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Vehicle driving cycle performance of the spark-less di-ji hydrogen engine

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ABSTRACT

The paper describes coupled CFD combustion simulations and CAE engine performance computations to describe the operation over the full range of load and speed of an always lean burn, Direct Injection Jet Ignition (DI–JI) hydrogen engine. Jet ignition pre-chambers and direct injection are enablers of high efficiencies and load control by quantity of fuel injected. Towards the end of the compression stroke, a small quantity of hydrogen is injected within the spark-less pre-chamber of the DI–JI engine, where it mixes with the air entering from the main chamber and auto-ignites because of the high temperature of the hot glow plug. Then, jets of partially combusted hot gases enter the main chamber igniting there in the bulk, over multiple ignition points, lean stratified mixtures of air and fuel. Engine maps of brake specific fuel consumption vs. speed and brake mean effective pressure are computed first. CAE vehicle simulations are finally performed evaluating the fuel consumption over emission cycles of a vehicle equipped with this engine.

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1. Introduction

Australia's annual green house gases emissions through to the 2009 June quarter for energy – transport amount to 89 Mt CO₂-e [1], or about 14.5% of the total. Development of more energy-efficient and environmentally friendly highway transportation technologies based on heavy and light duty truck and passenger car gas engines is a key factor for reducing fuel consumption, CO₂ production and pollutants emissions within Australia, therefore improving national energy security, environment, and economy. Improving the efficiency of internal combustion engines is the most promising and cost-effective approach to increasing vehicle fuel economy in the next 10 to 20 years, or until such time still far to forecast when plug-in hybrid electric or fuel cell hybrid vehicles will dominate the

market [2]. Advanced combustion engines have still great potential for achieving dramatic energy efficiency improvements, with the primary hurdles that must be overcome to realize increased use of advanced combustion engines being the higher cost of these engines requiring expensive R&D when compared to conventional engines, and compliance with particularly stringent new emission regulations with the catalytic emission control technologies much less mature than gasoline engine catalysts. In the near future, Euro 6 regulations will introduce particularly tough emission limits. Implementation of these stringent emission standards is anticipated to cause a reduction in fuel efficiency due to the exhaust emission control devices needed to meet emissions regulations for both NO_x and PM without introduction of advanced combustion technologies.

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The hydrogen fuelled internal combustion engine is now receiving large attention because of the opportunity operating lean of stoichiometry ($\lambda > 2.25$) to achieve top brake efficiencies over 45% while permitting below EURO 6 emissions without any after treatment [3–12]. Advanced combustion engine technologies being developed by the Author for gaseous fuels, not only hydrogen but also propane and methane, include modes of low-temperature lean combustion (LTC) increasing the efficiency beyond current diesel engines and reduce engine-out emissions of nitrogen oxides (NO_x) and particulate matter (PM) to near-zero levels. In addition to these combustion regimes, reduction of heat transfer, and control of load by quantity of fuel injected and a wide range of waste heat recovery technologies are also being considered to further improve engine efficiency and reduce fuel consumption.

The jet ignition pre-chamber is central to the definition of the always lean burn direct injection jet ignition engine [13–18], aimed at increased top brake efficiencies and reduced efficiency penalty changing the load. The jet ignition device is made up of a pre-chamber, connected to the main chamber through calibrated orifices, accommodating a pre-chamber fuel injector. In the standard spark plug version, the jet ignition device also includes a spark plug that ignites a pre-chamber mixture slightly rich that then bulk ignites the ultra lean, stratified main chamber mixture through the multiple jets of hot reacting gases entering the cylinder. In the glow plug version, the spark plug is replaced by a glow plug to increase durability and reduce maintenance costs, improve packaging and avoid occurrence of locally fuel rich conditions reducing the formation of nitrogen oxides. In the glow plug version, an even smaller amount of fuel is injected in a even smaller pre-chamber and then auto ignites after impinging on the hot glow plug surface that keeps the temperature within the pre-chamber very high. Fuel is injected directly within the cylinder by the main chamber DI injector operating single 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 is reduced in size to achieve mean chamber average mixtures ranging from $\lambda = 2.25$ to $\lambda = 7$. This mixture is then ignited by jets of reacting gases that issue from the pre-chamber. Fig. 1a presents a sketch of the cylinder head layout for a sample four valve pent roof combustion chamber application of the DI-JI engine, while Fig. 1b presents a picture of the jet ignition assembly in the versions with a glow plug replacing the traditional spark plug.

With reference to homogeneous DI or port fuel injection (PFI) and main chamber spark ignition, non homogeneous DI and jet ignition offer the advantage of much faster, more complete, much leaner combustion, less sensitivity to mixture state and composition, and reduced heat losses to the main chamber walls. This is because of better fuel to air ratio of the combusting mixture 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, multiple simultaneous ignition sites igniting the bulk of the in cylinder gases, and large concentrations of partially oxidized combustion products initiated in the pre-chamber accelerating the oxidation

a Jet ignition nozzles

b

Fig. 1 – a. Cylinder head layout of the 4 valve Direct Injection Jet Ignition engine (from [16]). b. Jet ignition assembly for the 4 valve Direct Injection Jet Ignition engine in the version with a glow plug (from [16]).

of fresh reactants. The concept is an original evolution of the idea of using jet-style ignition to enable the operation of a flame-propagation engine with very lean mixtures explored many times, mostly in the large engine natural gas industry.

The major differences of the present concept are the direct injector to the main chamber creating there mixtures from lean homogeneous to lean stratified to explore the many options of low temperature combustion, and the small size pre-chamber fitted with a second fuel injector and a spark or a glow plug, enabling start of combustion by multiple jet of hot reacting gases originating from ignition of a small fraction of the total fuel.

The volume of the jet ignition pre-chamber less than 1 cm^3 is definitively small if compared with main chamber combustion chamber volumes at top dead centre of about 130 cm^3 in a 11 liter in-line 6 truck engines, or about 60 cm^3 in a 3.6 liter V6 passenger car engines, totaling respectively the 0.8 and the 1.6% (indirect injection Diesel engine combustion chambers were not less than 40–50% of the main chamber combustion chamber volumes at top dead centre). This small size volume of the pre-chamber and the requirement to inject within the pre-chamber only a very small fraction of the total fuel is supposed to keep low NO_x production otherwise a major detriment of traditional pre-chamber engines even at very lean operating conditions.

Spark plug life within the pre-chamber is generally not viewed as a major issue so long as cooling considerations are taken into account when designing the pre-chamber housing. However, the limited amount of space available to accommodate a spark plug and the therefore very far from optimal conditions may suggest replacement of a spark plug with a much smaller glow plug. Replacement of the spark plug with a glow plug not only increases durability and reduces maintenance costs, but also improves packaging and avoid occurrence of globally fuel rich conditions carefully controlling auto ignition and pre-chamber injection (The best operation of the spark ignition jet ignition pre-chamber is achieved injecting in the pre-chamber an amount of fuel slightly exceeding the stoichiometric required for the amount of air [19–25]). The operation of the glow plug pre-chamber is on the other hand more complicated, because the pre-chamber fuel injection and auto-ignition processes are strongly interrelated and some additional studies are needed to further develop the concept. While the spark plug pre-chamber has been studied for more than one decade [19–25], the glow plug pre-chamber concept is relatively new, and focus is due not only on the much more demanding direct injector, but also on the use of the glow plug to control auto ignition.

CAE engine simulations obtained on the small high-tech four cylinders, 1.5 liter, and highly turbocharged engine fuelled with propane and hydrogen [16]. This engine has displaced volume $V_D = \pi \cdot B^2/4 \cdot S = 375 \text{ cm}^3$ (B is the bore and S the stroke of the engine), pre-chamber volume $V_{PC} = 1.5 \text{ cm}^3$, true compression ratio of the engine $\rho^* = (V_{PC} + V_{MCC} + V_D)/(V_{PC} + V_{MCC}) = 13.8$ (V_{MCC} is the main chamber combustion chamber volume at top dead centre) and reference compression ratio $\rho = (V_{MCC} + V_D)/(V_{MCC}) = 14.5$. This engine shows very interesting BSFC and brake efficiency results. In the range of engine speed 3500–7500 rpm, BSFC at WOT and MBT or knock limited spark timing has a minimum of 165 g/kWh with propane and less than 65 g/kWh with hydrogen about 3500 rpm, corresponding to brake efficiencies of almost 48%. These results clearly show the potentials to achieve even better brake efficiencies exceeding the 50% mark in the engine

redesigned for lower speeds, where friction losses are lower and air-to-fuel equivalence ratios may be even leaner.

Diesel pre-chamber engines have almost disappeared after the introduction of high pressure direct fuel injection systems because of the disadvantage of an increased combustion chamber wall surface area, the resulting increased heat losses, the restriction of the combustion burn, and the increased NO_x formation for the locally richer conditions due to the injection of all the fuel within the pre-chamber. The proposed jet ignition system uses a very small pre-chamber having a very small volume compared not only to the main chamber displaced volume, but also to the main chamber combustion chamber volume, to ignite there only a very small amount of the total fuel, with the most part of the fuel being delivered directly to the main chamber. The jet ignition concept was originally developed as a replacement of standard spark plugs in port fuel injected spark ignition engines for running lean homogeneous [19–25]. The overall size of the jet ignition unit was designed such that it was possible to screw into the block using the standard spark plug hole. The volume of the jet ignition pre-chamber has been so far only 0.75 to 1.5 cm^3 depending on the particular design. The operation of the direct injection jet ignition engine can not therefore be assimilated to the operation of a Diesel pre-chamber engine. Compared to normal direct injection H_2 engines, the direct injection jet ignition engine has the advantage of a much faster main chamber combustion initiated in the bulk of the cylinder gases by multiple jet of hot reacting gases rather than by a spark discharge close to the cylinder head wall, with reduced heat losses because the burning fuel richer area may be an inner region not bounded by cylinder head or cylinder liner walls. Furthermore, the jet ignition permits lean main chamber air-to-fuel ratios that can not be normally achieved with a standard spark plug, with complete combustion events even in case of very small amount of fuel injected in the main chamber close to the jet ignition nozzles, and therefore throttle-less load control Diesel like. The main chamber injection process must deliver the amount of fuel needed downstream of the jet ignition nozzles. This is accomplished with fast actuating, high pressure and high flow rate injectors permitting main chamber injections to occur towards the end of the compression stroke (In the simulations presented, the end of injection is placed at top dead centre.). The bowl in piston helps with containment of the gas fuel jet stratifying the mixture close to piston wall but far from head and liner walls. The complete system therefore delivers top and part load brake efficiencies better than spark plug ignited direct injection engines at the expenses of the additional complexity of the jet ignition device.

Purpose of the paper is to explore the potential of the proposed concept before building a prototype engine and a prototype car for a final experimental product validation. The paper couples Computational fluid dynamic (CFD) and Computer Aided Engineering (CAE) engine and vehicle performance simulations to describe the operation of the hydrogen fuelled direct injection jet ignition engine stand-alone over the full range of speed and load and over a driving cycle installed on a vehicle. CFD simulations are used to study the mixture formation within the pre-chamber and the main chamber, the auto ignition process within the pre-chamber,

and the subsequent jet ignition of the main chamber mixture and the combustion evolution within the main chamber. These descriptions will permit selection of direct injectors to main chamber and pre-chamber and glow plug, set-up of injection timings and flow profiles for injectors and definition of time scales of heat release processes within pre-chamber and main chamber needed in CAE simulations of engine performances. These latter simulations will finally provided engine brake mean effective pressure and specific fuel consumption over the full range of load and speed. Finally, CAE vehicle simulations will be performed by using these computed engine maps to compute the fuel economy over driving cycles of a vehicle equipped with a DI-JI hydrogen engine.

2. Direct injector selection

Selection of the fuel injectors is critical to the development of the DI-JI engine concept with hydrogen fuel. The fuel injector selection is already an issue in “normal” direct injection hydrogen engines. The additional constraints posed to the injection processes within the main chamber and the pre-chamber to fully exploit the potentials of the DI-JI engine concept with hydrogen fuel make the selection more difficult.

The amount of fuel to be introduced by the direct injector within the pre-chamber is quite small. If η_V is the volumetric efficiency $\eta_V = (m_a)/(\rho_{a,i} \cdot V_D)$, where m_a is the mass of air trapped within the cylinder when the intake valves close and $\rho_{a,i}$ is the reference air density, then the mass of fuel to be injected within the pre-chamber is roughly given by:

$$m_{f,PC} \approx \left[\frac{(F/A)_s}{\lambda_{PC}} \right] \eta_V \rho_{a,i} (CR - 1) V_{PC} \quad (1)$$

where $(F/A)_s$ is the stoichiometric fuel to air ratio, and λ_{PC} is the pre-chamber operational air to fuel equivalence ratio. As a first assumption, the mass of air within the pre-chamber at top dead centre is assumed to be equal to the total mass of air trapped within the cylinder multiplied by the ratio of pre-chamber volume to main chamber combustion chamber volume at top dead centre. In the detailed operation of the jet ignition pre-chamber described in [41], following the compression stroke the main chamber air (and residuals) mixture flows towards the pre-chamber through the jet ignition nozzles, with a process further complicated by the injection of fuel within the pre-chamber towards the end of the compression stroke, the following start of combustion, and the option to have back flows towards the main chamber even before the start of the expansion stroke. The actual mass of air (and residuals) within the pre-chamber at top dead centre is therefore different from this reference value, used to provide just a first guess of the amount of fuel to be introduced within the pre-chamber. η_V is about unity for naturally aspirated engines, but can reach values up to 2 in highly turbo-charged versions with charge cooler, while ρ may range from 10:1 to 15:1 depending on the boost provided by the turbo charger, and $(F/A)_s$ is 0.0294 for H_2 .

In the spark plug version, all the pre-chamber fuel has to be introduced before the spark discharge starts combustion, λ_{PC}

is representative of the fuel-to-air ratio at the start of combustion, and values slightly smaller than unity (i.e. slightly fuel rich) provide the best results. In the glow plug version, auto ignition starts before all the fuel is injected, and λ_{PC} is now just representative of the total fuel that will be injected within the pre-chamber. This parameter may reach values $\lambda_{PC} = 2$ to 3. Therefore, the pre-chamber DI injector has to introduce less fuel than the main chamber DI injector in general, and this amount is less in the glow plug vs. the spark plug version. In case of a turbo charged engine with unit displacement 375 cm^3 , compression ratio 14.5:1, volumetric efficiency 1.9, pre-chamber volume 1.5 cm^3 , the mass of hydrogen fuel to be introduced within the pre-chamber for stoichiometric conditions is 1.3 mg, and in case of a naturally aspirated engine with unit displacement 600 cm^3 , compression ratio 11:1, volumetric efficiency 1, pre-chamber volume 1.5 cm^3 it is 1 mg.

The auto ignition process set constraints to the injector pulse width duration and therefore to the flow rate and the opening and closing times. In the spark plug version, injection has to be completed before the spark discharge ignites the pre-chamber mixture, and it may start almost any time during the compression stroke and it may have almost any duration. In the glow plug version, fuel injection has to be faster with much higher flow rates to be effective. Enough fuel has to be introduced before the combustion evolution within the pre-chamber will increase there the pressure up to the very high values that will finally force the hot partially combusted products and radicals to move towards the main chamber. In the glow plug version, even if the quantity of fuel injected is much smaller, the flow rate has to be much larger and the opening times much shorter than in the spark-plug version. During the injection time, the nozzles are very unlikely to be choked, because the needle lift is opening and closing, with the minimum area being very likely the needle seat area over the most part of the injection process.

A proper estimation of the ignition delay is central to the development of the auto ignition glow plug pre-chamber. Published measured data obtained in shock tubes or rapid compression machines experiments [26–28] only partially help because not only composition, pressure and temperature differ, but also averaged and turbulent transport and diffusion are different. As a rough guideline, the auto ignition time is given in [28] as follows:

$$\tau_{ign} = A [X_{H_2}]^x \phi^y p^z \exp[E/RT] \quad (2)$$

where τ_{ign} is the ignition delay time, X_{H_2} the H_2 mole fraction in the overall fuel–air mixture, ϕ the fuel-to-air equivalence ratio, p is the pressure, T the temperature, R the gas constant and E , A , x , y , and z are model constants. The constant E in this equation is commonly referred to as the ignition activation energy. A , x , y and z are dimensionless. Values of E , A , x , y , and z as well as better details of the derivation of kinetic time models in Arrhenius-type formulas as functions of equivalence ratio, temperature, pressure, and molar fraction of H_2 are given in [28].

This equation provides auto ignition times of about 0.2 ms with $p = 1$ bar, $T = 1000$ K, $\phi = 0.5$, that are well below the time for complete opening and closure of today's fastest GDI piezo injectors that require times to achieve full opening lifts of

about 0.04 mm of not less than 0.3 ms. On the other hand, these injectors can also be operated part lift, with reduced pulse width and flow rates, having the minimum flow area the choked needle seat area.

Injectors should operate with not less than 200 bar of pressure. The hydrogen gas flows from an upstream higher stagnation pressure to a much lower downstream pressure is choked in the minimum effective area. Assuming ideal gas behavior, steady state choked flow occurs when the ratio of the absolute upstream pressure to the absolute downstream pressure is equal to or greater than $[(k+1)/2]^{k/(k-1)}$, where k is the specific heat ratio of the gas. The equation for the mass flow rate per unit effective area is:

$$\dot{m}^* = \frac{\dot{m}}{A_e} = \sqrt{k p_0 \rho_0 \left[\frac{2}{(k+1)} \right]^{(k+1)/(k-1)}} \quad (3)$$

where ρ_0 is the upstream stagnation density, p_0 the upstream stagnation pressure and A_e is the effective throat area (product of geometrical area and flow coefficient). For hydrogen at 2×10^7 Pa of pressure and 300 K of temperature, we may assume $\rho_0 = 14.4$ kg/m³, $c_v = 20.857$ J/(mol K), $c_p = 29.658$ J/(mol K), $k = c_p/c_v = 1.422$ and therefore $\dot{m}^* = 1.17\text{E}+04$ kg/(s m²) or 11.7 g/(s mm²), i.e. a flow rate of 4.09 g/s with a minimum effective area of 0.35 mm².

Equations (1)–(3) set constraints on pulse width and flow rate that suggest testing of fast actuating high pressure GDI injectors [29,30] or specific hydrogen injectors [31] as the potential glow plug pre-chamber direct injector. Less demanding low pressure GDI injectors [32] may be used in the spark plug pre-chamber. The main chamber direct injector has to be a specific hydrogen injector [31].

The fast single coil Direct injector in [29] provides (with gasoline fuel) flow rates up to 40 g/s at 200 bar, up to 3 multiple injections, hydraulic separation at multiple injection ≤ 0.2 ms, and a hollow cone pattern with cone angles as required by the application. The double acting multi holes Direct injector in [31] has much larger areas, with equivalent flow areas of 0.7 mm² through 16 holes, and may deliver up to 20 g/s with methane at 200 bar, with response times within 0.1 ms and minimum injection duration 0.5 ms. This latter injector has also been used with hydrogen in prototype applications [33].

3. CFD engine simulation results

Computations of the pre-chamber and cylinder mixture formation and combustion evolution have been performed by using CFD and CAE tools. A CFD tool is used to simulate the detailed fluid dynamic and combustion of the cylinder plus pre-chamber in 3D, while a CAE tool is used to describe the full cyclic engine operation including in cylinder and pre-chamber. CFD simulations are performed by using STAR-CCM [34], while CAE simulations are performed by using GT-POWER [35] and WAVE [36].

STAR-CCM [34] injection and combustion simulations have been performed for a single engine cylinder of a larger 3.6 liters, naturally aspirated six cylinders, gasoline engine fuelled with hydrogen. This engine has $V_D = 600$ cm³, $V_{PC} = 1.5$ cm³, $\rho^* = 10.8$ and $\rho = 11.0$. Computations start at

intake valve closure when initial conditions are set by using results of CAE simulations, and end at exhaust valve opening. Piston moves following the compression and expansion strokes, and the computational domain made up of the cylinder volume contract or expands accordingly, while layers are added and removed. The computational grid, made up of 300,000 polyhedral cells to keep the computational time and the internal memory requirements. Morphing is used to change the grid density to the variable in cylinder space aiming to produce computationally effective mesh elements in size and shape. Main chamber and pre-chamber injections are performed with very basic single holes injectors where up to sonic velocity is set during injector opening times. Simulations have been performed neglecting the residual gases within the cylinder and the pre-chamber at intake valve closure.

The flow is considered turbulent, compressible, reacting, multi species. Turbulence is modeled by using a Reynolds-Averaged Navier–Stokes (RANS) turbulence model; in particular 2 equations $K-\epsilon$ model with a two layer all y^+ wall treatment [34]. The $K-\epsilon$ RANS model is preferred for simplicity, generality and reliability.

Kinetics equations are obtained by using DARS-CFD [37]. The kinetics equations of the 21 elementary step mechanism used here are presented in Table 1 [37,41]. A , n and E_a are the Arrhenius rate constants:

$$k = AT^n e^{-E_a/RT} \quad (4)$$

where T is the temperature and R the gas constant.

Transport and diffusion equations are solved for the nine chemical species, namely for O₂, H₂, H₂O, H, O, OH, HO₂, H₂O₂. STAR-CCM solves the Partial Differential Equations (PDEs) for energy and species conservation [34]:

$$\begin{aligned} \frac{\partial}{\partial t} \rho Y_k + \frac{\partial}{\partial x_j} (\rho u_j Y_k + F_{k,j}) &= 0 \\ \frac{\partial}{\partial t} \rho h + \frac{\partial}{\partial x_j} (\rho u_j h + F_{h,j}) &= \frac{\partial}{\partial t} p + u_j \frac{\partial}{\partial x_j} p + \tau_{ij} \frac{\partial}{\partial x_j} u_i \end{aligned} \quad (5)$$

where t is the time, x_j are the spatial coordinates, ρ is the density, h is the enthalpy, p is the pressure, u_j are velocity vector components, Y_k are the species mass fractions, $F_{k,j}$ are species diffusion vector components, $F_{h,j}$ are enthalpy diffusion vector components and τ_{ij} are stress tensor components. DARS-CFD solves the Ordinary Differential Equations (ODEs) for chemical kinetics [37]:

$$\frac{\partial}{\partial t} Y_i = \frac{\omega_i}{\rho} \quad (6)$$

where ω_i is the species production rate.

When chemical kinetics is the limiting factor of the reacting system under investigation, near-perfect mixing of reactants and products is usually achieved. However, normally these mixing mechanisms have to rely on fluid motion or large-scale eddies and turbulence to provide the mixing. Local turbulence is particularly important as it promotes micro-scale mixing among the gas species. If the turbulence is too weak to provide fast mixing among the gas species, the micro-mixing process will interfere with the chemical kinetics. The previous model already implicitly addresses both situations. However, to further strengthen the kinetic-turbulence

Table 1 – DARS Preprocessor H₂/O₂ kinetic mechanism (units are cm³ mol s cal K).

Reaction		Arrhenius coefficients		
		A	n	E _a
r1f:	H ₂ + O ₂ = 2OH	1.700E+13	0.000E+00	1.999E+02
r1b:	H ₂ + O ₂ = 2OH	2.223E+10	3.877E–01	1.202E+02
r2f:	H ₂ + OH = H ₂ O + H	1.170E+09	1.300E+00	1.517E+01
r2b:	H ₂ + OH = H ₂ O + H	7.980E+10	9.726E–01	8.200E+01
r3f:	H + O ₂ = OH + O	2.000E+14	0.000E+00	7.029E+01
r3b:	H + O ₂ = OH + O	6.712E+11	3.742E–01	–1.190E+00
r4f:	O + H ₂ = OH + H	1.800E+10	1.000E+00	3.693E+01
r4b:	O + H ₂ = OH + H	7.014E+09	1.014E+00	2.866E+01
r5f:	H + O ₂ + M ₁ = HO ₂ + M ₁	2.100E+18	–1.000E+00	0.000E+00
r5b:	H + O ₂ + M ₁ = HO ₂ + M ₁	6.276E+20	–1.660E+00	2.142E+02
r6f:	H + 2O ₂ = HO ₂ + O ₂	6.700E+19	–1.420E+00	0.000E+00
r6b:	H + 2O ₂ = HO ₂ + O ₂	2.002E+22	–2.080E+00	2.142E+02
r7f:	H + O ₂ + N ₂ = HO ₂ + N ₂	6.700E+19	–1.420E+00	0.000E+00
r7b:	H + O ₂ + N ₂ = HO ₂ + N ₂	2.002E+22	–2.080E+00	2.142E+02
r8f:	OH + HO ₂ = H ₂ O + O ₂	5.000E+13	0.000E+00	4.184E+00
r8b:	OH + HO ₂ = H ₂ O + O ₂	4.033E+14	7.798E–02	2.972E+02
r9f:	H + HO ₂ = 2OH	2.500E+14	0.000E+00	7.950E+00
r9b:	H + HO ₂ = 2OH	3.867E+10	7.930E–01	1.544E+02
r10f:	O + HO ₂ = O ₂ + OH	4.800E+13	0.000E+00	4.184E+00
r10b:	O + HO ₂ = O ₂ + OH	2.212E+12	4.189E–01	2.221E+02
r11f:	2OH = O + H ₂ O	6.000E+08	1.300E+00	0.000E+00
r11b:	2OH = O + H ₂ O	1.050E+11	9.591E–01	7.510E+01
r12f:	H ₂ + M ₂ = 2H + M ₂	2.230E+12	5.000E–01	3.874E+02
r12b:	H ₂ + M ₂ = 2H + M ₂	6.310E+10	7.542E–01	–5.301E+01
r13f:	O ₂ + M = 2O + M	1.850E+11	5.000E–01	3.998E+02
r13b:	O ₂ + M = 2O + M	4.508E+07	1.115E+00	–1.038E+02
r14f:	H + OH + M ₃ = H ₂ O + M ₃	7.500E+23	–2.600E+00	0.000E+00
r14b:	H + OH + M ₃ = H ₂ O + M ₃	1.808E+27	–3.182E+00	5.073E+02
r15f:	H + HO ₂ = H ₂ + O ₂	2.500E+13	0.000E+00	2.929E+00
r15b:	H + HO ₂ = H ₂ + O ₂	2.956E+12	4.053E–01	2.292E+02
r16f:	2HO ₂ = H ₂ O ₂ + O ₂	2.000E+12	0.000E+00	0.000E+00
r16b:	2HO ₂ = H ₂ O ₂ + O ₂	5.131E+13	–1.776E–01	1.553E+02
r17f:	H ₂ O ₂ + M = 2OH + M	1.300E+17	0.000E+00	1.904E+02
r17b:	H ₂ O ₂ + M = 2OH + M	2.622E+09	1.630E+00	–3.268E+01
r18f:	H ₂ O ₂ + H = HO ₂ + H ₂	1.600E+12	0.000E+00	1.590E+01
r18b:	H ₂ O ₂ + H = HO ₂ + H ₂	7.375E+09	5.829E–01	8.682E+01
r19f:	H ₂ O ₂ + OH = H ₂ O + HO ₂	1.000E+13	0.000E+00	7.531E+00
r19b:	H ₂ O ₂ + OH = H ₂ O + HO ₂	3.144E+12	2.556E–01	1.453E+02

interactions, following [38] the Kong-Reitz model there described is used to scale the previously defined reaction rates s_i through a function of the kinetic and mixing times τ_{kin} and τ_{turb} given as follows:

$$s_i^t = s_i^l \frac{\tau_{kin}}{\tau_{kin} + f \tau_{turb}} \quad (7)$$

where

$$\tau_{turb} = C \frac{K}{\varepsilon} \quad (8)$$

with C a constant, K the turbulence kinetic energy and ε the turbulence dissipation rate, while

$$f = \frac{1 - \exp(-r)}{0.632} \quad (9)$$

$$r = \frac{m_{H_2O} + m_{H_2}}{1 - m_{N_2}}$$

and m mass fractions of the relevant species.

Default values are used for the all the constants involved in STAR-CCM. Initial and boundary conditions are obtained by

using CAE simulations. The main chamber and the pre-chamber injectors are modeled as $\phi = 0.9$ mm and $\phi = 0.3$ mm diameter orifices where up to sonic velocity is set during opening period. Opening and closing dynamic is considered through a fixed opening and closing time providing a trapezoidal velocity distribution. The glow plug has a temperature of 1200 K. The pre-chamber walls have a temperature of 600 K, while the remaining main chamber walls have a temperature of 550 K with the exception of the cylinder liner having a temperature of 500 K.

Simulations presented here have been obtained for operation at 7500 rpm. Diesel engines are well known being unable to run engine speed exceeding 4500 rpm because of diffusion and kinetics controlled Diesel combustion. The DI–JI engine without a spark-plug has a kinetic controlled start of combustion within the pre-chamber, but then turbulence controlled main chamber combustion following the jet ignition. However, thanks to the high rates of reaction for hydrogen, the kinetic controlled glow plug assisted start of combustion within the small jet ignition pre-chamber may be

effective also at the higher engine speeds of spark ignited engines. During operation at 7500 rpm with the glow plug pre-chamber, a quite difficult test for auto ignition engines, the start of injection (SOI) for the main chamber injector is located 40° crank angle before top dead centre (TDC), and end of injection (EOI) is located at 5° crank angle after TDC. The SOI for the pre-chamber injector is 20° crank angle before TDC, and EOI is located at 5° crank angle after TDC. The air-to-fuel equivalent ratio is $\lambda = 2.25$ for the main chamber and about same for the pre-chamber.

Temperature fields within the cylinder at different crank angle positions about firing top dead centre are presented in Fig. 2a and b. Interval between pictures is 2° crank angle or 4.44×10^{-5} s. From top to bottom of Fig. 2a, piston is approaching top dead centre, while from top to bottom of Fig. 2b, piston is moving far from top dead centre. The blue on the left of the scale identifies low temperature zones where the cold hydrogen fuel is injected, while the red on the right of the scale identifies areas where hot combustion products are displaced following the start of combustion.

Following injection, combustion starts almost immediately in hot spots with fuel available about the glow plug, but it takes a finite time have a considerable flamed volume within the pre-chamber, during which the fuel continues to enter within the pre-chamber. The strong flow from the main chamber following the compression stroke pushes the gases towards the top of the pre-chamber where combustion starts. When a significant quantity of fuel within the pre-chamber is combusted or being combusting, combustion quickly propagates to the rest of the pre-chamber volume. Finally, when combustion within the pre-chamber is fully initiated, the jet of partially combusted, hot products then rapidly spread combustion all over the main chamber through multiple jets, with help from the expansion stroke that contributes to the flow pre-chamber to main-chamber. Combustion within the main chamber then completes within a very short time despite of the lean composition, because almost all the fuel is located behind the jet ignition nozzles. These computations allow definitions of injection timings for the main chamber and pre-chamber injector, as well as prescription of combustion evolution within the pre-chamber and the main chamber.

For what concerns the combustion within the main chamber of major interest, it occurs shortly after firing TDC, when almost all the ignitable fuel mixture is reached by the multiple jets of hot combusting products and combustion then evolves very quickly. There is therefore no pressure build up during compression, and all the fuel energy is released during the expansion stroke within a very short time frame. The previous combustion evolution may obviously change varying the pre-chamber injector fuel flow rate and start of injection as well as the glow plug temperature, and in general all the other parameters affecting pressure, temperature, mean and turbulent velocity and composition of the pre-chamber mixture. In this particular case, the multiple jets of hot reacting gases enters the main chamber only about top dead centre, combustion starts within the main chamber only following the main chamber ignition, and there is therefore no pressure build-up within the main chamber during compression. The combustion duration 10–90% mass fuel burned is less than 10° crank angle in the simulated operating point

7500 Rpm, and it is expected to be even less than that reducing the engine speed, the processes being determined by both speed independent kinetic effects (temperatures not changing with mean piston speed) and speed dependent turbulence effects (turbulence fluctuations proportional to mean piston speed).

Simulations and experiments have been previously performed on port fuel injected engines with spark plug controlled jet ignition, hydrogen as the pre-chamber fuel and hydrogen, methane, propane and gasoline as the main chamber fuel [19–25]. These results are generally in good agreement showing a much faster rate of combustion with jet ignition. The proposed CFD simulation results are in line with what was previously measured and computed.

4. CAE engine and vehicle simulation results

CAE engine performance simulations have been finally performed by using the WAVE software [36]. These simulations may provide a first estimation of performance of an engine fitted with the DI–JI technology. CAE results are presented for a production HSDI Diesel engine converted to hydrogen and fitted with a DI–JI system for main chamber injection and ignition.

The engine is 2 liters, in-line four, 16 valves, fixed geometry turbo charged, with inter cooler and cooled Exhaust Gas Recirculation (EGR), full load boost of 1.5 to 2.6, bore $B = 85$ mm, stroke $S = 88$ mm, displaced volume per cylinder $V_D = 500$ cm³, compression ratio $\rho = 19.5$, and operates full load with $\lambda = 1.55$. The converted hydrogen engine also has the piston redesigned for a compression ratio $\rho = 14$ and containment of the hydrogen jet. All the other engine parameters are unchanged. The configuration optimal for a Diesel in terms of diameters, lifts and opening timings of valves, shapes of ports and diameters and lengths of pipes, and turbo charger selection, is certainly not optimal for a hydrogen engine fitted with the DI–JI technology, which in principle can be designed for much higher engine speeds and specific power outputs. Full load operation is also considered with $\lambda = 2.25$, then load is reduced changing the amount of fuel injected. The spark advance considered for the hydrogen engine is the maximum brake torque or knock limited. Combustion duration 10–90% mass fuel burned is set by using the results of the CFD simulations of the naturally aspirated engine previously described, while the point of 50% mass fuel burned is shifted to get maximum brake torque with normalized knock intensity computed with an empirical induction-time correlation model [39] below reference values for gasoline engines. Actual combustion rates in the smaller displaced volume, higher compression ratio, turbo charged engine are expected to be faster thus leaving space for further improvements. Results of CFD simulations provide values of combustion duration 10–90% below 10° of crank angle in the worst scenario. Even significant percentage variations about these values do not affect too much engine performances. The option to use different profiles of combustion duration is therefore not explored.

The knock estimation is based on an assumed octane rating for hydrogen of 120 following [3]. The octane rating is

Fig. 2 – a. Computed temperature fields within the cylinder of the DI–JI hydrogen engines about TDC with intervals 2° crank angle or 4.44×10^{-5} s. b. Computed temperature fields within the cylinder of the DI–JI hydrogen engines about TDC with intervals 2° crank angle or 4.44×10^{-5} s.

a measure of the resistance of petrol and other fuels to auto-ignition in spark-ignition internal combustion engines. It is well known that hydrogen does not fit well into the normal definitions of octane number, having a very high Research Octane Number (RON) but a low Motor Octane Number (MON),

or, if preferred, high resistance to knock and low resistance to pre-ignition. Knock is defined as auto-ignition of the hydrogen–air end-gas ahead of the flame front that has originated from the igniting jets. The high auto ignition temperature, the finite ignition delay and the high flame velocity of hydrogen

means that knock, as defined above, is less likely for hydrogen relative to gasoline, and this the effect described by the induction time correlation. The global effect of both knock and pre-ignition is nearly indistinguishable, and this is the primary reason for the lack of a clear distinction between the two phenomena in hydrogen engines. The distinction is made on the basis of the controlling phenomena. Pre-ignition can be avoided through proper engine design, while knock is an inherent limit on the maximum compression ratio. Knock can be controlled by retarding the spark timing in general, and the fuel injection in the jet ignition pre-chamber in the particular case, while pre-ignition cannot be controlled by adjusting spark timing or fuel injection in the jet ignition pre-chamber. The previous results have therefore validity in the assessment of the maximum compression ratio of the hydrogen engine as well as the knock limited start of pre-chamber injection.

Fig. 3a presents the brake efficiency and the brake torque of the hydrogen and Diesel engines full load. The DI–JI hydrogen engine has better than Diesel efficiency, and despite of the lower fuel-to-air equivalence ratio, it also provides better torque. These pictures demonstrate the opportunity to produce a car fun-to-drive powered by a lean combustion hydrogen engine. Load has then been changed by changing the quantity of fuel injected for the hydrogen engine. Fig. 3b presents the brake efficiency for operation with air-to-fuel equivalence ratio $\lambda = 2.25$, 4.5 and 6.75 or brake mean effective pressure BMEP = 2, 4 and 6 bar, and brake mean effective pressure for variable air-to-fuel equivalence ratio, $\lambda = 2.25$, 4.5 and 6.75. High efficiencies are obtained over the most part of engine loads, demonstrating the opportunity for a car equipped with the DI–JI engine to be also fuel efficient.

A modified form of the Chen–Flynn correlation is used to model friction [36]. The correlation has a constant term (for accessory friction), a term which varies with peak cylinder pressure, a third term linearly dependent on mean piston velocity (for hydrodynamic friction) and a fourth term quadratic with mean piston velocity (for windage losses). The same four constants are used for the H_2 and Diesel engines, with small differences in friction mean effective pressure that may therefore arise from different peak pressures. While the Diesel engine is calibrated to meet stringent NO_x and particulate emission limits, the only pollutant relevant to the H_2 engine are the nitrogen oxides. The selected ignition timings and the operation with air-to-fuel equivalence ratios $\lambda = 2.25$ and above produces low combustion temperatures and therefore negligible production of nitrogen oxides.

The original Woschni correlation is used to model heat transfer [36]. The Woschni model views the charge as having a uniform heat flow coefficient and velocity on all surfaces of the cylinder, and calculates the amount of heat transferred to and from the charge based on these assumptions. It is the most commonly used heat transfer model and can be applied to all cylinder elements. It uses multipliers to tune the model to the particular geometry, plus prescribed averaged wall temperatures and a swirl ratio. This model has been selected for the simplicity and the small amount of data needed to tune.

The Diesel CAE simulations are validated simulations with the pertinent fuel injection and combustion models [36]. The H_2 CAE simulations follow modeled replacement of the fuel injection system, modifications to the piston and the addition

of the jet ignition device, and introduction of combustion rates derived from previous CFD simulations in a Wiebe function. These results have therefore been only indirectly validated, and full engine experiments would certainly provide a better estimation.

The drop of brake efficiency running higher engine speeds reflects the design of the engine flow passages and valve lift profiles and the selection of the turbo-charger to maximize the low speed brake efficiencies of the Diesel (the engine operates mainly at low speeds and brake mean effective pressure during driving cycles). While the Diesel engine operating with $\lambda = 1.55$ has a mass flow of air through the compressor of 265 kg/h at 3000 rpm, at same speed the hydrogen engine operating with $\lambda = 2.25$ has a mass flow of air through the compressor of 430 kg/h.

First European test cycle with extra urban driving cycle (NEDC) simulations have then been finally performed for a large passenger car sedan with the Lotus Vehicle Simulation software [40]. The car has weight 1810 kg, frontal area 2.250 m², drag coefficient 0.298, rolling tyre radius 0.3160 m, 5-speed automatic transmission with transmissions ratios 3.22/2.29/1.55/1.00/0.75, final drive ratio 2.730. The 4 liter, in-line six cylinder, throttle body controlled, naturally aspirated gasoline engine with maximum power 190 kW and maximum torque 380 N m is replaced by the 2 litres, turbocharged, DI–JI hydrogen engine described above, having 140 kW maximum power and 245 N m maximum torque. Vehicle, tyres, driveline and gearbox data are kept constant, with the only exception of the final drive ratio reduced to 2.4. Fig. 4 presents the brake specific fuel consumption map (g/kWh) used in vehicle simulations.

The brake efficiency map of the $\lambda = 2.25$ 2 litres Turbo-charged H_2 DIJI compares favorably with the brake efficiency map of the $\lambda = 1.55$ 2 litres Turbocharged Diesel DI engine. This latter engine is already much better for vehicle fuel economy than the $\lambda = 1$ 4 litres naturally aspirated and throttle controlled gasoline engine, that however is still representative of power trains covering large market shares. The displacement effect shifts up by a factor of 2 the operating BMEP. The naturally aspirated gasoline engine works the most of the time at 1.5 bar BMEP and 1500 rpm, while the turbo-charged engine works the most of the time at 3 bar BMEP and 1500 rpm. The gasoline engine uses 936 g of a fuel having LHV = 43.2 MJ/kg to cover over the 1180 s total cycle time the 11.028 km distance travelled of the NEDC, for a fuel consumption of 8.487 kg or 366.7 MJ of fuel energy per 100 km. Even if the transmission is not optimized for the new engine, this latter engine only uses 213 g of a fuel having LHV = 119.95 MJ/kg, for a fuel consumption of 1.931 kg or 231.7 MJ of fuel energy per 100 km.

In terms of fuel energy, the DI–JI hydrogen engine therefore uses almost 40% less fuel energy than one large naturally aspirated low tech gasoline engine. This is due to the higher BMEP permitted by downsizing (2 times larger operating BMEP following the displacement ratio), the larger top and part load brake efficiencies permitted by the DI–JI concept, the higher compression ratio, the high boost from turbo charging partially recovering the exhaust waste heat, the spark advances closer to maximum brake torque because of the better resistance to knock of hydrogen than gasoline, the removal of the throttle.

Fig. 3 – a. Computed full load brake efficiency and torque for the HSDI Diesel and the DI-JI hydrogen engines. b. Computed brake mean effective pressure and efficiency for the DI-JI hydrogen engines changing the load.

Fig. 4 – Brake specific fuel consumption map (g/kWh) used in vehicle simulations.

5. Conclusions

Jet ignition pre-chambers are enablers of very fast ignition and combustion of main chamber mixtures. Their evolution is central to the development of the always lean burn direct injection jet ignition engine aimed at increased top brake efficiencies and reduced penalties changing the load. A first detailed description of the operation of a spark-less jet ignition pre-chamber has been provided in the paper.

The complex operation of the pre-chamber and the cylinder, including mixture formation, auto ignition, pre-chamber combustion evolution, jet ignition of the main chamber mixture and main chamber combustion evolution has been described using detailed chemistry libraries coupled to turbulent flow computations. Use of the STAR-CCM CFD code coupled with the DARS chemical package has proved to be fast and reliable permitting user to focus on the application rather than in the details of chemistry or turbulence. The combustion evolution within the main chamber is then much faster than with spark plug ignition, with combustion angles 10%–90% of about 10° running 7500 rpm with air-to-fuel equivalence ratios of 2.25.

CFD simulations integrated with CAE engine performance simulations have provided guidelines for selection of pre-chamber and main chamber fuel injectors and glow plug. Assembly of a prototype always lean burn direct injection jet ignition engine running hydrogen fuel appears to be possible by using off-the-shelf components for glow plug and direct

injectors, even if some changes are needed especially in the tip area of the injectors to better exploit the advantages of the concept.

CAE engine performance simulations properly set up with the help of CFD have provided engine maps over the full range of speed and load for a 2 liters HSDI Diesel engine modified to fit the DI–JI fuel injection and ignition system and run hydrogen fuel. These maps show the DI–JI always lean burn hydrogen engine has better than Diesel full load efficiency and torque, and a reduced efficiency penalty reducing the load.

The DI–JI hydrogen engine has top brake efficiencies of 43% running $\lambda = 2.25$, while the Diesel engine has a top brake efficiency of 38% running $\lambda = 1.55$. The DI–JI hydrogen engine also has better torque outputs, respectively 243 N m vs. the 222 N m of the Diesel engine, and about same power output, respectively 77.5 and 78.9 kW. The DI–JI hydrogen engine also exhibits a small penalty in efficiency reducing the load from full to a few bars of BMEP, with brake efficiencies still approaching 35% at 2 bar BMEP.

A passenger car fitted with the DI–JI hydrogen engine could therefore be fun to drive delivering good performances being at the same time fuel efficient. A large sedan with the 2 liters DI–JI hydrogen engine replacing a large naturally aspirated throttle-controlled stoichiometric gasoline engine could have a 40% improvement in fuel efficiency over the NEDC (MJ of fuel energy to complete the test).

The ability for H2ICEs to operate with near-zero engine-out emissions is primarily owed to the coupled effect of two characteristics unique to hydrogen [3]. First, nitrogen oxides are the only undesirable engine out emissions, formed by the thermal dissociation and oxidation of N_2 in air during combustion. Second, the low flammability limit of hydrogen allows stable combustion at highly dilute conditions. The DI–JI concept further enhances the always lean burn operation for stable and complete combustions even at very low fuel-to-air ratios. During the ultra-lean operation, combustion temperatures are low enough such that NO_x formation rates are too slow and engine-out emissions are near zero, but the combustion process always completes.

The proposed combustion concept is fuel-neutral and may be (and has been) applied to other gaseous fuels like propane and methane. This novel technology, does not have in general major drawbacks, if not the necessity to develop up to industrial standards jet ignition devices built so far as prototypes. For the particular application to hydrogen, compliance with specific fuel properties of main chamber and pre-chamber injectors also require further development of injectors for faster actuation and higher flow rates and injection pressures.

Even if the Hydrogen Assisted Jet Ignition (HAJI) concept from which the DI–JI concept originates has been previously validated with some experiments, validation with experiments of the DI–JI concept is desirable.

This work still in progress is aimed at reducing and capturing emissions in transport and energy generation. Benefits of the technology includes reduced greenhouse and other emissions and reduced consumption as well as encourage the increased uptake of alternative fuels, thus potentially enhancing national energy security and reducing greenhouse gas emissions.

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