hydrogen gas.

Detector Requirements

The requirements for a practical hydrogen leak detector are listed in Table 2A. The detector must be sensitive enough to warn of hydrogen leaks well before the concentration reaches the ignition limit (about 4% in air). In the event of a hydrogen leak, the sensor must respond fast enough to allow automatic safety devices to operate before a dangerous concentration develops. The optimum speed of this response depends upon the location and size of the leak and will be dictated by automobile system design considerations that are not yet known. The detector should be long-lived, durable (or cheap and easy to replace) and above all, reliable.

The reliability requirements for the detector can be discussed in terms of its response table (Table B). If the detector falsely indicates the presence of a hydrogen leak (a Type II error), it will cause an inconvenience. On the other hand, if the detector causes a Type I error, a serious accident may occur. Detector failure should cause Type II errors (a "fail safe" condition). Similarly, interference from other gases should cause safe, Type II errors.

The characteristics of the fiber-optic chemochromic sensor seem to favor reliable operation. If the fiber were to break or the light source fail, a safe Type II error would occur. Interferences from hydrocarbon gases will also tend to cause safe, Type II errors.

Table 2A. Requirements for Hydrogen Sensor

Sensitive	<<4% H_2 in air
Fast	(Few seconds?)
Reliable	Zero type I errors*
Insensitive to interfaces	Few type II errors*
Long life	~10 years (or easy replacement)
Low cost	(cents per sensor; few dollars per system)

*Table B. Sensor Response

Leak\Response	H_2 detected	H_2 not detected
$H_2 > 4\%$	no error	type I error
$H_2 << 4\%$	type II error	no error

Approach

Transition metal oxide thin films have been studied extensively at NREL for use in electrochromic, energy conserving window coatings. When small positive ions such as H^+ or L^+ are electrochemically inserted into tungsten oxide, the same kind of insertion compound, H_xWO_3 or L_xWO_3, with the same optical absorption spectra are formed as during the chemochromic coloration discussed above for the hydrogen sensor. Similar reversible electrochromic, insertion compounds are formed with oxides of vanadium, molybdenum, chromium, niobium, manganese, cobalt (Granquist 1994) and some mixed oxides such as tungsten-molybdenum oxide (Faughnan 1977). In all of these cases, it appears that the coloration is due to optical absorption by electron transitions in the vicinity of metal ions with reduced valence (e.g. W^{+5} in $W^{+6}O^{-2}_3$, Faughnan 1980) although the details of this process remain controversial. The kinetics of the ion migration in these materials is strongly dependent upon the morphology of the metal oxide which can be controlled by the details of its deposition as a thin film (Zhang 1993a and 1993b). In general, the fastest electrochromic response is obtained with nano-porous oxide films which have a fractal pore structure. The lower the fractal dimension, the faster is the ion transport. Films deposited at low temperatures in partial pressures of water vapor (10^{-4} torr) have fractal dimensions of about 2.65 and fast electrochromic responses.

Initially, chemochromic films will be prepared by thermal evaporation onto glass substrates and tested in carefully controlled environments as we optimize the design of the sensors. Our approach to optimizing the chemochromic sensor will be to adjust the composition and morphology of the oxide layer to achieve needed response speed and sensitivity and to adjust the composition and thickness of the overlying catalytic metal layer to increase selectivity (if necessary). Once desirable performance has been demonstrated on glass substrates, the same sensor construction will be tested on polymer substrates and finally applied to the ends of polymer optical-fibers. A bench-scale, detector system will then be constructed with these polymer optical-fiber sensors for engineering-scale testing.

Progress

The apparatus for exposing the sensor films to controlled atmospheres has been adapted from an existing, ultra-high vacuum system with integral mass-spectrometry and excellent gas mixing capabilities (Fig. 3). This apparatus has been modified to accept small sensor-coated substrates which can be optically monitored as its gaseous environment is changed (Fig. 4). A fiber-optic reflectometer will be used to monitor the change in optical reflection of a light beam that passes through one of the chamber windows, through the chemochromic oxide film and reflects off of the catalytic film. This same fiber-optic reflectometer will be used later in the project as part of the bench-scale fiber-optic hydrogen leak detector system.

Conclusions

A potentially advantageous method for detecting hydrogen leaks safely and economically has been identified. The solid-state physics of the hydrogen sensor operation is very similar to a very well studied electrochromic phenomenon. We have just begun to apply our knowledge of the electrochromic effects in metal oxides to the optimization of a hydrogen sensor. The sensor measurement apparatus has been constructed and samples have been prepared but results await delivery of a new fiber-optic reflectometer.

Acknowledgements

This work was supported by the U.S. Department of Energy under contract No.DE-AC36-83CH1009.

References

Benson, D. and J. S. E. M. Svensson 1988. "Plasma enhanced CVD of W and Mo Oxides.", In *Large-area Chromogenics: Materials and Devices for Transmittance Control,* 215-229. Hamburg, Federal Republic of Germany: SPIE Volume IS 4.

Faughnan, B. W. and R. S. Crandall. 1980. "Electronic Displays Based on WO_3."In *Display Devices* (J. I. Pankove, ed.), *Topics in Applied Physics* 40:181-211, Springer, Berlin.

Faughnan, B. W. and R. S. Crandall. 1977. "Optical Properties of Mixed Oxide WO_3/MoO_3 Electrochromic films." *Appl. Physics Lett.*, 31:834-836.

Granqvist, C. G. 1994. "Electrochromic oxides: a bandstructure approach." *Solar Energy Materials and Solar Cells* 32:369-382.

Ito, K. and T. Kubo 1984. "Gas Detection by Hydrochromism." In *Proceedings of the 4th Sensor Symposium, 1984,* 153-156.

Ito, K., T. Ohgami and T. Nakazawa. 1993. "Effect of water on hydrogen-sensitive tungsten oxide films." *Sensors and Actuators B*, 12:161-167.

Ito, K. and T. Ohgami. 1993. "Hydrogen detection based on coloration of anodic tungsten oxide film." *Appl. Phys. Lett.* 60: 938-940.

Oh, Y., J. Hamagami, Y. Watanabe and M. Takata. 1993. "Preparation and characterization of an optically-detectable hydrogen sensor consisting of Pd/WO_3 thin films." *Sensors and Actuators B*, 13-14:547-548.

McCarty, R. D., J. Hord and H. M. Roder 1981. "Selected Properties of Hydrogen (Engineering Design Data)." *National Bureau of Standards Monograph* No. 168: 6-290.

Shaver, P. J. 1967. "Activated Tungsten Oxide Gas Detectors." *Appl. Phys. Lett.* 11:255-256.

Zhang, J-G., C. E. Tracy, D. K. Benson and S. K. Deb. 1993a. "The influence of microstructure on the electrochromic properties of Li_xWO_3 thin films: Part I. Ion diffusion and electrochromic properties." *J. Mater. Res.* 8:2649-2656.

Zhang, J-G., D. K. Benson, C. E. Tracy, and S. K. Deb. 1993b. "The influence of microstructure on the electrochromic properties of Li_xWO_3 thin films: Part II. Limiting mechanisms in coloring and bleaching processes." *J. Mater. Res.* 8:2657-2667.

Figures

1. Typical optical spectra of a tungsten oxide thin film after exposure to various concentrations of hydrogen.
2. Schematic diagram of the fiber-optic, chemochromic hydrogen detector.
3. Diagram of the vacuum/controlled atmosphere test chamber for measuring sensor sensitivity to hydrogen and to interference gases.
4. Partial cut-away diagram of the sensor test chamber showing the use of a fiber-optic reflectometer for monitoring changes in the sensor inside the test chamber.

Optical Absorption in H_xWO_3 Films

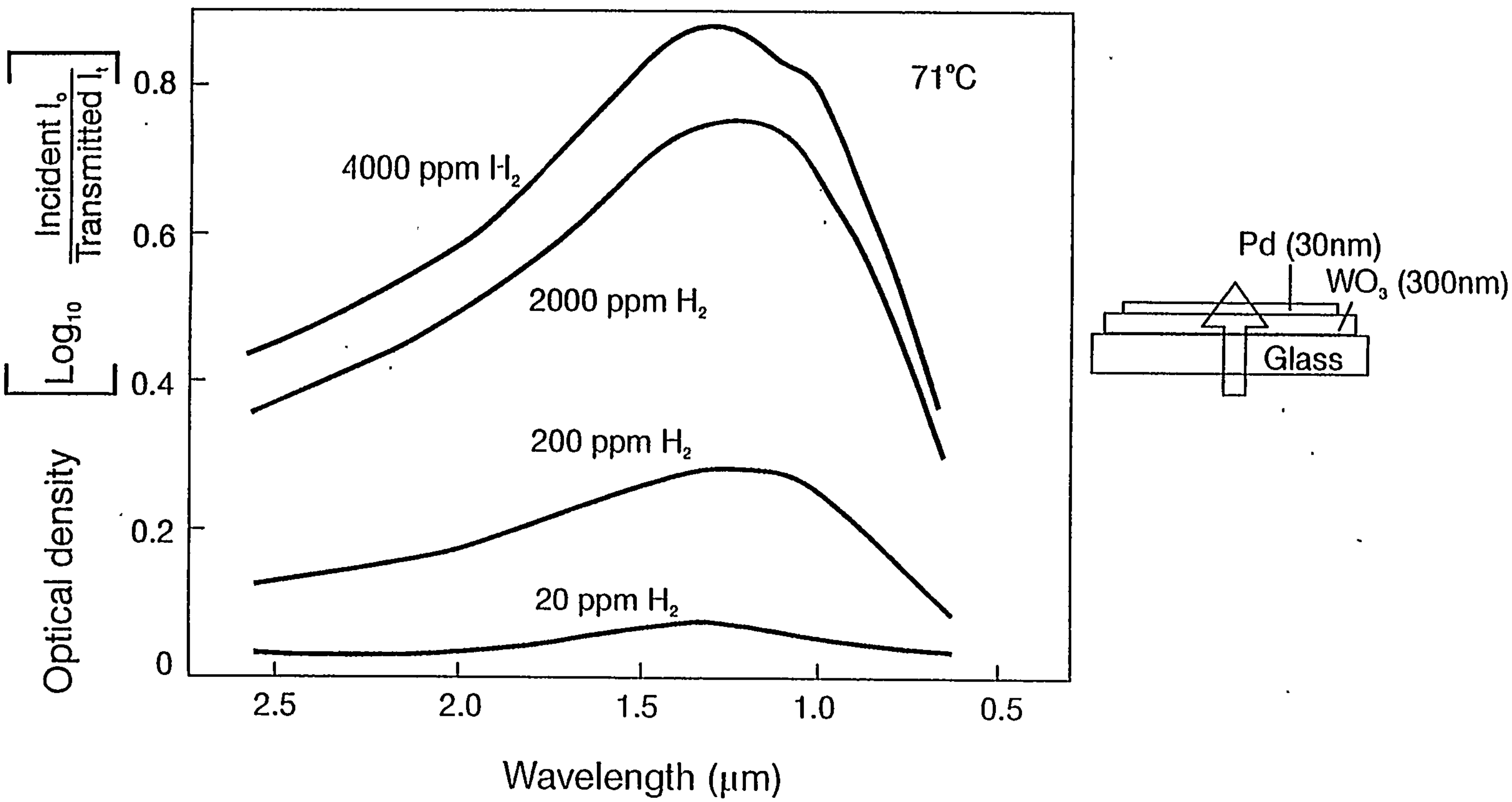
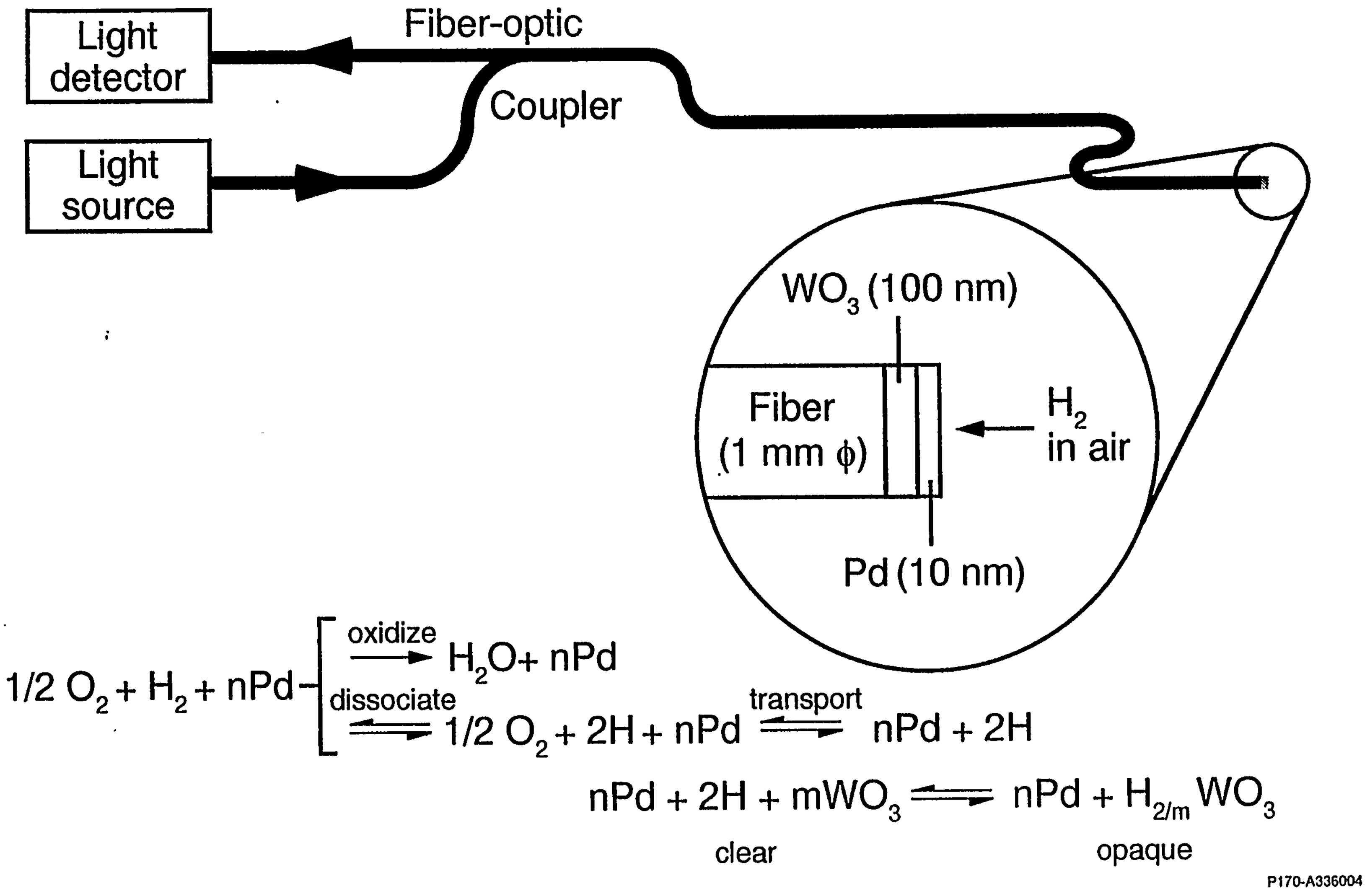


FIG. 1

K. Ito and T. Kubo (1984)



$$1/2\ O_2 + H_2 + nPd - \left[\begin{array}{l} \xrightarrow{\text{oxidize}} H_2O + nPd \\ \overset{\text{dissociate}}{\rightleftharpoons} 1/2\ O_2 + 2H + nPd \overset{\text{transport}}{\rightleftharpoons} nPd + 2H \end{array}\right.$$

$$\underset{\text{clear}}{nPd + 2H + mWO_3} \rightleftharpoons \underset{\text{opaque}}{nPd + H_{2/m}WO_3}$$

FIG. 2

Instrument System

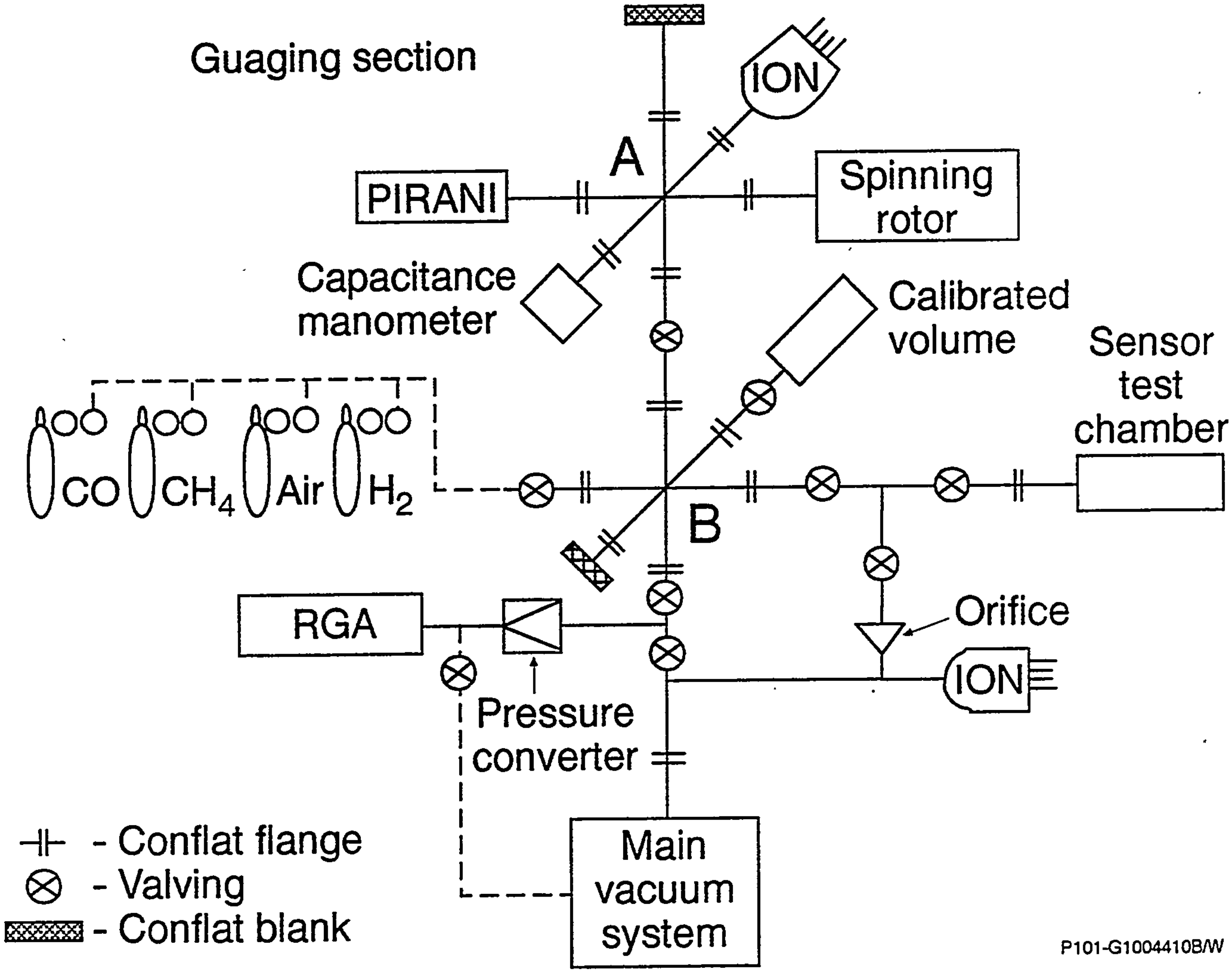


FIG. 3

Sample Holder

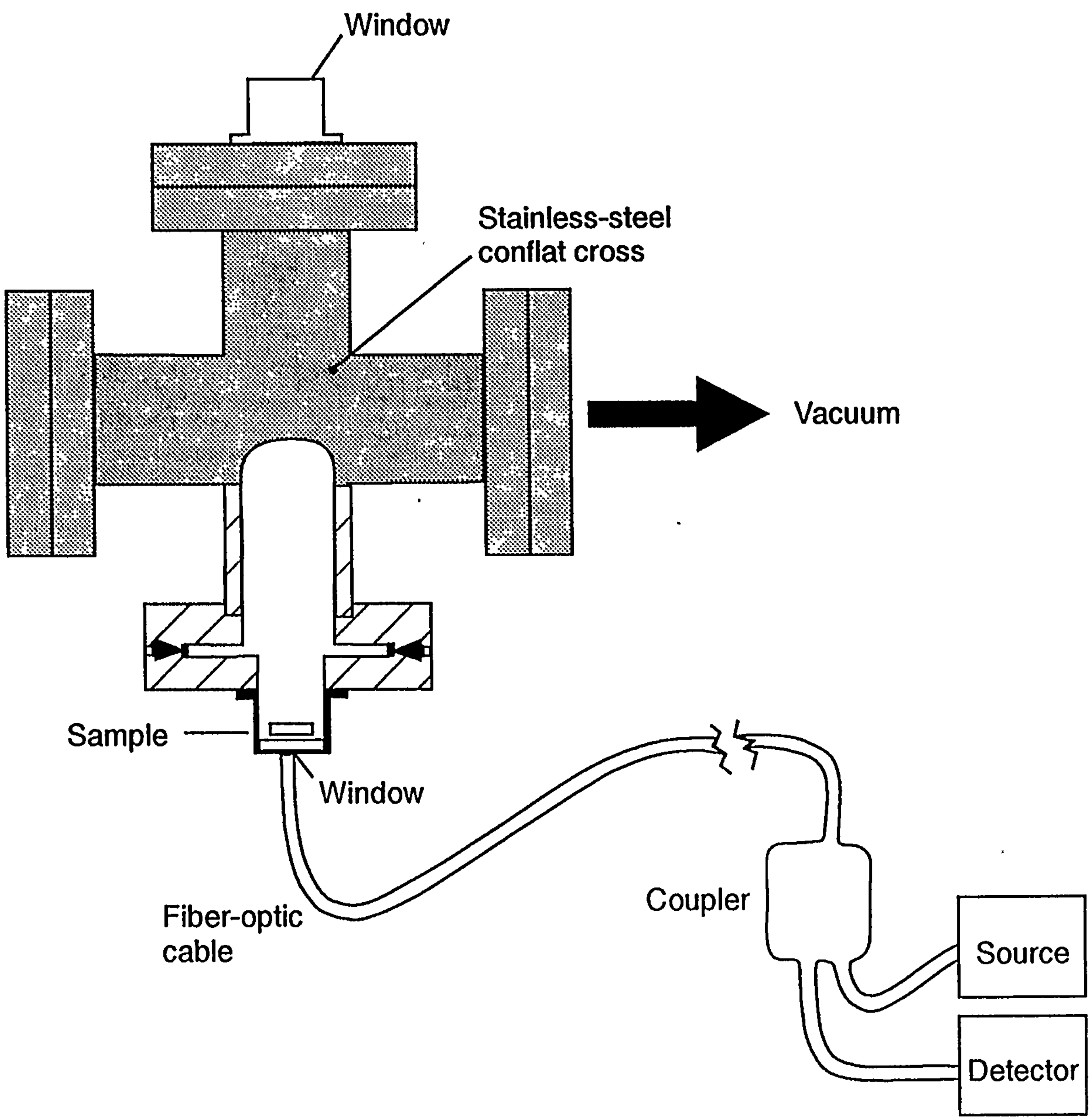


FIG. 4

A POLYMER ELECTROLYTE FUEL CELL STACK FOR STATIONARY POWER GENERATION FROM HYDROGEN FUEL

Shimshon Gottesfeld
Materials Science and Technology Division
Los Alamos National Laboratory
Los Alamos, NM 87545

Abstract

The fuel cell is the most efficient device for the conversion of hydrogen fuel to electric power. As such, the fuel cell represents a key element in efforts to demonstrate and implement hydrogen fuel utilization for electric power generation. The low temperature, polymer electrolyte membrane fuel cell (PEMFC) has recently been identified as an attractive option for stationary power generation, based on the relatively simple and benign materials employed, the zero-emission character of the device, and the expected high power density, high reliability and low cost. However, a PEMFC stack fueled by hydrogen with the combined properties of low cost, high performance and high reliability has not yet been demonstrated. Demonstration of such a stack will remove a significant barrier to implementation of this advanced technology for electric power generation from hydrogen.

Work done in the past at LANL on the development of components and materials, particularly on advanced membrane/electrode assemblies (MEAs), has contributed significantly to the capability to demonstrate in the foreseeable future a PEMFC stack with the combined characteristics described above. A joint effort between LANL and an industrial stack manufacturer will result in the demonstration of such a fuel cell stack for stationary power generation. The stack could operate on hydrogen fuel derived from either natural gas or from renewable sources. The technical plan includes collaboration with a stack manufacturer (CRADA). It stresses the special requirements from a PEMFC in stationary power generation, particularly maximization of the energy conversion efficiency, extension of useful life to the 10^4 hours time scale and tolerance to impurities from the

reforming of natural gas.

Background

The fuel cell is the most efficient device for the conversion of hydrogen fuel to electric power. As such, the fuel cell represents a key element in efforts to demonstrate and implement hydrogen fuel utilization for electric power generation.

The high efficiency combined with very low environmental emissions and modular construction have fostered continued interest for the last thirty years in fuel cell technology for utility, customer-side-of-the-meter and transportation applications. Among the family of fuel cell technologies, polymer electrolyte (PEM) fuel cells have some uniquely attractive features, including a combination of high power density and high chemical-to-electric energy conversion efficiency, fast and easy start-up, high reliability and highly durable and benign materials of construction. Nevertheless, the application of PEM fuel cell technology for utility and/or stand alone applications was judged in the past to be too expensive for any terrestrial applications and also to be too sensitive to low levels of carbon monoxide in reformed carbonaceous (most likely natural gas) fuel feed streams. Both of these barriers for implementation of PEM fuel cells in utility and/or stand-alone applications have been significantly lowered in the last few years, in large part as a result of work done at Los Alamos National Laboratory. This work has shown a clear way to the lowering of the cost of PEM fuel cell stacks and has demonstrated an effective technique for the elimination of anode catalyst deactivation effects resulting from low levels of CO or other organic impurities. These recent technical developments now allow to take advantage of some very attractive features of the PEM fuel cell technology in utility and stand-alone applications. Demonstration of hydrogen fueled PEM fuel cell stacks of intrinsic ally low cost and of high performance and durability is the subject of this project.

The PEM technology provides a compact system with demonstrated power densities of 0.2 kW/liter and a good potential for increase in power density to 1 kW/liter. It's operating temperature is typically 80°C, with significant power generated at room temperature. In the early 1980's, DOE initiated an exploratory research program to develop the core technology of the PEM fuel cell. The objective of the program was to enhance the performance and reliability and reduce the cost of the PEM fuel cell stack. Over the last few years, progress in this area has been quite spectacular in showing very effective routes for cost reduction and for application of steam-reformed carbonaceous fuels as the source of hydrogen for the PEM fuel cell stack.

In addition to these significant developments in the technology base, recent demonstration efforts in the transportation sector have been very effective in raising the profile of the PEM fuel cell technology and in demonstrating it as a potentially viable technology for transportation. However, it is quite clear that, because of somewhat less stringent cost and space requirements in stationary power generation applications (as well as easier answers for the source of hydrogen fuel), implementation of the hydrogen-fueled PEM fuel cell stack for the latter family of applications is likely to precede it's implementation in transportation applications.

Let us return now to some specific recent achievements at Los Alamos that advanced PEM fuel cell technology to the point of readiness for the demonstration of a low-cost hydrogen-fueled stack for stationary power generation.

- Low cost membrane-electrode assemblies with ultra-low platinum loadings of 0.2 gr/kW have been demonstrated in 5000 hours life tests, generating areal power densities of 0.6 kW/ft^2 (Wilson, 1992-1995).
- Complete sets of membrane/electrode assembly and other cell functional and structural components have been identified such as to lower the total materials cost to 45$/kW under mass production conditions.
- Effective water management principles have been identified, based to large extent on advanced membrane electrolytes evaluated jointly with membrane manufacturers (Springer 1991, Zawodinski 1993).
- Detailed evaluation of losses in the PEM fuel cells has been based on investigation of fundamental processes in the cell, including all electrocatalytic and transport phenomena (Springer, 1993).
- Based on the above evaluation, an effective code and set of experimental diagnostics for the PEM fuel cell has been established (Springer, 1993).
- Tolerance to carbon monoxide levels expected from steam reforming of natural gas has been achieved. Whereas, in previous work we have shown that air bleeding into the anode takes care of CO levels as high as 50-100 ppm under normal operation conditions (Gottesfeld, 1988 and 1990), we have recently identified at LANL ways to increase CO tolerance to 300-600 ppm without any bleeding of air.

These achievements place the technology developed at LANL at an excellent position for demonstration in a hydrogen-fueled PEM fuel cell stack for stationary power applications.

Approach

This project is based on a two-year program of a joint LANL/Industrial Partner effort. The industrial partner has had significant experience in the development of fuel cell stack and fuel cell system technology. The project will include the following main tasks:

(1) Exchange membrane/electrode (M&E) assemblies between LANL and the industrial partner and their testing

(2) Optimize fabrication of M&Es of larger area (100 cm^2 or above)

(3) Optimize flow field and backing materials

(4) Apply diagnostics and code for loss analysis in cells

(5) Test 3-5 cell baseline stack with different MEAs and existing hardware

(6) Hardware component design and fabrication

(7) 3-5 cell prototype stack fabrication and testing

(8) 20-cell, 120 cm^2 prototype stack, fabrication and testing

(9) Peripheral devices installed in assembly to provide 4-5 kW system

(10) Testing of system with hydrogen/air and simulated reformate/air

Progress

Funding for this project started February 1995. Since that starting date, the following progress has been made:

(1) A CRADA agreement has been negotiated based on a detailed joint work statement. At this point, the agreement has been approved by DOE/Albuquerque and requires only final signatures by LANL and the industrial partner.

(2) In preparation for Tasks (1) and (2) described above, work at LANL has been pursued for the automated fabrication of membrane/electrode assemblies of larger surface areas. A novel technique has been developed to apply the catalyst ink directly to the ionomeric membrane automatically, using a computer controlled X-Y recorder. This has enabled well controlled preparation of membrane electrode assemblies of 100 cm^2 area, to be compared with cells of 5-25 cm^2 active area used in most of the LANL work in the past. This automated application of the catalyst to the membrane has demonstrated the good potential for scale-up of the process developed at and patented by LANL. Figure 1 shows the equipment employed for the automated preparation of membrane/electrode (M&E) assemblies of large surface areas.

The 100 cm^2 M&Es were subsequently tested in some preliminary tests performed with new short stack hardware built for this purpose. The hardware has been based on some novel concepts for the flow field and on metal (titanium or stainless steel) bipolar plates. In these preliminary tests, a single cell of 100 cm^2 active area repeated the performance per cm^2 obtained before in 5 cm cells, demonstrating the uniformity of the M&E of larger area fabricated by the new automated process. Figure 2 shows the testing equipment and the new 100 cm^2 cell, generating above 100A at 0.5V when operating on slightly pressurized air and hydrogen. Preliminary experiments with a two-cell stack showed (per cell) 90% of the single cell performance, highlighting some need for more optimized humidification.

Conclusion

Having completed the preparation of a CRADA agreement with our industrial partner and having demonstrated, for the first time, automated fabrication of membrane/electrode assemblies based on the Los Alamos thin-film technology, this project is now ready to continue as a joint effort to manufacture a prototype PEM fuel cell stack fueled by hydrogen for stationary electric power generation of low cost and high performance and reliability. The preliminary results obtained at LANL with short stacks, based on such automatically fabricated M&Es and on metal bipolar plates, have been quite encouraging. The project is planned to yield within a period of two years from the beginning of active collaboration, a 4-5 kW system for utilization of hydrogen in the generation of electric power by means of a highly efficient energy conversion system of low cost and high performance and reliability.

References

1. M. S. Wilson and S. Gottesfeld, J. Appl. Electrochem., 22, 1-7 (1992)

2. M. S. Wilson and S. Gottesfeld, J. Electrochem. Soc., 139, L28-:30 (1992)

3. M.S. Wilson, US Pat Nos. 5,211,984 and 5,234,777 (1993)

4. M.S. Wilson, J. Valerio and S. Gottesfeld, Electrochim. Acta, 40, 355-363 (1995)

5. T. E. Springer, T. A. Zawodzinski and S. Gottesfeld, *J. Electrochem. Soc.,* **138,** 2334- 2442 (1991)

6. T. A. Zawodzinski, T. E. Springer, F. A. Uribe and S. Gottesfeld, *Solid State Ionics*, **60**, 199-211 (1993);

7. T. E. Springer, M. S. Wilson, and S. Gottesfeld, *J. Electrochem. Soc*. **140,** 3513 (1993).

8. S. Gottesfeld and J. Pafford, J. Electrochem. Soc. 135, 2651-2652 (1988)

9. S. Gottesfeld, US Patent No. 4.910,099 (March 1990)

Automated Printing of Catalyst on Membrane

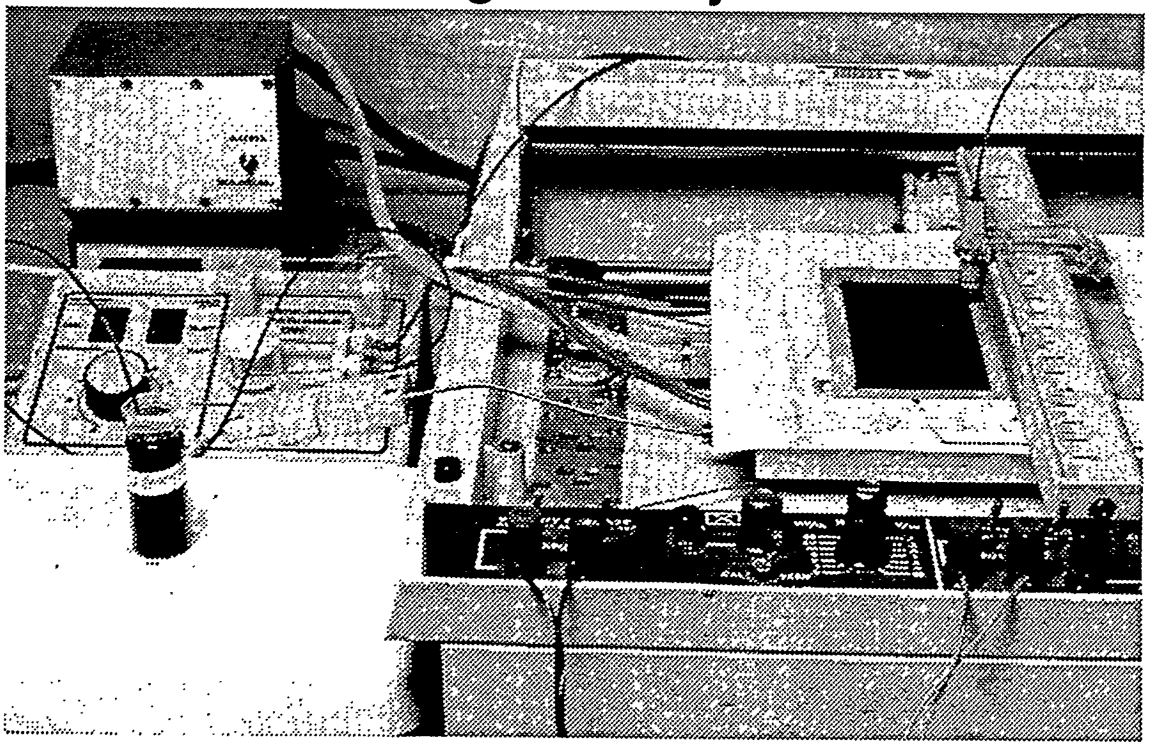


Figure 1

LANL 100 cm^2 PEFC

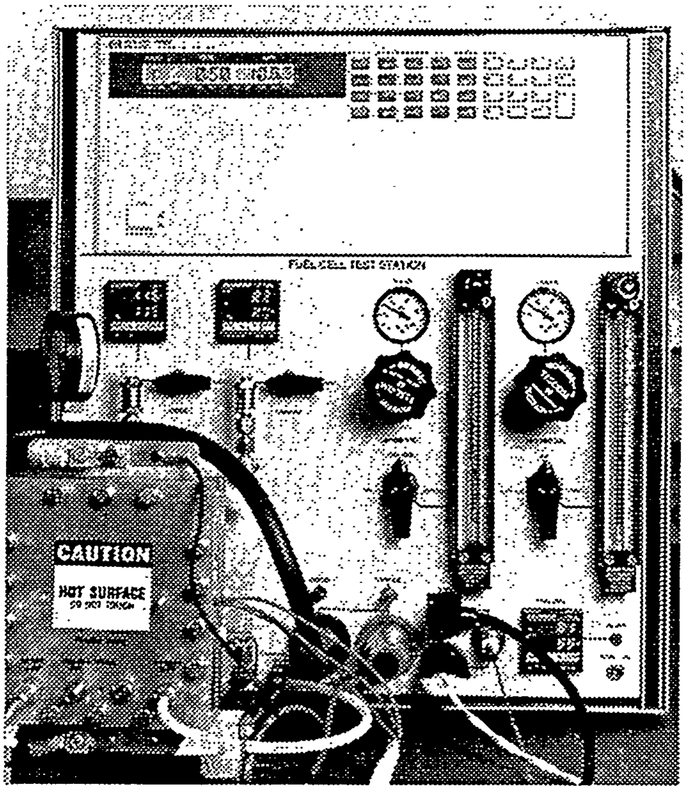
0.13 mg Pt/cm^2 each side, 80°C

$P_{air} = P_{H_2} = 30$ psig

Air Util. = 50%

H_2 Util. = 90%

Figure 2



SAFETY ANALYSIS OF HIGH PRESSURE GASEOUS FUEL CONTAINER PUNCTURES

Dr. Michael R. Swain
University of Miami
Coral Gables, FL 33143

Abstract

The following report is divided into two sections. The first section describes the results of ignitability tests of high pressure hydrogen and natural gas leaks. The volume of ignitable gases formed by leaking hydrogen or natural gas were measured. Leaking high pressure hydrogen produced a cone of ignitable gases with 28° included angle. Leaking high pressure methane produced a cone of ignitable gases with 20° included angle. Ignition of hydrogen produced larger overpressures than did natural gas. The largest overpressures produced by hydrogen were the same as overpressures produced by inflating a 11 inch child's balloon until it burst.

Introduction

The first section of this report is the result of a full scale study to assess the risk of storing hydrogen in compressed form as opposed to storing natural gas in compressed form. Risk includes two components, the likelihood of combustion and the severity of combustion. The size of the combustible cloud produced by the leaking gas is used as an indication of the likelihood of combustion. The overpressure produced by ignition of the cloud is used as an indication of the severity of combustion. This study has direct applicability to vehicular storage and stationary storage of hydrogen. The second section of the report is an example of the effect that the risk assessment results have on vehicle design.

Experimentation

Flame Visibility

The initial experimental work was centered around finding a suitable method for making a pictorial record of the ignitable boundaries of the combustible clouds. Previous experiments had shown the hydrogen flames to be clearly visible at night though there was some question as to whether the entire flame was visible. It should be pointed out that the hydrogen used was commercially available compressed hydrogen. The visibility of hydrogen flames at night or in artificial light has been noted with all commercially available compressed hydrogen tested to date. In an effort to verify that the visible boundary corresponded with the actual flame boundary, Kodak High Speed Infrared film was used (with a Wratten filter) to photograph the ignition of hydrogen-air flames. Hydrogen was vented, at night, at a constant flow rate and a propane ignitor flame was moved closer to the hydrogen jet until ignition occurred. The infrared photographs clearly showed the hydrogen flame extending up to, but not past, the propane ignitor flame. This demonstrated that the location of the combustible cloud boundary corresponded with the location of the edge of the visible flame. The flame position recorded was the same using Wratten 87 (780 Å and up) or 87C (850 Å and up) filters. This was also seen to be the case in photographs taken with standard color film (visible light). Since the High Speed Infrared film was only available from Kodak at extremely high cost, in 16mm motion picture format, video imaging was chosen as an alternative. A video camera with CCD imaging element was selected and the video taped flame ignitions showed the same flame boundary positions as did the infrared and visible light photographs.

Experimental Technique

The experiments consisted of simulated tank puncture as follows. Compressed gas storage cylinders were fitted with pneumatically actuated valves of sufficient capacity to provide minimal restriction to the flow when open. The outlet side of each valve was connected to an orifice (a simulated punctured container wall). Opening the valve initiated the leak, simulating tank rupture. The size of the resulting cloud of hydrogen or natural gas was quantified by testing ignitability at the periphery of the cloud with electric arcs or propane flames much the same way it had been done in the previous work. Additionally, measurements of overpressures were made and video recordings were used to document the combustion.

The simulated tank ruptures were made by venting either hydrogen or natural gas, horizontally or vertically, at pressures ranging from 2400 psi to 100 psi. The vent hole was 0.15 inches in diameter. The ignition source was then used to locate the ignitable boundary. Figures 1-4 show the results of the ignition tests. Next to each symbol on figures 1-4 is the initial pressure at which the test began. Multiple pressures listed represent multiple tests at that location. A description of the design of the experimental apparatus and electrical arc ignitor are found in the next section.

Experimental Apparatus

A high energy automotive type ignition system was modified to be used as the arc ignitor for the work. A digital timer and control circuit was used to sequence both the release of the combustible gas and the firing of the ignitor. When the start button on the sequencer was pressed the circuit actuated the pneumatic valve releasing the gas and then, a specified time later, fired the ignitor. The sequencer could be configured to fire the ignitor in single arc mode or continuous (rapid multiple arc) mode. Figure 5 shows how the apparatus was configured. Ignition was also initiated with a one half inch propane flame.

The orientation of leak orifice (direction of leak) could be varied from horizontal to vertical. Data was primarily taken either horizontally or vertically.

Overpressures were measured with a PCB Pieziotronics 106B pressure transducer. The signal from the transducer was recorded with a Nicolet digital oscilloscope.

Computer Model of Leakage Rate

The flow rate of gases leaking from a punctured compressed gas container is limited by sonic throttling in the passageway of the leak. The gas flow rates produced during sonic throttling are independent of the exit pressure or in this case atmospheric pressure outside the container. The velocity of the gas exiting the puncture is a function of the ratio of specific heats, molecular weight, and temperature of the gas. The initial pressure and temperature of the gas in the container was known and then the expansion of the gas in the container was assumed to be either isothermal of isentropic to bracket the possible conditions. The following equation defines the mass flow rate of the gas assuming sonic throttling:

$$\frac{\dot{m}}{A^*} = \frac{P_0}{\sqrt{T_0}}\sqrt{\frac{k}{R}}\,\frac{1}{\left(\frac{k+1}{2}\right)^{\frac{k+1}{2(k-1)}}}$$

Where:

$\dot{m}$ - *mass flow rate*
A^* - *effective area of throat*
P_0 - *gas pressure in tank*
T_0 - *gas temperature in tank*
k - *ratio of specific heats*
R - *gas constant*

A model was constructed comparing the leakage of hydrogen and pure methane from compressed gas containers. Since both hydrogen and methane are non-ideal gases at the high pressures used in compressed gas storage, tables of the properties for each gas compiled for the appropriate pressures were used in the modeling (Armstrong 1976, Dean 1961, Kunkle 1969).

The results of the model are presented in figures 6-9. The results were a strong function of whether the process was assumed to be isothermal or isentropic. The real process is somewhere between the two. As gas is allowed to escape from the container the remaining gases in the container must expand. This expansion lowers the internal energy, and therefore the temperature, of the remaining gases. The lowered gas temperature allows for the two following scenarios:

1. Enough heat is transferred from the container to the gases to return them to their original temperature. If this continues throughout the process the process is termed isothermal.

2. No heat is transferred from the container to the gases and the process is termed isentropic.

The two extremes are shown in the data presented. The real process yields data that lies between the two curves and is a function of the heat transfer coefficient between the container and the gases, the surface area of contact between the container and the gases, the heat capacity of the container, the heat capacity of the gases, and the heat transfer between the container and the environment.

Ignition Tests

The data from the ignitability testing is shown in figures 1-4. Hydrogen leaking from the high pressure container produced a combustible cloud in the shape of a cone of 28° included angle. Any ignition source placed outside the 28° cone failed to ignite the cloud. As can be seen from the data almost the entire interior of the cone shaped cloud was ignitable. The behavior of the flames produced from various ignition sites was markedly different depending on the location of the ignition site. Ignition high in the cloud grows at a relatively slow rate and tends to move upward with the bulk gas flow. As the flame front grows and begins to penetrate to the richer mixtures lower in the cloud, the flame speed increases. This leads to rapid flame growth and as hydrogen-air mixtures can burn at up to 74% hydrogen by volume the flame propagates down to the source of the leak and a stable flame is produced.

The data from the ignitability testing with natural gas shows the cone of combustible gases for natural gas under the same conditions to have a 20° included angle. The combustible cloud formed by natural gas differed noticeably from that of hydrogen in that the interior of the cone contained a sizable volume of gases that were too rich to burn. Because of the high flow rate of gases associated with leakage from high pressure compressed gas storage the rich limit of combustion for natural gas was exceeded through the center of the cone. In the case of natural gas the flame speed was not high enough to propagate downward to the source of the leak from a high pressure container. This resulted in periodic extinction of the flame.

Overpressures

Figure 10 shows the pressure trace from the largest overpressure measured. The pressure was measured at a location 3 feet from the leak and reached a peak value of 0.25 psi. Maximum values at 6 feet dropped to 0.07 psi. The high pressure gas leak produced an overpressure of 0.04 psi without ignition. To convey these values in a pragmatic way, it was found that inflating a standard 11 inch child's balloon until it burst produced similar overpressures at similar distances as did the hydrogen cloud combustion, within balloon to balloon repeatability. The balloons used were helium quality 11 inch balloons made by CTI Industries, Gary, Indiana.

The magnitude of the overpressure was a function of the location of ignition. The maximum overpressure occurred for ignitions close to the source of the leak. A short delay between opening the leak and ignition would produce accumulation of a large vertical cone of combustible hydrogen-air mixture. Additional delay to allow accumulation of additional hydrogen did not appreciably effect the value of the maximum overpressure or the duration of the overpressure.

Ignition near the top of the cloud which eventually produces flame propagation downward through the cloud to the leak source produced lower overpressures than an ignition location near the source. Overpressures produced by ignition of natural gas were even lower than hydrogen for all geometries.

Radiation

Measurements were made of the trunk skin temperature during the venting and ignition of 50 SCF of hydrogen. This is representative of the volume of hydrogen storage in one of the 3000 psi 4.35 inch OD compressed hydrogen containers used in the vehicle conversion design exercise in section 2. The surface temperature of the truck rose from 70°F to 101°F by the completion of the burn.

Conclusions

1. The volume of ignitable gases caused by hydrogen leaking from a compressed gas container is larger than those caused by natural gas. Both produce cone shaped clouds principally aligned along the axis of the leak direction.

2. The overpressures caused by ignition of hydrogen-air clouds are greater than those caused by natural gas but both are small.

3. Venting low density gaseous fuel upward reduces the likelihood of contact with ignition sources during an accident. Venting upward also reduces the likelihood that gases will be trapped in the vehicle during an accident. Venting upward allows the natural buoyancy of hydrogen to carry the gas away from the vehicle.

4. Storage of compressed gases in multiple small containers rather than fewer large containers can reduce the amount of gas released if one container is ruptured in an accident.

Application to Vehicle Conversion

The following is an exercise incorporating the previous conclusions in the conversion of an existing gasoline powered vehicle to hydrogen fueled operation. The design criteria used were:

1. Use many small high pressure compressed hydrogen containers rather than a few large containers.
2. Provide for hydrogen, that may escape due to an accident, to vent upward.
3. Provide large crush distances to protect the compressed hydrogen containers during an accident.

Vehicle Choice

A vehicle of an initial weight between 2000 to 2100 pounds was chosen as the subject vehicle for conversion to hydrogen fueled operation. This choice was made because vehicle weight increases with the addition of a compressed gas storage system. Computer modeling has previously been done (Swain, et al; 1983) for a hydrogen powered vehicle of 2800 pounds total weight. Total weight included the weight of a driver. A 1992 Toyota Tercel was chosen which has an initial weight of 2055 lbs.

Compressed Gas Storage

The ideal position for the hydrogen storage containers, consistent with both the desire to vent upward and provide ample crush distance during an accident, is the forward most part of the trunk. Placing the containers in the front of the trunk still allows the tops of the containers to be behind the bottom of the rear window. This allows upward venting (criteria 2) to be accomplished by providing a panel above the containers that can pop off if the hydrogen begins to escape. The location at the front of the trunk also provides the largest crush distance between the containers and the rear bumper in the event of an accident (criteria 3). Working within the dimensions of the frame in the rear of the vehicle (Fig 11) a storage system of thirty-two 4.35 inch OD 3000 psi compressed gas containers was incorporated. Assuming that pointing the end of the tank containing the outlet valve mechanism upward best satisfies criteria 2, the tank length is limited by the vehicle body dimensions to approximately 35 inches.

Hydrogen Container Weight and Storage Capacity

Two types of containers were investigated to determine what effect the use of multiple small containers has on vehicle weight and size. The specifications provided by Pressed Steel Tank Company, Inc. and EDO Canada Ltd. were used to make the investigation.

In both cases equations were derived that fit the provided specifications for container storage capacity and weight as a function of container length and outside diameter. The fit of resulting empirically derived equations to the provided specifications is shown in figures 12-15. Figures 16-17 are plots of the storage capacity to weight ratio as a function of both length and outside diameter. A large ratio indicates large storage capacity per container weight. The general trend shown in figure 16-17 is that small diameter and long length yields the best storage to weight ratios. As was indicated in the previous section the container length for this application needed to be approximately 35 inches. The specifications provided by the two manufacturers indicated that the average size of available storage containers is approximately 14 inches in diameter and 50 inches long. From figure 16-17 it can be seen that a storage container approximately 4 to 5 inches in diameter and 35 inches long has the same storage capacity to weight ratio as the "average" available storage container. Working within the dimensions of the frame in the rear of the vehicle (Fig 11) a storage system of 13 containers 4.35 inches OD by 35 inches long, 6 containers 4.35 inches OD by 34 inches long, 7 containers 4.35 inches OD by 33 inches long, and 6 containers 4.35 inches OD by 32 inches long, was incorporated.

The fuel system designed in this manner had a storage capacity of 1434 SCF of hydrogen for the Pressed Steel Tanks Co., Inc. system and 1412 SCF of hydrogen for the EDO Canada Ltd. system. Using the specifications for Pressed Steel Tank Company, Inc. containers produced a fuel system weight of 417 pounds (Fig 18). Using the specifications for EDO Canada Ltd. containers produced a fuel system weight of 140 pounds (Fig 19).

Fuel Economy and Exhaust Emission Calculations

Engine performance calculations were based on data gathered at the University of Miami using a Toyota 2TC 4 cylinder engine with a compression ratio of 9.0:1. A high efficiency low NO_x hydrogen fueled engine configuration utilizing the following criteria was assumed:

1. The equivalence ratio is held constant at $\phi = 1.0$ for all operating conditions.

2. Load is controlled by operating unthrotted and recycling varying amounts of condensed exhaust gases into the inlet system. At light load conditions (BMEP less than 30 psi) some throttling is desirable.

3. A NO_x reducing catalyst is employed to reduce NO_x. A W.R. Grace Co. Davex 178 catalyst has been tested at the University of Miami and will reduce NO_x by 90% at equivalence ratios as lean as $\phi = 0.98$.

Vehicle Weight

Vehicle performance is a function of vehicle weight. Figure 20 shows the calculation of vehicle weight. The weight of the gasoline normally held in the vehicle (71 lbs) was subtracted from the initial weight (2055 lbs). The weight of the hydrogen fuel storage system (either 417 or 140 lbs) was added. 30% of the fuel storage system weight was added as an estimate of the weight of supports and firewall for the fuel storage system (either 125 or 42 lbs). 30 pounds was added to account for lengthening the trunk 6.7 inches to increase the crush distance. Finally, 33 pounds was added due to the larger displacement hydrogen fueled engine needed to replace the gasoline fueled engine originally installed.

Vehicle Comparison

Figure 21 compares the original gasoline powered vehicle with three modified vehicles. Two of the modified vehicles are hydrogen powered vehicles following the design guidelines in the previous discussion and the third is a state of the art conversion of a vehicle to electric (battery) power built by BMW. The first of the two hydrogen powered vehicles utilizes a 2.2 liter high efficiency low NO_x hydrogen fueled engine with 14.0:1 compression ratio and reduced internal engine friction, a manual transmission, and the EDO Canada Ltd. containers to reduce vehicle weight. The performance numbers for the first of the two hydrogen powered vehicles were not felt to be conservative or optimistic while the performance numbers for the second of the two hydrogen powered vehicles were felt to be feasible but optimistic.

The predicted NO_x emissions from the first hydrogen powered vehicle are 0.05 grams/mile over the federal driving cycle. Insufficient data was available to make a prediction for the second hydrogen powered vehicle's NO_x emissions.

Figures 22 and 23 are drawings of the original gasoline powered vehicle before and after conversion to utilize hydrogen. In figure 23 the required 6.7 inch extension of the trunk is shown.

Acknowledgements

We would like to acknowledge the support of the Department of Energy and National Renewable Energy Labs without whose support this work would not have been done.

References

Angus, S., Armstrong, B., and de Reuck, K.M., 1976, *International Thermodynamic Tables of the Fluid State - 5 Methane*, International Union of Pure and Applied Chemistry, Pergamon Press.

Dean, J., 1961, *A Tabulation of the Thermodynamic Properties of Normal Hydrogen from Low Temperatures to 300°K and from 1 to 100 Atmospheres*, National Bureau of Standrds Technical Note 120

Kunkle, J., Wilson, S., and Cota, R., 1969, *Compressed Gas Handbook,* NASA SP-3045, Office of Technology Utilization, National Aeronautics and Space Administration

Swain, M., Adt, R., and Pappas, J., 1983, *Experimental Hydrogen-Fueled Automotive Engine Design Data-Base Project*, U.S. Department of Energy, Office of Vehicle and Engine R&D

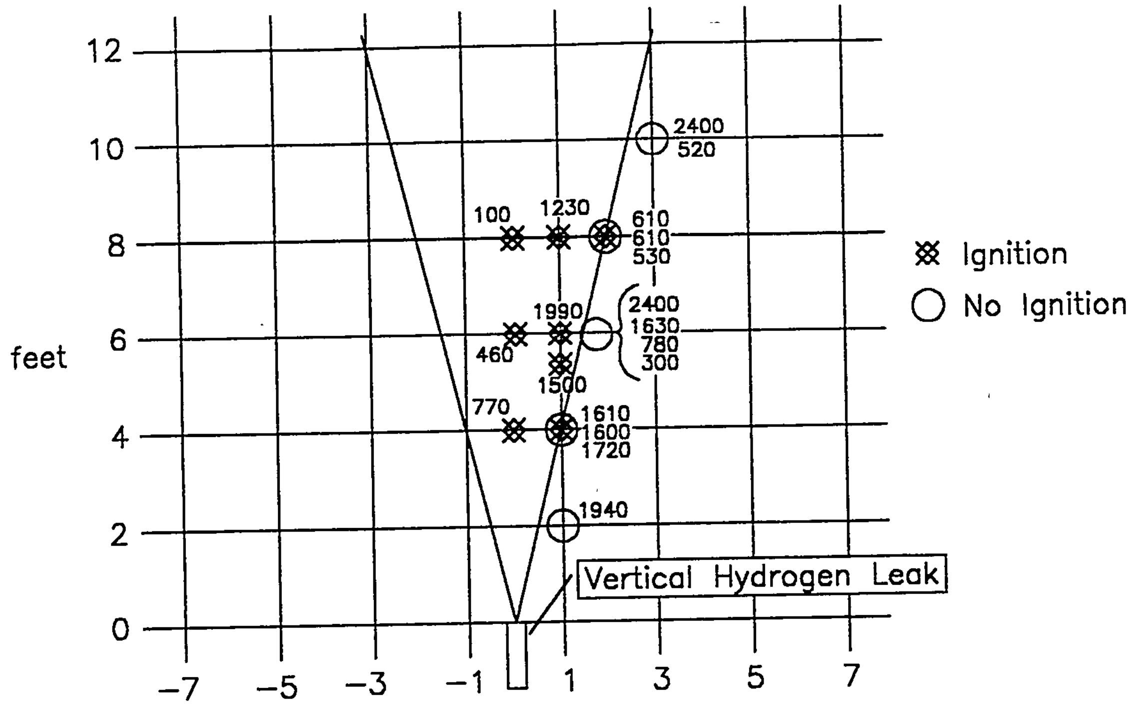


Figure 1 - Vertical hydrogen leak data

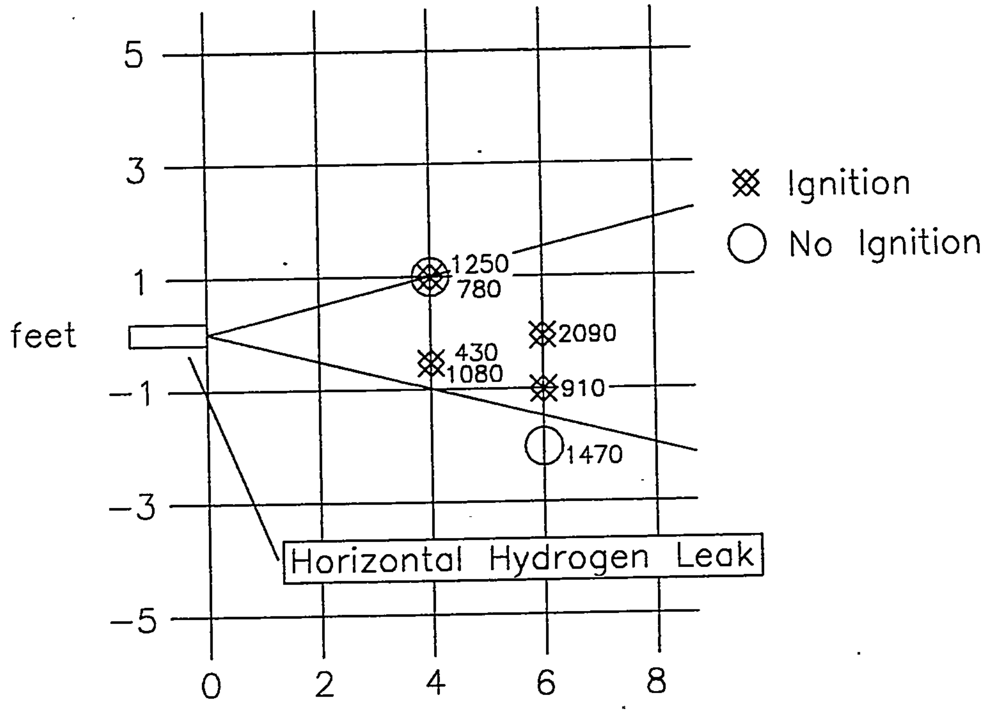


Figure 2 - Horzontal hydrogen leak data

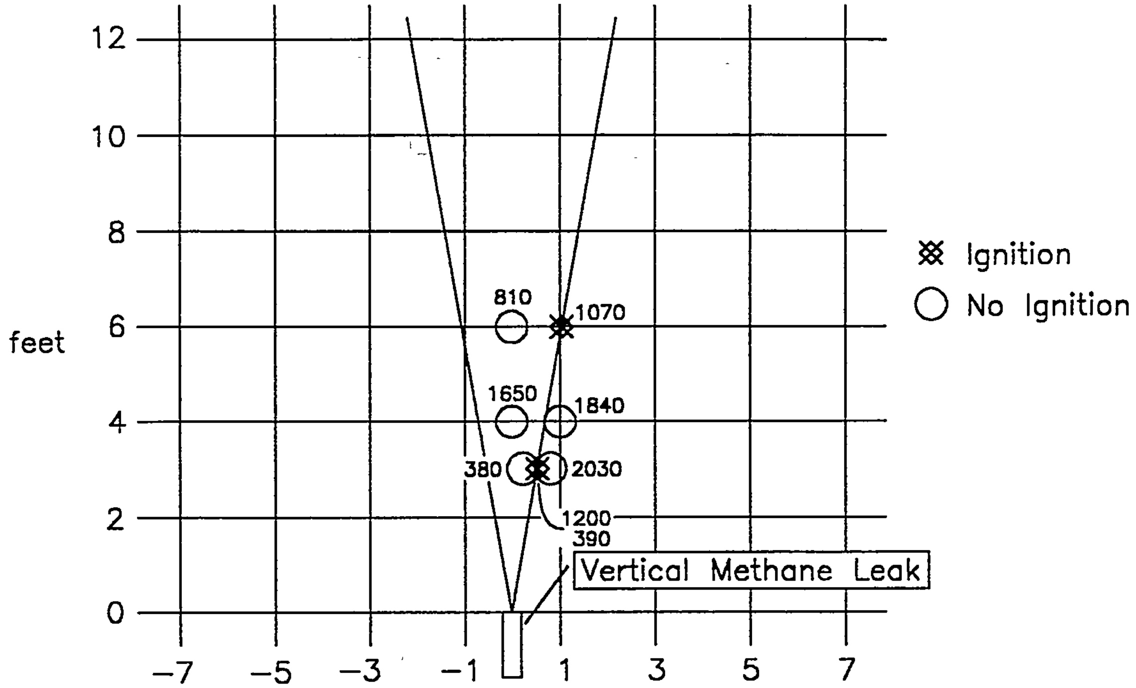


Figure 3 - Vertical methane leak data

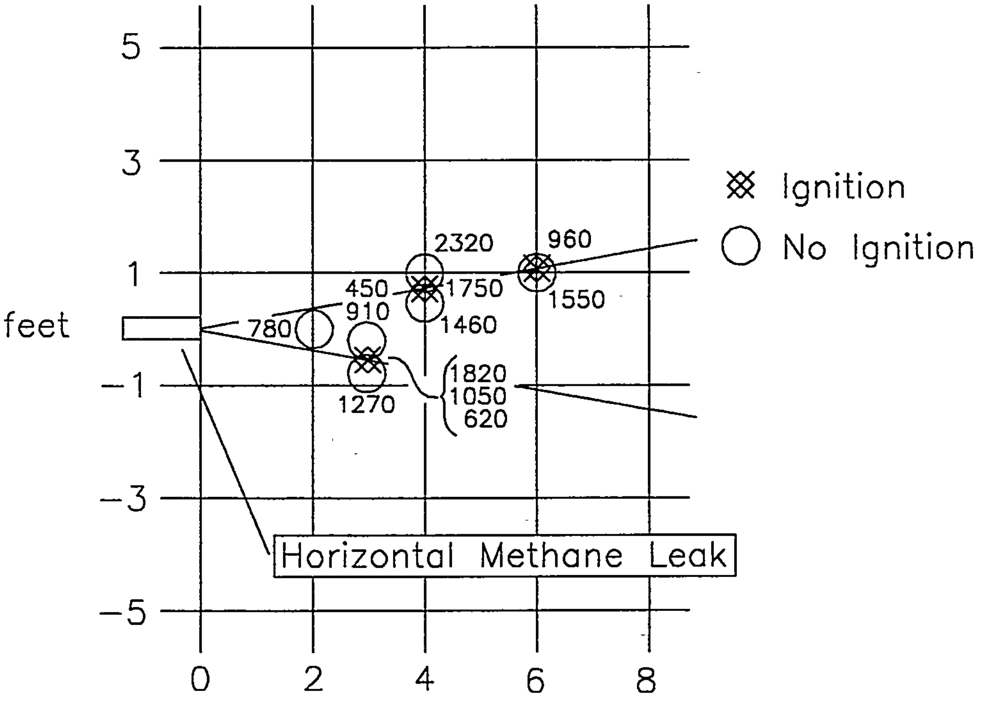


Figure 4 - Horizontal methane leak data

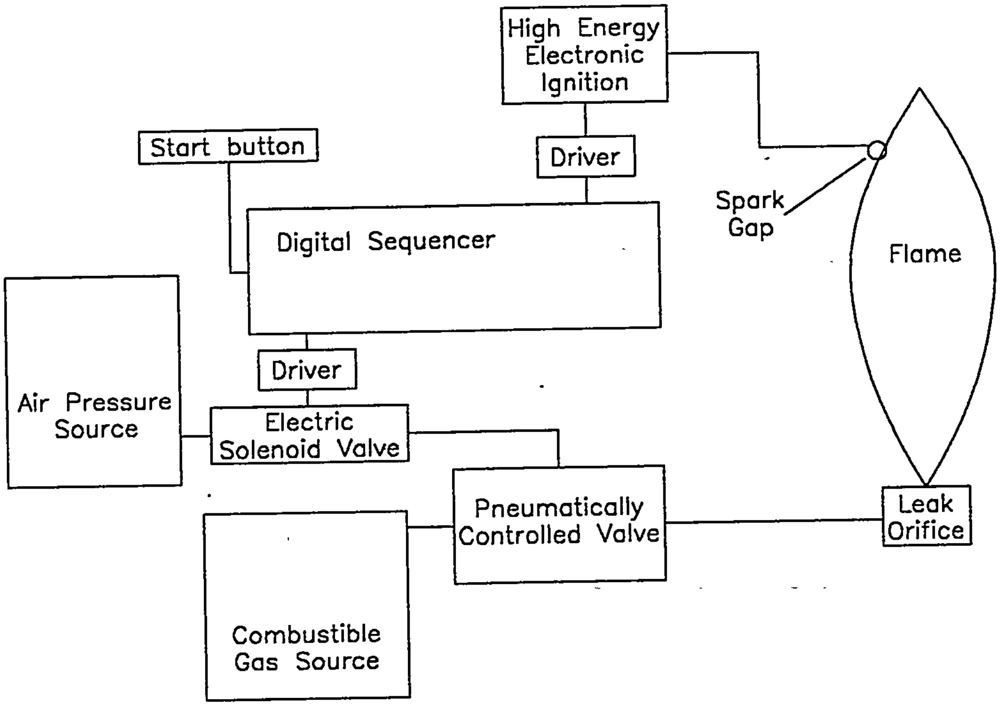


Figure 5 - Leak testing control apparatus

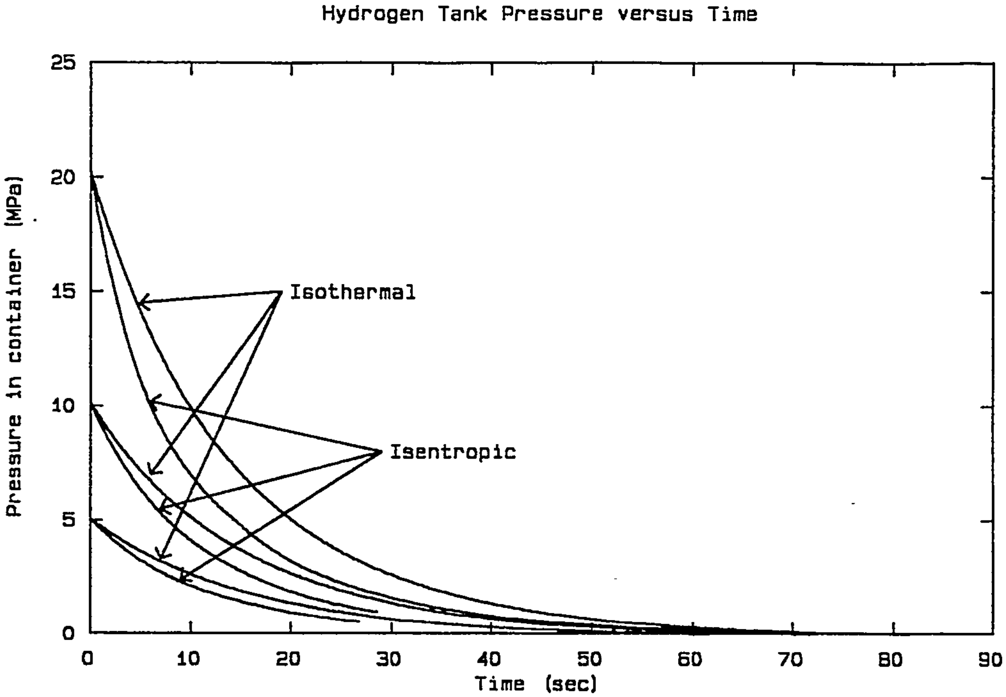


Figure 6 - Hydrogen pressure versus time in high pressure container leak

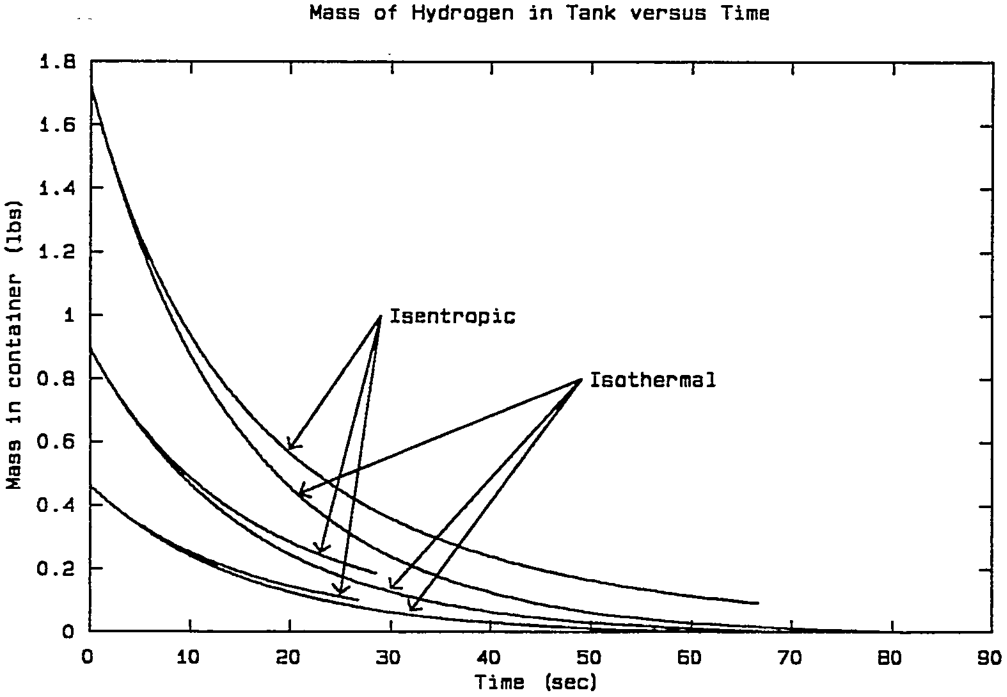


Figure 7 - Hydrogen mass remaining versus time in high pressure container leak

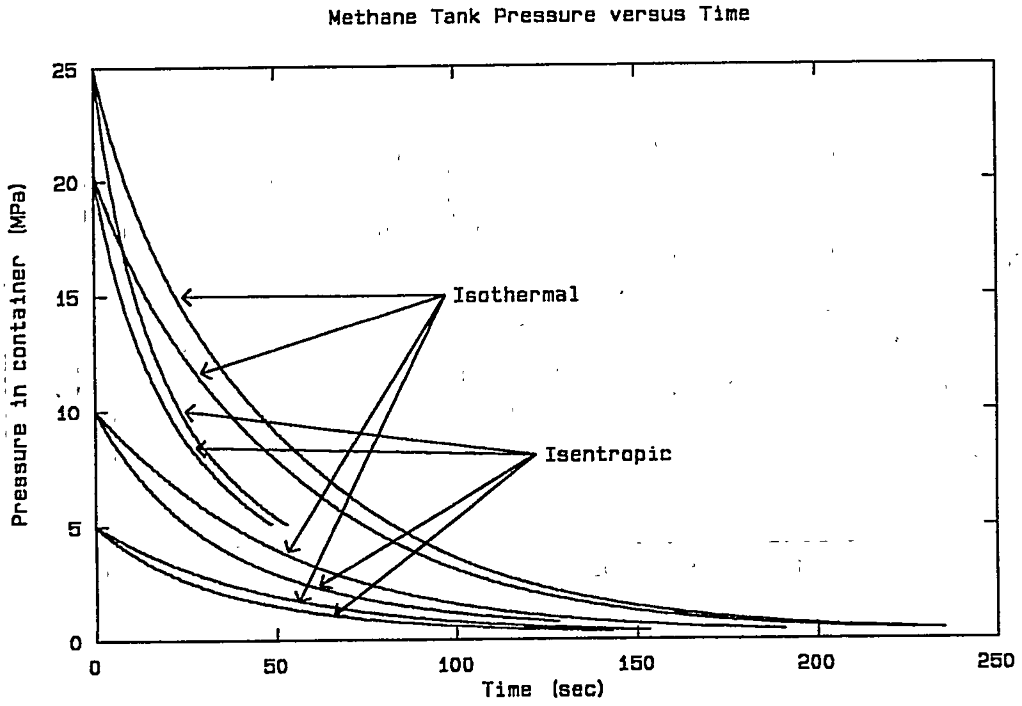


Figure 8 - Methane pressure versus time in high pressure container leak

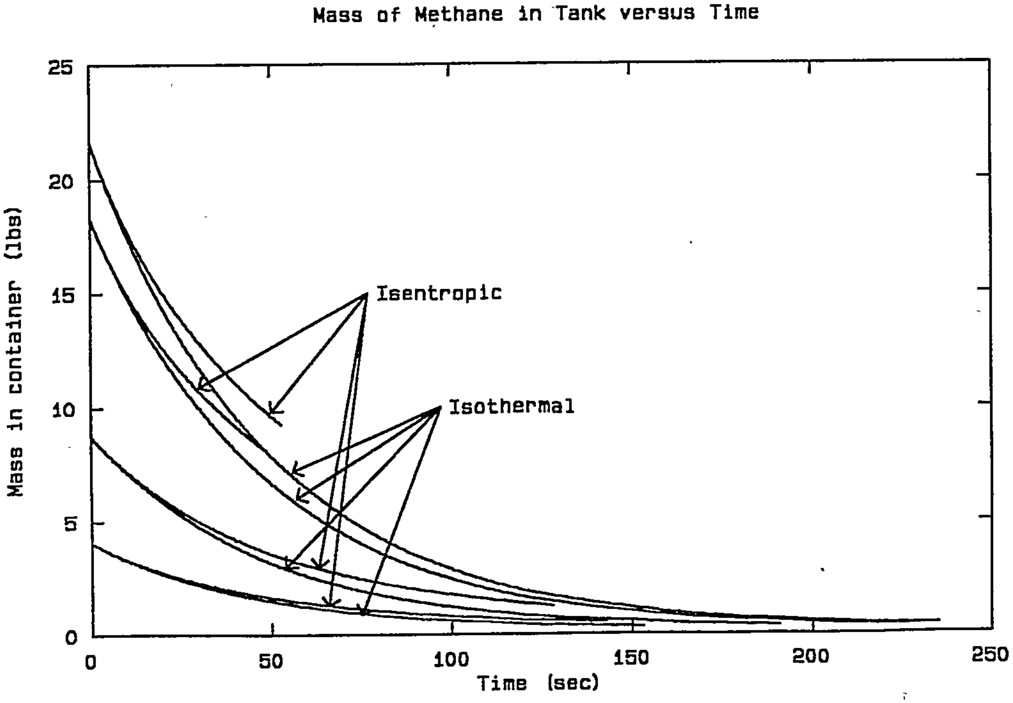


Figure 9 - Methane mass remaining versus time in high pressure container leak

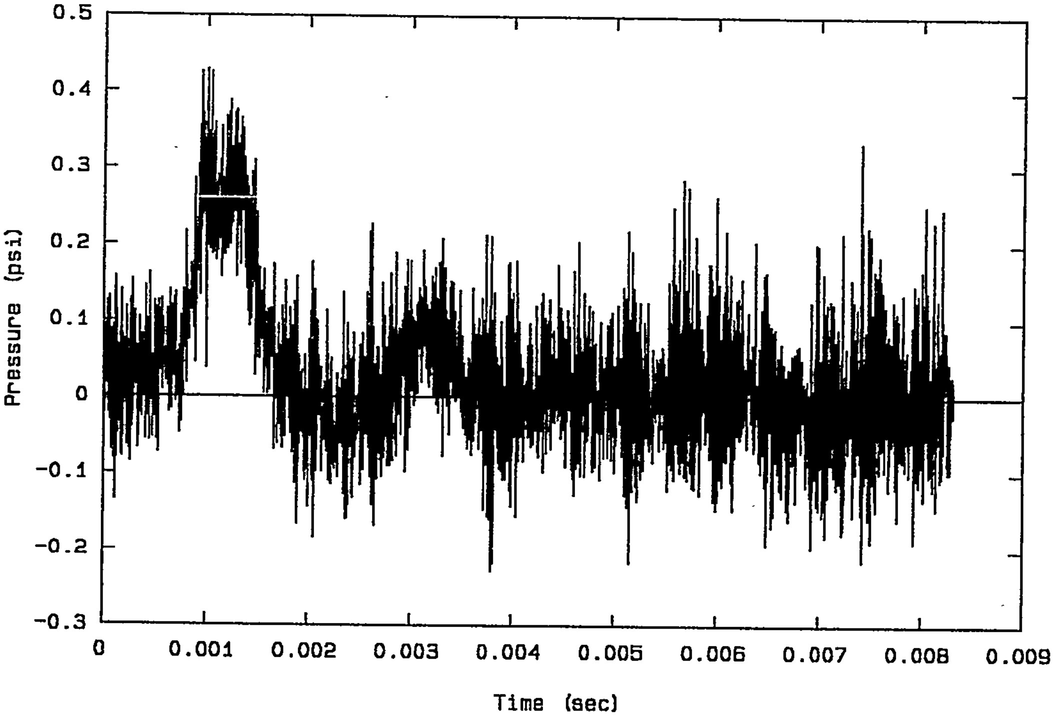


Figure 10 - Overpressure trace

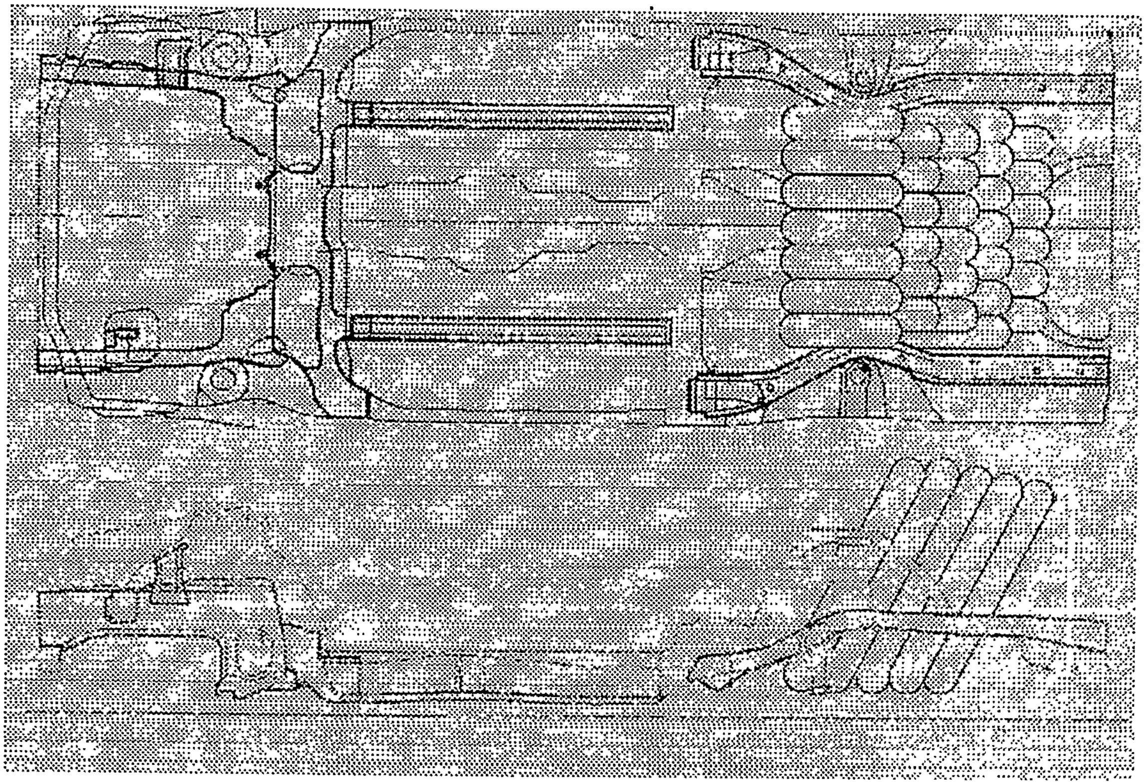


Figure 11 - Hydrogen powered vehicle frame with high pressure fuel storage containers installed

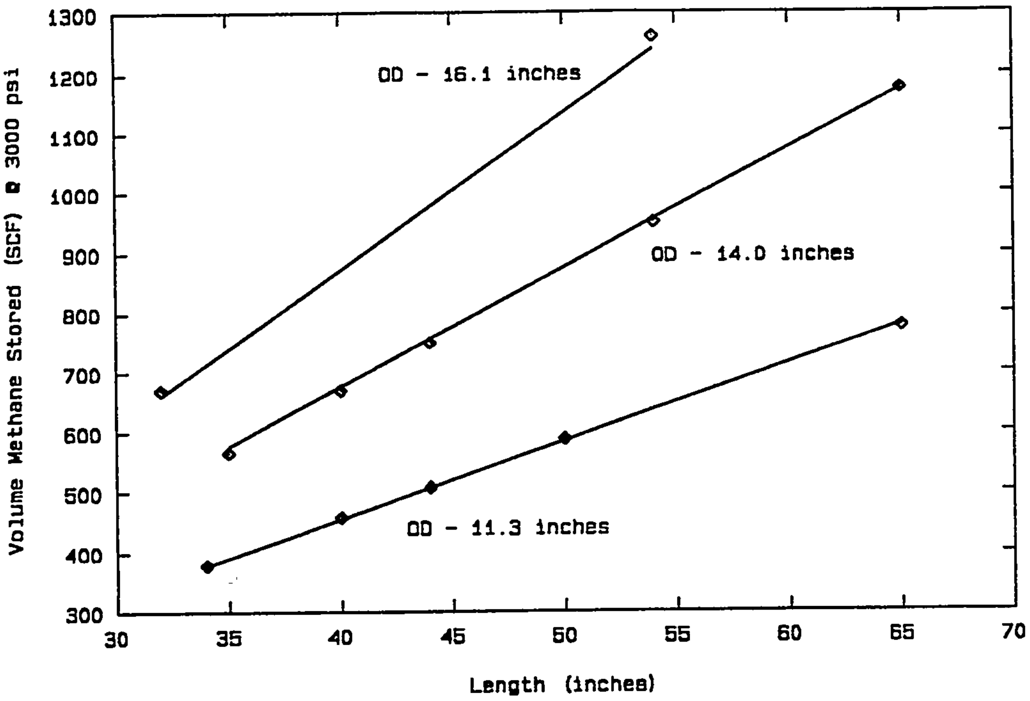


Figure 12 - Container storage capacity versus length for Pressed Steel Tank Co.

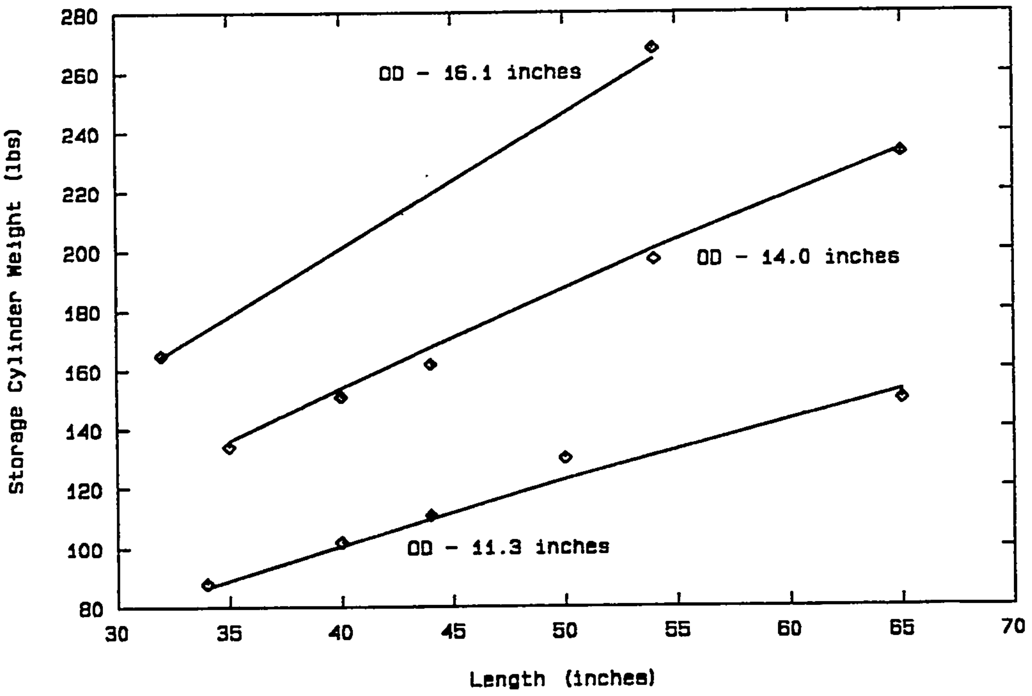


Figure 13 - Container weight versus length for Pressed Steel Tank Co.

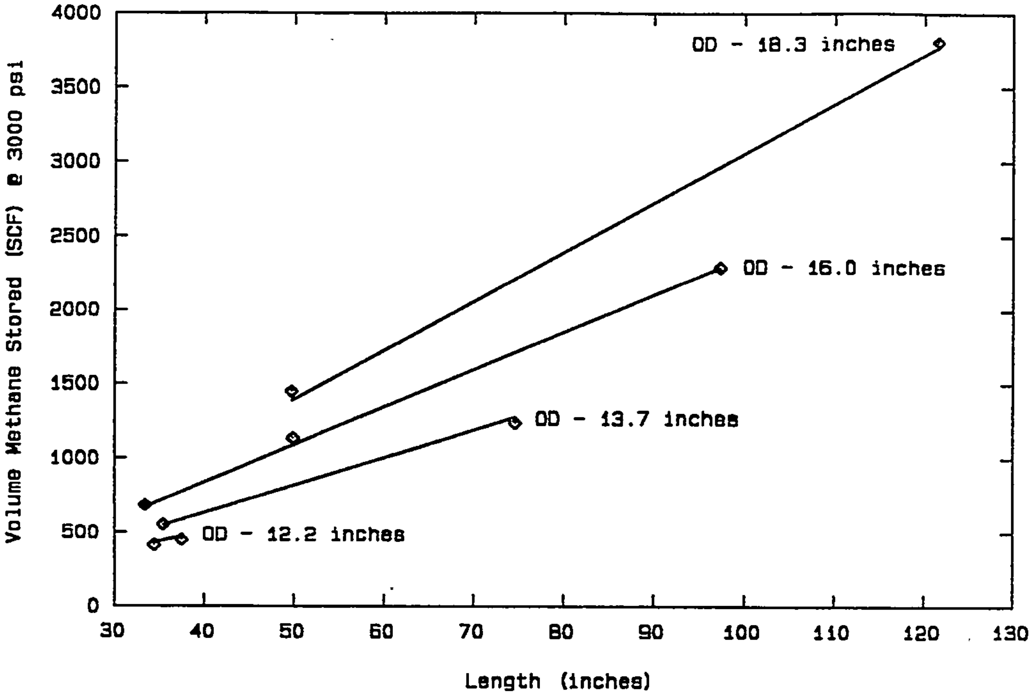


Figure 14 - Container storage capacity versus length for EDO Canada Ltd.

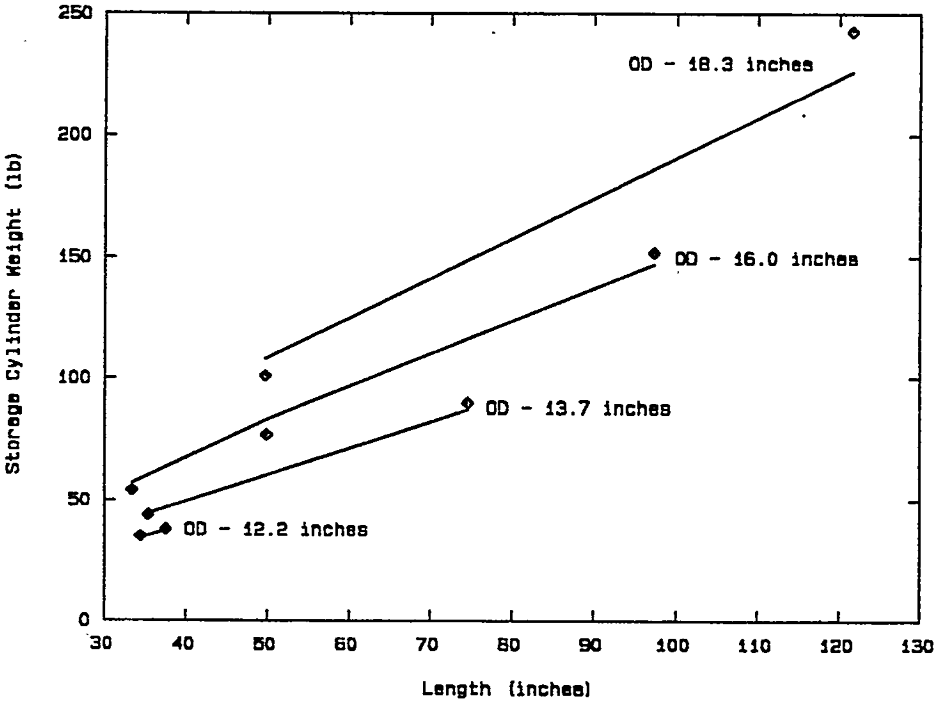


Figure 15 - Container weight versus length for EDO Canada Ltd.

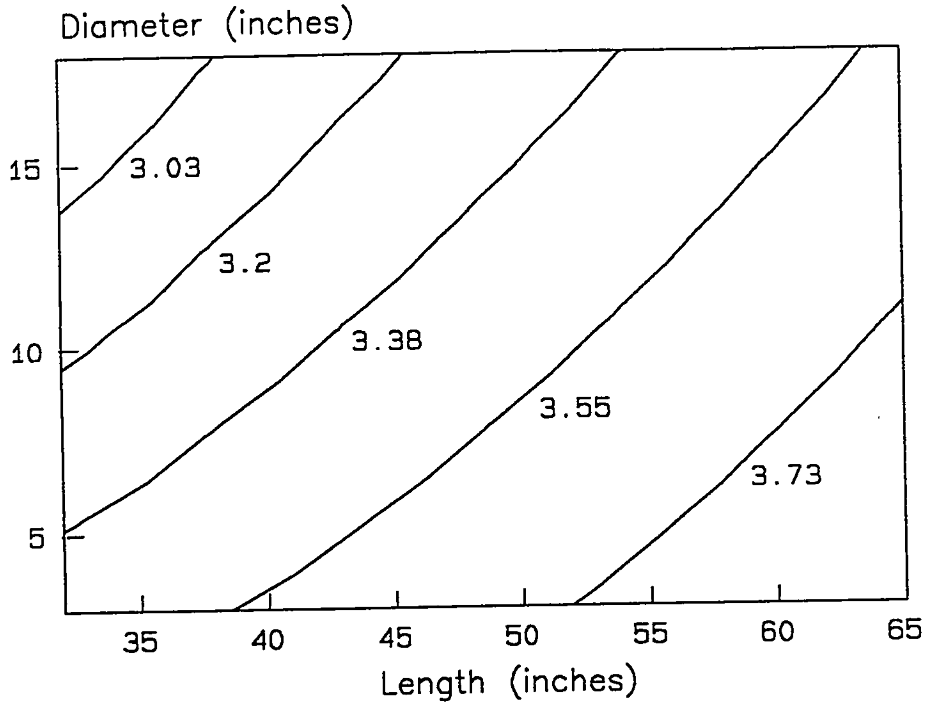


Figure 16 - Storage capacity/weight (SCF/lb) vs length and diameter for Pressed Steel Tank Co.

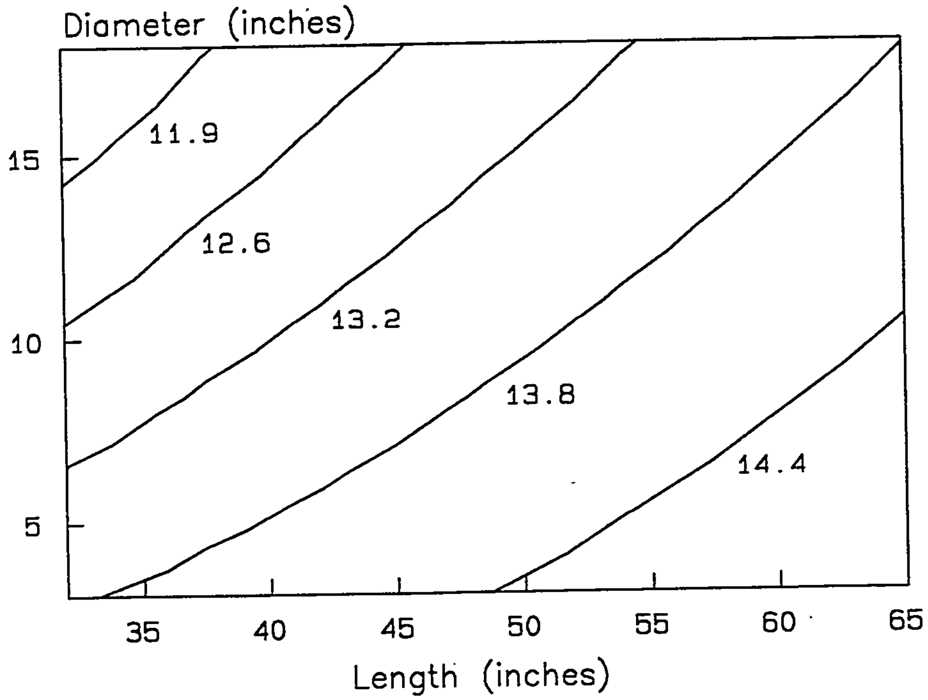


Figure 17 - Storage capacity/weight (SCF/lb) vs length and diameter for EDO Canada Ltd.

Pressed Steel Tank Co. Fuel Storage System

Cylinders used	Storage cylinder description	Volume hydrogen stored	Weight per cylinder
13	35 inch by 4.35 inch diameter 3000 psi	46.5 SCF	13.4 lb
6	34 inch by 4.35 inch diameter 3000 psi	45.1 SCF	13.1 lb
7	33 inch by 4.35 inch diameter 3000 psi	43.7 SCF	12.8 lb
6	32 inch by 4.35 inch diameter 3000 psi	42.3 SCF	12.4 lb

Total of 1434 SCF of Hydrogen weighing 417 lbs

Figure 18 - Description of Compressed Hydrogen Fuel Storage System

EDO Canada, Ltd. Fuel Storage System

Cylinders used	Storage cylinder description	Volume hydrogen stored	Weight per cylinder
13	35 inch by 4.35 inch diameter 3000 psi	45.8 SCF	4.53 lb
6	34 inch by 4.35 inch diameter 3000 psi	44.4 SCF	4.41 lb
7	33 inch by 4.35 inch diameter 3000 psi	43.0 SCF	4.29 lb
6	32 inch by 4.35 inch diameter 3000 psi	41.6 SCF	4.17 lb

Total of 1412 SCF of Hydrogen weighing 140 lbs

Figure 19 - Description of Compressed Hydrogen Fuel Storage System

Weight of Vehicle

Component	Weight (lbs)	Weight (lbs)
Original weight of 1992 Toyota Tercel	2055	2055
Weight of 11.9 gallon fuel tank (removed)	-71	-71
32 hydrogen cylinders (3000 psi)	Pressed Steel Co cylinders 417 lbs	EDO carbon fiber cylinders 140 lbs
Supports and firewall	125	42
Additional weight due to lengthened trunk	30	30
Replacement of stock engine with 90 HP hydrogen fueled engine	2.2 liter 9.0:1 CR Auto transmission 33 lbs	2.0 liter 14:1 CR Manual transmission 33 lbs
Total new weight	2589	2229

Figure 20 - Estimation of vehicle weight

Vehicle Comparison

	Stock gasoline powered 1992 Toyota Tercel	1992 Toyota Tercel converted to hydrogen fueled operation	1992 Toyota Tercel converted to hydrogen fueled operation	BMW E-2 dedicated electric vehicle sodium-sulfur batteries
Weight	2055 lbs	2589 lbs	2229 lbs	2200 lbs
Range	309 miles	103 miles	150 miles	160 miles
Horsepower	82 HP	90 HP	90 HP	45 HP
Equivalent Gasoline Mileage	26 mpg	30 mpg	45 mpg	N/A
0-60 MPH elapsed time	11.2 sec	12 sec	11.2 sec	19 sec

Figure 21 - Comparison of vehicles dicussed

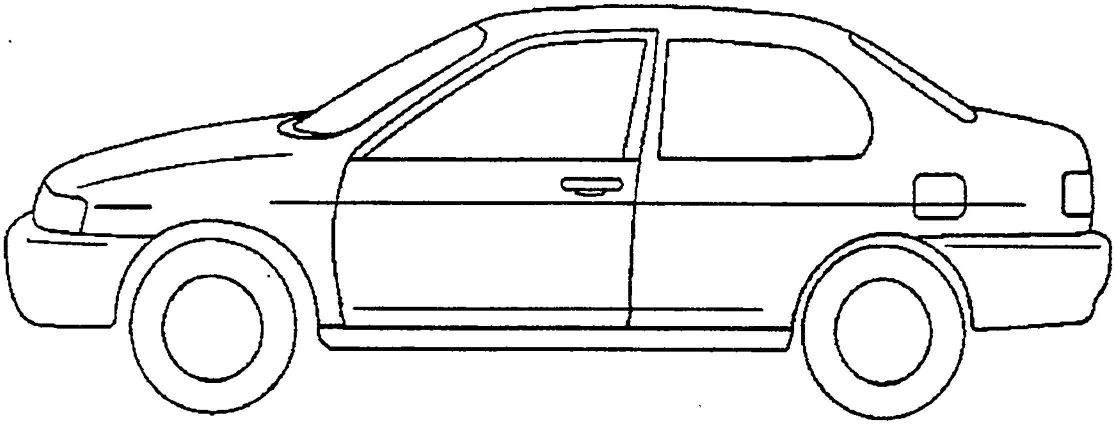


Figure 22 - Original gasoline powered vehicle

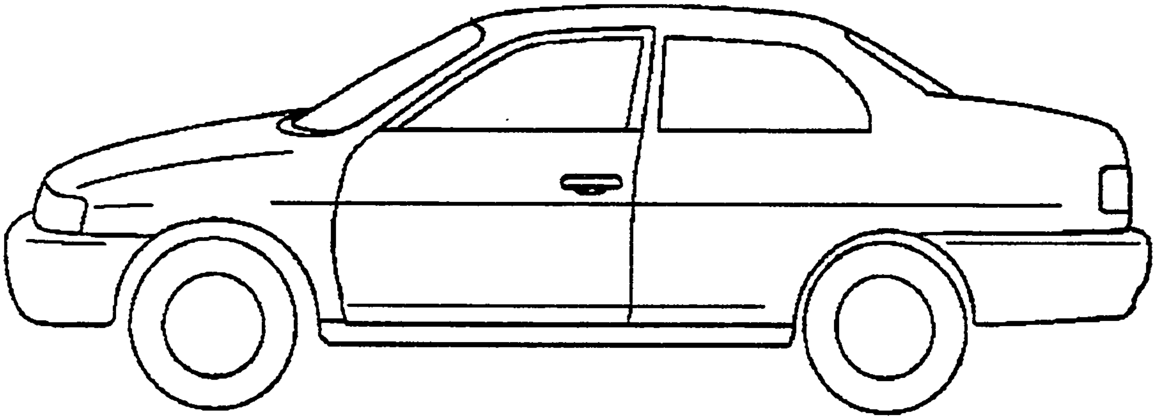


Figure 23 - Vehicle converted to hydrogen powered operation