# Recent progress in the use of hydrogen as a fuel for internal combustion engines

S. Verhelst

Ghent University, Department of Flow, Heat and Combustion Mechanics, Sint-Pietersnieuwstraat 41 B-9000 Gent, Belgium

#### Abstract

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Hydrogen-fueled internal combustion engines (H<sub>2</sub>ICEs) have been the topic of research for many decades, and contemporary reviews have surveyed the relevant literature. Because of a number of relatively large R&D projects that have been ongoing recently, much progress has been made that is worth reporting. Specifically, this paper reviews the advancements made in plotting the possibilities offered by direct injection of hydrogen, in-cylinder heat transfer, modeling and combustion strategies (on an engine as well as vehicle level). These efforts have resulted in impressive efficiency numbers, both at peak and part load operation, while keeping emissions far below regulatory

limits and reaching satisfactory specific power outputs. New demonstration vehicles have been put on the road showing the relatively low barriers (on a vehicle level) to introduce hydrogen engined transportation and these are briefly described. The paper discusses the merits of H<sub>2</sub>ICEs but also what makes them potentially unfit as a realistic alternative. Finally, the paper

concludes with the main areas of research that require further efforts.

*Keywords:* internal combustion engine, hydrogen, efficiency, emissions, direct injection, optical, experimental, numerical

# 1. Introduction

## 25 1.1. Why?

It is clear that the transportation sector is in need of other energy carriers and/or prime movers. Currently it is almost exclusively dependent on fossil fuels, leading to major contributions to anthropogenic emissions of carbon dioxide and pollutants. This in itself is enough of a reason to search

<sup>\*</sup>Corresponding author. Tel.: +32(0)92643306; Fax: +32(0)92643590 Preprint submitted to Elsevier Email address: sebastian.verhelst@ugent.be (S. Verhelst) October 5, 2013

- <sup>30</sup> for alternatives, but in addition fossil fuels' usage is still increasing, while reserves are finite, so prices continue to rise and many countries are looking for ways to secure their energy supply. This has led to investments in renewable energy and non-conventional fuels, and policies aiming at increasing energy efficiency. Hydrogen, as a means to chemically store energy, has been
- <sup>35</sup> advanced as an interesting energy storage or carrier. Given the wide variety of ways to produce hydrogen, and the possibility of producing energy from hydrogen with no or ultra-low emissions, hydrogen has the potential to be used for buffering renewable energy. One way is to produce hydrogen when renewable energy production exceeds energy demand, and convert it back to (electrical) energy when demand outweighs production (energy storage).
- Another way is to top off excessive renewable energy through producing hydrogen, and use it as a fuel for powering transportation (energy carrier).

With hydrogen possibly available as a fuel, there are two main options for using it to power vehicles. Arguably to most investigated one is the fuel cell powered vehicle (FCV). Fuel cells using hydrogen are attractive for their potential efficiency, particularly at part load (important for passenger cars), their emissions (only water vapor), quiet running and modularity. On the other hand, they are currently compromised due to cost and durability concerns. The second option is to use hydrogen in an internal combustion 50 engine.

Using the ubiquitous internal combustion engine (ICE) to produce motive power from hydrogen is attractive for a number of reasons, with perhaps the most obvious one being the possibility of relying on a mature industry and a vast production infrastructure. A second advantage lies in the fuel flexibility <sup>55</sup> of ICEs. An ICE can be run on different fuels, provided the engine control unit is suitably adapted and material compatibility with the different fuels is ensured. This makes H<sub>2</sub>ICEs prime candidates for introducing hydrogen as a transportation fuel: clearly, fueling stations cannot be extended with a hydrogen pump overnight, so in the event hydrogen is deployed on a large <sup>60</sup> scale, vehicles with "flex-fuel" capability offer the user much more comfort

- during the transition period (being able to switch to e.g. gasoline when no hydrogen pump is around). This feature, that could aid in the development of a hydrogen infrastructure, was the main reason for the  $H_2ICE$  being the subject of a Department of Energy funded program (see below).
- <sup>65</sup> Other attractive features of the  $H_2ICE$  are the lower requirements for hydrogen purity compared to fuel cells, leading to cheaper fuel; the potential for ultra-low emissions (quantified in this paper); and the increased peak and

part load efficiency compared to most commonly fueled ICEs (also described more fully in the following). Finally, the fact that it does not rely on rare materials [1] could broaden its potential application beyond that of a "bridging the gap" technology. Both FCVs and BEVs (battery-electric vehicles) rely on materials of which the supply, in the large quantities as required for making an impact on the transportation fleet, could potentially limit or prevent the widespread adoption of these alternatives. For fuel cells the bottleneck is the availability of platinum. This material is also the reason for the high cost of current fuel cells, with prices potentially increasing even further once demand increases. For BEVs, making rare earth elements available in large quantities is a challenge. Contrary to what their name suggests, these elements are not that rare, but ramping up their production has been reported

to potentially be too slow [2].

To summarize,  $H_2ICEs$  are attractive for:

- reducing local pollution,
- reducing global emissions of carbon dioxide,
- increased efficiency compared to current, fossil-fueled ICEs;
- <sup>85</sup> These being shared advantages with the fuel cell; and additionally as they:
  - can be made fuel-flexible,
  - do not rely on rare materials, i.e. can be made in large quantities and affordably,
  - are tolerant for fuel impurities, enabling them to use hydrogen from most sources, without the need for expensive purification,
  - can be introduced relatively easily, with the possibility of retrofitting engines [3, 4, 5, 6, 7].

## 1.2. Why not?

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Although many papers on  $H_2ICEs$  limit the introduction to why  $H_2ICEs$ are attractive, it is important to be realistic and also pay attention to potential show-stoppers. The most important question is probably whether hydrogen can be justified as an energy carrier. Next to the attractive features listed above, it cannot be forgotten that there are enormous hurdles to overcome. Much of them are down to the low density of hydrogen, rendering
distribution and storage difficult, costly and inefficient [8]. When hydrogen would be produced from fossil sources, as is the case for the majority of the hydrogen produced today, the losses in producing, distributing and storing hydrogen ("well-to-tank") have been reported to potentially be offset due to the higher efficiency ("tank-to-wheel") when used in fuel cells, resulting in an overall decrease in CO<sub>2</sub> emissions. According to Shelef and Kukkonen , this is not the case for H<sub>2</sub>ICEs [9]. However, given this statement was based on (efficiency) numbers available two decades ago, this will be revisited later in this paper.

In any case, it can be safely stated that the eventual use of hydrogen relies on the abundant availability of renewable energy. Even if this would be the case, the difficulty in storing hydrogen currently means that on-board storage is limited and expensive. It is hard to see hydrogen vehicles competing with conventional vehicles in terms of price, although one could argue that there are a lot of hidden, societal costs of present-day vehicles [10].

<sup>115</sup> Coming to  $H_2ICEs$ , it is currently not yet possible to combine high efficiency, low emissions, adequate specific power output and durability all in one concept. As will be touched upon later, there are a number of mixture formation concepts for hydrogen, with the port fuel injection (PFI) and direct injection (DI) spark-ignited ones being the most investigated. In the

- case of PFI, part load efficiency can be quite high, with ultra-low emissions, but low power output. DI engines have been demonstrated to offer very high efficiencies, with controllable emissions, but rely on DI injectors that still have to prove their durability. Moreover, full freedom in optimizing injection strategies asks for high injection pressures. This effectively limits on-board hydrogen storage options: either liquid hydrogen is stored in cryogenic tanks, and injection pressures are generated on-board [11], or compressed hydrogen is stored but then the full tank capacity cannot be utilised (unless there would be a "limp home" mode once tank pressures have dropped below the
- highest injection pressures). Compressing gaseous hydrogen on-board would <sup>130</sup> negate the efficiency benefits of DI.

This explains the viewpoint of a number of authors that the best way of using hydrogen is to chemically convert it to a fuel that is liquid at atmospheric conditions, making it much easier to handle. The extra processing step upstream, with associated losses, can be compensated by the lower losses of distributing and storing the resulting liquid fuel, as calculated by Specht

et al. [12] for the case of methanol. In some cases, dissociating the fuel on-

board using exhaust heat to generate a hydrogen-rich gas has been reported to benefit part-load efficiency or help with cold start [13, 14].

Clearly, the balance between this section and the previous one is undecided and is not solely dependent on technical considerations. Policies can affect whether the H<sub>2</sub>ICE powered vehicle is competing against liquid fueled ICE powered cars, or FCVs, or BEVs; e.g. if local authorities ban carbonemitting vehicles from entering city centers. In the remainder of the paper, we focus solely on the technical progress that has been made on H<sub>2</sub>ICEs, reviewing data that can then be used to quantify lifecycle energy use and emissions for vehicles using H<sub>2</sub>ICEs, to shed further light on the question whether we should continue to invest in them or not.

## 2. A review of reviews

As stated above, H<sub>2</sub>ICEs have been around for quite some decades and <sup>150</sup> many excellent period reviews have been published. Here, we refer to these papers for the fundamentals of hydrogen combustion, the basics of H<sub>2</sub>ICE operation and the progress in its development up to 2009. The present paper will then focus on the progress made since and pinpoint remaining areas in need of further research.

In his 1990 paper [15], Das reviewed H<sub>2</sub>ICEs, going back to the 1930s and pointing out the main features of hydrogen combustion, such as the potential for very low emissions, the load control through varying mixture richness (enabled by the wide flammability limits) but also the propensity for abnormal combustion phenomena such as backfire, preignition and knock. Both spark ignition as compression ignition work was reported. In 1998, a paper was authored by Peschka [11], which although not a review, is important as it contains many of the ideas on DI operation later explored in more detail, such as by Eichlseder et al. [16] who offer a good summary of the theoreti-

cal basis before reporting the first 'modern day' experimental comparison of PFI and DI and a discussion on load control strategies for the best tradeoff between efficiency and (oxides of nitrogen) emissions.

In 2006, White et al. [17] and Verhelst et al. [18] wrote review papers, which combined cover the most important findings of a wealth of literature. Finally, Verhelst and Wallner offer perhaps the most comprehensive review

<sup>170</sup> in their 2009 paper [19]. One of the last sections of that paper, summarizing the important research and development questions still to be resolved, is used as the starting point for the present paper. In particular, the following gaps in knowledge were identified:

- fundamental data: as pointed out by Verhelst and Wallner, there is a shortage of data of hydrogen ignition and combustion properties especially at engine conditions of pressure and temperature
- hardware: the maximum flow rate and durability of hydrogen DI injectors were put forward as the main challenges for injector development
- further exploration of possibilities of DI operation: at the time of writing, the many possibilities offered by DI engines were just starting to be explored
- simulation tools: initial work was reviewed, ranging from zero-dimensional to full CFD type models
- demonstration: the more complex control strategies had not yet left the laboratory environment

In the following, after a short description of the main research projects that were recently finished, the progress on these issues will be checked.

## 3. Recent progress

#### 3.1. R&D projects worldwide

<sup>190</sup> Before we delve into the details of the recent work on  $H_2ICEs$ , we give a short overview of the major R&D projects recently finished or ongoing, as in many cases the publication of important new findings results directly from these larger coordinated efforts.

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• In Europe, a three-year (2004-2007) Integrated Project called HyICE [20] resulted in the demonstration of engine concepts exceeding a specific power output of 100kW/l and a peak efficiency of 42%. The project was funded in the 6th Framework Programme of the European Commission and coordinated by BMW. The consortium consisted out of industrial and academic partners and investigated hydrogen's potential on single and multicylinder engines, with DI as well as cryogenic PFI; developed 1D and CFD modeling tools; DI injectors, and looked at optical measurement techniques to elucidate the particularities of

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hydrogen combustion in engines. While the project precedes what we mentioned to be the starting point in time for this review paper, it is explicitly mentioned as it initiated a number of research directions and as such laid the foundations for much of the recent work.

Other regional activities in Europe resulted in the conversion of passengers cars [4, 5] (Fig. 1 shows a converted VW Polo [5]) and a fork lift truck to  $H_2$ ICE operation [21] (see Fig. 2), in the framework of demonstration programs.

In Japan work was sponsored under the Next-generation Environmentally Friendly Vehicle Development and Commercialization Project (EFV21) of the Ministry of Land, Infrastructure, and Transport (MLIT). This project was coordinated by the National Traffic Safety & Environment Laboratory (NTSEL) and ran in two terms between 2005 and 2010. It aimed at reducing  $CO_2$  emissions from heavy duty engines and focused on H<sub>2</sub>ICEs as opposed to FCVs or BEVs in order to obtain high specific power outputs. It resulted in the development of DI injectors, mapped combustion strategies in single cylinder engines (metal and optical), evaluated a multicylinder engine towards the project target power out-220 put and looked at different ways of reaching  $NO_X$  emission standards [22, 23, 24, 25, 26].

• In the U.S., between 2004 and 2011 the Office of Energy Efficiency and Renewable Energy of the Department of Energy's FreedomCAR and Vehicle Technologies Program sponsored work at the Argonne and Sandia National Laboratories targeted at reaching specific peak and part load efficiencies, and  $NO_X$  emissions. In order to reach these targets, experimental work was undertaken on metal and optical single cylinder engines supported by numerical work (CFD simulations) [27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41].

Apart from these projects, some other smaller research efforts (in terms of the team involved) and demonstration activities are worth mentioning:

• Parallel to the work performed within the NTSEL project, Tokyo City University was also involved in research leading to the demonstration of 2 hydrogen vehicles. Iwasaki et al. [3] report the conversion of 2 engines to turbocharged PFI operation on hydrogen. These were used in a light duty truck with a hybrid powertrain (with the electric drive used to fill

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in low speed torque), see Fig. 3, and a 'microbus' (19 passengers, see Fig. 4), with the latter serving for over 2 years and covering more than 15000km at the time of the publication (it was put out of service in March 2013 - personal comm.). Lean operation was used to avoid the formation of  $NO_X$ , so that aftertreatment was not necessary; and turbocharging recovered most of the power loss due to the lean mixtures used, a strategy reported previously [19, 42]. Both vehicles were tested on the JE05 test cycle and emitted  $NO_X$  emissions far below the Japan Post New Long Term Regulation. The authors devoted much work to devising measures for avoiding abnormal combustion (backfire in particular), primarily through changes in the ignition system. The final conclusion of their paper reads "The hydrogen engines and hydrogen vehicles were manufactured for this study by combining existing parts and techniques, leaving nothing to be desired in durability and reliability. Because they can be manufactured at a low cost, it is believed that these are readily put to practical use with a commercial vehicle as an alternative engine.", which endorses the final bullet point in section 1.1.

• Dennis et al. [6] published the findings of work undertaken by the University of Melbourne and Ford Motor Company of Australia, on a PFI engine converted to hydrogen operation. The base strategy is the same as used by Iwasaki et al. [3], lean burn turbocharged, but additional control on air flow is achieved through fully variable valve timing on both intake and exhaust. The work thus presents new insights in the effects of gas dynamics and air flow on brake thermal efficiency (up to 38%) and occurrence of backfire, compared to other work that focussed on the use of a variable intake valve timing for optimizing the strategy where one switches from a lean burn wide open throttle operation to a stoichiometric throttled operation when high loads are demanded [43].

• In Delhi, India, 15 hydrogen-fueled three wheelers (rickshaws) were launched [7]. This was realized within a pilot project of the United Nations Industrial Development Organization (UNIDO), co-funded by its International Centre for Hydrogen Energy Technologies (UNIDO-ICHET) and the Indian Institute of Technology - Delhi, Air Products, Indian Trade Promotion Organization (ITPO) and Mahindra&Mahindra as project partners. 10 of the 15 vehicles are for passenger transport,

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5 are for carrying load. The original single cylinder, air-cooled, carbureted bi-fuel gasoline/CNG engines were converted to electronically controlled PFI hydrogen operation using relatively lean mixtures to avoid backfiring. Evidently, operation on hydrogen immensely reduced all pollutant emissions, compared to the original carbureted engines (with no aftertreatment).

- These works illustrate that progress is still being made also for PFI engines. Alternatives to restrict  $NO_X$  formation while enabling sufficient power output have also been reported, e.g. by Younkins et al. [44] who investigated the  $NO_X$ reducing potential of direct injection of water into a PFI engine, reporting a 20% increase in bmep is possible at a given  $NO_X$  limit.
- 285 3.2. Research themes

Much of the work reported in the following sections was performed within the framework of one of the major projects mentioned above. The recent progress can be grouped into a couple of research themes: direct injection, in-cylinder heat transfer, modeling and combustion strategies (on engine as well as vehicle level). Compared to the list of areas needing further re-290 search, put forward by Verhelst and Wallner [19] and summarized above, there has been little progress in increasing the dataset on fundamental properties. Some further work was devoted to determining the laminar burning velocity of hydrogen mixtures, but this involved mostly generating correlations from chemical kinetic computations [45, 46, 47], looking in more detail 295 at previously reported conditions [45] or repeating conditions with other measurement techniques [48] rather then expanding the data to more engine-like conditions. It is proving quite hard to surmount the challenges for accurate measurements at these conditions [19].

The overarching focus of recent research has been primarily to improve the trade-off between engine efficiency and  $NO_X$  emissions. Referring to the load control strategies reviewed previously [19], if homogeneous mixtures are used then  $NO_X$  control either relies on working lean (mostly above an air-tofuel equivalence ratio  $\lambda$  of 2), or using stoichiometric mixtures and reducing

NO<sub>X</sub> emissions in a three-way-catalyst (or more precisely: a two-way catalyst, using trace  $H_2$  to reduce  $NO_X$ ). However, working lean implies a low specific power output, which decreases efficiency as the mechanical efficiency will be quite low, next to indicated efficiencies suffering from relatively slow combustion. Still, efficiencies can be higher than on gasoline [6, 49]. Working

at  $\lambda = 1$  also leads to relatively low efficiencies, or in any case not higher than on gasoline [49], which has been ascribed to heat losses and will be further treated below.

While injection timing also impacts the performance of PFI engines [50], clearly it has a bigger impact for DI operation. Direct injection offers the theoretical possibilities of keeping combustion more or less confined, away from combustion chamber walls, decreasing heat loss; of stratifying the fuel/air mixtures for lower NO<sub>X</sub> when using relatively rich mixtures, or for faster combustion for relatively lean mixtures. The next section will offer a review of the work done to put theory in practice.

- Another way of speeding up combustion for (very) lean mixtures, increasing efficiency while avoiding  $NO_X$  formation, is homogeneous charge compression ignition (HCCI). HCCI operation on H<sub>2</sub> is far from straightforward because of its high autoignition temperature. Lee et al. [51] have succeeded in operating an engine on H<sub>2</sub> under HCCI conditions, but this necessitated extremely high compression ratios (up to 42) and was only possible within a
- very narrow window of equivalence ratio. This window is limited on the rich side because of knocking combustion or backfire, and on the lean side for lack of successful ignition. The special engine necessary for enabling HCCI engine and the narrow operating window mean that there is still a long way to go before H<sub>2</sub> HCCI operation could be part of any operating strategy. Aleiferis
- and Rosati used negative valve overlap (increasing internal EGR levels up to 42%) and air preheating to get hydrogen to autoignite [52]. The authors used OH LIF measurements to demonstrate that even at these conditions, once ignition occurs, there is still flame propagation, leading them to prefer the term controlled autoignition (CAI) as a better moniker than HCCI.

#### 3.3. Direct injection

As was described in detail by Verhelst and Wallner [19], direct injection offers the possibility to increase the power density of hydrogen engines and prevent the occurrence of abnormal combustion (backfire in particular). In earlier review papers, it was already reported that these advantages had been demonstrated. As mentioned in the previous section, subsequent work focused mostly on improving the efficiency-NO<sub>X</sub> trade-off. At the start of the projects listed in Section 3.1, some ambitious targets were set:

• the DOE program aimed at demonstrating a peak brake thermal efficiency (BTE) of 45%; a part-load BTE of 31%, with the part load

point set at 2 bar brake mean effective pressure (bmep) at 1500 rpm; and "Tier II Bin 5" emissions (which limit  $NO_X$  emissions to 0.07 g/mile) [53].

• the NTSEL project targeted a peak power output of 100 kW from the selected 4-cylinder naturally aspirated engine, with less than 0.5 g/kWh of NO<sub>X</sub> on the JE05 transient emission testing cycle.

Meeting these targets necessitated a profound study of DI combustion, with investigations of diverse combustion strategies, optical measurements in constant volume combustion chambers and optically accessible engines and CFD simulations of the mixture formation. Next to this, further work was devoted to the development of hydrogen DI injectors to increase their maximum flow rate and durability. These topics will be discussed in the following sections.

- 3.3.1. Optical techniques for measuring mixture formation and combustion in hydrogen-fueled engines
- <sup>360</sup> Before recent contributions to furthering the understanding of mixture formation and combustion in hydrogen engines will be reviewed, we first give a brief description of some of the measurement techniques that have enabled this progress.

Laser induced fluorescence (LIF) techniques have been developed for studying mixture formation in DI engines on hydrogen, partly within the HyICE project [54, 55]. Acetone [29, 30, 32], triethylamine [55] and trimethylamine [56] have been used as tracers. The technique is used to determine local hydrogen concentrations and thus local equivalence ratio, to determine the extent of mixture stratification. Salazar et al. [29] studied the quantitative planar LIF method using acetone tracer in detail to improve its precision and accuracy.

Shudo and Oba [57] developed the LIBS technique, laser induced breakdown spectroscopy, for measuring the hydrogen concentration distribution. To test the feasibility of the method, it was first used in an optically accessible constant volume combustion vessel equipped with a DI injector. The measured spectrum was then calibrated, relating equivalence ratio to atomic emission intensity ratio.

Roy et al. [58] determine local equivalence ratios through the use of 'SIBS', or spark-induced breakdown spectroscopy, a further development of the LIBS technique. Here, the spark itself is used as the light source and the equivalence ratio in the spark plug gap can be estimated. The spectrum was mea-

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sured through an optical fiber housed in the center electrode of the spark plug, which in principle makes this technique suitable for measuring the equivalence ratio in the spark gap, at ignition timing, in production engines. Although the technique has relatively large experimental uncertainty, the

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measured local equivalence ratio and its coefficient of variation corroborated the findings from the flame images and heat release analysis reported below. Finally, observation of flame propagation in hydrogen-fueled engines has

been done using several techniques such as shadowgraphy [26], schlieren [37], <sup>390</sup> direct imaging [59], flame chemiluminescence [60, 52] and OH LIF [60, 52].

### 3.3.2. DI injectors

The development in DI injectors for hydrogen is summarized elsewhere [61]. One of the goals within the NTSEL project was the development of an electrohydraulically operated injector capable of injection pressures up to 200 bar. This development is described by Yamane et al. [25], who also report successful durability testing of several hundred hours, including testing on an injector test stand as well as installed in an engine. Another important development has been the demonstration of a piezoelectric injector [62], which through its faster actuation compared to previous solenoid actuated injectors has enabled added optimization freedom (further discussed below).

#### 3.3.3. Understanding mixture formation and combustion in DI engines

While initial measurements with varying start of injection (SOI) timing, on single cylinder DI engines, pointed out that the trade-off between efficiency and  $NO_X$  emissions could be improved through careful mapping of SOI relative to ignition timing (IT) [63], a more detailed understanding of the mixture formation process and subsequent combustion was desired. A number of papers reported contributions based on optical measurements.

Within the DOE project mentioned above, Sandia National Laboratories operated a single cylinder optical engine on hydrogen to elucidate the mixture formation and subsequent flame propagation processes in DI engines. First, the in-cylinder flow field in the engine was characterized using PIV [27]. This initial work also showed the profound impact of the direct injection of hydrogen on this flow field and the significance of jet-wall interaction. Subsequent work focusing on the mixture formation and resulting equivalence ratio distribution reports on the influence of injection timing, different nozzle designs,

<sup>415</sup> tribution reports on the influence of injection timing, different nozzle designs, injector location (side or central) and tumble ratios [30, 32, 35, 37], in great detail. This work helped explaining the range of injection timings resulting in stable operation previously obtained on the all-metal single cylinder engine
with the same geometry, operated at Argonne National Laboratory [64]. The
stratification through late DI was shown to result in insufficient fuel at the
location of the spark plug for some conditions, causing unstable operation. It also demonstrated how the direct injection interacted with the in-cylinder
flow field and intake-generated tumble flow [32, 35]. Finally, the impact of
the interaction between the hydrogen jet and the tumble ratio on flame propagation was described [37]. This showed that, as for gasoline engines, the
initial flame speed has a major effect on the main combustion phase and
the combustion stability. Interestingly, no direct evidence was found for any
tumble breakdown, supposed to result in speeding up combustion through
generation of small scale turbulence around top dead center (TDC).

In work by Wimmer et al. [65] and Shudo and Oba [57], it was pointed out that decreasing heat transfer to the cylinder walls was a prerequisite for increasing efficiencies. While this seems like a general and logical statement, it is particularly important in the case of hydrogen, as will be explained in more detail in a subsequent section. Shudo and Oba investigated how direct injection could be used to stratify the mixture, with high equivalence ratios (relative to the mean equivalence ratio) close to the spark plug and low equivalence ratio close to the walls. They used the LIBS technique to look at the equivalence ratio distribution obtained with different injection strategies. They found that, while hydrogen diffuses more quickly than methane, a split injection (injecting hydrogen in two phases) could be used to slow down the diffusion and looked promising as a strategy for improving stratification.

The various DI injection strategies, including early and late DI, multiple DI before or after spark, etc., described by Wallner et al. [28], were the subject of experimentation in a number of papers. Various names have been used to discern the different strategies. Oikawa et al. [26] talk about a "plume ignition combustion concept" (PCC) denoting the ignition of a rich mixture plume during or right after an injection event. Roy et al. [59] use the terminology 'tail ignition', 'late ignition', 'center ignition' and 'head ignition' for the various possibilities. In both cases, the option of igniting a very rich mixture is looked at, being a unique capability with hydrogen DI as there are no fears of a sooting flame because of the lack of carbon. The wide flammability limits, with extremely rich mixtures still capable of reliable ignition and combustion [19] are another enabler for this strategy.

Shioji et al. were among the first to provide fundamental data of hydrogen jets being ignited at varying time relative to SOI, and at varying location relative to the injector [66]. They used high-speed shadowgraphy to observe the flame development, next to recording instantaneous pressure to calculate heat release rates. The results indicated the potential of using the degrees of freedom offered by a DI system for optimizing efficiency and emissions.

Within the NTSEL project mentioned higher, much effort was devoted 460 to further explore this concept. Oikawa et al. [26] report measurements in an optically accessible engine, using different injector nozzles, including single and multihole. The injector was mounted close to the spark plug, with the jet being directed towards the spark plug. Igniting the mixture shortly after the end of injection was shown to substantially reduce  $NO_X$  emissions with 465 minimal effect on the efficiency, with further potential through advancing ignition relative to SOI. Perhaps more importantly, the experiments helped in the understanding of the trade-offs with this technique. For example, igniting the jet can lead to impingement of the flame on the combustion chamber walls, due to the high jet velocities. This increases heat loss and 470 decreases efficiency. On the other hand, if the jet velocity is too low, the flame can also spread out towards the injector side and again increase heat loss because of the flame's proximity to the walls. Also, care has to be taken in order to maintain combustion efficiency, as unburned hydrogen can result from excessively lean regions, which would also decrease efficiency. The 475 findings of this study contributed to optimizing the engine for achieving the project goals, as discussed further below.

Roy et al. [59] report measurements on a constant volume combustion chamber and a single cylinder engine, both optically accessible, of jet penetration, flame propagation, pressure and heat release rate. The measurements in the combustion chamber were targeted at determining the jet characteristics (penetration and cone angle) as a function of fuel injection pressure and ambient pressure. The subsequent measurements in the engine recorded flame and pressure development for varying injection timing relative to ignition timing. The flame development was derived from direct combustion images, which allowed to study the differences in early kernel growth between the different injection modes. The 'tail ignition' case, with injection ending at TDC, and ignition occurring at TDC, resulted in the fastest flame propagation and most stable combustion.

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Finally, Aleiferis and Rosati made an important contribution to furthering our understanding of the impact of the direct injection of hydrogen on the in-cylinder flow field and the resulting combustion [60]. They used chemiluminescence and laser-induced fluorescence (LIF) to study flame propagation of hydrogen and compared against gasoline, as well as comparing PFI to
<sup>495</sup> DI operation. The flame images were processed to derive burning velocities, which were compared to values reported in literature. In most of the reported cases, the SOI for the DI cases was right after the intake valves has closed, i.e. an early injection strategy which would imply a fairly homogeneous mixture at ignition.

Some of the key findings are as follows. First, they noted that flame propagation is much more spherical in nature for hydrogen compared to gasoline, which can be explained by hydrogen's higher burning velocities, leading to the flame being less affected by in-cylinder bulk flow. This also implies less cyclic variability compared to gasoline, which was confirmed by the measurements. Secondly, the peak flame expansion speeds were quite a bit higher on hydrogen compared to gasoline: for the PFI case, in the range of 10-20 m/s for  $\phi = 0.50 - 0.83$  (hydrogen) compared to 8-12 m/s for  $\phi = 0.83 - 1.0$  (gasoline); for the DI case these were even higher, in excess of 35 m/s for  $\phi = 0.67 - 0.83$ . The flame expansion speeds were further

<sup>510</sup> processed leading to estimates of the corresponding burning velocities. The PFI values for hydrogen corresponded quite well with values reported for combustion in constant volume combustion chambers, with the DI values being much higher. This led the authors to suggest that in the DI case, the high velocity gas jet must have a profound impact on the in-cylinder flow and turbulence, greatly speeding up the combustion. Upon delaying SOI, even faster flame growth was observed.

It must be noted that perhaps the difference between PFI and DI is at least partly down to the methodology used by the authors. The engine speed and the intake pressure were fixed. While for gasoline this approach is justified, in the case of hydrogen this leads to a large difference in the amount of air that is aspirated, between the PFI and DI cases [33], and thus in a large difference in the resulting amount of mixture and therefore power output. Unfortunately, the authors do not show recorded cylinder pressure data which would allow to verify this.

525 3.3.4. Combustion strategies

Port fuel injection results in homogeneous fuel/air mixtures. The influence of engine settings (equivalence ratio, ignition timing, ...) has been reported in previous reviews (see Section 2). PFI is still being used for demonstration vehicles [3, 4, 5, 7, 67], as this is the most straightforward <sup>530</sup> way of converting a gasoline engine to hydrogen operation, but results in limited power output [19]. With direct injection the specific power output exceeds that of gasoline while it also offers more degrees of freedom, through the start of injection as well as through split injection. As reviewed above, CFD simulations and optical measurements have resulted in a better understanding of how this can impact mixture formation and flame development. Here, we discuss the work undertaken to take full advantage of the flexibility

offered by DI.

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As reviewed elsewhere [19], initial work done by BMW and TU Graz [16, 65] showed how using stratification at higher loads (through late SOI), resulting in a distribution of equivalence ratios, could lead to a substantial decrease in NO<sub>X</sub> emissions compared to homogeneous operation (early SOI) where all the mixture is around the equivalence ratio of peak NO<sub>X</sub>. This initial work also showed increasing emissions of unburned hydrogen, leading to a trade-off between low NO<sub>X</sub> emissions and high efficiency, which the authors suggested could be improved with further optimization. In recent years, a number of teams have put much effort in exploring the potential of DI strategies for improving this trade-off.

Within the NTSEL project, a single cylinder engine was used to explore different combustion strategies after which these were implemented on the target multicylinder engine. Kawamura et al. [22] and Naganuma 550 et al. [23] report sweeps of injection pressure, injection timing and ignition timing across the engine map and the resulting efficiency and  $NO_X$  emissions. The switch from PFI to DI greatly increased the maximum power output but also increased  $NO_X$  emissions. These were brought within the target limits in different steps. Use was made of the insights gained from the 555 optical work reported above, with varying SOI relative to ignition timing. At low load, low speed conditions, early SOI was confirmed to lead to the best compromise between efficiency and emissions. At high speed and high load conditions, a 'plume-tail ignition' strategy, with ignition at the end of the injection period, using high injection pressures (200 bar) resulted in a 560 significant improvement of the trade-off. A loss analysis [23] indicated this was down to a faster burn rate, leading to a more isochoric combustion, while

was down to a faster built fate, leading to a more isochoric combustion, while wall heat losses remained more or less constant. Further reductions of  $NO_X$ emissions, of around 50%, while preserving (indicated) efficiency at a high 45%, were achieved through the use of exhaust gas recirculation (EGR). As will be explained below, additional  $NO_X$  reduction was accomplished through

the use of aftertreatment.

The most promising strategies - early injection resulting in a homoge-

neous mixture at ignition timing, plume tail ignition and plume tail ignition

with EGR - were then further explored over the whole engine speed and load range, recording  $NO_X$  emissions and efficiency. This allowed the rough definition of engine mappings using the most optimal strategy depending on the operating condition. Further work on determining optimal injection and ignition timings was reported by Kawamura et al. [24].

During the DOE project, two generations of single cylinder research en-575 gines were used in order to find the best engine and combustion chamber geometry, and engine settings, for obtaining the DOE goals [33]. The original engine geometry, on which most of the CFD and optical work mentioned in the previous section was performed, was changed in an effort to increase efficiency. The compression ratio was increased (11.5 to 12.9) as well as 580 the stroke, the latter resulting in a more favourable bore to stroke ratio, for a lower combustion chamber surface area to volume ratio around TDC. Initial experimental results, supported by new CFD calculations of mixture formation [33] confirmed the gain in efficiency, with initial sweeps of SOI and ignition timing leading to a peak indicated efficiency of 45.6%. Another 585 important change going from the 1st to the 2nd generation engine was the switch from a solenoid actuated to piezo actuated injector, with the faster acting piezo injector enabling a wider range of SOI timings relative to IT.

A detailed analysis of losses enabled a step-by-step optimization of injection strategy [39]. It was shown how delaying SOI has the benefit of reduced compression work, but is limited to allow sufficient time for mixture formation to result in an ignitable mixture and stable combustion. The optimal SOI was found to increase (relative to TDC) linearly with engine speed, and resulted in an increase in peak efficiency as well as enlarging the area of high efficiencies in the engine map. Further testing and CFD analysis using different injector nozzles finally resulted in a peak brake thermal efficiency of 45.5%, exceeding the DOE target. Perhaps more importantly, high efficiencies were obtained over most of the engine map, with the authors reporting the engine to operate above 35% BTE over 80% of the tested operating range.

The part load efficiency target of 31% (at 1500 rpm and 2 bar bmep) set by DOE was also exceeded (with an efficiency of 33.3%). Figure 5 shows the map of engine efficiency using optimal SOI and injector nozzle, with Fig. 6 showing the corresponding brake specific NO<sub>X</sub> emissions. The work is particularly useful for its thorough description of the loss mechanisms and how their balance changes throughout the engine map and as a function of SOI.

Finally, recent work by Younkins et al. [68] shows that the freedom offered

by DI is far from fully explored. They compared 2 cylinder heads, one with a single centrally placed spark plug and one with two spark plugs placed diametrically opposite, close to the cylinder liner; and two nozzle geometries, one 5 hole injector as also used by Matthias et al. [39] and a 6 hole injector with three holes on each side of the nozzle; and their combinations. Using the 6 hole injector with each 3 hole group aimed at one of the spark plugs of the dual spark head, they recorded a net indicated thermal efficiency of 47.7% with NO<sub>X</sub> emissions of only 51ppm. Much of this is down to the highly stratified operation and the reduced burn duration, resulting from this setup.

## 3.4. Heat transfer

As mentioned above, Wimmer et al. [65] and Shudo and Oba [57] pointed out that decreasing heat transfer to the cylinder walls is a prerequisite for increasing efficiencies of hydrogen-fueled engines. Measurements of instantaneous heat flux through the combustion chamber wall, for stoichiometric 620 PFI operation on hydrogen, gasoline and methane have shown that the heat fluxes recorded for hydrogen were much higher than for gasoline or methane [69, 70, 71]. This explains why, although combustion is much faster, the resulting efficiency is only as high or even lower for hydrogen compared to gasoline or methane (see also [49]), due to the higher heat losses. The bal-625 ance becomes a lot better if lean mixtures are used, to take advantage of the wide flammability limits of hydrogen. For moderately lean mixtures, flame speeds remain higher than for gasoline or methane, while heat losses decrease substantially, leading to increased efficiencies. If part load points are then compared between lean hydrogen using wide open throttle, and stoichiomet-630 ric gasoline or methane using throttled operation, efficiencies on hydrogen are much higher [71] as the decrease in pumping losses also contributes to higher efficiency.

Stratified operation using DI is another way of decreasing heat transfer to the walls. As analyzed by Obermair et al. [33] and Matthias et al. [39], decreasing wall losses was one of the main contributors towards achieving the efficiency goal set out by DOE. Next to stratification, the 2nd generation engine used by these authors, with a lower surface to volume ratio, inherently reduces wall heat transfer. Results by Younkins et al. [68] also point at heat loss being an important factor in determining optimal mixture stratification.

Given the importance of wall heat transfer, it is perhaps surprising to learn that current engine modeling tools fail to properly predict heat transfer on hydrogen [72, 73]. The heat transfer models of Annand and Woschni have

been shown to be inadequate for hydrogen [72], but are still sometimes used. Demuynck et al. [73, 74, 75] show that predictions can be improved when 645 properly accounting for the changing gas properties when using hydrogen, but that more is needed to capture the physics of the heat transfer process in engines. Clearly, this is an area requiring further research.

#### 3.5. Numerical work

Some progress was made in improving computational tools for under-650 standing mixture formation and combustion in hydrogen engines. Sukumaran and Kong focused on numerical simulation of hydrogen DI [76]. They pointed out that calculation of mixture formation for hydrogen DI is very challenging, because of the high velocity gas jet, leading to a complex structure of shock waves, a Mach disk etc. The high velocities imply that mixing 655 with air mostly occurs after the jet impacts on a wall. This would mean that stratification is quite hard to achieve, but the authors focused mostly on early SOI (i.e. when in-cylinder density is still quite low), aiming at improving mixture homogeneity. After developing a numerical technique based on an adaptive mesh refinement, reconciling accuracy with computational effi-660 ciency, they investigated spray angle, SOI and injector location. Their results confirm the previously reported experimental trends of improving homogeneity by using early SOI. The authors then use the CFD model to determine the optimal location, spray angle and SOI for a particular injector and engine geometry. 665

Whitesides et al. [77] extended the 'gaseous sphere injection model' to better capture the particularities of under-expanded  $H_2$  direct injection in engines. The model allows a courser grid than what would be needed from a Eulerian injection simulation, as it does not need to resolve the injector nozzle, resulting in much faster computation. The criteria for a computational 670 cell to be defined as being in the jet region were refined so that the model works better in the case where forced flows are present, such as in engines. Model results were compared against the measurements by Shudo and Oba reported higher [57], showing reasonable correspondence for jet penetration and axial hydrogen mass fraction, but also that improvements were needed 675 to better reproduce the radial mass fraction.

The highly detailed local flow velocity and mixture equivalence ratio data measured by Sandia National Lab [30, 32, 35, 37] were used to evaluate and improve numerical simulation performed by Scarcelli et al. at Argonne [31, 34, 36, 38, 41]. CFD results accurately predicted the intake flow and the

mixture formation process for simple nozzle geometries (single-hole nozzle or multi-hole nozzle with non-interacting jets) [34], nevertheless the agreement with the experimental data got worse when strong jet-to-jet interaction was expected immediately downstream of the nozzle exit, due to more complex geometries [38]. Scarcelli et al. [41] state that in order to improve the accuracy of CFD predictions of mixture formation, the characteristics of high-pressure gaseous jets need to be investigated in greater detail, since it was shown that the structure of pressure shocks in the under-expanded region significantly affects the mixing of the jets with the surrounding gas and ultimately the jet-to-jet interaction. Still, the work resulted in a sufficiently accurate CFD tool to help in optimizing the DI engine towards achieving the DOE goals, as Figs. 7 and 8 illustrate.

The above illustrates that CFD tools now offer sufficient accuracy at relatively low computational cost for calculating mixture formation in hydrogen

- <sup>695</sup> DI engines, a very useful contribution given the complex interaction of nozzle geometry, in-cylinder flow field and combustion chamber geometry that needs to be resolved in order to create desired fuel stratification. However, much work is still needed in order to come to an accurate prediction of combustion. Verhelst and Wallner [19] reviewed thermodynamic and CFD models, with
- <sup>700</sup> particular examples of both model types resulting in satisfactory agreement for PFI or DI homogeneous operation. The DI strategies aimed at fuel stratification, reviewed above, are much more challenging though. Igniting a jet while it passes the spark plug with high velocity or injecting into a burning mixture, lead to partially premixed or non-premixed combustion, or both. <sup>705</sup> Models that are able to simulate these combustion models are still in their

infancy and computationally demanding [78].

Also, as mentioned in the previous section, heat transfer models need to be improved. While this would allow a better prediction of how heat transfer affects efficiency, it is of even more importance for accurate calculations of  $NO_X$  emissions, these being very temperature dependent.

## 3.6. Vehicle and engine strategies

The combustion strategies explored in the works reviewed above have been used to choose the optimal strategy for an engine to be used in a vehicle. The single cylinder test data obtained within the NTSEL project were used to estimate fuel consumption and  $NO_X$  emissions on a JE05 test cycle [23]. The engine data was converted to data maps for a six cylinder hydrogen engine powering a heavy-duty vehicle. It was shown that the application of EGR, combined with optimized injection timings, was necessary to get  $NO_X$  emissions below the emission limit.

<sup>720</sup> Next to using EGR for decreasing engine-out emissions, the possibility of NO<sub>X</sub> aftertreatment was also investigated. Kawamura et al. [22] describe the motivation for choosing a NO<sub>X</sub> storage-reduction catalyst. Using such a catalyst, NO<sub>X</sub> emissions are stored until a NO<sub>X</sub> sensor placed downstream of the catalyst detects the storage capacity being reached, at which point a hydrogen injector placed upstream of the catalyst injects hydrogen which serves as a reducing agent. Kawamura et al. [22] used a six-cylinder engine converted to PFI hydrogen operation to test the catalyst system. Steady state testing showed the potential of 98% NO<sub>X</sub> conversion rate with a fuel penalty of less than 0.5%, meaning a negligible influence on brake thermal

efficiency. An oxidation catalyst was used to oxidize any remaining hydrogen. The authors report emission of ammonia when an excess of reducing agent (i.e. hydrogen) is used. Furthermore, N<sub>2</sub>O emissions were also detected but in this case no significant correlation with the amount of injected reducing agent was observed.

Testing of the lean  $NO_X$  trap continued on the final engine chosen within the project, a four cylinder 4.7 liter heavy duty engine converted to naturally aspirated DI hydrogen operation [24]. The engine equipped with the aftertreatment system is shown schematically in Fig. 9 and was run on the JE05 test cycle. The aftertreatment system resulted in large reductions of

 $^{740}$  NO<sub>X</sub> emissions. However, the transient testing also showed how NO<sub>X</sub> spikes occurred due to the non-optimized control system, so further NO<sub>X</sub> reduction potential remains. An optimized transient control system should also address the outbreaks of N<sub>2</sub>O emissions that were measured after supply of the reducing agent.

Again, based on the measured engine data, vehicle simulations were run to estimate the  $NO_X$  emissions on the JE05 test cycle of the final medium duty truck for which the engine was intended [79]. Results showed that further optimization of the combustion strategy including EGR should enable to meet the  $NO_X$  emission limit without the need for aftertreatment, while adding the aftertreatment system with lean  $NO_X$  trap and oxidation catalyst has the potential for emission levels far below the limit, if a rich spike control procedure is added.

An alternative approach was taken within the DOE project [40]. Based on the obtained engine data, discussed above, a (simulated) turbocharged lean engine operating strategy was chosen. The equivalence ratio was fixed at  $\phi = 0.3$  ( $\lambda = 3.3$ ), with throttling at engine loads below 4 bar bmep and turbocharging at higher loads. The engine data was recalculated to a 3 liter engine powering a passenger car and used in a vehicle simulation on the Urban Dynamometer Driving Schedule (part of the FTP cycle). NO<sub>X</sub> <sup>760</sup> emissions were calculated to be within the SULEV II range, i.e. well below the target set by DOE, without any aftertreatment. Further calculations showed that downsizing the engine could result in increased efficiency while still meeting the DOE target for NO<sub>X</sub> emissions, albeit with a smaller margin. This again illustrates the trade-off between efficiency and NO<sub>X</sub> emissions. The authors suggest advanced powertrain layouts (hybridization) could be looked at in future to take full advantage of the high efficiency and ultra-low emissions regimes.

Figure 10, reproduced from Kawamura et al. [24], illustrates the different routes taken within the NTSEL and DOE projects. Going from port fuel injection to DI greatly increases the power output potential but can also increase  $NO_X$  emissions substantially. Optimizing SOI and IT, as explained above, can decrease  $NO_X$ , but additional measures are mostly needed to get  $NO_X$  emissions within target limits. EGR may bring emissions within these limits. If not the case, a lean  $NO_X$  trap can reduce  $NO_X$  emissions further. Alternatively, keeping the engine operation lean enough to limit combustion temperatures can avoid  $NO_X$  formation altogether, which then requires turbocharging to meet the target power output.

### 4. Conclusions

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Looking back at the research results and demonstrations reported in re-<sup>780</sup> cent years, it is clear that much progress has been made in advancing the maturity of hydrogen engines. New data has been published on PFI operation: on the effects of the ignition system on backfire occurrence, and the potential of variable valve timing and direct injection of water for improving the power-efficiency-emissions trade-offs. New demonstration vehicles have <sup>785</sup> been put on the road, from three wheelers over passenger cars to medium duty trucks.

Most work however was devoted to furthering the exploration of direct injection. It has been shown that the theoretical advantages of DI engines can be translated to practice, with very promising results in terms of power density as well as peak and part load efficiencies, and this at ultra-low emissions. Moreover, given the degrees of freedom in nozzle geometry, timing and number of injection events, single or dual ignition, combustion chamber geometry, ..., it is very well possible that even better results can be reached. For example, strategies with split injection have been suggested to aid in stratification [57] but have only been tried out for a limited range of engine conditions [28].

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However, this brings us to an area of research where less progress has been made, namely computational tools for hydrogen engines. That large degree of freedom also means it is becoming much more difficult to 'guess' optimal geometries or experimentally sweep all possible engine settings, so there is a strong need for such tools. There have been very useful contributions, in the form of models allowing the calculation of mixture formation in DI engines within practical computation time. These can now be used to numerically 'scan' the most promising nozzle and combustion chamber geometry and indicate the best timing for injection and ignition events, saving hardware cost and testbed time. In contrast, tools efficiently allowing accurate calculation of combustion and emission formation are lacking. The good news is that the wealth of data collected on mixture formation and flame propagation in optical engines can be used for validating model predictions.

Experimental data has also been published on in-cylinder heat transfer, albeit only for PFI. Initial steps have been taken to improve heat transfer models for hydrogen. Extending the heat flux measurements to DI would allow to validate the models for DI operation and enable heat transfer to be part of the design of optimal mixture stratification (minimizing heat loss to the walls).

Coming back to DI, one of the concerns raised by Verhelst and Wallner [19] was on injector durability. There was one recent paper reporting durability testing of an electrohydraulically actuated injector, checking wear over several hundred hours, with fairly positive results. Such testing has not been reported (yet) for injectors with piezoelectric actuation. This type of actuation is needed when multiple injection events per cycle are wanted, as response times are fast enough. Unfortunately, it can be expected that the injector lifetime is inversely proportional to the total number of injections, so going to multiple injection would decrease durability.

Finally, we revisit the statement by Shelef and Kukkonen. These authors claimed the efficiency benefit of hydrogen fueled engines over gasoline engines was too low to result in any well-to-wheel benefits, whereas the efficiency benefit of fuel cells resulted in an overall positive balance. It is informative to have a look at the assumptions taken to come to these conclusions. For hy-

- drogen engines, a relative improvement in efficiency of 15-25% over gasoline operation was assumed, whereas fuel cell efficiency was taken to be 45% irrespective of load. With the efficiencies demonstrated on hydrogen engines reviewed above, and taking the efficiency drop of fuel cells at higher loads into account, another picture may emerge. Namely, while the assumption on
- relative efficiency over gasoline turns out to be correct for the peak efficiencies, much larger relative gains can be reached for part load, which is much more important for driving cycles. On the other hand, updating this exercise should also use more recent data on the losses incurred by the production, distribution and on-board storage of hydrogen. Only then will we have a better idea whether Shelef and Kukkonen were pessimistic in their views, or realistic.

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Figure 1: Bi-fuel (gasoline/hydrogen) VW Polo demonstrated by the University of Navarre [5]. Permission to reproduce requested.



Figure 2: Forklift truck equipped with a  $H_2ICE$ , part of the demonstration activities within the Hydrogen Region Flanders - South-Netherlands project [21]



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