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Editorial

The role of hydrogen for future internal combustion engines

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Introduction

In order to successfully cope with the trend of mitigating climate change as outlined in the recommendations of Paris (COP21) and Glasgow (COP26) Climate Agreements, propulsion technologies must be able to achieve the highest CO_2 reduction, within very short time scales. To achieve this challenging goal, electric powertrains powered by batteries charged using renewable energy represents not only a public mandate but also the focus of research efforts of the relevant academic and industrial communities. However, this technology cannot answer all the various needs concerning personal mobility, sustainability and feasibility. Hence, in parallel an important role will be played by internal combustion engines (ICE) fed with non-fossil hydrocarbons and hydrogen (H_2).[1] Today, internal combustion engines using fossil fuels generate about 25% of the world's power and they are responsible for about 17% of the world's greenhouse gas (GHG) emissions,[2] while producing other main pollutant emissions such as carbon monoxide (CO), carbon dioxide (CO_2), nitrogen oxides (NO_x) and particulate matter (PM) with strong negative impact on air quality in urban spaces.

In the current energy landscape, hydrogen[3–9] is perceived as a flexible energy carrier with potential applications across all energy sectors. Hydrogen represents a promising energy carrier to store renewable electric energy when available in excess during peak production, due to the typical intermittent character of renewable wind and photovoltaic energy plants. Hydrogen may be used to feed fuel cells (FCs). The current state, hydrogen FC technology is expensive and requires pure hydrogen and a high specification compressor to supply the compressed air. In addition, large batteries would be needed to store the electricity required to cope with the transient nature of power demands for vehicle applications. As a result, the overall current FC-based powertrain efficiency is much lower than that of the FC alone.[10] A recent study showed how the overall efficiency of a FC powertrain system is very similar to that of ICE system for commercial vehicles.[11,12]

Furthermore, a PEMFC-based powertrain system rejects nearly all of its heat loss via the coolant, which also needs to be kept at a significantly lower temperature than the coolant of an ICE, and hence mandates significantly larger radiators and cooling systems. This is particularly critical for heavy-duty vehicles operating at low speeds, which is relevant considering that this is the most promising short-term application for FC powertrain systems.

A detailed analysis of benefits and costs could highlight the impact of different hydrogen mobility technologies with respect to alternative solutions in terms of societal and private costs and gains, taking into account a variety of socioeconomic and infrastructural contexts.[13] In the transport sector, which has very few near-zero emission energy carriers (i.e. electricity and advanced biofuels), hydrogen has the potential to address some of the key emission reduction challenges when combined with ICE technologies. In particular, the H_2 fuelled ICE (H2ICE) is the only alternative keeping the ICE powerplant that does not produce any tank-to-wheel CO_2 emissions at the tailpipe (as well as IC engines fed with ammonia,[14] however more suitable for ship applications). Contrarily to FC powertrain systems, H2 ICEs can be fuelled with non-purified hydrogen, resulting in significantly lower production cost of hydrogen fuel. H2ICEs can take advantage of the existing advanced combustion and engine control technologies, such as direct injection, Miller cycle, lean/diluted combustion, pre-chamber ignition, etc. Thus, the thermodynamic efficiency of direct injection H2ICEs can be similar to the overall efficiency to the FC powertrain.

In terms of pollutant emissions, a certain amount of NOx is generated during combustion, with traces of particulates due to the combustion of very small portions of lubricating oil, but all these can be reduced to zero-impact by means of a lean mixture and a suitable after-treatment system, together with the choice of a specific lubricating oil.[15] In particular, advanced hydrogen SCR catalysts[16] and particulate filters can remove these pollutant emissions. The availability of hydrogen on-board as a reducing agent can represent an innovative and convenient approach for NOx reduction, eliminating the need of urea/NH_3 storage in tanks and the possible ammonia slip at the tailpipe.

The H2ICE is attractive because it takes advantage of the current advanced state of ICE technologies, such as reliability, durability, existing supply chain, existing manufacturing plus recycling infrastructure and affordability, which makes it a near-term, widespread solution to accelerate the large-scale introduction of H_2 into transportation market, for both transitional and long-term usage. In fact, the existing worldwide know-how on ICEs and the widespread large-scale manufacturing and supply-chains can continue to be utilised, without any critical interruption. The H2ICE could provide a reliable, durable and cost-efficient solution based on a well-known existing technology, contributing to a fast transition towards carbon-free mobility. Moreover, it is characterised by low total cost of ownership total cost of ownership (TCO), especially in the field of heavy-duty on-road and off-road applications. It can be argued that H2ICE technology can be less expensive than the current state of technology for EV powertrains, due to its minor dependence on low available and expensive materials as rare earth metals. Last but not least, considering that H2ICEs are manufactured in the same production facilities and following the same manufacturing processes as the conventional fossil-fuel ICEs, they contribute to secure jobs by providing sustainable industrial and employment opportunities in the automotive industry.

Hydrogen can be produced from diverse resources. It is abundant in our environment, stored in water (H_2O), hydrocarbons (such as methane, CH_4), and other organic matter. One challenge of using hydrogen as a fuel is the efficiency of extracting it from these compounds. More specifically, hydrogen can be produced by several methods: the most widely used is steam methane reforming, for which the relevant efficiency of hydrogen production is very high (65%–75%) and the production cost is relatively low. Nevertheless, it results in high levels of CO_2 emission. Another widely used method of hydrogen production is coal gasification. In this case, however, the efficiency of hydrogen production is low (45%) while the CO_2 emissions are still high, if the CO_2 is not sequestered at the production site.

Electrolysis of water is another method of producing hydrogen, but it requires the use of large amounts of electricity and therefore this becomes expensive. In this case, the level of CO_2 emissions depends on the electricity source. Less common methods can also be used to produce hydrogen, such as biomass gasification, biomass-derived liquid reforming, or microbial biomass conversion.[17] However, only the solar–hydrogen and wind-hydrogen system allows emission-free—but expensive—hydrogen production. The universal applicability of hydrogen for modern energy needs has boosted significant investment and development of renewable hydrogen production in many countries.

Developments in storage

Several breakthrough developments of hydrogen technologies have included production and use, as well as advanced materials and methods for hydrogen storage.[18,19] In the meantime, global, cross-sectoral, hydrogen demand is increasing, with a current worldwide consumption of approximately 70 million metric tons per year. To meet the demand, a range of hydrogen production technologies are being developed

As hydrogen has a very low density ($0.089\,kg/m^3$) at atmospheric pressure, the physical storage requires ultra-high pressure in gas bottles or extremely low temperatures in liquid. The current applications require that hydrogen is pressurised between 35 and 70 MPa, and between 11% and 13% of the hydrogen energy content is expended to reach these pressure levels.[3] The liquification of hydrogen would consume about 30% of its total energy content. In addition, the hydrogen storage capacity with the physical storage methods is only 4.5 wt%. Solid-state materials can reversibly absorb and release hydrogen, and the reported highest storage capacity is 7.6 wt%, but at an operating temperature of 600 K. Therefore, the extreme complexity and substantial cost of hydrogen storage systems and relatively low gravimetric storage capacity have prevented the wider use of hydrogen for the long-distance road and marine applications, as well as the aviation sector, which have extremely high requirement on the gravimetric energy density of fuels to be used.

Besides the direct use of hydrogen, another alternative is to run through subsequent reaction processes in order to produce low carbon synthetic liquid fuels from hydrogen, with a large variation of fuel specifications possible from different process routes. These hydrogen-based low carbon liquid fuels generated through renewable sources have been increasingly applied to speed up the CO_2 reduction in existing combustion engines for long-distance vehicles and vessels. For example, both methanol and ethanol can be produced from renewable sources and used in ICE with zero life-cycle carbon emissions. Other potential hydrogen-based alternative fuels are polyoxymethylene dimethyl ether, short: OME (POMDME) and paraffinic diesel fuel (PDF) – either purely synthetic from Fischer-Tropsch processes or derived from biogenic sources through hydrogenation like HVO (hydrogenated vegetable oil). Due to its paraffinic nature, PDF is free of aromatics, resulting in a significantly reduced tendency to form soot compared to conventional diesel fuel. OME fuels are usually produced from a reaction of methanol and formaldehyde through a trioxane route.[20]

Storing hydrogen in hydrogen-dense liquid fuels also has the added benefit of being compatible and synergic with grid storage and the transportation of renewable energy around the world, for example, production of methanol from solar powerplants in one part of the world and transporting it to another part of the world, to meet renewable energy needs and mandates. Therefore, new methods of storing and using hydrogen in liquid fuels would provide the following two benefits towards low and zero-carbon transport: (1) immediate and wider use of hydrogen in existing engines and (2) improved engine performance and lower emissions of engines fed with a blend of synthetic fuel achieved by better atomisation and faster combustion. An emerging approach for storage of H_2 is through the use of gaseous bubbles in liquids. This approach has been studied for applications in aquaculture, water treatment and biomedical engineering. Bubbles have shown to remain stable in liquid for months[21] and have extremely high internal gas density (30–340 kg/m^3).[22] It has been reported that the concentration of hydrogen bubbles in liquid can achieve up to ~2e13 bubbles/m^3.[23] Their high stability, internal density and concentration make it possible to store considerable amounts of hydrogen in liquid fuels. The increase in the volume ratio of dissolved hydrogen bubbles can further increase the hydrogen storage capacity in liquid fuels. Because of the 4x higher calorific value of hydrogen (120 MJ/kg) compared to that of methanol (15.9 MJ/kg) and gasoline (46 MJ/kg) for example, hydrogen fuel blend will have a higher energy density compared to the base liquid fuel, which makes it appealing for improving the engine performance, and reducing CO_2 pollutant emissions.

Developments in injection strategies

Most H2ICE prototypes use a Port Fuel Injection (PFI) system, benefiting from a straightforward conversion from existing gasoline engines.[24,25] However, the drawbacks of hydrogen PFI are also well known, including pre-ignition, knocking, backfiring, low volumetric efficiency and compression loss problems. This limits the engine's achievable load and efficiency, so engine brake thermal efficiencies up to 37% at medium loads were reported.[26] The negative impact on volumetric efficiency results in a decrease of the engine power density, which can be mitigated by the use of a turbocharging system, or by port injection of cryogenic hydrogen at very low temperatures (around 90 K),[27,28] with some drawbacks due to possible ice formation in the intake pipe and the requirement of liquid hydrogen stored on board.

Controlling backfire and surface ignition restricts the injection timing as it should be set carefully, allowing a suitable air-cooling period during the early stages of the intake stroke and assuring that all the hydrogen is inducted into the cylinder before the end of injection, with no hydrogen in the intake manifold after the intake valve closing. The valve timing is also restricted, as negative valve overlaps are usually required to avoid hot exhaust gases flowing towards the intake manifold.

The previous drawbacks are mitigated by switching to a Direct Injection (DI) system. To avoid abnormal combustion, injection, ignition, and mixture formation are key factors. DI and dedicated injection strategies that avoid hydrogen backflow towards the intake manifold, are efficient levers to avoid backfire. The potential of a DI system has already been demonstrated by BMW in 2009.[28] A hydrogen DI system with up to 300 bar injection pressure has been integrated and developed into an SI engine, achieving a maximum efficiency of 42%. Recent work funded by the U.S. Department of Energy in hydrogen DI[29–35] obtained thermal efficiency up to 45% at 2000 rpm and a high load condition of 13.5 bar brake mean effective pressure. Because of this, it seems highly probable that the future of SI engines will rely on direct injection, so mid to high pressure DI is very probably the key to successfully implement hydrogen combustion.

In Compression Ignition (CI) hydrogen engines operating with mixing-controlled combustion systems the high-pressure injection system is obviously mandatory, with minimum pressure levels almost doubled compared to the maximum levels required in SI engines, in the range of 600 bar. In fact, the lack of commercially available injection systems is one of the key factors limiting the expansion of hydrogen CI engines. Big players are currently developing hydrogen DI systems for large HD CI engines with application to the maritime transport sector. The development and industrialisation of these systems is critical for enabling the integration of hydrogen as single fuel in CI engines.

Developments in combustion

Focusing on the combustion of hydrogen-air mixtures in IC engines, it is important to highlight that H_2, in contrast to commonly used hydrocarbon fuels, exhibits peculiar combustion properties due to its higher reactivity and diffusivity, such as large flame speeds and wide flammability limits, tendency of transition from deflagration to detonation, short quench distances and instabilities. Therefore, rather than making small adjustments to existing designs, internal combustion engines for H_2 should be redesigned for this specific application.

Hydrogen has several physical, chemical, and thermal properties making it superior to conventional fuels, but at the same time also challenging in practical applications. Since hydrogen emits zero carbonaceous emissions, it is the ideal environmentally friendly ICE fuel for the future. Moreover, the high flammability range of H_2 allows ultra-lean operation, enabling low engine-out NOx emissions. Therefore, its usage reduces harmful emissions into the environment. Also, because of higher flame speed,[36] higher auto-ignition temperature and octane number (Table 1), the risk of knock is

Table 1. Main properties of gaseous hydrogen and gasoline.[37,38]

	Hydrogen	Gasoline
Formula	H_2	$C_nH_{1.87n}$
Density (kg/m^3)	0.09 @ 0°C, 1 bar	720–780
Energy content (MJ/kg)	120.0	44.0
Energy content (MJ/l)	8	32.0
Octane number (RON)	$\geqslant 120$	92–98
Latent heat of vaporisation (kJ/kg)	461	305
Boiling point (°C)	-252.9@ 1 bar	27–225
Flame speed (m/s)	1.85	0.37–0.43
Lean equivalence ratio	0.1	0.6
Ad. flame temp. at 1 atm (K)	2380	2300
Ad. flame temp. at 100 atm (K)	2490	2405
Auto-ignition temp. (K)	858	550
Stoichiometric A/F ratio (by mass)	34.3	14.8
Quenching distance at stoich. (mm)	0.64	2.84
Min. ignition energy (J)	2×10^{-5}	5.5×10^{-4}

reduced and the engine compression ratio can be consequently increased, allowing a better thermal efficiency.

Some properties of gaseous hydrogen and gasoline are given in Table 1 for comparison. It is evident that hydrogen has extremely wide flammability limits, with a lean limit equivalence ratio around 0.1 and a typical high laminar flame speed around four times that of gasoline.

Overall, several challenges need to be overcome, which are linked to the properties of hydrogen as a fuel.[39] The first one is the prevention of abnormal combustion. The large flammability range and the low ignition energy of hydrogen can cause pre-ignition due to hot spots in the chamber, as well as backfiring in the intake in case of indirect injection engines. Abnormal combustion strongly affects efficiency and engine durability. The second challenge is the efficiency. Some hydrogen properties like high laminar flame speed are favourable. Others are disadvantageous, like low quenching distance, contributing to increased wall thermal losses. The capacity to reach high thermal efficiency also means optimum combustion phasing and high theoretical efficiency. Both depends on the behaviour of hydrogen regarding occurrence of abnormal combustion and on the maximum in-cylinder capacity. Moreover, high combustion speed tends to increase the rate of heat release and so the maximum temperature in the chamber, with a negative effect on NOx production.

In addition, as seen in Table 1, hydrogen has a much lower energy per unit volume relative to gasoline. Hence, the low volumetric energy density of hydrogen requires injection of a large volume of hydrogen in a short time to reach high load. This results in a clear limitation for power density of the engine. In general, the power developed by an engine running solely on a hydrogen-air mixture is expected to be lower than an equivalently sized gasoline-fuelled engine. Therefore, slight changes in design, such as higher compression ratio, are requested.[39,40] However, to prevent the engine from knocking, the engine compression ratio should be optimised, proper mixture formation should be achieved, and hydrogen-rich mixtures should not be used,[41–43] especially at high engine speeds.

As already mentioned, one major problem with hydrogen engines is the occurrence of backfire in richer fuel-air mixtures. This severely limits the performance of a hydrogen engine. Because of the relatively smaller flame quenching distance, hydrogen flames can propagate through much smaller gaps than flames of other fuels. This increases the chances of engine backfire because flames can propagate into the intake manifold via very small gaps between the intake valve and the valve seat, leading to an explosion of the mixture present in the intake manifold. One primary source of backfire in conventional hydrogen-fuelled engines is the spark plug's hot electrode surface, acting as an ignition source for the hydrogen-air mixtures. In addition, the effect of piston liner crevices, where hydrogen can be stacked, is an issue especially for PFI engines.

To overcome the challenges related to hydrogen combustion in ICEs, several technological solutions can be considered to benefit from the positive impacts of hydrogen on engine performances, and to minimise the negative ones, as illustrated by Figure 1.

First of all, to avoid abnormal combustion, injection, ignition and mixture formation are key factors. Direct injection and dedicated injection strategies which eliminate back-flow are efficient levers to avoid back firing. Another way to control the abnormal combustion is the increase of air dilution. With the large flammability range of hydrogen, it is possible to run the engine at very low Fuel-Air Equivalence Ratio. This lean hydrogen combustion has the further advantage of drastically decreasing NOx emissions. Dilution with water injection or Exhaust Gas Recirculation (EGR) is an additional lever to limit the occurrence of abnormal combustion, and to further reduce NOx emissions. On top of that, lean burn will reduce thermal losses. Due to hydrogen's properties compared to those of gasoline, especially its high flame speed, low quenching distance, low density leading to low injected pulse momentum, the required levels of flow turbulence could be lowered to reduce thermal losses, but might impact the quality of the fuel air mixture. If abnormal combustion could be avoided, the compression ratio and so efficiency, would be further increased. The spark plug can play a role in the appearance of abnormal combustion, by being one of the hot spots in the cylinder. Finally, an optimised lean burn turbocharger is required, and its up-sizing can help to reach the targeted performances.

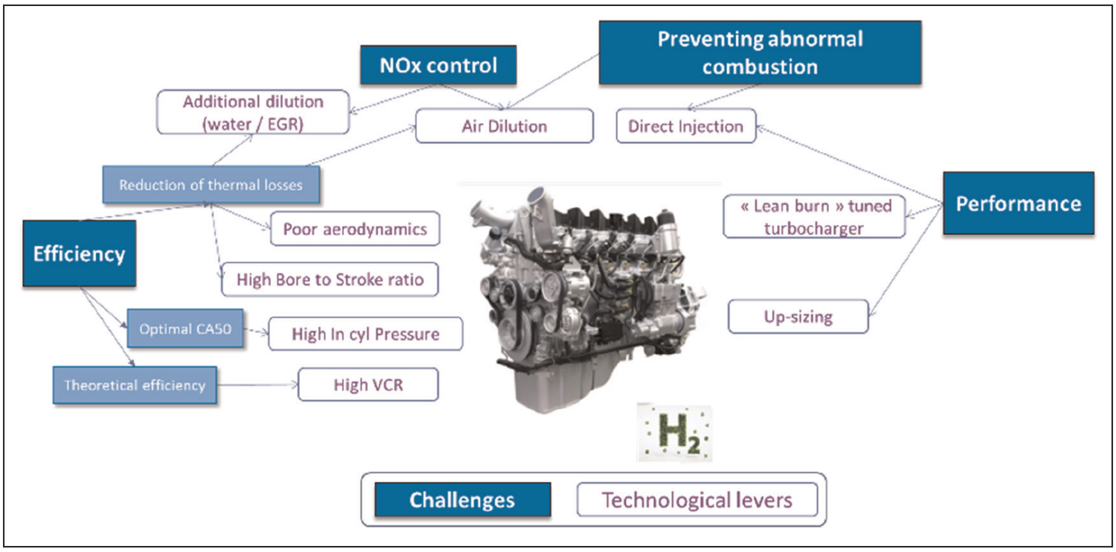

Figure 1. Technological assembly with respect to key challenges. Reproduction from Duffour et al.[45]

Today several research activities have started and currently grow worldwide, to demonstrate the applicability of hydrogen as a fuel of ICEs, with clear advantages and high potential.

A single-cylinder engine with a displacement of 0.5 L, high compression ratio of 14, high and low tumble air motion, central cold spark plug, direct injector[44] has been set-up as a technological demonstrator and described in Duffour et al.,[45] with the aim of investigating the impact of these technological levers previously described. Experimental and numerical results highlighted the potential of H2ICEs, with the possibility to reach zero NOx emissions at part load with a high indicated efficiency above 47%. Challenges of H2ICEs have been pointed out, in particular the pre-ignition control and the NOx emissions.

As an example, the engine tests have confirmed the occurrence of pre-ignition. Figure 2 shows an operating point at 2000 rpm mid load, at a fuel equivalence ratio of 0.5. Pre-ignition starts to appear at about 150 Crank Angle Degree (CAD) BTDC. To understand the cause of this pre-ignition event, 3D CFD simulations were carried out and compared to another setting of operating conditions without pre-ignition, also shown in Figure 2. The results of the 3D CFD calculations show that local rich mixture zones are witnessed near the spark plug and near the exhaust valves in the case of significant pre-ignition, while a better fuel homogeneity is observed in the case without pre-ignition. This result confirmed that the presence of local rich mixture near hot spots is a very probable cause of pre-ignition.

However, some solutions exist to avoid abnormal combustion, in particular pre-ignition: a suitable optimisation of the mixture preparation itself can be achieved acting on injection parameters (SOI, injection pressure) and internal aerodynamics. In addition, a careful reduction of hot spots in the combustion chamber can be obtained resorting to a cold sparkplug or introducing piston cooling improvement and a dedicated lubricant.

Because of their stronger aerodynamics and higher turbulence kinetic energy, gasoline engine baselines are well suited to reach high efficiency hydrogen combustion. Nevertheless, a diesel engine baseline could also be adapted for optimum hydrogen combustion system. For both architectures, air fuel mixture quality is a key focus area, not only for controlling the abnormal combustions but also to reduce the NOx emissions. The mixing process highlights a trade-off between multiple phenomena: residence time, turbulence, interaction between the hydrogen jet and the in-cylinder aerodynamic field, injector design and positioning, injection timing.

In this context, 3D CFD is a relevant tool for developing new hydrogen combustion systems or to adapt existing ones. Rapidly increasing computational resources further support this approach. This is reflected in internal combustion engines, for example, by the transition from URANS to LES.[46] These simulations rely on well-established numerical methodologies and physical modelling approaches that were previously developed for hydrocarbon combustion.[47] In particular, in the case of pure hydrogen as fuel, although the kinetics of H_2 combustion is mostly well understood, some special challenges exist. In fact, this diatomic, very light and fast diffusing gas features very specific molecular transport properties, leading to large flame velocities, wide ignition limits, and in conclusion to massive differences in combustion properties and related safety issues (explosions, detonations) compared to hydrocarbons. Hence, the high diffusion rates of hydrogen coupled with the ambient flow dynamics change the internal structure of the reaction zone (microstructure) and thus the local reaction rate. The resulting heat release couples with the flow field and influences the macroscopic flame and flow structures.

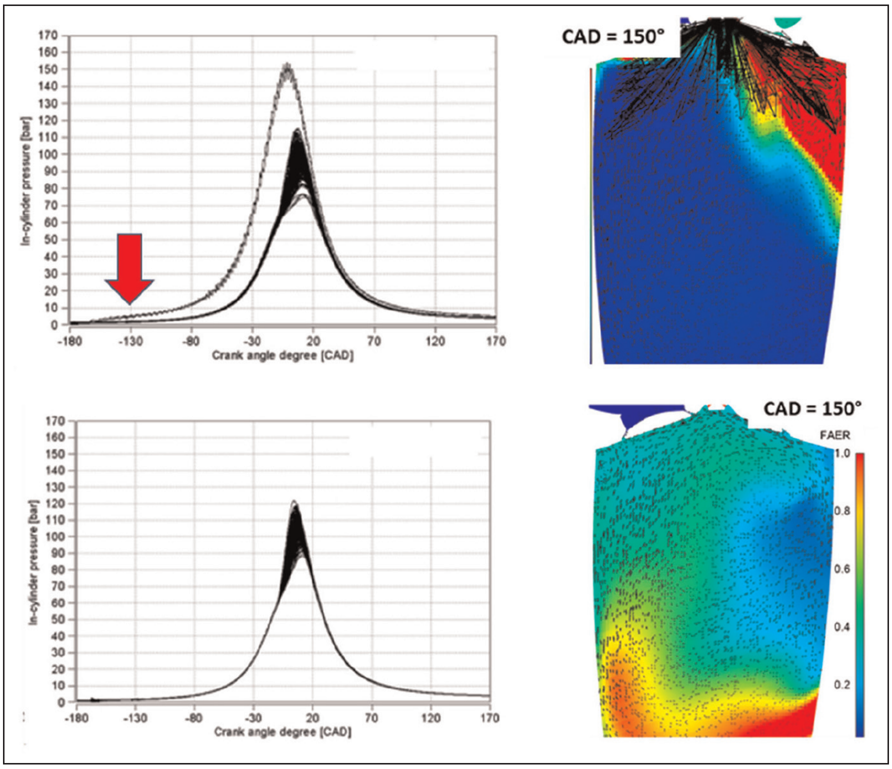

Figure 2. Impact of fuel distribution on occurrence of pre-ignition, 2000 rpm, mid load, lambda = 2. Reproduction from Duffour et al.[45]

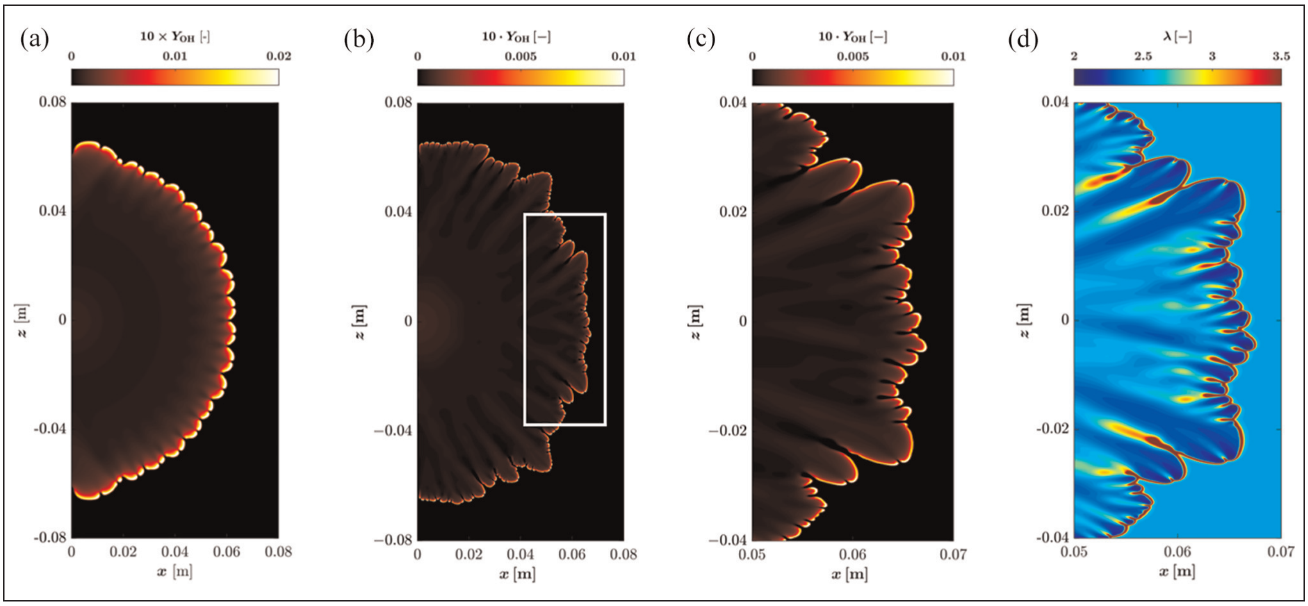

Figure 3. Thermo-diffusive instability in laminar spherically outwards propagating lean H_2/air flame illustrated by a simulation fully resolving transport and chemistry. From left to right. Left: (a) reaction zone visualisation by the hydroxyl radical highlighting cell formation at 1 atm, (b) reaction zone visualisation by the hydroxyl radical highlighting cell formation at 5 atm, (c) zoom of the local reaction zone at 5 atm and (d) zoom of the local air-to-fuel ratio at 5 atm. Figures adapted from Wen et al.[48,49]

One particularly prominent example for H_2 combustion is the so-called thermo-diffusive instability. This is demonstrated in Figure 3 for a simulation of a lean premixed H_2/air flame. Early on, cell formation occurs along the reaction zone, made visible by the hydroxyl radical (OH), which becomes increasingly strong as the flame spreads outward, resulting in a highly wrinkled flame structure. Figure 3(a) (1 atm) and (b) (5 atm) clearly show a strong pressure influence. A more detailed analysis of the local structure, see zoom in

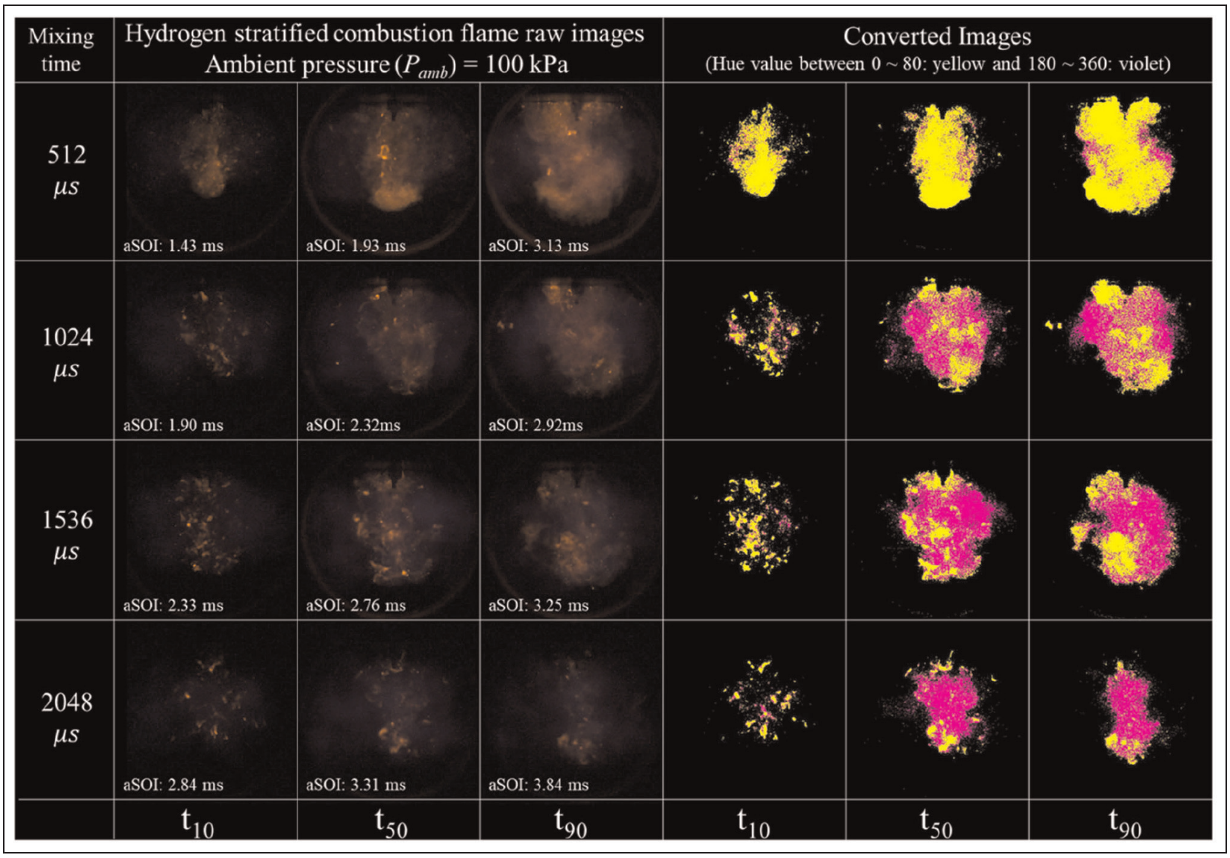

Figure 4. Direct flame images and Hue-based flame division converted images at different mixture formation times. Figure adapted from Lee et al.[51]

Figures 3(c) and (d), show that in areas of very high negative curvature, that is, towards the burned gases, there is a depletion of hydrogen and corresponding increase in the air-to-fuel ratio. The flame propagates more slowly, locally even extinction, that is, negligible heat release, is observed. In the areas of positive curvature there is an enrichment of hydrogen (reduced air-to-fuel ratio), so that the flame propagates faster. This thermo-diffusive instability is based on the higher diffusion coefficient of light hydrogen compared to heat (more than a factor of three). Further, this phenomenon becomes even more relevant with increasing pressure, as shown above.

All of these phenomena must be considered in simulations and looking in particular at turbulent combustion, comprehensive models for engine conditions do not yet exist. They cannot be devised simply as an extension of the well-established and validated numerical methods that have been developed for hydrocarbon combustion in recent decades.

A very promising combustion mode is based on high-pressure direct injection (DI) of hydrogen with stratified charge. In fact, stratified charge combustion can be used to highly extend the lean limit, without particulate emission generated by the ignition from a highly rich-fuel mixture, which is the typical hurdle for the stratified charge in classical GDI engines. In general, hydrogen DI is fundamental to achieve a highly efficient engine operation. The investigation of a high-pressure hydrogen jet is required by means of both experimental optical diagnostics and numerical CFD modelling. Some preliminary research on the evolution of a hollow-cone-shaped hydrogen jet is described in Lee et al.[50,51] and Roy et al.[52] The formation of hydrogen mixture fraction by laser-induced breakdown spectroscopy is described in Roy et al.[52] It was observed that hydrogen rich-combustion emits a visible range of wavelengths, as shown in Lee et al.,[51]Shudo and Oba[53] and Schefer et al.[54] and presented in Figure 4.

The combustion behaviour is strongly dependent on the mixture formation time and heat loss is the dominant factor for the indicated thermal efficiency, as shown in Lee et al.[55] In this work, although a highly diluted in-cylinder mixture was formed (lambda ~2.5), NOx was generated by the combustion of a locally rich-fuel mixture. Therefore, lean boosting or EGR should be equipped to approach the zero-emission vehicles.

Another useful technology for advanced hydrogen spark ignition engines is represented by laser ignition. It employs a pulsating laser beam passing through an appropriate optical arrangement, to focus it tightly on a small spot and generate high energy intensity, where plasma formation occurs. Adequate energy density leads to the formation of plasma-based ignition, followed by shock waves, leading to flame kernel evolution and propagation in the combustible mixture.[24]

Of all these processes, the ignition delay and the flame kernel development affect the combustion duration significantly. The ignition begins leading to plasma formation. The high temperature and high pressure generated by plasma formation develops a shock wave that guides the flame kernel evolution.

Laser ignition is an electrode-less ignition; therefore, chances of surface ignition, pre-ignition and backfire decrease significantly in the case of the hydrogen-fuelled engine. Plasma position and location inside the combustion chamber can also be adjusted using the laser ignition technique, which can shorten the combustion duration.[56]

There is also a possibility of stretching the ignition limit to burn relatively leaner fuel-air mixtures, which a conventional spark plug ignition system cannot ignite.[57] Igniting leaner mixture leads to lower in-cylinder temperatures, resulting in lower NOx formation. A laser ignition system can achieve precise ignition timings, and shows excellent potential of laser ignition in hydrogen fueled engines.

Developments in turbocharging

For H2 IC engines the power output compared to a conventional gasoline engine is significantly lower, especially for port fuel injection (PFI) type hydrogen engines. This is mainly due to the low density of hydrogen (15% lower than gasoline at stoichiometric conditions) which reduces volumetric efficiency.[58] In addition, H2ICEs operating at lean to very lean levels bring operating and performance challenges, requiring either increased displacement or increased levels of forced induction, since more air mass flow is required to compensate for the power deficit and for lean combustion. One of the effective ways to supply such a high air mass flow is to introduce a turbocharging system in order to achieve comparable power to current state-of-the-art gasoline engines. A turbocharging system can improve the power output by pushing more air into the combustion chamber; however, incorrect matching results in lower levels of power output compared to what can be achieved from a careful H2ICE-turbocharger system match.[59]

Compared to stoichiometric gasoline ICEs, the air consumption level of a lean H_2 engine is expected to be about 50% higher. To supply such a high mass flow, it is expected that high boost pressure is necessary in the H2ICE application. In the case of PFI H2ICE, it has been shown that in addition to 50% higher mass flow, a 90% higher boost pressure compared to the turbocharged gasoline engine is required. This in turn means that a single-stage charging system is not able to supply the required boost and mass flow over the wide range of operation required. Instead, a two-stage boosting system with Variable Geometry Turbocharger[60] is mandatory. The boost and mass flow demand are mainly influenced by the operational lambda (λ) and target performance which should be considered carefully when designing the boosting system for the PFI SI type H2ICE. Curiously, even though the hydrogen engine exhibits low exhaust enthalpy with lower exhaust temperature, nevertheless, the total mass flow is increased by lean mixture operation. Hence, the amount of the available energy at the turbine would be similar or higher under the same power output.

Moreover, it has been observed that by boosting the engine with a supercharger, a lower pumping loss and higher indicated mean effective pressure can be obtained, when compared to turbocharger boosted engines under low-load conditions.[60,61] However, a single stage is unlikely to produce the required boost pressure, twin-charger combinations are suggested in order to achieve beyond Euro VI type certifications (and its equivalents around the world).

Of course, challenges for turbocharging can be improved by combining hydrogen-diesel in conventional (commercial) engines with hydrogen being port-fuel injected at the expense of a more conventional and, therefore, larger carbon footprint compared to pure H2ICEs. Even for such configurations, a Variable Geometry Turbocharger for the provision of higher boost pressure during the engine run has been deemed necessary according to Taghavifar.[62]

The two other main requirements from an H2ICE system are NOx reduction (since other emissions are largely suppressed or non-existent in an H2ICE) and combustion stability. For NOx, the previously mentioned study by Nguyen et al. (2020) showed that at an optimisation point of air excess ratio between 1.4 and 1.8, NOx emissions were lower than that of an equivalent turbocharged engine.[61] With respect to combustion stability, there is a clear correlation between boost pressure increase (up to 40 kPa in this case) and a Coefficient of Variation of IMEP (COV_{IMEP}) reduction of more than 15%. This shows that the relatively more stable in-cylinder combustion conditions support the increase in engine power.[63] The same authors indicated that an increase in NOx emissions with increasing boost pressure is detrimental to the environmental-economic indicators of the H2ICE. Therefore, it is necessary to carry out a careful selection of engine tuning parameters (combustion duration, start of injection, valve timing, possible inclusion of water injection etc), to achieve the targeted engine performance and NOx mitigation, depending on individual engine classification and type. Finally, a dedicated after-treatment system is the key technology to reach the requested zero-impact NOx emissions.

Engine-out emissions and after-treatment systems

One critical issue with H_2 combustion in IC engines is certainly the generation of NOx pollutant emissions due to stoichiometric/lean combustion. NOx must be removed from the exhaust gas by an efficient catalytic conversion process in a dedicated after-treatment system, to guarantee zero-impact emissions.

One possibility could be to exploit an SCR after-treatment system based on the injection of urea ($CO(NH_2)_2$) to produce ammonia (NH_3). The drawback would be the production of CO_2 emissions as a side product of the urea conversion reaction, which is clearly unwanted, since the H_2 engine should not produce any CO_2, of course. As an alternative, it is possible to directly use H_2 as reducing agent to convert NOx to N_2 and H_2O. In this case, selective catalytic reduction can be achieved on active catalytic substrates loaded with Pt and supported by γ-Al_2O_3, SiO_2, TiO_2, which have been demonstrated to be suitable in the low temperature range, typical of hydrogen-fuelled engines running in lean/stoichiometric conditions.[64–67] Moreover, in the literature there are some examples of the combination of different catalysts, in particular Pt and Pd based catalysts supported on CeO_2 and MgO,[65] which provide a good solution for the whole 100–400°C temperature range.

The presence of high concentration of water vapour in the exhaust gas can result in a reduction of the catalytic activity, due to competitive adsorption of H_2, O_2, NO and H_2O on the active surface, which can also lead to an increase of N_2O production, which is obviously a drawback.

However, in some cases, the addition of water vapour can lead to a positive effect on the catalytic reactions in terms of NO conversion, for example with a Pt/Mg-Ce-O catalyst in the low 100-200°C range; the N_2 selectivity appears to be only affected at temperatures higher than 200°C.[64–66]

Generally, a higher hydrogen concentration in the exhaust gas results in an increase of both catalyst activity and N_2 selectivity. On the other hand, this high H_2 concentration could favour the NH_3 production mechanism, so that N_2 selectivity is reduced.[64] In other papers[66,67] it is remarked that also a dependency on temperature has to be considered, when looking at the concentration of H_2 in the feed gas. In fact, in the 170°C–220°C range, the high conversion of NO resulting from a higher H_2 concentration, is accompanied by a significant ammonia formation. In addition, a higher hydrogen concentration in the gas leads to high water production.

Oxygen concentration largely influences the reduction of NOx; in particular, if oxygen concentration is reduced, NO conversion increases. Moreover, the reduction of NO starts at lower temperature and the conversion remains high for a broader range, even at temperatures above 200°C. In contrast with this benefit, if less oxygen is present in the feed, the selectivity of N_2 reduces and a promotion of side reactions is observed.[66]

As suggested in Liu et al.,[67] new catalyst based on transition metals added to the noble ones to form alloys or other new structures should be investigated in order to reduce the cost and to improve the catalytic performances.

Final remarks

The transition towards a sustainable, secure and equally accessible energy system requires a radical transformation of the mobility system including road as well as industrial and off-road, naval and aeronautical transportation sectors.

Considering the trend of mitigating climate change worldwide, the contribution of a widespread, reliable and affordable propulsion technology like the IC engine can be significant, once a renewable fuel is used as replacement of typical fossil fuels. Hydrogen and hydrogen-dense liquid fuels can play a relevant role in this sense, allowing zero CO_2 emissions and zero-impact pollutant emissions from IC engine powertrains.

The main issues are related to the availability and production of H_2 and its safe storage at the point of use. These factors involve economic considerations that must be balanced against the costs to society, associated with the potential reduction of carbon emissions from existing hydrocarbon fuels.

As a matter of fact, hydrogen represents a promising energy carrier to store renewable electric energy when available in excess during peak production, due to the typical intermittent character of renewable wind and photovoltaic energy plants.

The H_2 fuelled IC engine is a viable alternative to rely on the thermal powertrain without producing any tank-to-wheel CO_2 emissions at the tailpipe. Moreover, H2ICEs can be fuelled with non-purified hydrogen, resulting in significantly lower production cost of hydrogen fuel. High boost pressures, direct injection, advanced combustion modes, deployment of laser ignition, and dedicated after-treatment SCR systems will guarantee a competitive, high efficiency propulsion technology. Considering the possible developments of the next generation of H2ICE, the resulting thermodynamic efficiency will be similar to that of a modern Fuel Cell powertrain.

Overall, the H_2 (and H_2-dense fuel) IC engines will provide a reliable, durable and cost-efficient solution based on a well-known existing technology, contributing to a fast transition towards carbon-free mobility. The low total cost of ownership, especially in the field of heavy-duty applications, as well as its negligible dependence on low available and expensive materials such as rare earth metals, make this solution appealing and convenient in some application fields.

References

1. Desantes JM, Molina S, Novella R, et al. Comparative global warming impact and NOx emissions of conventional and hydrogen automotive propulsion systems. *Energy Convers Manag* 2020; 221: 113137.
2. Reitz RD, Ogawa H, Payri R, et al. IJER editorial: the future of the internal combustion engine. *Int J Engine Res* 2020; 21(1): 3–10.
3. Kansu S, Kahraman N and Ceper B. Experimental study on a spark ignition engine fuelled by methane-hydrogen mixtures. *Int J Hydrogen Energy* 2007; 32(17): 4279–4284.

4. Sohret Y and Gurbuz HA. Comparison of gasoline, liquid petroleum gas, and hydrogen utilization in a spark ignition engine in terms of environmental and economic indicators. *J Energy Resour Technol* 2021; 143(5): 052301.
5. Huang Z, Liu B, Zeng K, et al. Experimental study on engine performance and emissions for an engine fueled with natural gas-hydrogen mixtures. *Energy Fuels* 2006; 20(5): 2131–2136.
6. Catapano F, Di Iorio S, Sementa P and Vaglieco BM. Analysis of energy efficiency of methane and hydrogen-methane blends in a PFI/DI SI research engine. *Energy* 2016; 117: 378–387.
7. Prasad RK and Agarwal AK. Development and comparative experimental investigations of laser plasma and spark plasma ignited hydrogen enriched compressed natural gas fueled engine. *Energy* 2021; 216: 119282.
8. Li G, Yu X, Jin Z, et al. Study on effects of split injection proportion on hydrogen mixture distribution, combustion and emissions of a gasoline/hydrogen SI engine with split hydrogen direct injection under lean burn condition. *Fuel* 2020; 270: 117488.
9. Sarikoc S. Effect of H2 addition to methanol-gasoline blend on an SI engine at various lambda values and engine loads: a case of performance, combustion, and emission characteristics. *Fuel* 2021; 297: 120732.
10. Desantes JM, Novella R, Pla B, et al. Impact of fuel cell range extender powertrain design on greenhouse gases and NOx emissions in automotive applications. *Appl Energy* 2021; 302: 117526.
11. Simon JM. *Heavy duty hydrogen ICE: Production realisation by 2025 and system operation efficiency assessment in Powertrain Systems for Net-Zero Transport*. London: CRC Press, 2021.
12. Klepatz K, Konradt S, Tempelhagen R and Rottengruber H. Systemvergleich CO2-freier Nutzfahrzeugantriebe [System comparison CO2-free commercial vehicle drives]. In: Berns K, Dressler K, Kalmar R, Stephan N, Teutsch R and Thul M. (eds) *Commercial vehicle technology 2020/2021*. Wiesbaden: Springer Vieweg. DOI: 10.1007/978-3-658-29717-6_13
13. Cantuarias-Villessuzanne C, Weinberger B, Roses L, et al. Social cost-benefit analysis of hydrogen mobility in Europe. *Int J Hydrogen Energy* 2016; 41(42): 19304–19311.
14. Frrankl S, Gleis S, Karmann S, et al. Investigation of ammonia and hydrogen as CO2-free fuels for heavy duty engines using a high pressure dual fuel combustion process. *Int J Engine Res* 2021; 22(10): 3196–3208.
15. Heid B, Martens C and Orthofer A. *How hydrogen combustion engines can contribute to zero emissions*. McKinsey report, 25 June 2021. McKinsey & Company. https://www.mckinsey.com
16. Koch D, Eßer E, Kureti S, et al. H2-DeNOx-Katalysator für H2-Verbrennungsmotoren. *MTZ Motortech Z* 2020; 81: 32–39.
17. Stepien Z. A comprehensive overview of hydrogen-fueled internal combustion engines: achievements and future challenges. *Energies* 2021; 14: 6504.
18. Beduneau JL, Kawahara N, Nakayama T, et al. Laser-induced radical generation and evolution to a self-sustaining flame. *Combust Flame* 2009; 156: 642–656.
19. Zheng J, Liu X, Xu P, et al. Development of high-pressure gaseous hydrogen storage technologies. *Int J Hydrogen Energy* 2012; 37: 1048–1057.
20. Schmitz N, Burger J, Ströfer E, et al. From methanol to the oxygenated diesel fuel poly(oxymethylene) dimethyl ether: an assessment of the production costs. *Fuel* 2016; 185: 67–72.
21. Oh SH, Han JG and Kim JM. Long-term stability of hydrogen nanobubble fuel. *Fuel* 2015; 158: 399–404.
22. Sun Y, Xie G, Peng Y, et al. Stability theories of nanobubbles at solid–liquid interface: a review. *Colloids Surf A: Physicochem Eng Aspects* 2016; 495: 176–186.
23. Ohgaki K, Khanh NQ, Joden Y, et al. Physicochemical approach to nanobubble solutions. *Chem Eng Sci* 2010; 65(3): 1296–1300.
24. Dharamshi K, Pal A, Agarwal AK. Comparative investigations of flame kernel development in a laser ignited hydrogen–air mixture and methane–air mixture. *Int J Hydrogen Energy* 2013; 38(25): 10648–10653.
25. Verhelst S. Recent progress in the use of hydrogen as a fuel for internal combustion engines. *Int J Hydrogen Energy* 2014; 39: 1071–1085.
26. White CM, Steeper RR and Lutz AE. The hydrogen-fueled internal combustion engine: a technical review. *Int J Hydrogen Energy* 2006; 31: 1292–1305
27. D'Errico G, Onorati A and Ellgas S. 1D thermo-fluid dynamic modelling of an S.I. Single-cylinder H2 engine with cryogenic port injection. *Int J Hydrogen Energy* 2008; 33(20): 5829–5841.
28. BMW. *BMW hydrogen engine reaches top level efficiency*. Munich, Germany: BMW, 2009
29. Salazar VM, Kaiser SA and Halter F. Optimizing precision and accuracy of quantitative PLIF of acetone as a Tracer for hydrogen fuel. *SAE Int J Fuels Lubr* 2009; 2: 737–761.
30. Kaiser S and White C. PIV and PLIF to evaluate mixture formation in a direct-injection hydrogen-fuelled engine. *SAE Int J Engines* 2009; 1: 657–668.
31. Wallner T, Scarcelli R, Nande AM, et al. Assessment of multiple injection strategies in a direct-injection hydrogen research engine. *SAE Int J Engines* 2009; 2: 1701–1709.
32. Scarcelli R, Wallner T, Salazar VM, et al. Modeling and experiments on mixture formation in a hydrogen direct-injection research engine. *SAE Int J Engines* 2010; 2: 530–541.
33. Scarcelli R, Wallner T, Matthias N, et al. Mixture formation in direct injection hydrogen engines: CFD and optical analysis of single- and multi-hole nozzles. *SAE Int J Engines* 2011; 2: 2361–2375
34. Matthias NS, Wallner T and Scarcelli R. A hydrogen direct injection engine concept that exceeds U.S. DOE light-duty efficiency targets. *SAE Int J Engines* 2012; 5: 838–849
35. Wallner T, Matthias NS, Scarcelli R, et al. A Evaluation of the efficiency and the drive cycle emissions for a hydrogen direct-injection engine. *J Automob Eng* 2013; 227: 99–109.
36. Iafrate N, Matrat M and Zaccardi JM. Numerical investigations on hydrogen-enhanced combustion in ultra-lean gasoline spark-ignition engines. *Int J Engine Res* 2021; 22(2): 375–389.
37. Varde KS. Combustion characteristics of small spark ignition engines using hydrogen supplemented fuel mixtures. SAE paper 810921, 1981.

38. Bae C and Kim J. Alternative fuels for internal combustion engines. *Proc Combust Inst* 2017; 36: 3389–3413.
39. Verhelst S and Wallner T. Hydrogen-fueled internal combustion engines. *Prog Energy Combust Sci* 2009; 35: 490–527.
40. Li H and Karim GA. Knock in spark ignition hydrogen engines. *Int J Hydrogen Energy* 2004; 29: 859–865.
41. Szwaja S, Bhandary KR and Naber JD. Comparisons of hydrogen and gasoline combustion knock in a spark ignition engine. *Int J Hydrogen Energy* 2007; 32: 5076–5087.
42. Kawahara N and Tomita E. Visualization of autoignition and pressure wave during knocking in a hydrogen spark-ignition engine. *Int J Hydrogen Energy* 2009; 34: 3156–3163.
43. Chen Y and Raine R. Engine knock in an SI engine with hydrogen supplementation under stoichiometric and lean conditions. *SAE Int J Engines* 2014; 7(2): 595–605.
44. Hoffmann G, Dober G, Piock WF, Doradoux L, Meissonnier G, Cardon C, et al. BorgWarner's injection system solutions for natural gas and hydrogen. In: *Proceedings of 30th Aachen Colloquium Sustainable Mobility 2021*. https://www.aachener-kolloquium.de/
45. Duffour F, Walter B, Ternel C, et al. *Potential and challenges of the hydrogen internal combustion engine from experimental and numerical investigation*. Plenary lecture at SIA Powertrain & Power Electronics Digital Edition 2021. Springer
46. Hasse C. Scale-resolving simulations in engine combustion process design based on a systematic approach for model development. *Int J Engine Res* 2016; 17: 44–62.
47. Peters N. Multiscale combustion and turbulence. *Proc Combust Inst* 2009; 32(1): 1–25.
48. Wen X, Zirwes T, Scholtissek A, et al. Flame structure analysis and composition space modeling of thermodiffusively unstable premixed hydrogen flame | Part I: atmospheric pressure. *Combust Flame* 2022; 111815. https://doi.org/10.1016/j.combustflame.2021.111815
49. Wen X, Zirwes T, Scholtissek A, et al. Flame structure analysis and composition space modeling of thermodiffusively unstable premixed hydrogen flame | Part II: elevated pressure. *Combust Flame* 2022, 111808. https://doi.org/10.1016/j.combustflame.2021.111808
50. Lee S, Kim G and Bae C. Behavior of hydrogen hollow-cone spray depending on the ambient pressure. *Int J Hydrogen Energy* 2021; 46: 4538–4554.
51. Lee S, Kim G and Bae C. Lean combustion of stratified hydrogen in a constant volume chamber. *Fuel* 2021; 301: 121045.
52. Roy MK, Kawahara N, Tomita E, et al. High-pressure hydrogen jet and combustion characteristics in a direct-injection hydrogen engine. SAE technical paper 2011-01-2003, 2011.
53. Shudo T and Oba S. Mixture distribution measurement using laser induced breakdown spectroscopy in hydrogen direct injection stratified charge. *Int J Hydrogen Energy* 2009; 34: 2488–2493.
54. Schefer RW, Kulatilaka WD, Patterson BD, et al. Visible emission of hydrogen flames. *Combust Flame* 2009; 156: 1234–1241.
55. Lee S, Kim G and Bae C. Effect of injection and ignition timing on a hydrogen-lean stratified charge combustion engine. *Int J Engine Res*. Epub ahead of print 21 August 2021. DOI:10.1177/14680874211034682
56. Prasad RK, Jain S, Verma G, et al. Laser ignition and flame kernel characterization of HCNG in a constant volume combustion chamber. *Fuel* 2017; 190: 318–327.
57. Prasad RK and Agarwal AK. Experimental evaluation of laser ignited hydrogen-enriched compressed natural gas-fueled supercharged engine. *Fuel* 2021; 289: 119788.
58. Verhelst S, Maesschalck P, Rombaut N, et al. Increasing the power output of hydrogen internal combustion engines by means of supercharging and exhaust gas recirculation. *Int J Hydrogen Energy* 2009; 34(10): 4406–4412.
59. Natkin R, Tang X, Boyer B, et al. Hydrogen IC engine boosting performance and NOx study. SAE technical paper 2003-01-0631, 2003.
60. Kim J and Rajoo S. A numerical study on turbocharging system for PFI-SI type hydrogen combustion engine. SAE technical paper 2021-24-0094, 2021.
61. Nguyen D, Choi Y, Park C, et al. Effect of supercharger system on power enhancement of hydrogen-fueled spark-ignition engine under low-load condition. *Int J Hydrogen Energy* 2021; 46(9): 6928–6936.
62. Taghavifar H, Nemati A, Salvador FJ, et al. 1D energy, exergy, and performance assessment of turbocharged diesel/hydrogen RCCI engine at different levels of diesel, hydrogen, compressor pressure ratio, and combustion duration. *Int J Hydrogen Energy* 2021; 46(42): 22180–22194.
63. Gürbüz H and Akçay IH. Evaluating the effects of boosting intake-air pressure on the performance and environmental-economic indicators in a hydrogen-fueled SI engine. *Int J Hydrogen Energy* 2021; 46(56): 28801–28810.
64. Savva PG and Costa CN. Hydrogen lean-DeNOx as an alternative to the ammonia and hydrocarbon selective catalytic reduction (SCR). *Catal Rev Sci Eng* 2011; 53(2): 91–151.
65. Alghamdi NM, Restrepo Cano J, Anjum DH, et al. Hydrogen selective catalytic reduction of nitrogen oxide on pt- and pd-based catalysts for lean-burn automobile applications. SAE technical paper 2020-01-2173, 2020.
66. Borchers M, Keller K, Lott P and Deutschmann O. Selective catalytic reduction of NOx with H2 for cleaning exhausts of hydrogen engines: impact of H2O, O2, and NO/H2 Ratio. *Ind Eng Chem Res* 2021; 60(18): 6613–6626.
67. Liu Z, Li J and Woo SI. Recent advances in the selective catalytic reduction of NOx by hydrogen in the presence of oxygen. *Energy Environ Sci* 2012; 10: 8799–8814.

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