Conf-9410256--1

UCRL-JC- 116894
PREPRINT

Optimized Hydrogen Piston Engines

J. R. Smith

This paper was prepared for submittal to the
Society of Automotive Engineers'
Convergence '94
Detroit, MI
October 18, 1994

May 10, 1994

Lawrence Livermore National Laboratory

DISCLAIMER

Optimized Hydrogen Piston Engines

J. R. Smith
Lawrence Livermore National Laboratory
University of California, Livermore, CA 94550

ABSTRACT

Hydrogen piston engines can be simultaneously optimized for improved thermal efficiency and for extremely low emissions. Using these engines in constant-speed, constant-load systems such as series hybrid-electric automobiles or home cogeneration systems can result in significantly improved energy efficiency. For the same electrical energy produced, the emissions from such engines can be comparable to those from natural gas-fired steam power plants. These hydrogen-fueled high-efficiency, low-emission (HELE) engines are a mechanical equivalent of hydrogen fuel cells. HELE engines could facilitate the transition to a hydrogen fuel cell economy using near-term technology.

INTRODUCTION

The long-term future energy economy will probably be based on electricity and hydrogen as energy carriers made from fission, fusion, or renewable primary sources. Electricity is already a major part of the energy economy of every developed country. Hydrogen, however, has yet to become significant as a fuel even in advanced countries. Currently, about 10 billion kg of hydrogen (about 1.1 quad energy equivalent) is produced in the United States. Approximately 60% of it is utilized within oil refineries in petroleum refining, 30% in chemical manufacturing, and the remainder in metal fabrication, oil and fat hydrogenation, rocket propulsion, and small industrial uses. [1] The two major questions on the hydrogen transition are when and how it will take place. Infrastructure studies at Lawrence Livermore National Laboratory indicate that the transition to hydrogen from current fuels is hindered by both the lack of hydrogen utilization devices and the lack of an extensive hydrogen distribution infrastructure. [2] This paper addresses one of the potential conversion devices—i.e., piston engines—in some detail. Use of the existing natural gas infrastructure as a feed stock to steam reforming or pyrolysis to produce hydrogen could circumvent the near-term distribution issue.* Most of the immediate motivation for move to hydrogen, especially in transportation, is the potential for improved urban air quality. However, other issues such as energy security, balance of payments, and reduction of greenhouse gas emissions also strongly support the need for a near-term hydrogen transition. Issues that hinder the transition are the low direct cost of fossil fuels, and the low energy efficiency of current automobiles. This last concern (low engine efficiency) makes the direct substitution of hydrogen as a transportation fuel a serious problem in on-board storage if comparable range is demanded.

This paper first discusses the application of high efficiency, low emission (HELE) hydrogen-fueled piston engines; then covers the issues and estimates of emissions from such engines; and finally makes some estimates and reviews issues concerning the likely thermal efficiency achievable. To the author's knowledge, no small piston engines have been optimized for hydrogen.

APPLICATIONS

HYBRID AUTOMOBILES — A recent comparison of various power-train efficiencies for vehicles of equal weight and drag concluded that considerable improvement over conventional automobile efficiency could be achieved through the use of the series hybrid-electric drivetrain concept. [3] In the series hybrid-electric power train proposed, all of the chemical energy of the fuel is converted to electrical energy by means of a piston engine coupled to an electrical generator. The electrical energy is stored in an advanced battery, ultracapacitor, or electromechanical battery (EMB). The EMB is a flywheel storage device that has 95% roundtrip efficiency and is the closest of these storage technologies to full-scale demonstration. [4] The stored electrical energy is extracted from storage as needed by the power demands for acceleration, cruise and accessories. An electric motor is coupled to the wheels by a single-speed transmission to complete the power train. Regenerative braking is accomplished by having the drive motor act as a generator with the energy going back to the storage device during braking. If the engine generator were sized just to replace average energy consumption, then this concept could be thought of as a range extender for an electric vehicle. However, if the engine generator is sized to supply power at a rate required for a fully loaded vehicle to climb hills at cruise speeds, it performs similar to today's gasoline powered automobiles.

Using an LLNL-developed hybrid vehicle simulation code as a guide for maximizing efficiency suggests that electrical storage of 1 to 2 kWh is needed, with 100 kW peak electrical power capability and about 30 kW electrical power from a hydrogen-fueled engine generator set that is sized for hillclimb. Assuming a drag coefficient of 0.24, a cross-sectional area of 2.04 m^2, and an engine brake thermal efficiency of 48%, in an 1,136 kg (2,500 lb) empty-weight vehicle yields a combined EPA urban/highway schedule energy equivalent mileage of over 85 mpg. A major premise of this paper is that electrical energy can be generated at efficiencies approaching 45% based on a 48% brake thermal efficiency engine and a 95% generator efficiency. (The prospects for this engine efficiency are addressed later in this

* Most hydrogen is produced today from the steam reforming of natural gas, but a pilot plant by Kvaerner of Lysaker, Norway, produces hydrogen and carbon black from any hydrocarbon by pyrolysis without any CO_2 emissions.

ne

paper.) This vehicle would require about 3.3 kg of hydrogen for a 480 km (300 mile) range. This is an extremely energy-efficient vehicle. To put it into perspective, the reader is reminded that a kilogram of hydrogen has roughly the same energy content as a gallon of gasoline. The combined high efficiency of this vehicle and the power train are necessary to make the hydrogen on-board storage problem tractable. Depending on the engine power output and the size of the electrical energy storage chosen, the duty factor for the engine is projected to be from 12 to 20% of the driving time on the combined driving schedule. That is, the engine does not idle — it is shut down each time the energy storage device is fully charged.

The combination of a lean-burn hydrogen engine and an electrical generator is the mechanical equivalent of the hydrogen fuel cell. It has been suggested independently [5] that this combination could act as a surrogate fuel cell for vehicle applications. Although such engine generator sets do not have the zero emissions of the fuel cell, their emissions can be quite low, and they represent a low-cost ($50 to $75/kW) near-term technology that could promote hydrogen distribution infrastructure. Clearly, the fuel cell is the "right technical choice" when it becomes an economic option. In an ideal transition, much of the hydrogen infrastructure would be in place when the fuel cell comes to market.

HOME-COGENERATION — Cogeneration, the simultaneous generation of electricity and low-grade heat from the same fuel, has been sucessfully applied in small towns, ships, large office buildings, motels, and apartment and industrial complexes. The generation and storage elements of the power-train of the series hybrid electric vehicle described above could also be used for home-cogeneration. The efficiency of electrical energy from a central power plant delivered to the home is only about 33% due to average power plant efficiency of approximately 36% and electrical transmission efficiency of 92%. [6] Use of the heat rejected from the cogeneration engine for domestic hot water, space heating or absorption air conditioning raises the overall fuel energy utilization. Total fuel decreases if the cogeneration electrical generation process is greater than about 25%. Efficient electrical generation in small systems improves the economics of home cogeneration systems because home applications do not typically require as much heat as is rejected. The major difference between the small-scale cogeneration application and the hybrid vehicle application is the durability requirement of the engine. Cogeneration use will require 30,000 to 40,000 hours of lifetime compared to perhaps 1,000 hours for the vehicle (recall that the duty factor for the vehicle is low). Fortunately, since the cogeneration engine requires only 15 to 20 kW, the durability may be achieved by derating the engine, as is done with current automotive-type cogeneration engines. [7] To be a viable option, the challenge for the home-cogeneration system is not so much efficiency as low capital cost and high reliability.

EMISSIONS

The major emissions from hydrogen-fueled engines are NO_X which consists of NO (nitric oxide) and NO_2 (nitrogen dioxide), and which can be considerably higher than the NO_X emissions from conventional gasoline-fueled engines due to its higher adiabatic flame temperature. [8] 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 spark-ignition engines, NO usually represents 98% or more of the NO_X, while in compression ignition engines (diesels) 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 Heywood [9].

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. [10] 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 and methane are shown in Fig. 1. 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, but the turbulence and burned gas expansion act as multipliers on the laminar flame speed.

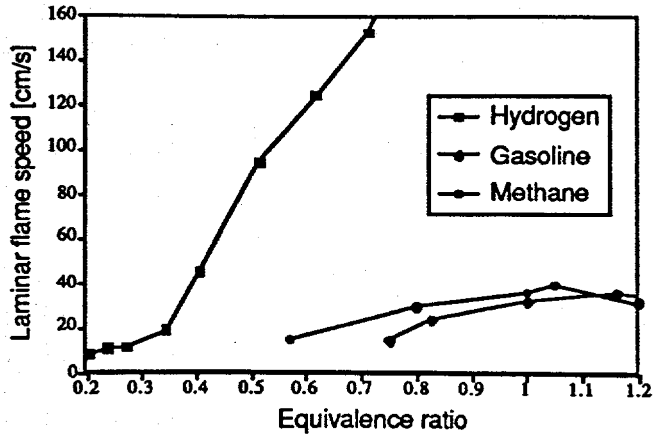

Figure 1. Comparison of the laminar flame speed of hydrogen (data compiled by M. Marinov, LLNL), with that of methane and gasoline (from Ref. 9, p. 403).

The extensive work of Homan [11] 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 kilowatt-hour of power produced using a spark-ignited hydrogen air mixture at equivalence ratio 0.38. [12] Das [13] measured the NO_X emissions from another hydrogen-fueled, research engine as a function of equivalence ratio at compression ratios up to 11:1. These emissions are shown in Fig. 2, and are consistent with the extensive measurements of Ref. 8.

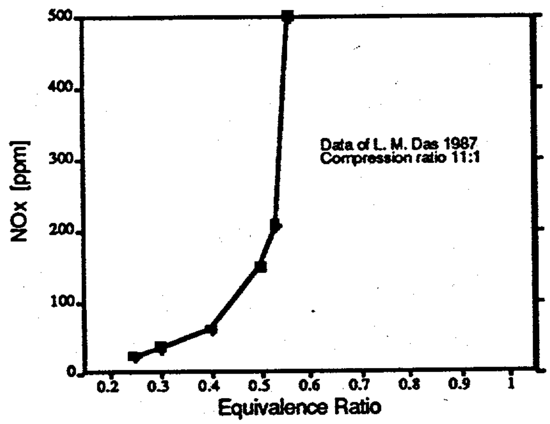

Figure 2 NO_X decreases dramatically as a hydrogen engine is leaned below 0.5 equivalence ratio.

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 [14] 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.

Although there is no carbon in the fuel, all piston 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. [15] 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. Since most of the HC comes from the walls of the cylinder, the emissions will be scaled by the engine displacement surface area, i.e., the ratio of the engine displacements raised to the 2/3 power. A 1.5 liter displacement engine, which is approximately the size envisioned for the hybrid vehicle described above, would have about 30% of the internal surface area of the 9 liter engine tested. Thus the estimated HC would be in the range of 0.003 g/kWh and the CO about 0.0053 g/kWh. 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 detail design of piston rings affects oil transport into the combustion chamber. [16] Experiments by Furuhama, Hiruma, and Enomoto [17] 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 in Ref. 15 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.

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 decade or so. The automotive storage problem is discussed in some detail by Robinson and Handrock. [18] 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 in Ref. 2.

The thermal efficiency as a function of compression ratio for a number of single-cylinder research engine experiments on hydrogen are shown in Fig. 3. Note that the efficiencies reported by Das [13] are for brake thermal efficiency whereas those of King et al. [19], Oemichen [20], and Homan [11] are reported as indicated thermal efficiency. It is probably more appropiate to report single-cylinder research engine efficiencies as indicated (net work done on the piston), because the high friction of most research engines are not representative of modern multicylinder engines.

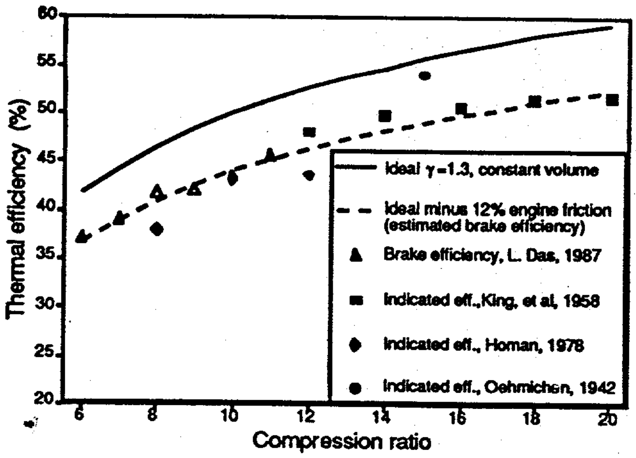

Figure 3. Thermal efficiency of various hydrogen-fueled research engines compared with an ideal efficiency and estimated brake efficiency theroetical curves.

Included in Fig. 3 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. [9] R_c is the compression ratio and γ is the ratio of specific heats, taken here to be 1.3. Also included is a plot of this ideal efficiency reduced by 12% to roughly account for engine friction. Note that this fits Das's data reasonably well. In contrast, the indicated (no friction) efficiency data by King for the most part is only slightly above this approximation to brake 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 [21], 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 TDC (Top Dead Center) 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 [22] 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 [23]. 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. 4, where the difference between the ideal thermal efficiency calculated from Eq. (1) and the measured indicated thermal efficiency (η) of King et al., is plotted against the surface-to-volume ratio which has been estimated from the engine schematic and dimensions provided in their paper.

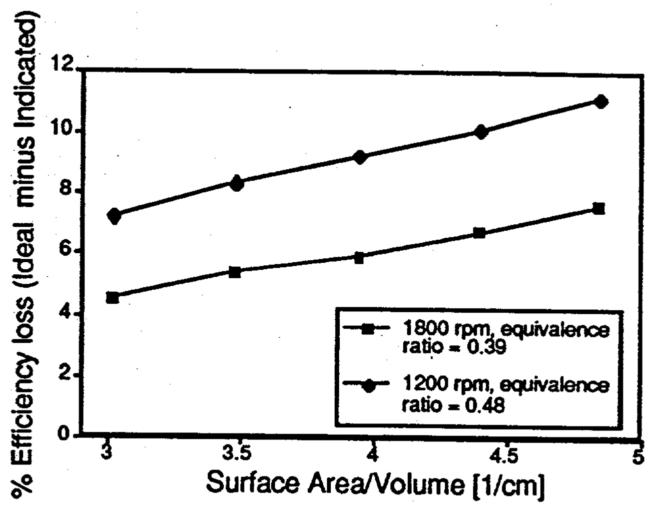

Figure 4 Efficiency loss (ideal minus indicated) versus estimated surface-to-volume ratio in King et al. experiments on a hydrogen engine.

Thus heat transfer losses are likely to be the main reason for experiments to fall well short of the ideal efficiency. This is further supported in Fig. 4 by the comparison of the 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 in Ref. 23 for stoichiometric gasoline can be reasonably well fit by:

$$Q_c/Q_f = 20\,(1400/N)^{0.5} \tag{2}$$

where Q_c/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 be 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 the proposed applications, there is an opportunity to reduce friction because intermittant high-speed operation is not necessary. 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 [24] as:

$$\text{fmep (bar)} = 0.97 + 0.15(N/1000) + 0.05(N/1000)^2, \quad (3)$$

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 30 kW (40 hp) for the hybrid vehicle application will probably require a 1.5 liter engine in a four-stroke version. A modern gasoline engine can produce 75 to 80 kW from a 1.5 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. Of course, these engine sizing issues are of little concern to the home cogeneration application. Combustion and engine models can guide our choices of the parameters for an optimized engine, but only experimental data can confirm our goals.

SUMMARY AND CONCLUSIONS

It is proposed that small, high-efficiency, low-emission engines be considered for hybrid automobile and home cogeneration applications. 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 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, depending on the application.

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

[1] *Chemical Economics Handbook*, SRI International, February 1990, p. 743.
[2] G. D. Berry, A. D. Pasternak, G. D. Rambach, J. R. Smith and R.N. Schock, "Hydrogen as a Future Transportation Fuel," LLNL, to be published.
[3] J. R. Smith, "The Hydrogen Hybrid Option," Proceedings of the Workshop on Advanced Components for Electric and Hybrid Electric Vehicles, Gaithersburg, MD, Oct 27-28, 1993, also available as LLNL preprint UCRL-JC-115425.
[4] R. F.Post, T. K.Fowler, and S. F.Post, "High Efficiency Electromechanical Battery," *Proceedings of the IEEE*, Vol. 81, No. 3, March 1993.
[5] J. Fulton, F. Lynch and R. Marmaro, "Hydrogen Engines as Surrogate Fuel Cells," presentation to the South Coast Air Quality Management District, June 1993, available from Hydrogen Consultants, Inc., Littleton, CO.
[6] *Hydrogen Program Plan FY1993-FY1997*, U.S. Department of Energy, Office of Conservation and Renewable Energy, Table C-1, June 1992.
[7] J. Dorn, CEO of Intellegen Solutions, Inc, Carson City, NV, a cogeneration system supplier, April 1994, private communication.
[8] M. R. Swain, R. R. Adt, Jr., and J. M. Pappas, *Experimental Hydrogen-Fueled Automotive Engine Design*

Data-Base Project, Vol. 1, May 1983, DOE Contract No. E(04-3)-1212, p. 20.
[9] J. B. Heywood, *Internal Combustion Engine Fundamentals*, McGraw-Hill, New York, 1988, Ch 11.
[10] Ibid p 583.
[11] H. S. Homan, "An Experimental Study of Reciprocating Internal Combustion Engines Operated on Hydrogen," PhD thesis, Cornell University, January 1978, p. 69.
[12] Ibid p. 174.
[13] L. M. Das, "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, 1990.
[14] L. A. Sinclair and J. S. Wallace, "Lean Limit Emissions of Hydrogen-Fueled Engines," *International Journal of Hydrogen Energy*, Vol. 9, No. 1/2, 00. pp. 123-128, 1984.
[15] J. C. Hedrick, "Advanced Hydrogen Utilization Technology Demonstration," Southwest Research, Inc., Final Report, Project No. 03-5080, November 1993.
[16] J. A. McGeehan, "A Survey of the Mechanical Design Factors Affecting Engine Oil Consumption," *Society of Automotive Engineers Transactions*, Vol. 88, SAE paper 790864, 1979.
[17] S. Furuhama, M. Hiruma and Y. Enomoto, "Development of a Liquid Hydrogen Car," *International Journal of Hydrogen Energy*, Vol. 3, pp 61-81, 1978.
[18] S. L. Robinson and J. L. Handrock, "Hydrogen Storage for Vehicular Applications: Technology Status and Key Development Areas," Sandia National Laboratories White Paper, Livermore, CA, February 1994.
[19] R. O. King, 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.
[20] M. Oemichen, "Hydrogen as an Engine Fuel," Engine Laboratory of the Technische Hochschule, Dresden, Germany, VDI-Verlag GmbH, Berlin NW, V.D.I. Paper No. 68, 1942 (English translation).
[21] D. F. Caris and E. E. Nelson, "A New Look at High Compression Engines," *Society of Automatic Engineers Transactions*, Vol. 67, pp. 112-124, 1959.
[22] See Heywood, *Internal Combustion Engines Fundamentals*, p. 697.
[23] S. Muranaka, Y. Takagi and T. Ishida, "Factors Limiting the Improvement in Thermal Efficiency of S. I. Engine at Higher Compression Ratio," Society of Automatic Engineers Transactions, SAE paper No. 870548, 1987.
[24] H. W. Barnes-Moss, "A Designer's Viewpoint," Passenger Car Engines Conference Proceedings, Institution of Mechanical Engineers, London, pp. 133-147, 1975.