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THE POTENTIAL OF HYDROGEN INTERNAL COMBUSTION ENGINES FOR HEAVY-DUTY APPLICATIONS

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Introduction

The importance of fast charging and high on-board energy storage capability

In a decarbonized future in which vehicles' carbon dioxide (CO_2) emissions are heavily constrained, hydrogen offers a direct solution to the problem of such emissions at point of use. Furthermore, compared with other major technologies proposed for land transport, namely, battery electric vehicles (BEVs), hydrogen vehicles can be rapidly recharged as well as configured so that more energy can be carried. The magnitude of the latter advantage is such that the higher inefficiency of the powertrain can be overcome to a significant degree, thereby extending the driving range. These two capabilities mean that vehicles using hydrogen as their primary energy storage medium may be superior to BEVs, particularly for heavy-duty (HD) applications.

Various hydrogen storage technologies exist, including physical and chemical. Chemical storage technologies have not yet been shown to be truly practical for vehicular use (and are not discussed further here). Meanwhile, physical storage technologies are the most advanced type. The two most commonly used technologies are pressurized and liquid storage. For pressurized gas applications, two storage pressures are commonly used: 350 bar and 700 bar. First, 700 bar is used by systems producing light-duty (LD) vehicles, including the systems of Toyota, Hyundai, and Honda. Second, 350 bar is used for HD applications, as the system volume is less challenging for trucks. Additionally, compression energy is saved by not having to double the pressure (Weber 2022). For example, BMW successfully trialed liquid hydrogen tank systems and developed a production process for them in collaboration with Magna Steyr (Amaseder and Krainz 2006).

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Without specifying which approach should be used, the US Department of Energy (DOE) has targeted an infrastructure-to-vehicle transfer rate of 5 kg of hydrogen in 2.5 minutes (i.e., 2 kg/min; US Department of Energy 2021). This value equates to a charging rate of 4 MW or 67 kWh/min (Turner 2020). This represents an energy transfer rate nearly six times that presently rolled out for BEV charging (e.g., 350 kW by Porsche). However, importantly, no thermal management issues exist under this approach. Such issues usually arise from the fact that battery charging efficiencies are typically 95% and that an electric system would simultaneously have to dissipate 17.5 kW of heat at a charging rate of 350 kW. In addition to these two commonly known physical storage methods, cryo-compressed storage offers twice the hydrogen density of 700-bar compressed storage and concomitantly the potential for very high energy transfer rates. Brunner and Kircher (2016) stated that BMW achieved transfer rates of 2 kg/min in 2012 by using cryo-compressed gas storage, equaling the then-long-term US DOE target (see Figure 29.7, page 9 of Brunner and Kircher 2016).

High energy transfer rates can help address the second point to some extent by overcoming the efficiency disadvantage all powertrain concepts suffer compared with pure electric propulsion. While the energy transfer rate differs from energy density, the ability to transfer energy quickly allows greater vehicle utilization; this is important for commercial applications, especially HD applications. To reinforce this, compare the charging inefficiency of a battery with that of chemical energy transfer. Filling any tank when fugitive emissions are absent is a 100% efficient process, as is its discharge process. However, as mentioned above, batteries suffer from significant charging losses as well as losses on discharge, both of which must be thermally managed and represent an erosion of the useful energy transferred.

Hence, when the refueling rate is important, the attraction of hydrogen over electricity as an energy storage medium is clear. However, hydrogen also has an advantage in terms of the amount of energy that can be stored in a given vehicle platform, although this depends on the amount of energy to be carried. Regarding the automotive sector, Pearson, Turner, and Peck (2009) compared the capability of various energy vectors when the mass or volume of the entire energy storage system is included. In this setting, 700-bar pressurized hydrogen is about 10 times better than Li-ion batteries on a gravimetric basis and about 2.5 times better in volumetric terms. The corresponding values for liquid hydrogen storage are 10 and 5 times, respectively. This calculation was based on LD requirements. However, the advantage of hydrogen increases for applications necessitating a greater energy storage capability such as long-distance HD vehicular use. This is because battery mass and volume linearly follow the amount of energy stored, whereas the mass of a torispherical hydrogen tank system with a constant wall thickness is *not* linearly dependent on the mass of gas contained. For this reason, liquid hydrogen has traditionally been the fuel of choice for larger rocket applications. Specifically, hydrogen's very high lower heating value becomes an increasingly major benefit over hydrocarbon fuels as the proportion of mass attributable to the tank system reduces.

This overview suggests that hydrogen is expected to play a major role in long-distance transport, as the physical advantages of its greater energy storage capability and more rapid refueling surpass those of BEVs for zero-tailpipe-CO_2 emission propulsion. This provides the energy efficiency advantage of electric propulsion can be mitigated at the system level.

The remainder of this chapter discusses this point in greater detail. Using thermal conversion via combustion in engines versus electrochemical conversion in fuel cells (FCs) is first discussed.

An alternative to FCs in the chemical energy conversion of hydrogen

In this section, we compare the internal combustion engine (ICE) with the FC type most commonly proposed for automotive applications, namely, the proton exchange membrane (PEM) cell. Here, we do not examine solid oxide fuel cells (SOFCs), as we limit our discussion to more near-term possibilities. SOFCs, which can reach very high efficiencies when compounded by a gas turbine (GT; Azizi and Brouwer 2018), have been discussed in the context of larger applications, and the solid oxide fuel cell-gas turbine (SOFC–GT) hybrid system has even been analyzed for aeronautical use (Collins and McLarty 2020).

The chemical energy stored in the bonds of molecules can be liberated via two main pathways. One pathway is their combustion to release heat, which is then converted to work in an engine. Another pathway is electrochemically in an FC. Practically, the types of fuel energy converters in both ICEs and external combustion engines require oxygen to react the fuel with, which is conventionally sourced from the atmosphere. However, for brevity, only the ICE type is discussed here.

ICEs have a vast manufacturing infrastructure. Their cost-effectiveness, combined with the historical use of liquid hydrocarbon fuels, has ensured their position as the dominant prime mover for a wide range of power requirements. This is despite their relative immaturity compared with batteries and FCs, both of which significantly predate them. Nevertheless, they have two major disadvantages compared with FCs and batteries. First, because they convert thermal energy, they are subject to the limitation of Carnot cycle efficiency. This states that the maximum efficiency obtained from such a thermal system depends on the maximum and minimum cycle temperatures, as shown in Equation (1):

$$\eta_{Carnot} = 1 - \frac{T_{Low}}{T_{High}}$$

where η_{Carnot} is the Carnot cycle efficiency, T_{High} is the maximum temperature in the cycle, and T_{Low} is the minimum temperature in the cycle.

Conversely, as electrochemical devices, both the FC and the battery are ostensibly *not* subject to this limitation. Nonetheless, the efficiency of any subsystem attached to them to facilitate their operation will be limited by the Carnot cycle efficiency if they depend on a temperature change. However, since these subsystems do not represent the bulk of the energy flow, they have minimal effect on the efficiency of the entire system. Hence, the ICE, where all the energy is converted thermally, is immediately at a significant disadvantage thermodynamically.

Second, the combustion of fuels with oxygen is a high-temperature process (referring to Equation (1), arguably, the higher the better considering the Carnot limitation). This can give rise to nitrogen oxide (NOx) emissions. For hydrocarbon fuels, we must also consider unburned hydrocarbons, carbon monoxide (CO), CO_2, and soot (or particulate matter) emissions. However, since these are non-carbonaceous, they are all theoretically eliminated with hydrogen (although the undesired combustion of lubricating oil must be avoided). Unfortunately, hydrogen has a very high adiabatic flame temperature, which exacerbates NOx formation. This leads to an operational challenge, albeit one for which solutions exist (see the later discussion on engine operating strategies). Neither batteries nor FCs suffer from such problems. In particular, FCs do not suffer from these problems because the mass transfer and molecular recombination occur via an electrode. This precludes the involvement of nitrogen in the process, and the temperatures involved are far lower than those in an engine combustion chamber.

In a future in which hydrogen is a major energy vector, ICEs may be assumed to be at an inherent disadvantage, but this is not necessarily the case. In addition to their cost advantage and the fact that they can be manufactured from abundant and readily recycled materials, ICEs have several other benefits. Owing to the method of energy conversion, the primary output of an engine involves mechanical work, whereas, similar to batteries, FCs only produce electricity and heat. The production of mechanical power output in turn means that more efficient transmissions can be used in vehicles, with or without electrical hybridization. Thus, at the system level, ICEs can begin to reverse the situation. Even in the case of older vehicle technologies in US mid-size cars, Rousseau et al. (2008) estimated that a hydrogen ICE could compete with a PEM FC in terms of fuel consumption. It is interesting to note that these estimations were based on engine and hybrid vehicle technology that was advanced then but of the norm now.

In the United States, Argonne National Laboratory found that the peak stack efficiency of a 2017 Toyota Mirai PEM FC vehicle was 66% (Lohse-Busch et al. 2018). By contrast, the peak system efficiency (i.e., fuel energy to electrical energy, accounting for air supply system losses) was 63.7% at the same loading (Lohse-Busch et al. 2018).[1] The latter value is extremely impressive compared with ICEs, where reaching 55% is a research goal for the production of HD engines. However, as these peak efficiencies occurred at 5%–10% peak power, several points must be made:

1 The efficiencies of FCs drop off monotonically beyond their peak. At a 100% load, stack efficiency reduces to 48% and FC system efficiency to below 40%. While the latter is still impressive at the 90 kW peak power level produced by the Mirai FC, it is not significantly better than that of many diesel ICEs.
2 The peak efficiency for ICEs is 40%–50% of maximum power.

3 For FCs, tank-to-wheel efficiency falls significantly under the requirement for an electric-only transmission. If such a transmission were 90%–95% efficient, tank-to-wheel efficiency at maximum power would then be 36%–38%. This is an important point when considering HD applications, which habitually operate at a much higher proportion of full load.
4 A parallel hybrid transmission can readily be employed with ICEs. Not only is the engine's highest efficiency in a more useful area of the map, but a hybrid transmission can also help raise it.

Reporting for the US DOE, Kurtz et al. (2017) stated that system efficiencies are generally around 57% at one-quarter power, whereas this drops to 43% at peak power (see also Lohse-Busch et al. 2018). In 2021, Toyota launched a new Mirai, and the efficiency of its FC is claimed to be higher. For optimized HD applications, tailoring the FC efficiency curve would benefit its use in that application. However, for engines, efficiency rapidly increases with size, primarily because of reduced thermal losses and reduced friction owing to the necessary lower rotational speeds. This effect is particularly true when moving from road-going LD to HD applications. Finally, because of their high exhaust temperatures, ICEs have significant further potential in waste heat recovery, whereas there is virtually no such opportunity for PEM FCs. However, this is not the case for SOFCs, which are higher-temperature devices than PEMs, as discussed in the subsection titled "The SOFC–GT engine."

The foregoing shows that for HD vehicles in which the engines are generally larger, hybridized ICEs should have an opportunity to compete with FCs on an energy-efficiency basis. This is already the case for hydrocarbon fuels, but further opportunities exist when optimized hydrogen use in ICEs is considered, as is now discussed.

Research on using hydrogen as a fuel for automotive ICEs

Verhelst and Wallner (2009), Verhelst (2013), and Yip et al. (2019) provided excellent overviews of the use of hydrogen in ICEs, explaining the challenges, applications, and research gaps. In an earlier paper, Das (1990) stated that the first commercial application of hydrogen in transport was in the 1930s, predating when ammonia was first used for transport purposes (Valera-Medina et al. 2018). Ammonia is mentioned here because it is another non-carbonaceous energy carrier that can be synthesized from renewable energy and is considered to be a potential hydrogen carrier. However, it is not discussed further because while it may have some storage advantages, it is a noxious and poisonous gas and its combustion characteristics are worse than those of hydrogen.

Characteristics of hydrogen in engine applications

Hydrogen is a more interesting fuel than common hydrocarbon alternatives for many reasons. These include its very high laminar burning velocity (LBV) and very wide flammability limits, which range from 4% to 77% by volume in air.

Given these limits and its extremely low ignition energy, hydrogen is extremely hazardous, and significant precautions must be taken when using it (Verhelst and Wallner 2009). As a fuel, its characteristics provide both opportunities and challenges in typical ICE systems (see Tables 23.1 and 23.2) compared with methane and iso-octane. Methane is considered to be representative of a gaseous fuel, while iso-octane represents a typical liquid hydrocarbon fuel.

The LBV of hydrogen is approximately six times higher than that of typical hydrocarbons. At its stoichiometric air/fuel ratio is 34.08, its combustion is shorter than that of gasoline by a factor of approximately 2.5. Its very high LBV also means that its dilution tolerance is very high, allowing very lean combustion. Eichlseder et al. (2003) stated that operation is possible at $\lambda = 10.5$, which corresponds to the lean combustion limit. Conversely, the rich limit is $\lambda = 0.125$. As a consequence of the ease of operation beyond $\lambda = 4$, mixture quality control is possible over most of the engine operating map, although some throttling may be necessary at very light loads to stay within acceptable combustion stability limits. Throttling is also typically necessary for the so-called lambda leap to control NOx (see the later discussion on engine operating strategies). With respect to full-load operation, the extremely low density of hydrogen displaces significant quantities of air (29.6% at stoichiometry). While this concomitantly reduces power output in naturally aspirated engines with external mixture preparation, it serves as part of the ability to control load through mixture quality.

The disadvantages of hydrogen in spark ignition (SI) engine operation include its very short flame quenching distance, which means that heat transfer to the engine structure is greater in homogeneous combustion systems. This not only reduces

TABLE 23.1 Properties of hydrogen compared with methane and iso-octane.

Property	*Hydrogen*	*Methane*	*Iso-octane*
Molecular weight (g/mol)	2.016	16.043	114.236
Density (kg/m^3)	0.08	0.65	692
Mass diffusivity in air (cm^2/s)	0.61	0.16	~0.07
Minimum ignition energy (mJ)	0.02	0.28	0.28
Minimum quenching distance (mm)	0.64	2.03	3.5
Flammability limits in air (vol%)	4–75	5–15	1.1–6
Flammability limits (λ)	10–0.14	2–0.6	1.51–0.26
Flammability limits (ϕ)	0.1–7.1	0.5–1.67	0.66–3.85
Lower heating value (MJ/kg)	120	50	44.3
Higher heating value (MJ/kg)	142	55.5	47.8
Stoichiometric air-to-fuel ratio (kg/kg)	34.2	17.1	15.0
Stoichiometric air-to-fuel ratio (kmol/kmol)	2.387	9.547	59.666
Specific heat at constant pressure (MJ/kgK)	14.307	2.2537	1.7113
Gas constant R (kJ/kgK)	4.124	0.5182	0.0729
Ratio of specific heats γ	1.405	1.299	1.044

Source: Verhelst and Wallner (2009), with additional data from Ohio University (2021).

Data given at 300 K and 1 atm.

TABLE 23.2 Properties of hydrogen/air, methane/air, and iso-octane/air mixtures.

Property	*H2/air* ($\lambda = 1, \phi = 1$)	*H2/air* ($\lambda = 4, \phi = 0.25$)	*CH4/air* ($\lambda = 1, \phi = 1$)	*C8H18/air* ($\lambda = 1, \phi = 1$)
Volume fraction fuel (%)	29.5	9.5	9.5	1.65
Mixture density (kg/m^3)	0.850	1.068	1.123	1.229
Kinematic viscosity (mm^2/s)	21.6	17.4	16	15.2
Autoignition temperature (K)	858	>858	813	690
Adiabatic flame temperature (K)	2390	1061	2226	2276
Thermal conductivity (10^{-2} W/mK)	4.97	3.17	2.42	2.36
Thermal diffusivity (mm^2/s)	42.1	26.8	20.1	18.3
Ratio of specific heats	1.401	1.400	1.354	1.389
Speed of sound (m/s)	408.6	364.3	353.9	334.0
Air-to-fuel ratio (kg/kg)	34.2	136.6	17.1	15.1
Mole ratio before/after combustion	0.86	0.95	1.01	1.07
LBV, ~360 K (cm/s)	290	12	48	45
Gravimetric energy content (kJ/kg)	3758	959	3028	3013
Volumetric energy content (kJ/m^3)	3189	1024	3041	3704

Source: Verhelst and Wallner (2009).

Data given at 300 K and 1 atm (with the exception of the LBV, given at 360 K and 1 atm).

efficiency but also increases thermomechanical stresses. Stratified or diesel-type mixing control can address this. Further, owing to the very low ignition energy, preignition (PI) and backfire have historically been problematic, particularly with external mixture preparation, although means of addressing this have been devised (see the next section). Verhelst, Sierens, and Verstraeten (2006) discussed the conflation of knocking behavior with PI for hydrogen, deducing that while its octane numbers, particularly its research octane number, may be high, PI obscures the truth in many cases.

The following sections discuss how these fuel characteristics are pertinent to work investigating the use of hydrogen as a fuel in engines.

Engine performance and operating strategies with port-fuel injection (PFI; external mixture preparation)

BMW has long researched the SI of hydrogen/air mixtures, and its PFI research program resulted in a limited-production vehicle employing a bi-fuel approach, the BMW Hydrogen 7 (based on the then-current 760iL mass production model).

One hundred of these vehicles were produced between 2005 and 2007 (Wikipedia 2021). This bi-fuel vehicle, which used a 6.0-liter V12 engine with two separate fuel systems, was designed to offer the same performance when operating on gasoline or hydrogen (Kiesgen et al. 2006). While the gasoline fuel system used direct injection (DI), the hydrogen fuel system used PFI. Liquid hydrogen was stored in a cryogenic tank in the boot of the vehicle, which was developed to production-ready status (Amaseder and Krainz 2006).

Much of the historical literature on the application of hydrogen in SI combustion systems comes from BMW's extended research program and the Technical University of Graz. Freymann, Pehr, and Strobl (2002) discussed BMW's early work. Given the improvement in combustion because of the fast LBV and high knock resistance, Eichlseder et al. (2003) stated that external mixture preparation hydrogen engines generally have a maximum power capability of approximately 80% that of gasoline despite the high level of oxygen displacement. However, this disadvantage is offset by the ability to control load using mixture quality, thereby reducing filling time markedly. The V12 engine in the Hydrogen 7 vehicle also used BMW's Valvetronic mechanically variable valve timing system to control load. While this was necessary for gasoline operation, it was only used at part load with hydrogen and to facilitate changing operation between fuels. Within this engine, operating on hydrogen necessitated reducing the compression ratio (CR) from the standard production value of 11.3–9.5 due to abnormal combustion as well as using calibration strategies to minimize NOx emissions. Owing to the very fast combustion rates and desire to run at maximum efficiency, the CR may have been reduced to limit the peak cylinder pressure seen during operation.

These very fast combustion rates mean that if knock and PI can be avoided, optimal ignition timings are very close to top dead center, provided peak cylinder pressure limits are not exceeded. Regarding the Hydrogen 7, Kiesgen et al. (2006) stated that when using hydrogen at full load, the optimal ignition timing was only 1° before top dead center. This reflects the observation regarding the combustion duration above, which is partly responsible for the fact that the power output for a PFI hydrogen engine is more than the oxygen displacement would lead one to expect.

Tang et al. (2002), who discussed the problem of PI, backfire, and knock, operated Ford Motor Company's PFI hydrogen engine with three satisfactory CRs up to 15.3. Generally, very lean equivalence ratios had to be used to limit backfire, together with a reduction in valve overlap because the incoming fresh charge is essentially ignited by concentrations of hot residuals in the combustion chamber. This is a significant disadvantage of external mixture preparation, which the BMW Hydrogen 7 engine mitigated by using its Valvetronic system. This approach limited both valve overlap and intake depression, thereby minimizing residual retention and showing that modern variable valve systems can help significantly. Nevertheless, the introduction of hydrogen into the intake runner in the BMW engine also had to be optimized to stop fresh hydrogen passing through on overlap, as discussed by Kiesgen et al. (2006). Tang et al. (2002) reported brake thermal efficiencies (BTEs) of around 38% despite operating lean. Conversely, the valve train of the BMW engine enabled stoichiometric operation. However, the highest efficiency was around that reported by the Ford researchers (Eichlseder et al. 2003). The use of the stoichiometric air/fuel ratio was important for full-load exhaust after treatment (EAT), as discussed under the subsection titled “Emissions control.” The peak BTE reported by Tang et al. (2002) is similar to what a conventional SI engine operating on gasoline using DI would be expected to achieve. However, SI engines following Miller cycle strategies would be expected to be more efficient.

Not all ICE research in this area has been conducted with reciprocating engines: several Wankel rotary engines have been operated on hydrogen. However, the Wankel design is peculiar in that its operating cycle is laid out sequentially around the housing. Hence, the definition of external and internal mixture preparation becomes somewhat blurred, and this engine type is discussed separately in the section on the Wankel engine.

In summary, reciprocating four-stroke engines employing external hydrogen mixture preparation are severely handicapped by PI and backfire. Indeed, either lean operation at full load or extra complications in the valve train must be employed. Knock is arguably less of a restriction, although these two main forms of abnormal combustion have not yet been definitively separated. The BTEs achieved with this mixture preparation method are no longer acceptable even for LD engines operating on gasoline. This is definitely the case for HD vehicles, where competition with FCs is likely to be strong in the future. Many of the limitations of external mixture preparation can be eliminated using hydrogen DI. This enables different operating strategies and greater operational flexibility, as discussed in the next section.

Engine performance and operating strategies with DI (internal mixture preparation)

Several research groups have published content on hydrogen DI combustion systems. This mixture preparation approach eliminates backfire since hydrogen is not introduced into the working chamber until after the exhaust valves have closed. Moreover, the hot residuals are diluted by fresh air through the homogenization of the in-cylinder temperature. Furthermore, higher specific outputs can be achieved when the hydrogen introduction is delayed until after closing the intake valves (17% higher than gasoline for naturally aspirated engines; Wimmer et al. 2005). However, injecting when the intake valves are still open enables a degree of dethrottling as well. All these strategies have been disclosed and discussed by the BMW–Graz research group since 2003 (Eichlseder et al. 2003; Rottengruber et al. 2004; Wimmer et al. 2005).

Increasing BTEs was a driver of this research. With DI, higher CRs are permitted because of the delayed introduction of hydrogen. Wimmer and Gerbig (2006) showed that in conjunction with stratification, raising the CR to 16–18 should allow a hydrogen DI SI engine to rival the efficiency of a diesel engine (providing heat rejection can be reduced as well). Eichlseder et al. (2003) showed that a 50% BTE should be achievable with such an engine. They also stated that this would rival an FC in vehicles (at the time the article was published). They showed that part of this higher efficiency with DI comes from delaying the hydrogen introduction as much as possible. As shown in Table 23.1, this reduces the increase in compression work resulting from the significantly higher constant pressure of hydrogen compared with air (the value of hydrogen is 14.23 times that of air). Operationally, this delay in the fuel introduction is permitted by the very high diffusivity of hydrogen in air. Wimmer et al. (2005) reinforced the findings of Eichlseder et al. (2003) in this respect.

Interestingly, under high diffusivity, the DI of hydrogen appears to be relatively insensitive to injector targeting. Rottengruber et al. (2004) investigated different numbers of holes in a direct injector. Even one hole was shown to work well in homogeneous operation, indicating the magnitude of the diffusivity mentioned earlier. They also investigated the effect of reducing injection pressure from 150 bar (their default setting) to 45 bar. Important combustion metrics such as the position of the 50% mass fraction burned and the coefficient of variation of the indicated mean effective pressure were constant across this range and efficiency declined only slightly. This reduction could be due to the increased compression work resulting from the longer injection periods necessary to introduce the same amount of hydrogen and its high constant pressure, as discussed above. Being able to operate at a lower injection pressure means that more of the volume of a pressurized tank can be used and “limp-home” strategies are possible below the “normal” minimum tank (i.e., injection) pressure.

Later work by the University of Michigan and Ford also investigated the effect of injection timing on compression work. Further, it discussed the fact that pneumatic work is recovered with late injection timings (i.e., the gas does not expand into a lower-pressure cylinder only to have to be compressed again). Younkins, Boyer, and Wooldridge (2013) estimated how much of the 110-bar injection pressure they used could be recovered. However, they also discussed the extent to which injection timing influences the significant trade-off between stratification, NOx emissions, and heat losses. These aspects are crucial for maintaining efficiency when operating on hydrogen. If injection is delayed, most of the fuel can be combusted in a relatively rich kernel around the spark plug, reducing the heat rejection because of the very lean areas near the walls. However, this brings more of the mixture volume into high-NOx-generating regions (see the subsection titled “Emissions control”). Throughout their work, they operated at $\phi = 0.4$ to limit NOx (this being $\lambda = 2.5$, the equivalence ratio, ϕ, being the reciprocal of λ). Nonetheless, they still achieved a 47.7% indicated thermal efficiency with the second iteration of their engine that used an unusual combustion system featuring a central injector and two side-mounted spark plugs. This was markedly different from BMW’s typical approach, which was to close-couple the injector and spark plug in the center of the combustion chamber, as is now common in its gasoline DI systems. The earlier version of the Ford engine of Younkins, Boyer, and Wooldridge (2013) used the close-coupled approach and provided an indicated thermal efficiency above 46.5%.

The cylinder head layout of the earlier version of Younkins, Boyer, and Wooldridge's engine had been used by researchers at the Argonne National Laboratory. By correcting for single-cylinder friction, these researchers had achieved a maximum BTE of 45.5% and a BTE above 35% across 80% of their tested range (Matthias, Wallner, and Scarcelli 2012). The Argonne engine had a longer stroke than that of Younkins, Boyer, and Wooldridge's (2013) engine, which, using the same cylinder head, resulted in a higher CR and better surface area-to-volume ratio (SVR), presumably helping account for its higher BTEs. Thus, the Argonne engine exceeded the DOE's targets for LD hydrogen engines (Matthias, Wallner, and Scarcelli 2012). These results suggest that as hydrogen DI/SI combustion systems develop, BMW's 50% BTE target may be realistic if operations at higher CRs can also be achieved.

More recently, researchers at Bosch and TU Graz have published results based on a simple conversion of an SI engine in which they replaced the gasoline DI system with a prototype hydrogen one (Seboldt et al. 2021). This research engine also had PFI; however, when operating on DI, it yielded the highest BTE of 39%, which, with a relatively low CR of 9.8, is above that expected of an engine of this specification operating on gasoline. Furthermore, the coefficient of variation of the indicated mean effective pressure was excellent across the map, as was the combustion phasing. This work suggests that existing engines could be simply converted to operate on hydrogen, with the uptake of such engines then leading to more optimized ones.

Given that BTEs of 45%–50% are possible for LD engines, higher efficiencies should be possible for HD engines owing to their potential for lower heat losses (due to a better SVR). However, stratification will be required, and knock will likely become increasingly problematic with larger bore sizes. Hence, moving to the mixing-controlled combustion of hydrogen in a diesel-type constant pressure combustion system would be advantageous. While Yip et al. (2019) discussed this, the ignition of the plumes can only practically be achieved using a diesel pilot injection, as discussed earlier. The need for technology that allows the use of monovalent diffusion-burning combustion systems is discussed in the section titled "Research gaps and opportunities." With the excellent results in SI combustion systems, however, in-vehicle efficiencies for HD hydrogen engines that rival PEM FCs should be possible (see the next section). This is especially since these diesel-type combustion systems can be produced and post-treatment issues can be resolved (see the subsection titled "Emissions control").

Case study: hydrogen as a fuel for HD trucks

Hydrogen represents a major opportunity for ICEs, with this technology reaching a 47% BTE for HD applications (Mayr et al. 2021). The higher efficiency for hydrogen ICEs is comparable with that of other emerging technologies such as

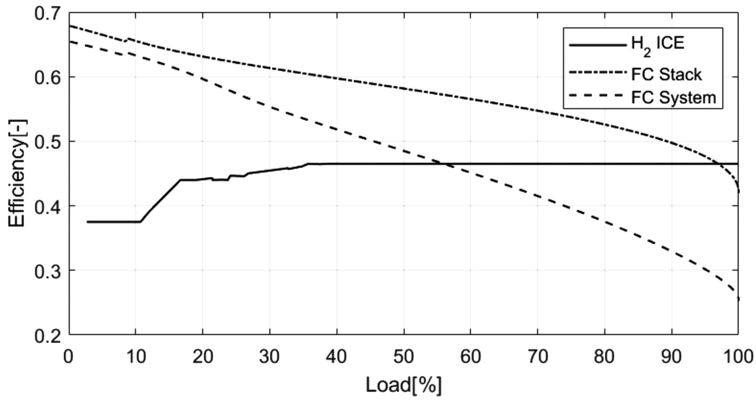

FIGURE 23.1 Hydrogen ICE, FC stack, and system efficiency for a HD truck.

Source: Authors.

FC powertrains. Recent studies of FCs have focused on automotive applications. These energy systems have shown potential efficiencies up to 60% (Lohse-Busch et al. 2018), and some vehicle manufacturers have built and tested working prototypes, including LD applications (e.g., Toyota Mirai) and HD road applications (e.g., XCIENT from Hyundai). Although FCs have high efficiency, their efficiency is highly dependent on load, decreasing by up to 30% at full load (including system auxiliaries such as pumps and compressors), as shown in Figure 23.1. By contrast, ICEs have high and almost constant efficiency at high loads, suggesting great potential for HD applications. Next, two powertrains, ICEs and FCs, are compared for an HD truck.

A full vehicle model is built for each powertrain (see Figure 23.2), and then the two are compared under real driving conditions, following a standard driving cycle for HD trucks. The full vehicle model used as a reference for the study is the Volvo FH4 truck in a 4 × 2 traction configuration with a load weight of 35,000 kg, as reported in Table 23.3. This model also includes a driver block to replicate the action of a real driver and follow the desired driving cycle. The FC model is based on a solid polymer electrolyte FC connected to a battery pack and then to a motor/generator to drive the truck. By contrast, the ICE powertrain is based on a series hybrid configuration. The ICE is attached to a generator connected to the battery pack, which finally powers the truck through a traction motor.

The FC model in this simulation is based on the solid polymer electrolyte FC reported by Lohse-Busch et al. (2018). This FC has 370 cells in the stack, reaching a maximum power of 114 kW, equal to the number in some HD prototypes (XCIENT from Hyundai; Linderl et al. 2021). On this scale, the fuel weighs around 100 kg and has a volume of 70 liters. The air and hydrogen supplies are modeled as a constant pressure source and the power consumption of the auxiliaries is modeled as a linear proportion of the electrical power consumption. The FC system is

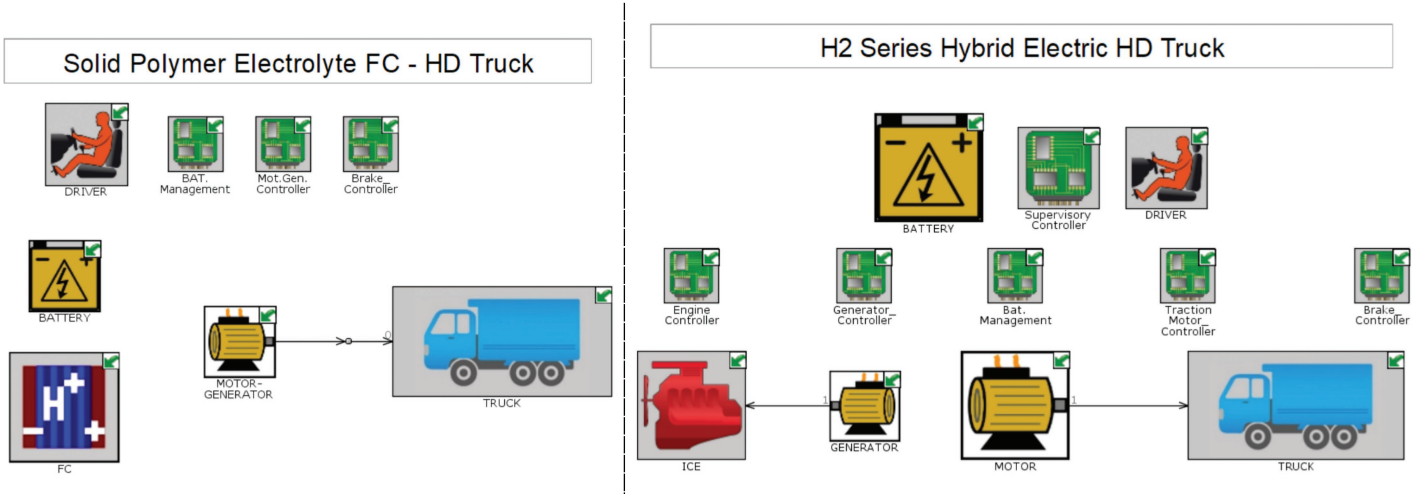

FIGURE 23.2 Simulation models: (left) FC powertrain, (right) hydrogen ICE series hybrid powertrain.

Source: Authors.

TABLE 23.3 Properties of the main simulation blocks for the two powertrains

Truck	
Reference	Volvo FH4
Drag coefficient	0.31 (–)
Traction	4 × 2
Load weight	35,000 (kg)
Battery	
Configuration	190 in series and 4 in parallel
Open circuit voltage	660 (V)
Capacity	400 (Ah)
Storage energy	263 (kWh) 950 (MJ)
Generator/Motor	
Max. power	210 (kW)
ICE	
Max. power	350 (kW)
Max. efficiency	46.5 (%)
Engine speed range	800–1,600 (rpm)
FC Stack	
Max. power	190 (kW)
Number of cells	620 (–)

connected to the battery pack with an open-circuit voltage of 660 V and a capacity of 400 Ah. Finally, a 210 kW electric motor receives the energy from the battery and drives the shaft of the truck.

By contrast, the ICE powertrain has a series hybrid configuration to improve the operating range of the engine efficiency. The ICE is a 13-liter engine running on hydrogen with a maximum output power of 350 kW (Mayr et al. 2021). This engine has a peak BTE of 47%, which is set as the operating region along with the whole operation of the powertrain. This reference engine uses the compression ignition principle coupled with a high-pressure DI system for hydrogen. Additionally, it may reduce NOx emissions by coupling with a customized post-treatment system. In this simulation model, the engine is coupled to an electric generator, which powers the battery pack. Then, the battery pack powers the traction motor that drives the truck. This aspect is the same as that of the FC powertrain for comparability purposes.

Both powertrains are tested under the same driving cycle to retain consistent conditions to improve comparability (see Figures 23.3 and 23.4). The selected driving cycle is the California HD cycle (Kasab and Strzelec 2020), which has a duration of 660 seconds and mixes low-load regions and high-load roads. This mixture allows us to compare the powertrains under large operating conditions, as shown by the power cycle in Figures 23.3 and 23.4. Additionally, the two simulation models aim to have a constant state of charge for the battery throughout the cycle, as shown in Figure 23.4. In these conditions, most fuel energy is

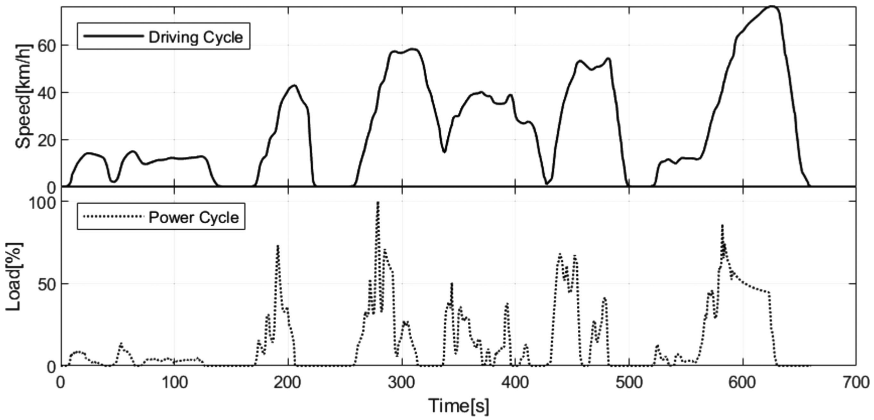

FIGURE 23.3 Driving and power cycles for the California HD legislation.

Source: Authors.

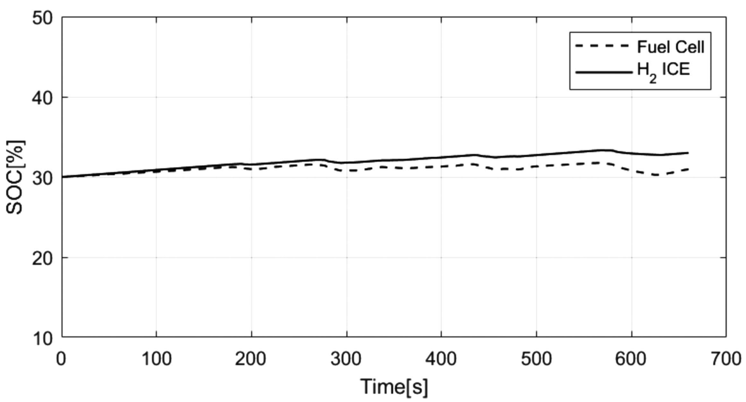

FIGURE 23.4 Battery's state of charge for the simulation of the two powertrains.

Source: Authors.

converted into traction energy on the truck, easing the energy flow and conversion in the two powertrains.

Figure 23.5 reports the efficiency of the powertrains. The ICE powertrain exhibits its higher efficiency than the FC powertrain. In this case, the simulated conditions with full load weight and constant state of charge (typical conditions for an HD fleet) represent a high-load condition for the powertrain. In the high-load region, the ICE has higher efficiency than FC powertrains with similar power requirement designs. A powertrain with an oversized FC (twice the reported power) could efficiently overcome the ICE powertrain. Nonetheless, from a technical and economic perspective, the size of FCs is incompatible with commercial purposes.

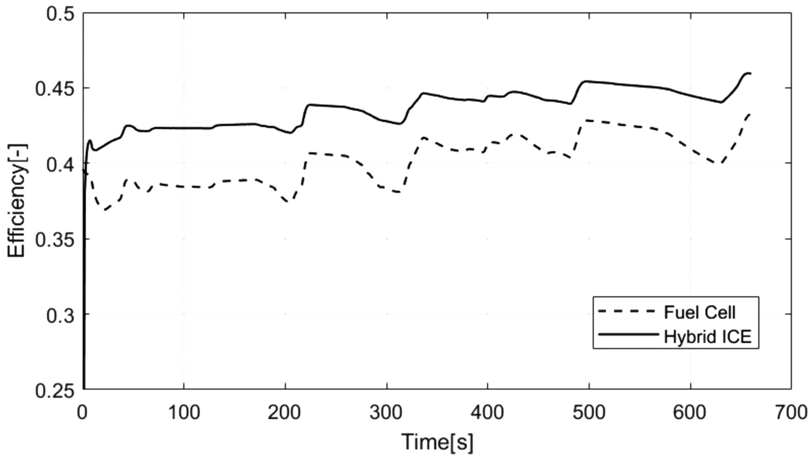

FIGURE 23.5 Powertrain efficiency throughout the California driving cycle.

Source: Authors.

Besides the higher efficiency in the high-load scenarios, ICEs have other benefits over FC powertrains. ICEs are considered to be a mature technology developed to the extent that they have low production prices and high reliability. By contrast, FCs still have some technical challenges to overcome before mass production, such as operating the cooling system of the powertrain at high loads. ICEs are also compatible with hybrid electric systems, which allow high-efficiency operation. One of the disadvantages of hydrogen ICEs is NOx emissions, which can be suppressed/controlled with the current technology, as discussed in more detail in the next section.

Emissions control

The ideal combustion of hydrogen would have no hydrocarbons, CO, or CO_2 emissions because no carbon would be involved in the combustion process. However, some combustion of the lubricating oil is likely. Fitting a catalyst suitable for stoichiometric operation could oxidize hydrocarbons and CO to water and CO_2 under all conditions assuming no rich mixture operation (i.e., lean to stoichiometric fueling only). Such a “three-way catalyst” (TWC), as termed in conventional gasoline combustion, could thus also be adopted for hydrogen engines. However, there would ideally be no emissions of two of the species such a catalyst usually converts. Because the oil consumption of modern engines is extremely low, original equipment manufacturers have had to address this issue to ensure emissions systems’ compliance over extended mileages. Hence, we do not discuss hydrocarbons, CO, and CO_2 emissions further except to state that the EU intends to mandate a limit of 1 gCO_2/km for a vehicle to be considered a zero-emissions vehicle. Owing to the amount of energy such a vehicle consumes, this limit would be harder for an HD vehicle to meet than for an LD one. However, this issue is expected to be overcome using modern piston rings and cylinder design. Recent work led by Bosch and TU Graz proposed a full EAT suite, including a particulate filter to eliminate any soot emissions from hydrogen ICE vehicles (Kufferath et al. 2021).

Consequently, NOx emissions are a challenge for hydrogen combustion in air. This is because its adiabatic flame temperature is high and the engine is habitually operated lean for optimal fuel consumption, as discussed above. Verhelst and Wallner (2009) found that operation at leaner than $\lambda = 2.2$ produces negligible NOx because the flame speed reduces due to the presence of excess oxygen, as shown in Figure 23.6. Operating at $\lambda = 1.3$ produces maximum NOx, approximately 2.7 times higher than that produced at $\lambda = 1$. The increase in NOx just lean of stoichiometric is due to the competition between increasing oxygen availability for its formation and a reducing gas temperature. This situation is not resolved in favor of declining heat availability until $\lambda = 1.3$.

Eichlseder et al. (2003) described research investigating the limits of operation and NOx emissions control; meanwhile, Berckmüller et al. (2003) and Rottengruber et al. (2004) discussed mixture preparation and emissions control, including the use of exhaust gas recirculation (EGR), which we discuss later in this section.

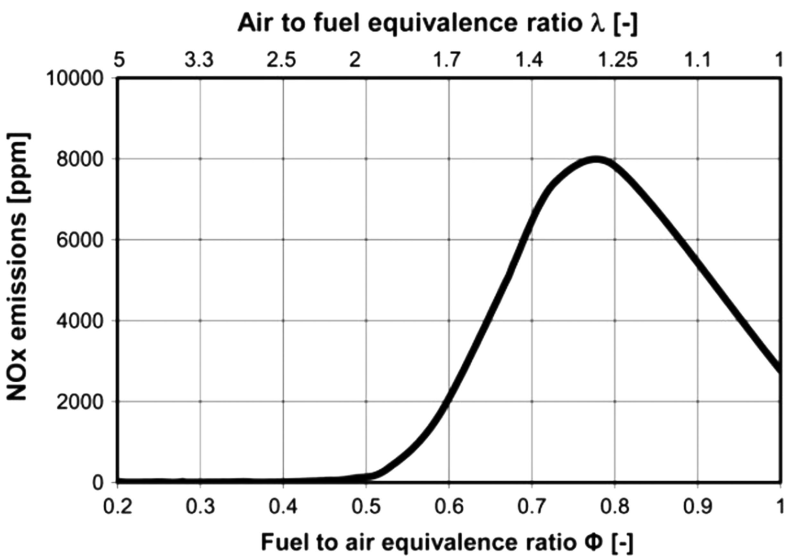

FIGURE 23.6 NOx emissions from hydrogen combustion in air compared with the air-fuel equivalence ratio λ and its reciprocal ϕ.

Source: Verhelst and Wallner 2009.

Stoichiometric operation permits the use of a TWC, which will itself not convert NOx in a lean gas stream, and near-zero NOx is emitted from the combustion chamber beyond $\lambda = 2.2$. Therefore, functionally, this necessitates a "leap" from one air/fuel ratio to another if maximum oxygen utilization is desired. This leap is problematic but achievable, especially when a variable valve train is fitted to the engine, as was the case with BMW's Hydrogen 7 engine. Kiesgen et al. (2006) described the control steps to ensure the switch is invisible to the driver. They also found that when operating at full load, the Hydrogen 7 engine reached $\lambda = 0.97$ (i.e., slightly rich) to provide excess hydrogen to reduce the NOx in the catalytic converter because hydrogen is a strong reducing agent. However, this does mean that some unburned hydrogen would escape into the exhaust system, leading to an efficiency penalty.

Kawamura et al. (2009, 2010) took a different approach to the EAT system. Instead of employing a TWC, they used a combination of a NOx storage reduction (NSR) catalyst in tandem with a diesel oxidation catalyst (DOC). This approach also used hydrogen as the reductant, but at a slightly lower fuel consumption penalty than Kiesgen et al.'s (2006) approach. Kawamura et al. (2009, 2010) reported a NOx reduction rate of 98% for an increase in hydrogen consumption of only 0.2%–0.5%. Although ammonia is usually used as a reductant in a selective catalytic reduction (SCR) system, hydrogen is a much stronger reagent in this respect. Hence, using the technology has less impact at the system level for a hydrogen vehicle than, for example, for a conventional diesel one. Nonetheless, reducing the fuel consumption penalty associated with employing it is clearly important. Naganuma et al. (2010) discussed how an NSR catalyst can be controlled by an occasional rich fueling spike within the engine. In counterpoint, Kufferath et al. (2021) recently proposed using an SCR system to control NOx, but with conventional urea used to reduce NOx. They argued that as SCR technology is now mature for diesel engines, the NOx loading rate would be lower for a hydrogen engine. Thus, further work is necessary to prove that using hydrogen as a reductant is as robust as using the now widely available "AdBlue" fluid.

Another means of controlling engine-out NOx emissions is to use EGR. Functionally, this is possible for the same reason that hydrogen engines can be operated at very lean air/fuel ratios: the very high LBV of the fuel means such engines will tolerate extreme dilution. Unlike the use of EGR in conventional SI engines, however, the operating strategy is more like that in diesel engines. This is because in a stoichiometrically operated SI engine, EGR is used as an inert diluent to maintain operation at $\lambda = 1$ to allow a TWC to function. Operation at $\lambda = 1$ is not always necessary for a hydrogen-burning engine because NOx emissions can be very low anyway. Thus, in a hydrogen engine with EGR, oxygen makes up a significant proportion of the gas being recirculated from the exhaust to the intake. Nevertheless, with EGR, operation much closer to $\lambda = 1$ is possible than with just air. Naganuma et al. (2010) showed that using EGR operation at $\lambda = 1.2$ is possible with significantly lower NOx emissions (up to 91%) than operation without EGR at $\lambda \leq 2.0$ in some areas of the operating map. In their work, while BTE reduced, this efficiency drop was presumably to some degree a result of the increased pumping work through the EGR loop. Importantly, they also investigated using an NSR catalyst and a DOC, the combination of which was capable of a further 92% reduction of NOx emissions.

Finally, one can use water injection to control NOx. Again, this water is a form of diluent. However, while there is a reduction in flame speed associated with the presence of water molecules in the combustion chamber, there is also a benefit in terms of base temperature reduction due to the latent heat of the liquid water. Hence, there are functional differences depending on how the water is introduced (i.e., indirectly via the intake ports or directly via a dedicated in-cylinder higher pressure injector). The latter is clearly more expensive to implement but ensures that the water vaporization effect occurs exactly where it is most beneficial. Water injection is arguably easier to implement for a vehicle fitted with a hydrogen engine, where there are no carbonaceous emissions that could lead to undesirable effects in the water harvesting, storage, and introduction systems. Böhm et al. (2016) discussed these issues for the application of the technology for a gasoline DI engine. They showed that the formulation of gasoline affects the condensate properties significantly. They added that acidity levels as high as pH 3 are possible for high-alcohol-content fuels (they stated that pH 5 is the minimum acceptable value). Straight condensation from the exhaust would seem more feasible for hydrogen engines. Clearly, the amount of water that can be injected is limited to less than that which can be harvested if an extra tank that has to be topped up by the operator is to be avoided.

Finally, the subject of catalyst protection must be addressed. As stated earlier, hydrogen combustion is very hot, with the heat flux to the catalyst concomitantly high, especially with operation at stoichiometric conditions. With gaseous fuels, the typical SI approach of fuel enrichment to limit exhaust temperatures will not work because such strategies primarily depend on the heat capacity of the unburnt fuel. Generally, slightly lean operation, with the unburnt oxygen absorbing some of the heat, can be used. However, this would put the engine into a high-NOx producing region, which a TWC would then not be able to process. BMW reported a strategy of switching a cylinder within a bank to the low-NOx range. Then, the resulting excess oxygen is available in the exhaust gas to bulk cool it before it strikes the catalyst. They reported that another cylinder (out of the six) could be switched, if necessary. Any power loss was considered to be equal to that potentially needed in extreme catalyst protection measures in a gasoline SI engine (Kiesgen et al. 2006). Although the BMW engine was naturally aspirated, it is assumed that such approaches would also be acceptable for turbocharged ones (in which the turbine is typically in front of the catalyst in the exhaust gas run). Future research on this should be conducted.

In summary, hydrogen combustion in engines presents many opportunities for reducing emissions. Those of hydrocarbons, CO, and CO_2 are eliminated (assuming lubricant consumption can be controlled), while particulate matter from fuel combustion is non-existent. Further, NOx, which easily forms since hydrogen combustion is very hot, can be controlled using the ultra-lean potential of hydrogen operation and relatively simple post-treatment systems. The latter can take advantage of hydrogen being an extremely strong NOx reductant, meaning a second fluid need not be carried for an SCR system. Further, the fuel consumption penalty is relatively low. Research in this area must aim to fully optimize such systems as well as determine component protection strategies. Nonetheless, emissions from hydrogen combustion systems seem to be entirely controllable.

Opportunities for applying hydrogen as a fuel for non-automotive engines

Generally, non-LD transportation applications must carry significant amounts of energy and often have a relatively controlled ecosystem in which they operate. The former makes the penalty of the non-linear mass/displacement trade-off of the tank system less of an issue as well as the fast recharge of hydrogen tanks significantly advantageous compared with batteries. Such a fast recharge can also limit the infrastructure challenge. Further, engines become more efficient with size. Hence, HD non-automotive applications of hydrogen engines have significant potential. Many universities and engine consultancies are announcing new projects related to hydrogen ICEs, with an emphasis on such HD applications.

HD off-road

On-road HD diesel engines, which typically have capacities of over 2.0 liters per cylinder, are targeting a BTE of 60%. Provided such levels can be achieved with hydrogen combustion, SI combustion in larger engines could then play a role. However, mixing-controlled diffusion burning combustion systems should be developed. While many of the characteristics of the fuel could be useful here, the challenge regarding NOx formation will still have to be surmounted. Some of the expected improvements will be hampered by the increase in fuel consumption associated with operating the EAT system. However, this is already accepted in many such applications with the complications of diesel SCR systems. Operating costs may also be affected due to the need to replenish AdBlue fluid in the emissions control system. Hydrogen operation could therefore be seen as a potential simplification.

Some applications for eliminating particulate matter emissions (e.g., in subterranean mining applications and warehouses) may be opened up by hydrogen engines. Until now, it has been assumed that such applications can only be serviced by FCs. As the size of machines increases, so does the efficiency of the larger engines necessary to power them. The ability to use mechanical transmissions with optimal hybridization may thus prove overwhelming compared with PEM

FCs. Research into the crossover point at which this occurs would be beneficial. However, assuming that parity can be reached, the engine would initially be expected to have a lower powertrain cost as well as reduced maintenance costs.

Railroad and maritime

Many of the points above apply equally to railroad and marine transport. As engines increase in size, the efficiency increase will become more important, as will the reliability associated with them. This advantage cannot be understated, especially in maritime applications, where replacing the propulsion system due to failures in the field is not viable for larger crafts. Although FCs could be made modular for swap-out purposes, the primary issue is that PEM devices are simply not efficient enough. The SOFC–GT hybrid system could be a longer-term potential prime mover for shipping. The efficiencies of this system are not only routinely predicted to be above those of large engines, but there is also the potential to have a mechanical power output for at least part of what is produced. However, until this technology matures, there is no real competitor to the ICE for marine use. Further, in addition to mitigating CO_2 emissions, it must be made considerably cleaner for emissions control areas. While hydrogen has advantages in combustion, ammonia is arguably a better energy carrier for marine applications. (Methanol may be ideal for marine use in that it is liquid, fully miscible with water, non-toxic to marine life, and can be stored easily aboard a vessel. However, the carbon used to make it would have to be sourced from the biosphere.)

Using waste heat recovery, ammonia could be converted into a mixture of hydrogen and nitrogen for use in an engine's combustion system, which could improve combustion. However, the complete conversion of two moles of (liquid) ammonia to three (gaseous) moles of hydrogen and one of nitrogen essentially makes this a hydrogen combustion system with extra nitrogen present. Hence, NOx emissions would need to be monitored closely. However, as discussed in the subsection titled "Engine performance and operating strategies with DI (internal mixture preparation)," ammonia or hydrogen could be used in an SCR post-treatment system to mitigate these emissions. Therefore, no extra fluids would have to be carried to achieve compliance in this regard.

The railroad application of the PEM FC is also being driven by emissions. For instance, Californian railroad emissions standards are being tightened considerably and are expected to reach Federal Tier 5 in 2025, severely limiting hydrocarbons, particulate matter, and NOx emissions (Hoffrichter 2019). Some of the technologies discussed above should allow adherence to all these limits using a combustion engine. Efficiency will then become the main issue. Since rail traction is generally performed using electric transmission, the FC now has an advantage over the ICE in this application for two reasons. The first reason is that it does not require a generator. Second, the associated losses are lower. Nevertheless, since locomotives generally operate at high power loadings, the efficiencies at those points do not make a compelling case for FCs (Kurtz et al. 2017). An opportunity for HD hydrogen ICEs might arise if the requirement to drive a generator can be offset by high engine efficiency such that the overall system efficiency is superior.

Aviation

While hydrogen has been used in rocketry, its use in conventional aviation is more restricted. Air-breathing hydrogen engines, however, are uncommon in aviation because small engines are not efficient enough for light aviation use. This is important because of the impact on how much hydrogen must be carried and the consequent mass of the storage system. Conversely, because they are more efficient at cruise speeds, PEM FC light aircrafts are being developed for short-range operation and applications where power must be modulated relatively quickly.

In larger applications, considering a long range, the SOFC–GT hybrid powertrain system is being studied for aviation use (also incorporating high-power battery usage), and these configurations promise very high efficiencies (Collins and McLarty 2020). Regarding fuel for combustion in aviation GTs, Pratt and Whitney successfully converted existing turbojet engines such that hydrogen can be used, as well as developed the Project 304 "Suntan" engine. This engine used a novel cycle in which liquid hydrogen was pressurized to 200 bar and then heated and expanded through a turbine to drive the engine's compressor (Mulready 2001). The remainder of the hydrogen not used for heating the heat exchanger was then burned in an afterburner. For more details, see Mulready (2001) on the Rae expander cycle and its novel approach to using the physical energy invested into hydrogen to make it storable.

Hydrogen is of interest in such aviation applications for a variety of reasons. When stored cryogenically, the very low temperature can be used to supercool motors and electronics to reduce conduction losses. As such, it offers a number of other benefits beyond being a zero-carbon energy carrier. Indeed, aircraft manufacturers such as Airbus are investigating how using liquid hydrogen as a fuel will allow or require changes in aircraft architecture, with real impetus behind its adoption in this domain (Airbus 2021).

Future potential of hydrogen in non-conventional engines

The Wankel engine

The potential synergies between hydrogen combustion and the Wankel engine have long been discussed (Salanki and Wallace 1996). The unidirectional nature of the rotor motion of the Wankel engine means that the four phases of the Otto cycle are spatially separated from each other (Yamamoto 1981). Being able to delay introducing hydrogen into the air until after the exhaust port has shut, thus eliminating backfire, is a potential advantage. Some hydrogen Wankel engines have employed a form of DI where the gas is introduced near the major axis. This approach takes advantage of the long intake phase (50% longer than that in a reciprocating four-stroke engine) and the fact that the injector is then shielded from maximum chamber pressure during combustion (Mazda 2021). Furthermore, the generally increased volumetric efficiency of the Wankel engine can compensate for the oxygen displacement effect of hydrogen owing to the porting arrangement and lack of valves. This also ensures that no hot exhaust valves exist in the combustion chamber to initiate PI and backfire. Instead of using one-piece injectors, dedicated hydrogen injection ports have been deployed (Salanki and Wallace 1996). Alternatively, Mazda's original HRX hydrogen rotary engine included a dedicated hydrogen intake port timed by a camshaft (Cranswick 2016). Hence, newly developed injection equipment offers advantages over the relative mechanical complication (compared with the simple Wankel engine) of using a dedicated extra mechanism.

The high LBV of hydrogen can overcome one of the problems of the Wankel engine, as it takes a very long time for the flame to traverse the long combustion chamber. This situation is compounded by the fact that the rotor is moving away from the advancing flame front. Using hydrogen leads to more rapid combustion and can also burn the mixture in the trailing part of the chamber more rapidly. The basic engine does, however, suffer from a very poor SVR. This combined with the short quenching distance of hydrogen means that the heat losses are likely to be significant, although this may actually help make the Wankel engine more tolerant to hydrogen. Salanki and Wallace (1996) cited Swain, Swain, and Adt (1988) in this respect.

The disposition of the operating phases around the periphery of the trochoidal housing can also permit more targeted cooling arrangements. In theory, the Wankel engine can readily adopt thermal barrier coatings, which could also help offset the heat loss issue (Kamo, Kakwani, and Hady 1986). These are all potential avenues for future research, as is perhaps the resurrection of the John Deere/NASA Direct Injection Stratified Charge (DISC) combustion system. Under this system, a pilot jet is ignited by a spark; this pilot then causes the main jet to ignite, combusting the fuel in a diffusion-burning manner. This would appear to be eminently suited to hydrogen combustion. Moreover, given that jets can be kept away from the walls, it might promise significantly improved efficiency. Modern computational fluid dynamics approaches could offer potential to assist in the optimization here.

In light of the above potentialities, after initiating a hydrogen rotary engine research program with the HRX, Mazda offered a Wankel-engined hydrogen RX-8 for lease in 2006. Instead of the eccentric shaft-driven camshaft used to time the introduction of low-pressure hydrogen into the working chambers, it combined DI and PFI (Mazda 2021). Mazda's offering just predated the BMW Hydrogen 7. A Premacy model with a series hybrid drivetrain powered by a version of this engine was also developed later. This suggests that the Wankel engine may be more easily converted to a hydrogen combustion engine than a reciprocating engine for all the reasons discussed in relation to both types. With further research, this could become an important option in the future, despite the current inefficiency of conventional gasoline versions. Nevertheless, significant potential exists for the Wankel engine, especially perhaps as a range extender engine for an electric vehicle. Another option would be a mixing-controlled combustion system such as the John Deere/NASA DI stratified charge arrangement, a more efficient device. In either case, further investigation is desirable.

The two-stroke engine

Synergies between the two-stroke cycle and hydrogen combustion

The two-stroke cycle is arguably better suited to road transport than the four-stroke, certainly when SI combustion is considered. This is because load control by throttling in the four-stroke increases pumping work considerably. By comparison, as the two-stroke lacks dedicated intake and exhaust strokes, it does not suffer from these losses. The disadvantage is that because of its poorer trapping efficiency, it is normal for two-stroke engines to lose charge down the exhaust. This increases both fuel consumption and emissions markedly in premixed charge engines.

DI can be used to offset these shortcomings by delaying the fuel introduction until after the ports close. However, a TWC cannot be used to convert NOx because some fresh air is inevitably lost, causing the catalyst feed gases to become lean overall. The two-stroke requires half the load from its complete cycle to match the torque of an equivalently sized four-stroke. This is a major advantage because the in-cylinder pressures and temperatures required to achieve the same flywheel output are lower, reducing NOx directly. Upon accepting that overall lean operation is an unavoidable factor and that hydrogen combustion is greatly simplified if it is constrained to lean conditions, a synergistic relationship between the engine and fuel appears. However, the reasons for this differ between the Wankel and hydrogen. While operating at $\lambda \geq 2$ in the cylinder necessarily reduces the output in each cycle, the twice as high firing frequency can mitigate this impact. Further, the same approach to NOx at higher loads can be used as that proposed by Kawamura et al. (2010), namely, adopting an NSR catalyst and a DOC. The fact that hydrogen combustion does not produce any emissions arising from the combustion of carbon (of course oil control must be robust) means that the emissions penalty of the two-stroke operating on conventional hydrocarbon fuels is eliminated by using hydrogen. Hence, the engine type and fuel appear to be peculiarly well suited, and further research is warranted. While heat rejection could remain an issue, a specific type of two-stroke engine could improve this significantly, as discussed next.

The opposed-piston two-stroke engine

This type of engine has exceptionally good thermodynamic properties, especially due to its very good SVR at top dead center (Wilson 1946; Pirault and Flint 2010). Further, with uniflow scavenging, the opposed-piston two-stroke engine can be expected to yield benefits in terms of trapping and exhaust lambda control (Turner et al. 2019). Its architectural problem, namely, that fuel and ignition have to be located on the circumference of the cylinder bore, is offset by the high diffusivity of hydrogen allowing it to mix more readily after introduction with its high burning velocity offsetting the position of the ignition source. Recall that Younkins, Boyer, and Wooldridge (2013) achieved higher thermal efficiencies using two spark plugs at the periphery of their engine's combustion chamber, while the injector was in the center. Mixing-controlled diffusion burning may also be simpler to achieve with the opposed-piston two-stroke scheme for two main reasons. The first is because of the high swirl maintained in the combustion chamber, and second, there is greater opportunity to direct fuel plumes across the chords of the cylinder within that swirling air flow. Further, since opposed-piston two-stroke engines typically have a larger swept volume, such a hydrogen-burning version could have potential for HD applications, from trucks to marine and stationary applications.

The free-piston engine

Besides all the advantages of combining the two-stroke cycle with hydrogen, free-piston engines (FPEs) generally use the cycle, meaning such a combination could form an excellent in-vehicle range extender. An FPE does not contain a cranktrain as such. The crankshaft and connecting rod are instead replaced by a "mover" that converts the expansion energy to work, with modern embodiments generally taking this work as electricity produced by a linear generator. Mechanical efficiency improves by removing side thrust and bearing friction, and there is an opportunity to vary top and bottom dead center positions, and with it, the CR. Van Blarigan and coworkers at Sandia National Laboratory proposed such a combination and conducted experiments to reinforce the adoption of hydrogen in a homogeneous charge compression ignition combustion system (Van Blarigan, Paradiso, and Goldsborough 1998; Goldsborough and Van Blarigan 1999). This system tends to result in highly reduced NOx emissions regardless of the fuel. Additionally, with the FPE's ability to vary its CR to control this, this could control NOx emissions within the combustion process. Indeed, a variable CR can allow sparkless combustion with a wide variety of fuels in two-stroke engines with conventional cranktrains. This is expected to be portable to FPEs in a similar manner to that reported by Sandia researchers (Blundell et al. 2010; Turner et al. 2010).

Overall, investigating hydrogen in two-stroke engine systems is highly desirable, especially if an opposed piston form could be made to work.

The SOFC–GT engine

In larger HD applications, the cyclic combustion engine should be capable of being developed to provide better in-vehicle fuel economy than a PEM FC. However, the same is not true in relation to the SOFC, particularly when it is compounded by a GT to create a SOFC–GT hybrid system. The SOFC operates at far higher temperatures than the PEM, which leads to operational challenges (i.e., very long start-up times). However, compounding it with a Brayton GT cycle (which can be either topping or bottoming) is logical. The higher operating temperature also means that the catalyst loading required for the electrochemical reaction does not have to be as high as it is in the PEM device, thus potentially providing some cost benefits.

Such SOFC–GT hybrid systems have been predicted to have extremely high thermal efficiencies (in terms of fuel energy into electrical power), with 65%–70% forecasted for larger applications (Cunnel, Pangalis, and Martinez-Botas 2002; Azizi and Brouwer 2018). These systems are being studied for a variety of larger applications, even with regard to aviation (Collins and McLarty 2020). In aviation, if liquid hydrogen is used, as mentioned above, there is an opportunity to use it to supercool electronics and motors and thus increase the efficiency of those components as well. Alternatively, when combined with a further steam bottoming cycle, overall efficiencies as high as 80% have been predicted (Azizi and Brouwer 2018).

This remarkable potential is a result of 80%–85% of the energy being converted electrochemically in the SOFC, a proportion therefore not limited in efficiency by the Carnot cycle. However, because SOFC–GT hybrid systems are high-temperature devices, a significant amount of high-temperature waste heat can be harvested by the compounding GT device. While the proportion of heat rejected is similar in the PEM and SOFC, it is very low grade in the PEM and essentially useless. The GT in a SOFC–GT plant instead produces 15%–20% of its total power. However, while the efficiency of this device is more limited, its contribution makes up a relatively small proportion of the overall contribution. Furthermore, the work from the turbine can be applied mechanically, which may raise in-vehicle efficiency if it can be used in such a manner.

When using hydrogen as the fuel, we can also envision an SOFC–GT hybrid power plant as part of an integrated power generation scheme in which renewable energy is used to electrolyze water. Moreover, the resulting hydrogen can be stored for later recombination in the power plant. The very high efficiency of the plant helps make this approach more practical. Hence, owing to its extremely high-efficiency potential, a SOFC–GT operating on hydrogen is worthy of further study.

Research gaps and opportunities

The foregoing discussion shows the vast potential for studying the use of hydrogen in combustion engines. However, some aspects require further research and development, primarily the fuel injection equipment. This must be of the DI type, since backfire and PI severely limit the potential in four-stroke engines and such DI equipment would be necessary for two-stroke engines anyway. Further, higher pressure equipment may be needed for mixing-controlled diffusion burning. The means of achieving this process should be researched because of the chance of increasing efficiency by reducing heat rejection and eliminating knock. However, this may require the development of high-pressure hydrogen pumps for some applications.

The two-stroke cycle engine merits study in conjunction with hydrogen since it promises greater efficiency and because of its synergy with hydrogen's combustion characteristics. The opposed-piston type would appear particularly well suited in many respects because of its beneficial heat rejection characteristics.

Post-treatment systems and control must also be analyzed further based on the operating strategy. In four-strokes employing a "lambda leap," the strategy will differ from that in engines that only ever operate lean to limit NOx emissions. In parallel, strategies to provide thermal protection for components in the exhaust stream need further investigation.

The opportunity to employ the Miller cycle (with a high expansion ratio) to limit knock would be worth researching. Another potential research direction would be to examine the use of water injection and associated water harvesting from the exhaust, especially whether the gathered water has a useful pH value. The issue of hydrogen building up in the crankcase also needs attention, as does whether it can be catalyzed on its way through the breather system. Moreover, with respect to very high energy conversion efficiencies in larger plants, the SOFC–GT hybrid system operating on hydrogen should be investigated further.

Finally, for larger applications that merit it, recovering some of the energy from storing hydrogen must be researched. Liquefying hydrogen or pressurizing it to 350 or 700 bar requires a significant energy input. As hydrogen's constant pressure is approximately 10 times that of air, a means to generate power from the process of feeding it from a tank to an engine system could improve overall vehicle system efficiency. This is at the root of the Rae expander cycle used in the Suntan engine, where the hydrogen turbine was considerably smaller than the air compressor to which it was attached. While energy systems use only the heating value of the fuel and overlook the associated physical energy, this can raise system efficiency at the expense of the hydrogen supplier.

Conclusion

This chapter reviewed many aspects of hydrogen as a fuel and its interaction with engines, specifically for HD applications. It was shown that with its use in combustion engines, in-vehicle efficiencies should be higher than those of a PEM FC. DI fuel systems will be a necessary technology to achieve this, with many further avenues to pursue once they are productionized. While post-treatment arrangements are understood, detailed work is needed to minimize the fuel consumption penalty associated with their operation. How best to apply any necessary component protection strategies to prevent them from being damaged by excessively high temperatures also demands future research.

There are interesting possibilities to improve in-vehicle efficiencies further as a result of the synergies between hydrogen combustion and alternative engine types. Among cyclic combustion types, the Wankel engine may have some potential, especially with mixing-controlled combustion systems. However, the two-stroke cycle could improve efficiency over its four-stroke equivalent, especially in the form of the opposed-piston architecture. Further improvements may also arise from using an FPE arrangement. This would have to be very high efficiency because it only generates electrical power in its modern incarnation.

A form of alternative engine that promises to significantly beat both the PEM FC and optimized HD engine is, almost ironically, another FC type. This is the SOFC–GT hybrid, for which extremely high efficiencies should be achievable. Operational challenges must be addressed due to the length of time it takes to heat up. Nonetheless, the potential efficiencies (around 65%–70% or higher) make attempting to address these worthwhile. The duty cycle of large ships would seem immediately suited to them, but they may also become practical for aviation. Stationary power generation as part of base load, perhaps employing hydrogen electrolyzed during the day using renewable power, also appears to be a significant opportunity.

Finally, we discussed the perceived research and technology gaps. This work shows the significant potential of hydrogen combustion engines, which could form an important part of the future technology mix for carbon-free transportation.

Abbreviations

BEV	Battery electric vehicle
BTE	Brake thermal efficiency
CO	Carbon monoxide
CO_2	Carbon dioxide
CR	Compression ratio
DOC	Diesel oxidation catalyst
DOE	Department of Energy
DI	Direct injection
EAT	Exhaust after treatment
EGR	Exhaust gas recirculation
FC	Fuel cell
FPE	Free-piston engine
GT	Gas turbine
HD	Heavy-duty
ICE	Internal combustion engine
LBV	Laminar burning velocity
LD	Light-duty
NOx	Nitrogen oxide
NSR	NOx storage reduction
PEM	Proton exchange membrane

PFI	Port-fuel injection
PI	Preignition
SCR	Selective catalytic reduction
SI	Spark ignition
SOFC	Solid oxide fuel cell
SOFC–GT	Solid oxide fuel cell–gas turbine
SVR	Surface area-to-volume ratio
TWC	Three-way catalyst
λ	Relative air/fuel ratio
ϕ	Equivalence ratio

Note

1 Low-temperature FC efficiencies are often quoted using the lower heating value of the fuel. However, this is not always the correct approach, since the exhaust temperature of a PEM cell is generally lower than the dew point of water. Therefore, the higher heating value should be used. For hydrogen, the ratio of the higher heating value to the lower heating value is the highest among that of all fuels, at 1.175, and this would cause a significant drop in quotable efficiency. While of little practical difference when the cost of operating a vehicle is considered, this remains a valid scientific point.

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