Computational analysis of the lean-burn direct-injection jet ignition hydrogen engine

A Boretti [1*], H Watson [1], and A Tempia [2]
[1]School of Science and Engineering, University of Ballarat, Ballarat, Victoria, Auatralia
[2]Robert Bosch (Australia), Pty Ltd, Clayton, Victoria, Australia

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Abstract: This paper presents a new in-cylinder mixture preparation and ignition system for various gaseous fuels including hydrogen. The system consists of a centrally located direct-injection (DI) injector and a jet ignition (J) device for combustion of the main chamber (MC) mixture. The fuel is injected in the MC with a new-generation fast-actuating high-pressure high-flowrate DI injector capable of injection shaping and multiple events. This injector produces a bulk lean stratified mixture. The J system uses a second DI injector to inject a small amount of fuel in a small pre-chamber (PC). A spark plug then ignites a slightly rich mixture. The MC mixture is then bulk ignited through multiple jets of hot reacting gases. Bulk ignition and combustion of the lean jet-controlled stratified MC mixture resulting from coupling DI with J makes it possible to burn MC mixtures with fuel-to-air equivalence ratios reducing almost to zero for a throttle less control of load diesel-like and high efficiencies over almost the full range of loads. Computations are performed with hydrogen as the PC and MC fuel.

Keywords: gas engines, direct injection, jet ignition, lean-burn stratified combustion, bulk ignition, combustion

1 INTRODUCTION

At standard temperature and pressure, hydrogen is a colourless odourless non-metallic tasteless, highly flammable diatomic gas H_2. With an atomic weight of 1.00794, hydrogen is the lightest element. Hydrogen is also the most abundant element in the universe, making up 75 per cent of normal matter by mass and over 90 per cent by number of atoms. Under ordinary conditions on Earth, elemental hydrogen exists as the diatomic gas H_2. However, hydrogen gas is very rare in the Earth's atmosphere because of its light weight which enables it to escape from Earth's gravity more easily than heavier gases. Hydrogen in chemically combined form is the third most abundant element on the Earth's surface. Most of the Earth's hydrogen is in the form of chemical compounds such as hydrocarbons and water.

*Corresponding author: School of Science and Engineering, University of Ballarat, PO Box 663, Ballarat, Victoria 3353, Auatralia.
email: a_boretti@yahoo. com

Despite the fact that hydrogen can be prepared in several different ways, the economically most important processes involve removal of hydrogen from hydrocarbons. Commercial bulk hydrogen is usually produced by the steam re-forming of natural gas. Hydrocarbons other than methane can be used to produce synthesis gas with various product ratios. Other important methods for H_2 production include partial oxidation of hydrocarbons. Hydrogen may also be produced from water by electrolysis at substantially greater cost than production from natural gas.

Hydrogen gas is highly flammable and will burn in air at a very wide range of concentrations between 4vol/% and 75vol/%. Hydrogen–oxygen mixtures are explosive across a wide range of proportions. Its autoignition temperature, the temperature at which it ignites spontaneously in air, is 858K. H_2 reacts with every oxidizing element.

A hydrogen internal combustion engine (H_2ICE) is a hydrogen-fuelled internal combustion engine providing efficiencies in excess of today's gasoline engines and operating relatively cleanly with nitrogen oxides (NO_x) being the only emission pollutant [1–3]. Table 1 (from references [1] to[5]) presents some properties of hydrogen to outline the unique combustion properties in internal combustion engine applications. These properties are beneficial at certain engine operating conditions and pose technical challenges at other engine operating conditions. The presented values are not all well accepted and may be slightly different in other references. The definition of the research octane number (RON) in particular is open to discussion. Rigorously, RON determination of H_2 with the conventional ASTM method is not possible. The value proposed in Table 1 (from references [1], [3], and [5]) simply indicates the decrease in knock tendency of hydrogen (when surface ignition and residual gas ignition are eliminated) with reference to gasoline fuel experimentally demonstrated in the limited number of engine tests performed so far.

Favourable properties of H_2 are the wide flammability range for ultra-lean operation, the high laminar flame speed for good stability, and the high octane number for high compression ratios with improved thermal efficiency. Unfavourable properties of H_2 are the high percentage stoichiometric volume fraction of the vapour with the consequent air displacement effects, the low minimum ignition energy with consequent propensity to pre-ignite, the small quenching distance for thin thermal boundary layers, and the low density that make it difficult to provide large injected mass flowrates.

Temperatures below 200K are collectively known as cryogenic temperatures, and liquids at these temperatures are known as cryogenic liquids. Boiling is the transition from liquid to gas. Hydrogen has the second-lowest boiling point of all substances, second only to helium. The boiling point of a pure substance increases with applied pressure up to a point. Unfortunately, hydrogen's boiling point can only be increased to a maximum of 33.145K through the application of a pressure of 12.964b ar, beyond which additional pressure has no beneficial effect.

The fuel properties play a key role in development of the direct-injection (DI) mixture preparation system. Figure 1 presents the fluid properties of methane, propane, and hydrogen along isothermal lines [6]. This picture clearly states the problems and opportunities of gas injection with variable pressure levels. Late DI overcomes the air displacement effects of port fuel injection (PFI) of gaseous fuels. However, development of a direct injector providing adequate flowrates is difficult. Propane (C_3H_8) has a critical temperature T_c 5 369.8K, critical pressue p_c 5 42.5b ar, and critical density r_c 5 220.0k g/m^3, while the normal boiling point is 231.1K. Methane (CH_4) has a critical temperature T_c 5 190.6K, critical pressure p_c 5 46.0b ar, and critical density r_c 5 162.7k g/m^3 while the normal boiling point is 111.7K. Hydrogen (H_2) has a critical temperature T_c 5 33.1K, critical pressure p_c 5 13.0b ar, and critical density r_c 5 31.3k g/m^3 while the normal boiling point is 20.4K. At a temperature T 5 300K, propane is a vapour for pressures below 10.0b ar, and liquid above. Conversely, methane is a vapour for pressures below 48.4b ar, and supercritical above. Hydrogen is

Table 1 Fuel properties at 25 uC (except when otherwise noted), 1b ar, and stoichiometry (when applicable) (from references [1] to[5])

Minimum ignition energy (MJ)	0.02
Flame velocity (m/s)	1.85
Adiabatic flame temperature (K)	2480
Minimum quenching distance (mm)	0.64
Fuel-to-air mass ratio	0.029
Vapour volume fraction (%)	29.53
Heat of combustion (MJ/(kg air))	3.48
Flammability limit (volume) (%)	4–75
Flammability limit w	0.1–7.1
Minimum autoignition temperature (K)	858
Research octane number	. 120
Vapour density at 20 uC (kg/m^3)	0.0838
Liquid density at normal boiling point (kg/m^3)	70.8
Lower heating value (MJ/kg)	119.93
Higher heating value (MJ/kg)	141.86

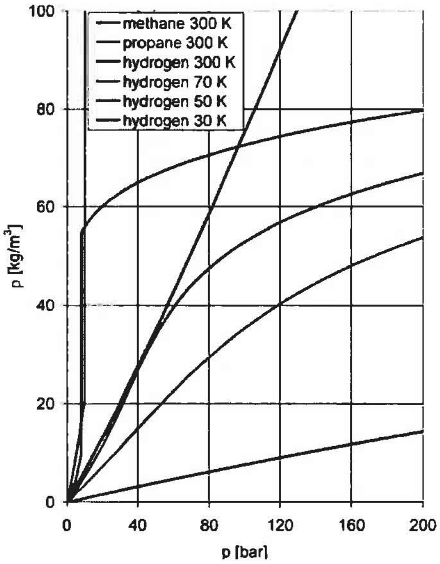

Fig. 1 Isothermal density data of propane, methane, and hydrogen [6]

a vapour for pressures below 13.5b ar, and supercritical above. Therefore, while a dedicated liquefied petroleum gas (LPG) engine may inject fuel in the liquid phase, a flexi-fuel LPG–compressed natural gas (CNG) engine would have injection in the vapour-phase if at a low pressure, and in the liquid or supercritical phase if at a high pressure. If high flowrates are possible with LPG, CNG is certainly much more demanding, even if not so challenging as hydrogen. Apart from fast actuation, pressure build-up in the injection line seems to be the key factor to deliver a high flowrate within short periods of time.

2 PROPOSED ADVANCED H_2ICES

Different design options and engine management strategies are available for advanced H_2ICEs with high power density to satisfy super-ultra-low emission vehicle (SULEV) emissions while providing high efficiencies and regular, smooth, and stable operation over the full range of engine speed and loads [1, 2]. The recent European Union (EU) HyICE project 'Optimization of a hydrogen powered internal combustion engine' [7] has shown cryogenic PFI and DI to be the best options currently available to develop H_2ICEs. HyICE developed and tested two concepts of mixture formation for specific hydrogen engines, DI at 10–200b ar and cryogenic PFI at about 2 200uC. In both methods the performance was doubled while consumption was reduced with reference to prior state-of-the-art hydrogen combustion engines designed for both gasoline and hydrogen usage. DI is also being used in the ongoing EU NICE project 'New integrated combustion system for future passenger car engines' [8] as the best option for gas engines. Hydrogen-assisted jet ignition (HAJI) devices have been designed, built, and tested at the University of Melbourne over more than a decade for enhanced combustion of homogeneous lean mixtures in single- and multiple-cylinder research engines [5, 9–17]. Some of the options for advanced H_2ICEs are now presented and reviewed.

SULEV operation may or may not require after treatment depending on the fuel-to-air equivalence ratio w. Operation at stoichiometry (w5 1) requires after-treatment with fuel-rich reduction catalyst. Lean operation (w< 0.7) requires a lean-NO_x trap (LNT). Operation in the ultra-lean region (w, 0.45) and below does not require after-treatment.

Hydrogen engines can be run stoichiometric to the ultra-lean (w, 0.45) region with very high rates of combustion. Backfiring (or back flashing) and pre-ignition are major problems especially at stoichiometry, and knock may limit spark advances up to ultra-lean operation and beyond. Backfiring, pre-ignition, and knock also depend on additional factors, including the combustion chamber surface materials, surface temperature, compression ratio, pressure boosting, charge cooling, and recirculation of exhaust gases. The power density, rate of combustion, and stability decrease by reducing the fuel-to-air equivalence ratio, while the efficiency at first increases and then decreases going towards leaner operation.

The combustion rate deteriorates moving from ultra-lean combustion (w, 0.45) to further ultra-lean combustion (w< 0.2). Moreover, ultra-lean combustion requires stratified charge with DI or jet ignition (JI) to ensure stability. High compression ratios and pressure boosting may help to keep the rate of combustion high.

The load can be reduced by lowering the fuel-to-air equivalence ratio rather than by throttling for better thermal efficiencies through the reduction in pumping losses. However, the rate of combustion decreases and stability worsens when the fuel-to-air equivalence ratio is reduced and, after certain values of fuel-to-air equivalence ratios, the efficiency drops significantly.

Conventional PFI engines with gaseous fuel are the most susceptible to pre-ignition and knock. This 'warm' PFI also has the disadvantage that the large displacement of air (stoichiometric volume fraction, 29.53 per cent) limits the air-based volumetric efficiency and therefore the power output. Cryogenic PFI with the embedded charge cooling significantly reduces displacement effects and sensitivity to knock and pre-ignition and dramatically improves the volumetric efficiency.

DI of gas-phase H_2 is also less susceptible to pre-ignition, produces reduced or even no displacement effects, and eliminates back flash. Displacement effects with early DI are not too far from those of PFI, while late DI may almost cancel these effects. DI enables stratified operation with the engine able to run in a more ultra-lean way for lower NO_x emission and higher efficiency. DI also considerably improves the fuel economy at part-load, mainly because of reduced pumping losses. Late DI has the penalty of needing to deliver H_2 at a pressure of 100b ar or more with consequent fuel pressurization work, which is less for cryogenic H_2.

The power density may be increased by introducing pressure boosting, supercharging or turbocharging. However, with pressure boosting, the temperature increases, the heat transfer increases, the knock tendency increases, and the maximum allowable compression ratio is reduced. With the addition of an intercooler, the temperature rise across the compressor can be significantly offset.

The rate of combustion (and therefore its stability) and the lean limit may be improved by replacing the standard spark ignition (SI) in the main chamber (MC) with ignition in a pre-chamber (PC). In the HAJI system, additional fuel is injected in a PC connected to the MC via calibrated orifices, creating fuel-rich conditions in the pre chamber. Following ignition by a conventional spark plug in the PC, the MC lean mixture is then ignited by the jets of hot products and radicals from the PC, enabling faster combustion of the lean MC mixture to occur. Flame speed enhancement of up to six times has been measured.

Exhaust gas recirculation (EGR) allows lean equivalent conditions with stoichiometric inflow. EGR allows after-treatment with a reduction catalyst, and the excess air is replaced by EGR dilution. EGR also mitigates pre-ignition effects in the case of warm PFI. Cool EGR controls the charge temperature within the cylinder and may also be beneficial for lean operation.

3 THE LEAN-BURN DIRECT-INJECTION JET IGNITION H_2ICE

MC DI of fuel with fast-actuating high-flowrate high-pressure injectors capable of injection shaping and multiple events, and MC J, with ignition by spark or autoignition in a small-volume PC providing minimal complication of cylinder head design with PC mixture preparation by PC DI [18, 19] has never been considered before for both stationary and transport applications. In large-volume PC ignition systems for large gas engines, the PC fuel is not negligible, the cylinder head design is strongly affected, and PC combustion is important also in itself and not just in initiating MC combustion whereas, in standard DI injectors, the DI injector is a traditional low-cost slow-actuating solenoid low-pressure low-flowrate injector; finally, with standard MC SI coupled to DI, combustion is wall initiated with a relatively small energy supply in just one location.

The new-generation fast-actuating high-pressure high-flowrate DI injector capable of injection shaping and multiple events produces a bulk lean jet-controlled stratified mixture. Late DI overcomes the air displacement effects of PFI of gaseous fuels. High-energy bulk ignition is then achieved by using PC J.

The proposed ignition PC is very small in size, just a few per cent of the combustion chamber volume at top dead centre (TDC) and about 1 cm^3; it is designed to be fitted within the traditional spark plug thread of diameter 14 mm. The ignition device therefore only marginally increases the level of complexity of designing a cylinder head with a standard spark plug.

The jets of reacting gases from the ignition PC enhance the rate of combustion of the MC mixture and allow bulk ignition and combustion for reduced heat losses and faster heat release.

The coupling of J and DI technologies allows development of an engine permitting operation with overall fuel-to-air equivalence ratios reduced to almost zero, because combustion is always started in the J PC provided that there is a very small amount of fuel, and the jets of hot reacting gases from the J PC may extend combustion to globally very lean MC mixtures provided that only a minimum amount of fuel is behind the J nozzle, thus replicating diesel-like light-load operation.

The lean-burn DI J engine uses a fuel injection and mixture ignition system consisting of the following:

(a) one MC DI fuel injector per engine cylinder;
(b) one J device per engine cylinder, the latter being made of one PC connected to the MC through one or more calibrated orifices, one PC DI fuel injector, and one PC (SI version) or one PC (autoignition version);
(c) all the ancillaries required to supply the fuel at the desired pressures by the DI injectors and to operate the DI injectors and the SI or the autoignition PC.

The fuel injection and mixture ignition system operation is as follows.

1. One fuel is injected directly within the cylinder by an MC direct injector operating one single injection or multiple injections to produce a lean stratified mixture. This non-homogeneous mixture is mildly lean in an inner region surrounded by air and some residuals from the previous cycle. The extension of the inner region may be reduced in size to achieve mean chamber average mixtures ranging from slightly to extremely lean.
2. This mixture is then ignited by one or more jets of reacting gases that issue from a PC connected to the MC via calibrated orifices, sourced from the same or an alternative fuel that was injected into

it by a direct injector and then ignited by a spark plug discharge (spark plug version).
3. Combustion which started slightly fuel rich in the very-small-volume PC moves to the MC through one or more J nozzles, with one or more jets of reacting gases bulk igniting the MC mixture. The jets of reacting gases enhance combustion of lean stratified mixtures within the MC through a combination thermal energy and the presence of active radical species.

With reference to homogeneous DI or PFI and MC spark ignition, non-homogeneous DI and J offer the following advantages:

(a) much faster, more complete, much leaner combustion;
(b) less sensitivity to mixture state and composition;
(c) reduced heat losses to the MC walls.

This is because of better fuel for same chamber-averaged lean conditions, combustion in the bulk of the in-cylinder gases, heat transfer cushion of air between hot reacting gases and walls, very high ignition energy at multiple simultaneous ignition sites igniting the bulk of the in-cylinder gases, aided by large concentrations of partially oxidized combustion products initiated in the PC that accelerate the oxidation of fresh reactants.

The advantages of the system are as follows:

(a) higher brake efficiency (ratio of the engine brake power to the total fuel energy) and therefore reduced brake specific fuel consumption (BSFC) (ratio of the engine fuel flowrate to the brake power) for improved full load operation of stationary and transport engines;
(b) efficient combustion of variable-quality fuel mixtures from globally near stoichiometry to globally extremely lean for load control mostly throttleless by the quantity of fuel injected for improved part-load operation of non-stationary engines.
(c) opportunity in the ultra-lean mode to produce near-zero NO_x.

4 COMPUTATIONAL PROOF OF CONCEPT

The concept has been applied to a 1.5l SI four-cylinder gasoline engine with double overhead camshafts and four valves per cylinder. This engine is a V-Four 1.5l engine, with a bore of 78mm, a stroke of 78mm, an intake valve seat insert inside diameter of 32mm, an exhaust valve seat insert inside diameter of 26mm, a connecting-rod length of 109mm, and a pent roof combustion chamber.

While much less than 0.08mg/cycle has to be introduced by the PC injector, and therefore a gasoline DI injector can be used as the PC injector for prototype applications where durability and dry run capability are not an issue, a specific hydrogen injector must be developed for the short injection time, high temperature, high injection pressures, high durability, and dry run capability of the MC injector having to introduce up to 14.8mg/cycle and to produce the charge stratification. Lean stratified mixtures would be possible by adopting charge motion controlled by jet and shaped piston surface–wall or fully jet controlled configurations depending on the injector performance.

Figure 2 presents a view of the in-cylinder plus PC volumes, while Fig. 3 presents a sectional view with a plane passing through the PC axis. The DI injector and the J device are placed at the centre of the cylinder head. A pressure sensor for combustion studies is also located in the centre. The J device is a six-nozzle type. The J device is designed to fit an standard spark plug thread of diameter 14mm. It accommodates one racing spark plug of diameter

Fig. 2 View of the in-cylinder and PC volumes

Fig. 3 Plane cut of the in-cylinder and PC volumes

10m m [20] and one solenoid gasoline DI injector [21–23] and features six equally spaced nozzles of diameter 1.25m m. The PC volume is 1.5c m^3. A bowl-in-piston is system used to produce a lean stratified mixture. Details of the MC DI injector tip are not included.

The engine has been modelled with GT-POWER [24–28]. GT-POWER is the industry standard engine simulation tool, used by most leading engine and vehicle makers and their suppliers. Fuller details of the model have been presented in references [25] to [28]. The model has been derived from a validated high-performance engine model with PFI of gasoline [29]. The main differences are the stroke and lengths of primary intake and exhaust pipes to accommodate reduced maximum torque and power engine speeds, compression ratios, valve events, the J replacing the standard spark plug, the DI injector producing lean stratified mixtures, and finally the fuel. Compression ratios have been selected on the basis of knock index computations. The selected compression ratio produces knock index results close to those obtained for the validated high-performance engine model with PFI of gasoline. This engine turbocharged with charge cooling has a compression ratio CR of 14.5.

The rate of combustion is computed with the predictive combustion model for stoichiometric homogeneous conditions. The rate of combustion is then imposed in lean stratified operation with air-to-fuel equivalence ratios I 5 1/w& 1 by using a Wiebe function with 50 per cent fuel burned anchored at 7.5u crank angle after TDC and 10–90 per cent combustion duration given as

$$h_{10(\;90}(I \& 1, s) \sim \frac{h_{10(\;90}(\sim 1, h)}{I^{b}}$$

where $h_{10\text{-}90}$ (I 5 1,h) is the value computed by the predictive model for stoichiometric I 5 1 homogeneous combustion, $h_{10\text{-}90}$ (I & 1, s) is the value used in the Wiebe function prescription for lean I & 1 stratified combustion, and b is a correlation coefficient smaller than unity. The rate of heat transfer is also decreased introducing a heat transfer multiplier proportional to I^{2c} where c is another correlation coefficient smaller than unity. This formulation produces very fast combustion with reduced heat losses, which in turn produces very high peak pressures also running very lean, namely 90–120b ar in turbocharged applications.

Results on the indicated mean effective pressure (IMEP), brake mean effective pressure (BMEP), friction mean effective pressure (FMEP), BSFC (ratio of the engine fuel flowrate to the brake power), and brake efficiency g_B (ratio of the engine brake power to the total fuel energy), (g_B ; 1/BSFC) obtained during the wide-open throttle (WOT) operation are presented in Figs 4, 5, 6, 7, and 8 respectively for operation with I 5 2, 3, 4, and 5. With I 5 2, the engine has a BMEP approaching 24b ar at 3500r / min, while the BSFC is as low as 65g/kWh , or brake efficiencies g_B as high as 46 per cent, approaching 3500r /min. Further improvements in brake efficiencies g_B of about 1–2 per cent are possible running slightly leaner than I 5 2 especially in the low-engine-speed range. When load variations are obtained by varying the air-to-fuel equivalence ratio from I 5 2 upt o I 5 5 without throttling the intake, high efficiencies and low BSFCs are possible from about 25 per cent load.

Internal combustion engines generally have different BSFC values at different speeds and loads. The brake efficiency g_B is given by

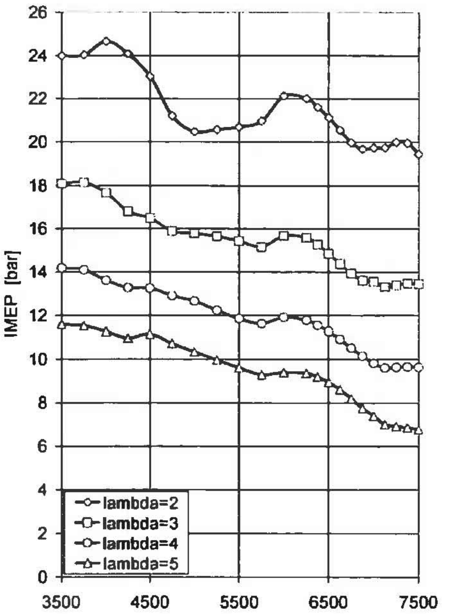

Fig. 4 IMEP results with I 5 2, 3, 4, and 5 at WOT and minimum best torque (MBT) or knock-limited spark timing

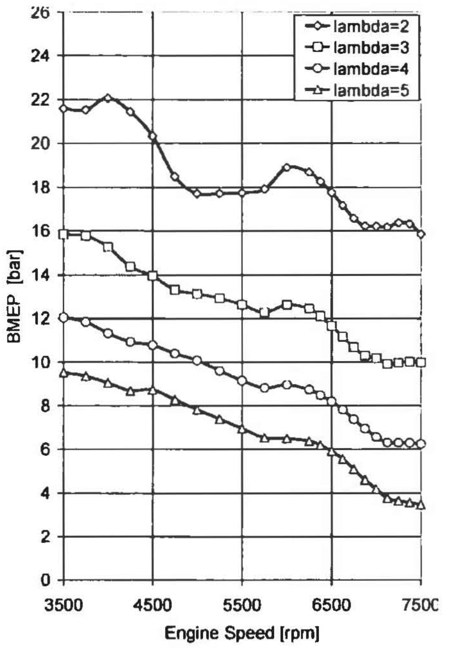

Fig. 5 BMEP results with l 5 2, 3, 4, and 5 at WOT and MBT or knock-limited spark timing

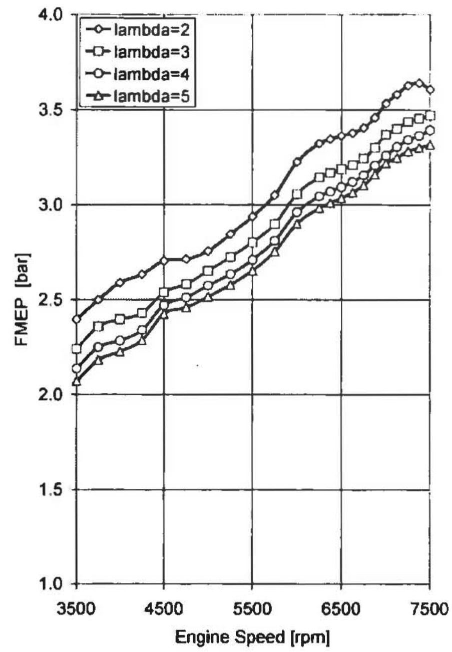

Fig. 6 FMEP results with l 5 2, 3, 4, and 5 at WOT and MBT or knock-limited spark timing

$$\begin{aligned} \eta_B &= \frac{1}{BSFC} \\ &= \frac{BMEP\,N}{FMR} \\ &\sim \frac{IMEP\,N}{FMR} - \frac{FMEP\,N}{FMR} \\ &= \frac{1}{ISFC} - \frac{1}{FSFC} \end{aligned}$$

where ISFC is the indicated specific fuel consumption, FSFC is the friction specific fuel consumption, N is the engine speed, and FMR is the fuel mass flowrate.

In a throttle-controlled homogeneous stoichiometric l 5 1 SI gasoline engine, the minimum BSFC is usually found about peak BMEP operation with the intake not throttled. If N increases, the BSFC increases mostly because of the rising FMEP while, if N is reduced, the BSFC increases mainly because of the increased time for heat transfer to cylinder walls, reducing the IMEP, and, if the intake is throttled, the BSFC increases for the larger pumping losses and therefore reduced IMEP.

In the DI JI engine, the fast, nearly adiabatic lean bulk combustion will deliver lower minimum BSFCs, while the load control by the quantity of fuel injected will keep the BSFCs low over most of the load range, because of the improved ISFC. Increasing l generally reduces the ISFC but also increases the FSFC, as FMEP is only weakly dependent on l. Increasing l therefore reduces the BSFC only up to a minimum with l ~ 2; then it increases the BSFC. Increasing l, the BSFC increase running higher engine speeds becomes more relevant as the ratio FMEP/IMEP increases with increasing l.

5 CONCLUSIONS

Coupling of JI and DI allows development of an engine permitting operation with overall fuel-to-air equivalence ratios that may be reduced to almost zero for diesel-like throttleless control of load and high-efficiency lean stratified bulk combustion.

The system delivers a higher brake efficiency (ratio of the engine brake power to the total fuel energy) and therefore reduced BSFC (ratio of the engine fuel

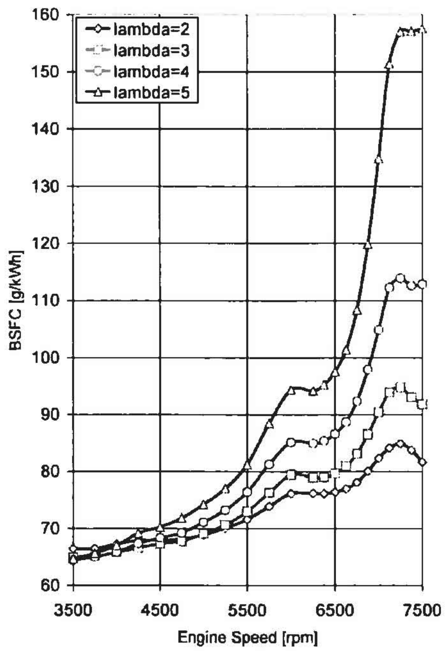

Fig. 7 BSFC results with l 5 2, 3, 4, and 5 at WOT and MBT or knock-limited spark timing

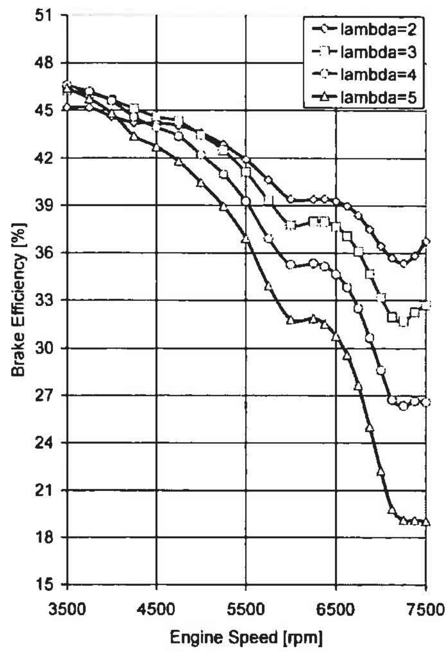

Fig. 8 Brake efficiency results with l 5 2, 3, 4, and 5 at WOT and MBT or knock-limited spark timing

flowrate to the brake power) for improved full-load operation. The system also offers the advantage of having an efficient combustion of variable-quality fuel MC mixtures from near stoichiometry to extremely lean for improved part-load operation.

The proposed technology significantly reduces fuel energy consumption with reference to traditional throttled PFI homogeneous l 5 1 gasoline engines at full load and much more at part-load. Improvements are also significant when reference is made to H_2ICEs developed as a slightly modified version of the traditional gasoline internal combustion engine burning fuel and being controlled in approximately the same manner as for gasoline engines.

With reference to the two concepts developed in the H_yICE project, the main advantage of the technique is the load control by the quantity of fuel injected, improving the part-load operation.

The turbocharged H_2ICE with charge cooling proposed here deliver very high efficiencies running at l 5 2 to l 5 4 with a power density even higher than naturally aspirated homogeneous combustion stoichiometric gasoline engines.

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