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Hydrogen combustion in piston engines: challenges and modeling approaches

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This article presents a comprehensive analysis of hydrogen combustion issues in reciprocating engines and the potential for numerical modeling in the context of developing low-emission technologies. The advantages and technical and environmental challenges associated with its use are presented, with particular emphasis on nitrogen oxides emissions, ignition control, and material requirements. This article takes a closer look at how advanced numerical modeling methods – such as computational fluid dynamics, large eddy simulation, and direct numerical simulation – help better understand the hydrogen combustion process in piston engines. These methods reveal flame behavior, combustion processes, and associated emissions. The authors compare various computational programs and demonstrate how simulation can aid in combustion chamber design, ignition timing, and mixture tuning. The article summarizes the most important findings in this field and outlines the direction hydrogen technology is headed. The analysis indicates that hydrogen addition (typically 10–30% by volume) can enhance combustion stability and indicated thermal efficiency under lean conditions, although excessive hydrogen fractions do not guarantee further performance gains. At the same time, challenges related to NO_x formation, pre-ignition, and mixture control require advanced injection strategies and precise combustion calibration. The reviewed studies confirm that high-fidelity numerical modelling is essential for capturing preferential diffusion and turbulence–chemistry interactions, making it a key tool in the optimization of hydrogen-fueled piston engines.

Key words: *hydrogen combustion, internal combustion engines ICE, numerical modelling, hydrogen-enriched fuels, CFD simulation*

1. Introduction

1.1. The importance of hydrogen as a fuel in the context of energy transformation

Contemporary transformations in the energy sector are driven not only by growing energy demand but also by the urgent need to reduce the impact of human activity on the natural environment. The depletion of fossil fuel resources and the greenhouse gas emissions associated with their combustion are driving the search for alternative solutions that can ensure energy security while also promoting the decarbonization of the economy. In response to these challenges, low-emission fuels such as biofuels, natural gas, and hydrogen are increasingly being utilized [38], which could play a significant role in shaping the future of energy.

Among all emerging clean-energy options, hydrogen stands out as one of the most promising. It combines high energy content, zero-emission combustion, and flexibility of use across industry, transport, and power generation, making it a strategic part of the global energy shift [61]. In 2024, world hydrogen use reached about 100 million tons – growth fueled more by overall economic activity than by climate policy. Even with stronger policy support, low-carbon hydrogen production may hit only 6 million tons by 2030, or roughly 10 percent of what's envisioned in the NZE 2050 scenario [48]. Hydrogen's role in the energy transition is clear, but unlocking its full potential will demand both new technologies and a broader, sustainability-oriented approach to future energy planning [74].

Due to the instability of renewable sources caused by weather conditions and seasonality, they cannot ensure a continuous energy supply at the desired level [59]. Therefore, systems for hydrogen production and storage are seen as a key element in the transition to emission-free energy technologies, replacing coal-fired power plants [39]. As the transition to climate neutrality speeds up, hydrogen is gaining attention as a strategic fuel for the future. By 2030, global demand could reach 150 million tons a year, with almost half expected to come from low-carbon production. Still, most hydrogen today is produced from fossil fuels, which emit around 920 million tons of CO_2 each year. Developing cleaner ways to produce hydrogen, such as renewable-powered electrolysis or carbon-capture reforming, is now one of the top priorities for decarbonizing energy and industry [48, 66]. In 2023, hydrogen consumption rose by 2.5%, hitting a record 97 million tons (Fig. 1).

Currently, China accounts for nearly one-third of global hydrogen demand, followed by the US at roughly 14%. The increase in global hydrogen demand has been driven mainly by its broader use in oil refining, chemical processing, and ironmaking via DRI technologies that utilize hydrocarbon-based syngas. Nevertheless, fossil-derived hydrogen still dominates production, mostly without carbon capture, resulting in nearly 920 Mt of CO_2 emissions per year – exceeding those of entire nations such as France or Indonesia [48].

According to the Net Zero Emissions 2050 scenario, hydrogen consumption is forecast to reach around 150 million tonnes annually by 2030. Approximately 45% of this total will come from low-carbon production routes, while roughly 40% of the growth will originate from emerging applications such as heavy transport, industrial decarbonization, e-fuel synthesis, and renewable-based power systems [48].

1.2. Hydrogen combustion characteristics compared to conventional fuels

Hydrogen, which produces only water vapor during combustion and no CO_2, has become one of the most promising alternatives to conventional fuels. Research interest in its use for powertrains has increased, especially in combustion and hybrid systems, where hydrogen offers a path to lower emissions without abandoning existing infrastructure. This trend is well-documented in the scientific literature, which emphasizes studies on the design, performance, and control of hydrogen-powered engines [70] and their implementation in hybrid configurations [4]. Comparative experiments involving spark-ignition engines operating on hydrogen and gasoline [56] demonstrate notable variations in efficiency, output performance, and pollutant emissions.

In addition, a growing body of work investigates hybrid engines operating on hydrogen-enriched conventional fuels [2, 3] and includes combined theoretical and experimental analyses evaluating these systems' effectiveness [62, 69].

Research consistently demonstrates that supplementing the intake charge with a hydrogen–oxygen mixture enhances energy efficiency and decreases CO and HC emissions, though it may simultaneously raise NO_x concentrations, particularly when used with low-ethanol gasoline blends [67]. At the same time, increasing research attention has been devoted to sustainable biofuels, which are now widely regarded as complementary energy carriers thanks to their advantageous combustion behaviour, often matching or even surpassing that of conventional fossil fuels [14]. Work in this area spans alcohols [7, 21], hydrogen [34], biogas [13], biofuels [28, 33], and dimethyl ether [45]. all of which display unique emission and performance profiles. Another promising line of investigation concerns nanoparticles [1], used as fuel additives, which appear to enhance flame propagation, improve thermal efficiency, and reduce pollutant concentrations.

Hydrogen's footprint in road transportation remains small but is expanding quickly. In 2023, global hydrogen demand for road transport reached approximately 60 kilotonnes, representing less than 0.1% of total consumption but marking a 55% increase from 2022. The most dynamic growth occurred in fuel-cell truck and bus fleets, particularly in China, where per-vehicle hydrogen usage is considerably higher than in passenger transport [48]. Data from 2021–2023 indicate that commercial vehicles – including trucks, delivery vans, and public buses – were the main drivers of this expansion, with hydrogen consumption nearly doubling over the course of one year. These results highlight that hydrogen currently has the greatest potential in high–energy–demand sectors of road transport, where continuous operation, practical refueling, and system efficiency best leverage its inherent advantages (Fig. 2).

Analysis of data from 2021–2023 clearly indicates that the increase in demand is primarily related to commercial vehicles. Although hydrogen consumption in the passenger car segment has been gradually increasing. In 2023, the largest share was accounted for by commercial vehicles including delivery vans and trucks, whose demand for hydrogen almost doubled compared to the previous year. The

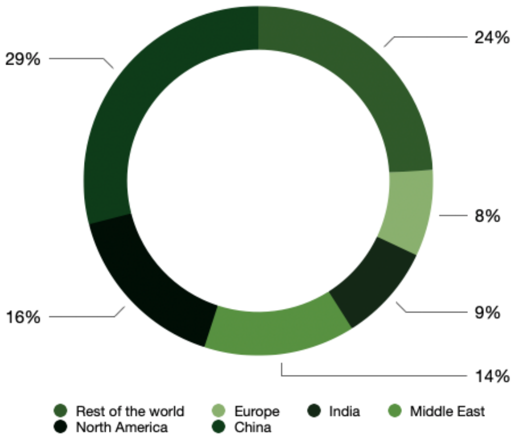

Fig. 1. Geographical differentiation of hydrogen consumption in 2023 [48]

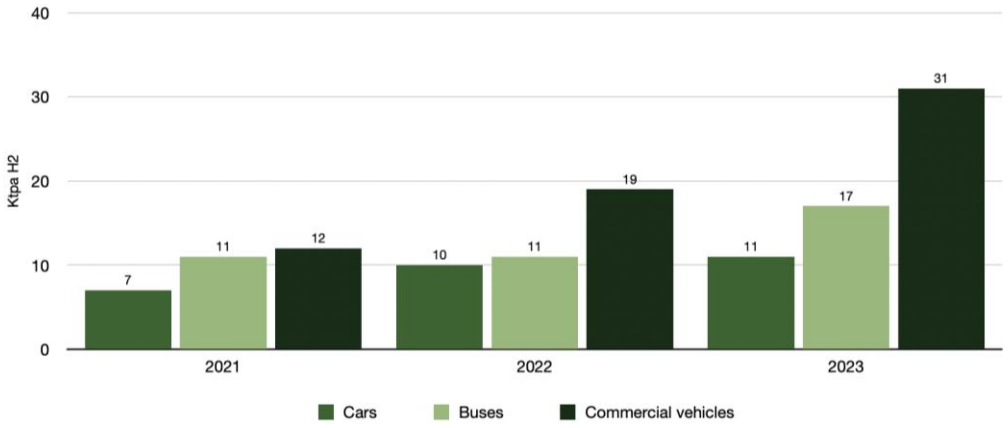

Fig. 2. Hydrogen consumption breakdown in road transport: global segment perspective [48]

bus segment also showed significant growth, reflecting the growing number of fuel cell-based urban public transport fleet projects (Fig. 2). These findings confirm that hydrogen use in road transport offers the greatest potential in sectors with high energy demands and intensive driving cycles, making buses and trucks the most natural and promising applications for this technology.

2. General overview of hydrogen as a fuel

2.1. Physicochemical properties of hydrogen affecting combustion

Hydrogen as a fuel has unique combustion properties compared to conventional fuels. Its very low ignition energy (approximately 0.02 mJ) and high combustion velocity (over 260 cm/s) make it possible to achieve ignition even with a small energy dose and in lean mixtures [19, 30, 69]. The high temperature of the hydrogen flame (approximately 2390 K) promotes efficient energy release, but can lead to increased nitrogen oxide (NO_x), emissions, requiring the use of combustion control systems such as exhaust gas recirculation or mixture cooling. [63]. Hydrogen, unlike traditional hydrocarbon fuels, does not emit carbon dioxide during combustion, making it an important contributor to efforts to reduce emissions in transport and the energy sector [30, 69].

Additionally, it is used as an admixture in alternative fuel blends, including methane (CH_4), biogas, LPG, CNG, ammonia (NH_3), and diesel fuel in dual-fuel solutions. Table 1 clearly shows that adding hydrogen, even in small to moderate amounts, has a strong positive effect on combustion. It leads to quicker ignition, greater mixture reactivity, and a faster-moving flame. When used with methane (CH_4), hydrogen allows the fuel to burn more rapidly and with less ignition energy. In ammonia-based blends, hydrogen serves to stabilize combustion by compensating for ammonia's low chemical reactivity, which results in smoother and more dependable engine operation. Likewise, in biogas-fueled setups, introducing H_2 increases the combustion rate and improves cycle-to-cycle uniformity. These effects are especially beneficial in micro-cogeneration systems, transport applications, and farm machinery. In dual-fuel systems (e.g., diesel–H_2), hydrogen as a secondary fuel not only reduces diesel consumption but also, thanks to its faster combustion, shortens ignition time. Table 1 shows that, regardless of the base fuel, H_2 admixture plays a key role in improving the efficiency and stability of combustion.

Fuel mixtures with hydrogen, so-called H_2-blends, are increasingly being analyzed as transitional solutions. Adding hydrogen to methane, biogas, LPG, or even ammonia significantly improves ignitability, increases flame speed, and combustion stability, which is particularly important in low-temperature engine operating conditions or in cogeneration technologies [47, 52]. Using hydrogen as an admixture not only reduces CO_2 and carbon monoxide emissions but also enables the combustion of more difficult fuels (e.g., ammonia) while maintaining stable engine operating conditions [52, 69]. Compared to conventional fuels, hydrogen blends demonstrate better combustion cycle repeatability, shorter ignition time, and the potential to significantly reduce harmful emissions [8].

Hydrogen also has an exceptionally high calorific value of approximately 120 MJ/kg, making it one of the most energetic fuels currently available [58]. For comparison, the calorific value of gasoline is approximately 44 MJ/kg, while that of natural gas is approximately 50 MJ/kg. Combustion of hydrogen with oxygen produces only water vapor, without the emission of carbon dioxide (CO_2), sulfur oxides (SO_x), or particulate matter [30, 31].

Due to its wide flammability range (4% to 75% by volume in air), hydrogen can be burned in very lean mixtures, making it an extremely flexible fuel across engine operating conditions [16, 30]. Moreover, hydrogen exhibits a high flame front velocity of approximately 2.65–3.25 m/s, several times higher than that of methane or gasoline. This property favors rapid and complete combustion (64), but in the absence of precise process control, it can cause undesirable phenomena such as combustion knock, flashback, or uneven reaction [69].

Storage and safety remain major limitations to the widespread use of hydrogen as a fuel. Due to its very low density under normal conditions, hydrogen must be compressed to high pressures or liquefied at low temperatures, which incurs additional energy and material costs [11, 15, 69]. Furthermore, hydrogen is colorless and odorless, and its very low ignition energy increases the risk of explosion in the event of a leak [11, 32, 67]. Despite existing limitations, hydrogen is a key element of the upcoming energy transformation. It is increasingly being treated not only as a fuel but also as an effective energy carrier and storage medium,

Table 1. Comparison of the physicochemical properties of hydrogen, methane, gasoline, and diesel [51, 57]

Property	Hydrogen	Methane	Gasoline	Diesel
Carbon content [mass%]	0	75	84	86
Density (at 1 bar & 273 K); [kg/m^3]	0.089	45.8	43.9	42.5
Molecular weight	2.016	16.043	110	170
Boiling point [K]	20	111	298–488	453–633
Auto-ignition temperature [K]	853	~813	~623	~523
Minimum ignition energy in air (at 1 bar & at stoichiometry) [mJ]	0.02	0.29	0.24	0.24
Stoichiometry air/fuel mass ratio	34.4	17.2	14.7	14.5
Quenching distance (at 1 bar & 298 K at stoichiometry) [mm]	0.64	2.1	2	–
Flammability limits in air [vol%]	4–76	5.3–115	1–7.6	0.6–5.5
Adiabatic flame temperature (at 1 bar & 298 K at stoichiometry) [K]	2480	2214	2580	2300
Octane number (R+M)/2	130+	120+	86–94	–
Cetane number [–]	–	–	13–17	40–55

capable of integrating various economic sectors: transport, energy, and industry [29]. Further progress, however, requires the development of production technologies such as electrolysis powered by renewable energy sources, the expansion of transmission and storage infrastructure, and the establishment of consistent safety standards [11, 72].

2.2. Selected technologies for the use of hydrogen in piston engines (blends)

Using hydrogen as an additive to traditional fuels in piston engines is currently considered one of the most promising solutions for reducing exhaust emissions, without requiring a complete modernization of the drive system. Hydrogen-fuel blends (H_2-blends) enable partial replacement of fossil fuels with gaseous hydrogen, reducing CO_2 and CO emissions while also affecting ignition and combustion characteristics. Due to its high reactivity, wide flammability range, and low ignition energy, hydrogen significantly alters flame front dynamics, enabling lean mixture operation and improving cycle repeatability. Depending on the base fuel used, such as methane, LPG, biogas, or diesel, various hydrogen injection strategies are used, including direct injection, sequential injection, dual-fuel systems, and premixing. To ensure stable, controlled combustion of the hydrogen-fuel mixture, it is crucial to properly develop a fuel strategy and optimize the component ratios. This helps avoid unfavorable phenomena such as combustion knock, flashback, and excessive NO_x emissions. Modern design processes increasingly use CFD numerical modeling, which enables detailed analysis of the mixture's behavior in the combustion chamber, accounting for the effects of geometry, turbulence, and gas residence time. The results of such simulations are essential for developing modern, efficient engines optimized for hydrogen fueling across diverse operating conditions.

Hydrogen as a fuel exhibits unique physicochemical properties that distinguish it from conventional hydrocarbon fuels [57]. Furthermore, its combustion rate in the engine chamber is approximately six times that of gasoline, resulting in a shorter combustion duration and reduced thermal losses. In mixtures of hydrogen with other fuels, especially gases such as methane or LPG, appropriate injection and ignition control strategies enable the exploitation of the synergistic properties of both components. Dual-fuel systems enable the adaptation of existing engines to co-combustion of hydrogen with a base fuel, but require precise control of stoichiometric ratio and ignition timing to avoid undesirable phenomena such as combustion knock, pre-ignition, or flashback [57, 74].

As shown in Table 1, hydrogen has unique physicochemical properties that significantly shape combustion in piston engines, particularly in dual-fuel systems. With its very low ignition energy (0.02 mJ) and wide flammability range (4–76% by volume), hydrogen is an exceptionally reactive fuel, capable of igniting even under conditions where traditional fuels fail. Its high flame temperature (2480 K) improves engine thermal efficiency but also increases the risk of NO_x emissions, requiring precise temperature and mixture control. Owing to its high stoichiometric air-to-fuel ratio [4, 38] and minimal flame extinction distance (≈0.64 mm), hydrogen supports very rapid combustion front movement, but also presents a higher risk of knock and flashback, notably in high-compression-ratio engines.

Its low density under normal conditions (0.089 kg/m³) limits the energy content per unit volume [MJ/m³], which is compensated for by appropriate design solutions, such as direct injection or systems operating at increased pressure [57]. Such properties require the use of advanced modeling methods, including CFD simulations, which include analysis of chemical kinetics, turbulence, and heat transfer, which allows for the prediction of the behavior of the fuel-air mixture containing hydrogen. To ensure high efficiency and low emissions with stable engine operation, precise optimization of the ignition strategy, combustion chamber shape and operating parameters is necessary depending on the type of base fuel (e.g. methane, LPG, diesel).

Controlling nitrogen oxide (NO_x) emissions remains a major challenge in operating hydrogen-fueled combustion systems. The inherently high flame temperatures of hydrogen promote NO_x formation; however, employing lean-burn mixtures, exhaust gas recirculation (EGR), and retarded ignition strategies can significantly lower emissions, keeping them within the limits of forthcoming regulatory standards. It is also worth emphasizing that hydrogen internal combustion engines (H_2-ICEs) are already close to industrial implementation, given their technological maturity and low dependence on critical raw materials, distinguishing them from fuel cell systems [4, 57].

The use of hydrogen-methane mixtures (so-called H_2–CH_4 blends) in piston engines allows for significant improvements in combustion parameters, such as flame propagation speed and shortened ignition delay time. The addition of hydrogen increases the heat release rate and shortens the time between ignition and the pressure peak, thereby improving the overall efficiency of the process. Studies show that even with H_2 contents of 10–40% by volume, flame speed can be increased by several dozen percent compared to pure methane [35]. Increasing hydrogen concentration not only accelerates the combustion reaction but also extends the mixture's ignition limits. Laboratory experiments have shown that the addition of H_2 shifts the maximum flame speed toward richer mixtures and broadens the φ range in both the lean and rich zones. For example, for a CH_4–H_2 mixture with 50% hydrogen, the ignition limit was extended from $\varphi = 0.5$ to $\varphi = 1.6$. This characteristic allows engines to operate under a wider range of load conditions [35, 62]. However, the technical aspects of combustion of such mixtures are complex and dependent on many parameters – pressure, initial temperature, gas composition, and combustion chamber geometry. Furthermore, the effect of pressure on flame velocity is not always intuitive; existing empirical relationships are subject to revision in light of the latest experimental data and CFD calculations. This demonstrates the importance of conducting further research both in laboratory conditions and in industrial-scale engines.

The introduction of hydrogen into natural gas fuel mixtures, known as HCNG (hydrogen–compressed natural gas), significantly alters their energy and combustion properties. As shown in Table 2, increasing the volumetric fraction of hydrogen from 10% to 30% leads to a gradual increase in the specific calorific value of the mixture (LHV [MJ/kg]), while simultaneously reducing the volumetric calorific value (LHV_{vol} [MJ/Nm³]). Increasing the hydrogen content leads to a lower volumetric calorific value and a slight decrease in the stoichiometric energy content of the mixture. This also increases the stoichiometric air/fuel ratio (AFR_{stoich}), meaning that more air is required for complete combustion. These modifications directly impact combustion process parameters and control strategies. Table 2 presents an analysis of the impact of HCNG mixtures on pollutant emissions, energy efficiency, and engine stability.

Table 2. NG and HCNG properties [30, 38, 55]

	Natural gas	HCNG10	HCNG20	HCNG30
H_2 [% vol.]	–	10	20	30
H_2 [% energy]	–	3.2	7.0	14.4
LHV [MJ/kg]	45.3	46.2	46.7	48.5
LHV_{vol} [MJ/kg]	36.0	34.3	31.7	29.2
AFR_{stoich} [–]	15.6	15.8	16.1	16.4

HCNG mixtures are being intensively researched as fuels for internal combustion engines, particularly in the automotive sector. Numerous analyses indicate that with an appropriate blend composition, CO_2 emissions can be reduced by up to 20–30% compared to gasoline, as well as significantly reducing particulate matter and nitrogen oxide emissions [37]. Furthermore, increased energy efficiency of the drive unit is observed, making HCNG fuels an attractive transitional solution on the path to zero-emission transportation. From a technical perspective, the presence of hydrogen in HCNG increases the laminar combustion velocity, requiring an adapted ignition strategy, including an earlier ignition timing to avoid efficiency degradation during the expansion phase [37]. Figure 3 presents the dependence of the laminar burning velocity on the equivalence factor (ϕ) for fuel-air mixtures containing hydrogen, based on data from various authors (Miao, Halter, Huang, Yu) [26, 27, 40]. The graph shows that the combustion velocity increases with ϕ, reaches a maximum in the range $\phi \approx 1.1–1.2$, and then decreases. This course indicates that hydrogen significantly improves combustion rate, especially at stoichiometric and slightly rich mixture conditions, which is important for engine efficiency and for optimizing ignition timing with variable mixture composition.

The presence of methane in HCNG blends helps maintain a smooth, stable combustion process while reducing the risk of detonation and flashback. Research shows that the best results are achieved when the hydrogen content in the blend is between 10% and 30%. This range enables better engine performance and safe, predictable system operation [36]. Road tests of dual-fuel vehicles have demonstrated that HCNG fueling results in lower fuel consumption [MJ/km], which translates into more uniform and stable combustion in subsequent engine cycles. Additionally, emission tests confirmed significant reductions in CO and HC emissions and lower NO_x levels compared to systems fueled with pure methane [37], making HCNG a viable alternative for commercial vehicles and stationary cogeneration units.

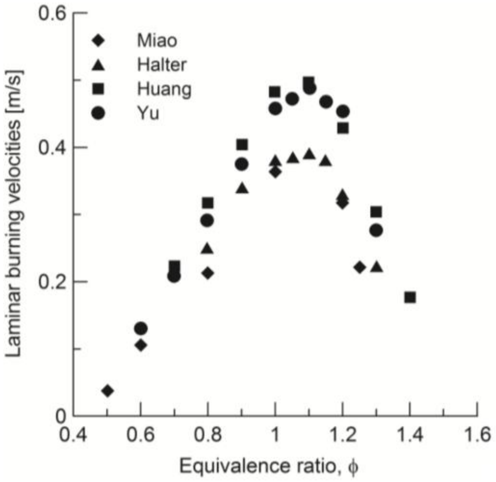

Fig. 3. Variation of unstreched laminar burning velocity with equivalence ratio (ϕ) for HCNG20 blend [37]

These results are confirmed by the analysis presented in Fig. 4, which illustrates the effect of the relative air-fuel ratio (λ) on the efficiency of an engine fueled with different fuel mixtures: pure natural gas (NG), HCNG10 (with 10% hydrogen), and HCNG20 (with 20% hydrogen). The measurement carried out at 3800 rpm, full throttle, and at MBT ignition advance showed that the addition of 10% hydrogen leads to a significant increase in engine efficiency compared to natural gas over the entire λ range [55]. At the same time, increasing the hydrogen content to 20% no longer brings additional benefits, suggesting that the efficiency improvement effect reaches a saturation point at higher hydrogen concentrations.

The influence of inert gas admixtures on hydrogen combustion in modern ignition systems is an important area of research for the development of emission-free propulsion technologies. One approach in this regard is the use of helium as a fuel mixture component, which allows for modification of the combustion process in turbulent ignition (TJI) engines. In the article [41], the influence of helium addition to hydrogen on the combustion process in a turbulent ignition (TJI) piston engine was analyzed. The studies were conducted on a single-cylinder AVL 5804 engine using H_2/He mixtures (from 100% H_2 to 60% H_2 with 40% He) at lean mixtures ($\lambda = 1.5–3.0$).

It was shown that increasing the helium content lowers the maximum combustion pressure, IMEP, and heat release rate, and also reduces the risk of combustion knock. For example, each additional 10% of helium resulted in an average 10% decrease in IMEP and up to a 75% reduction in combustion rate [41]. Further on, the authors analyzed the effects of hydrogen content, throttle opening, and excess air ratio (λ) on combustion characteristics. Figure 5 presents a three-dimensional map of these relationships, which indicates that increasing the hydrogen content in the fuel leads to the combustion of increasingly leaner mixtures (higher λ) and simultaneously increases the sensitivity of the process to changes in throttle position. Especially at H_2 content above 90%, small changes in the throttle valve caused nonlinear changes in IMEP–located in the lower part of the graph (blue).

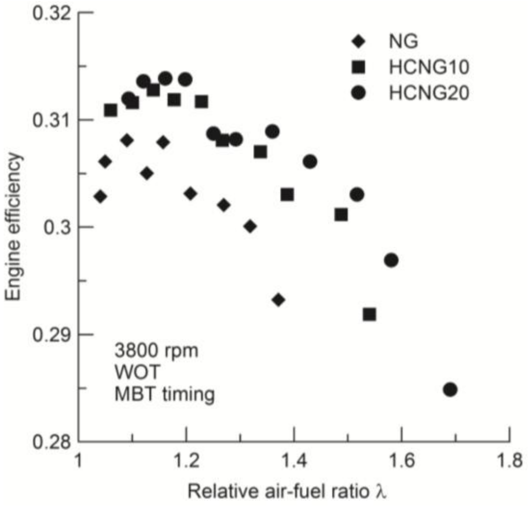

Fig. 4. Engine efficiency versus relative air-fuel ratio lambda for different fuels [55]

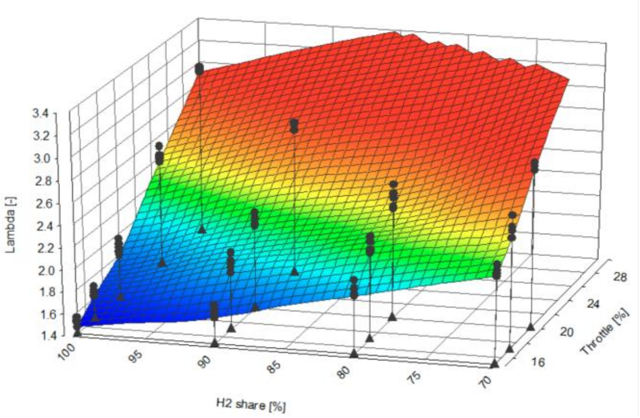

Fig. 5. Map of variations in the throttle position, hydrogen content of the mixture, and resulting excess air ratio (color-resulting excess air ratio; circles-excess air ratio values; triangles-projection onto the plane of λ-value) [41]

Research results show that both helium and hydrogen can effectively influence the combustion process. However, precise control of the mixture composition and throttle valve opening is crucial for the Turbulent Jet Ignition (TJI) engine to operate stably and efficiently when fueled with lean hydrogen mixtures.

The effect of hydrogen as a component of the fuel mixture manifests itself not only through changes in combustion dynamics but also through modification of the autoignition regime. In this article [17], a numerical analysis of autoignition was performed across various combustion systems, ranging from spark-ignition (H_2/CH_4) and compression-ignition (H_2/ON) engines to MILD technologies and detonation engines (RDE). The use of hydrogen results in a significant reduction in the mixture ignition time, but this effect is highly nonlinear and depends on thermodynamic conditions. The results of isolinear ignition delay analyses (iso-contours) showed that hydrogen can both accelerate and retard autoignition, depending on temperature and pressure, due to complex transition chemistry (e.g., the NTC effect in hydrocarbon fuels). This relationship is confirmed by the data presented in Fig. 6, which shows the effect of hydrogen in a methane (NG_2) mixture on the ignition delay time and the laminar combustion velocity under conditions typical of spontaneous ignition in a spark-ignition engine (T = 1000 K, P = 85 bar). Although pure hydrogen has a combustion velocity 6–8 times higher than methane, an increase in the hydrogen content to 50% only causes a two-fold increase in the mixture flame velocity. At the same time, a nonlinear but systematic decrease in ignition time is observed with increasing hydrogen content. The results confirm that the addition of hydrogen significantly changes the way fuel ignites. Therefore, this effect should be taken into account when developing combustion strategies and ignition calibration in engines operating on H_2/NG blends.

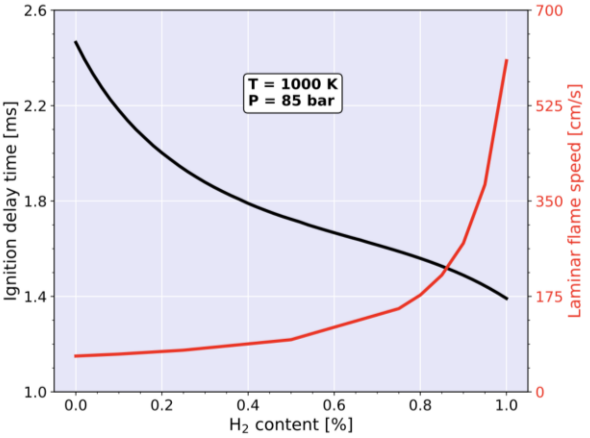

Fig. 6. Effect of hydrogen fraction in the H_2/NG_2 mixture on ignition delay time and laminar burning velocity under conditions characteristic of autoignition in a spark-ignition (SI) engine (T = 1000 K, P = 85 bar). A stoichiometric mixture (φ = 1.0) was used [17]

These conclusions are confirmed by DNS studies of hydrogen combustion under reheat combustion conditions, presented by Gruber et al. [23]. Numerical simulations in a diffusion-free system have shown that flame stabilization in the second combustion stage (e.g., in the two-stage system) can be achieved by spontaneous ignition. The key factor determining the reaction location and rate in this case is the inlet temperature of the reactants, not the mixture equivalence factor. Hydrogen reheat flames are highly sensitive to small temperature changes, which is associated with dynamic combustion instabilities and the potential occurrence of self-ignition waves in the velocity range between classical deflagration and detonation – the so-called spontaneous propagation zone.

As part of research on hydrogen co-combustion technologies in piston engines, a three-dimensional model of the Gasoline Direct Injection (GDI) engine was developed to analyze in detail the effect of hydrogen volume fraction (HVF) on combustion and emissions [18]. Simulation results showed that increasing the hydrogen content in the fuel mixture increases maximum cylinder pressure and heat release, accelerates ignition, and shortens combustion duration. It was also observed that, due to a higher OH radical content, combustion becomes more dynamic and approaches ideal isochoric combustion, which translates into an increase in the indicated efficiency (ITE). The highest efficiency increase (from 35.1% to 40.1%) was achieved with a 10% HVF and delayed ignition. However, the authors noted that too early ignition at low HVF can intensify combustion knock (KI > 3 MPa). Importantly, because hydrogen has a higher octane number, increasing HVF mitigates the mixture's susceptibility to autoignition. Ultimately, the work indicates that appropriate selection of HVF and ignition timing can optimize efficiency and reduce emissions while maintaining safe combustion in gasoline direct injection engines. Figure 7 illustrates that increasing HVF (up to 10%) increases ITE, particularly with delayed ignition (e.g., IT = 2°CA aTDC), while a decrease in efficiency is observed with premature ignition (e.g., IT = −11°CA aTDC). This effect highlights the importance of properly calibrated ignition parameters in engines burning gasoline-hydrogen mixtures.

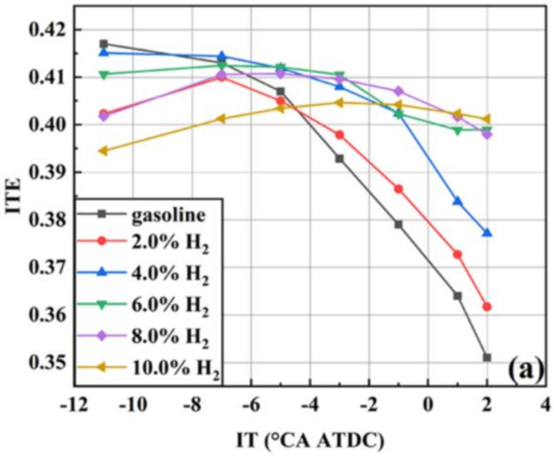

Fig. 7. Effect of hydrogen fraction in the fuel mixture (HVF) and ignition timing (IT) on the indicated thermal efficiency (ITE) of a GDI engine [18]

2.3. Technological and environmental challenges

The dynamic development of hydrogen technologies for internal combustion engines is driven by global efforts to reduce greenhouse gas emissions. Hydrogen-powered engines (H_2-ICEs) and versions powered by fuel blends, such as hydrogen with natural gas or gasoline, offer an alternative to traditional engines and fuel cells. Despite its many advantages – including the absence of CO_2 emissions in the TTW cycle, high calorific value, and rapid combustion kinetics the use of hydrogen poses numerous technical and environmental challenges. These require solutions for safety, combustion efficiency, NO_x emissions, and integration with the fuel infrastructure.

One of the main technological challenges with direct hydrogen injection remains precise control of injection timing and pressure. Late-cycle injection requires very high pressure up to 300 bar to overcome cylinder pressure and deliver fuel quickly. Injection too early leads to thermal losses and a too homogeneous mixture, while injection too late leads to incomplete fuel-air mixing, which increases NO_x emissions and reduces combustion efficiency [22]. Another limitation is that the displacement effect, the presence of hydrogen in the intake manifold, reduces the amount of air drawn into the cylinder, reducing volumetric efficiency. In conventional indirect injection (PFI) systems, additional boosting or cryogenic hydrogen injection is necessary to achieve performance similar to that of gasoline engines. Direct injection offers greater mixture control and shorter fuel preparation time, but it requires costly modifications to the fuel and control systems.

Adding hydrogen to gasoline in GDI engines improves combustion parameters by accelerating chemical reactions and increasing the proportion of active OH radicals. This shortens the ignition delay and overall combustion time. In practice, this translates into higher maximum cylinder pressure and thermal efficiency, which improve engine performance and reduce cyclic irregularities. However, increasing the hydrogen proportion in the fuel mixture can lead to early self-ignition, especially at advanced ignition angles. Additionally, despite improved knock resistance, the increase in combustion temperature with a high hydrogen content promotes NO_x generation, requiring the use of appropriate exhaust gas aftertreatment systems or lean combustion strategies [18].

In cogeneration systems, adding hydrogen to natural gas significantly alters the combustion process. At hydrogen contents up to 20% by volume, an increase in flame speed is observed, which shortens combustion time and allows for greater power with delayed ignition. However, excessive hydrogen content decreases mixture density, thereby reducing volumetric efficiency. At the same time, higher hydrogen content increases combustion temperature, leading to higher NO_x emissions. Furthermore, a shorter combustion process limits the recovery of exhaust heat energy in turbines. Therefore, it is necessary to appropriately adjust the ignition strategy and use a lean mixture to balance emissions and engine efficiency [9].

Although hydrogen is a clean fuel, its use in engines poses technological challenges, including pre-ignition, flashback, and the risk of leaks. Advanced materials resistant to operating conditions and appropriate safety systems are essential. Furthermore, producing "green" hydrogen requires significant capital expenditures, and its storage and transportation (e.g., at 700 bar) remain economically and technologically challenging. Due to hydrogen's high combustion temperature, nitrogen oxide emissions are a major environmental concern. The use of ultra-lean combustion, exhaust gas recirculation (EGR) systems, and SCR catalytic converters using hydrogen alone as a reducing agent can significantly reduce this problem, but requires precise control and matching the combustion strategy to load conditions [6].

The biggest problem with hydrogen-powered cars (H_2–ICE) is not the engine itself. Hydrogen requires special stations and tanks, which are expensive and must meet very stringent safety standards. Therefore, despite the ready-made technology, its widespread use is currently difficult. There is also the issue of safety, as hydrogen is highly flammable, so ventilation systems and leak detectors must be installed. Nevertheless, hydrogen has its advantages, H_2-ICE engines do not require rare metals and can be produced in existing factories, making them an excellent interim solution until zero-emission transport becomes the norm [70].

For engines to run on hydrogen, significant design changes are necessary. These factors impact not only the intake and exhaust systems but also the ignition method, the materials used, and the control systems. Properly selecting injection pressure and ignition timing is particularly crucial, as hydrogen has a very low ignition energy and is prone to premature combustion, which can damage engine components. From an environmental perspective, NO_x emissions remain the biggest problem, as they increase with increasing combustion temperature. Solutions could include lean fuel mixtures, modern exhaust gas aftertreatment systems, and hydrogen as a reducing agent in SCR catalytic converters. However, the effectiveness of these methods depends on precise engine control and compatibility with existing fuel infrastructure [38]. Although hydrogen has enormous potential as a future fuel, hydrogen-powered engines are not as volumetrically efficient as conventional gasoline engines. This is because hydrogen, in its gaseous state, has a lower energy density, and in indirect injection systems it occupies part of the space intended for air. As a result, the power of such engines is usually somewhat lower, especially under heavy load. Their advantage, however, is the ability to operate on very lean mixtures, which reduces nitrogen oxide emissions. The problem is that this makes it more difficult to maintain stable combustion and avoid knocking. Therefore, increasingly advanced combustion control and modeling systems are needed to fully utilize hydrogen's potential [69].

Table 3. Summary of the main technical and environmental challenges associated with the use of hydrogen in internal combustion engines and potential directions for their mitigation [6, 9, 18, 38, 51]

Challenge	Potential solution
Pre-ignition and flame backflow	Delayed ignition, advanced injection control
High NO_x emissions in richer mixtures	Lean-burn strategy, EGR, H_2-SCR systems, and NSC catalysts
Poor hydrogen–air mixing	High-pressure direct injection and stratified mixture formation
Lack of hydrogen refueling infrastructure	Expansion of the H_2 station network, public support
High hydrogen storage pressure	Advanced Type IV composite storage tanks
Increased wear and corrosion of engine components	Protective coatings, optimization of cooling systems
Complex material requirements for injection systems	Use of resistant materials and lubricants
Secondary emissions: N_2O and NH_3	Advanced exhaust gas after-treatment systems
Lack of standardized norms and regulations	Development of harmonized international standards
Pollution from hydrogen production based on fossil fuels	Development of ICE electrolysis and green hydrogen production

Table 3 presents the main technological and environmental challenges associated with using hydrogen as a fuel in piston engines, both in single-fuel systems and in blends. It addresses typical issues related to hydrogen combustion, such as the risk of pre-ignition, difficulties in properly mixing fuel with air, and demanding material requirements for injection system components. Additionally, it summarizes possible directions for technical and system solutions. The table also considers non-engine factors, including limited availability of hydrogen refueling infrastructure, secondary emissions (N_2O, NH_3), and the impact of its production method on the actual carbon footprint. Implementing the solutions presented in the table, including direct injection, advanced cooling and exhaust gas aftertreatment systems, and the development of green hydrogen production, can significantly increase the technological maturity and environmental efficiency of H_2ICE engines. However, these actions require close cooperation among industry, research institutions, and decision-makers, particularly in regulatory harmonization, component certification, and infrastructure development.

3. The role of numerical modelling in the analysis of hydrogen combustion processes

Numerical modelling is currently a key tool in the analysis of hydrogen combustion processes in piston engines. Due to extremely short chemical reaction times, high flame propagation speeds, and the strong dependence of ignition mechanisms on local conditions, the use of experimental methods that fully capture these phenomena is often limited. Simulation tools not only allow for the reproduction of engine operating parameters under various operating conditions but also enable the analysis of temperature distributions, mixture composition, NO_x formation, and flame front propagation with very high accuracy. Models based on chemical kinetics mechanisms and CFD techniques are particularly important, as they allow for the representation of the complexity of reactions occurring in real time, including the spatial distribution of thermodynamic and flow phenomena.

Currently, numerical modelling is one of the most important tools for studying hydrogen combustion in piston engines. Due to the very rapid chemical reactions, high flame propagation speed, and the strong influence of local conditions on ignition, traditional experiments do not always fully capture these processes. Computer simulations enable the analysis of engine operating parameters under various conditions and the precise tracking of changes in temperature, mixture composition, NO_x emissions, and flame propagation. The choice of software depends on the nature of the given study or application. Each available program has its advantages but also limitations, both technological and cost-related.

AVL FIRE is one of the most accurate combustion simulation tools available. It enables the analysis of complex engine phenomena, works with GT-Power, and supports a wide range of fuels, including hydrogen and its blends. This allows for the study of emissions and combustion behaviour under various operating parameters. The program's drawbacks include high licensing costs and demanding hardware requirements. GT-Power, on the other hand, is primarily used for one-dimensional analyses. It features an intuitive interface, a large component library, and the ability to interface with 3D solvers. GT-Power's limited ability to reproduce local physicochemical phenomena poses a significant challenge when conducting detailed analyses of hydrogen combustion.

ANSYS Fluent, on the other hand, thanks to its flexibility and advanced CFD modelling capabilities, is one of the most widely used and recognized tools for hydrogen combustion simulation. It allows for the consideration of real-world geometries and complex boundary conditions, but its use requires extensive experience and significant computa-

Table 4. Comparison of selected simulation tools used in combustion modelling in hydrogen-fueled piston engines – summary of key advantages and limitations of AVL FIRE, GT-Power and ANSYS Fluent [25, 43, 64, 68, 73]

Software	Advantages	Limitations
AVL FIRE	– Advanced combustion modelling – Integration with GT-Power – High accuracy – Support for various fuels (hydrogen, ammonia) – Extensive emissions and fuel consumption analyses – Professional technical support	– High license cost – High hardware requirements – Steep learning curve for beginners – Less flexibility than open-source tools – Time-consuming simulation setup – Smaller user community
GT-Power	– Fast 1D simulations – Integration with AVL FIRE and ANSYS Fluent – Full powertrain system analysis – Rich component library – Support for various fuels – Intuitive user interface	–Limited accuracy of 1D models – High license cost – No full 3D modelling capability – Dependence on other tools for detailed analyses – Requires highly accurate input data – Limited model flexibility
ANSYS Fluent	– Advanced CFD modelling capabilities – Dedicated hydrogen combustion models – High flexibility and customization options – Integration with other ANSYS tools – Large user community and extensive documentation – Support for HPC (High-Performance Computing)	– High license cost – High hardware requirements – Steep learning curve – Time-consuming model preparation – Challenges in modelling certain physical phenomena – Strong dependence on accurate data for stratified mixture formation

tional resources. Therefore, the selection of a simulation tool should always be preceded by an analysis of the research goals, available resources, and the required accuracy. These simulation tool features are summarized in detail in Table 4, which compares the advantages and limitations of the three most commonly used programs: AVL FIRE, GT-Power, and ANSYS Fluent. This comparison provides a practical reference point when selecting software for a specific type of hydrogen combustion analysis in piston engines.

When modelling hydrogen combustion, transport phenomena arising from its characteristic properties are particularly important, especially preferential diffusion, which affects flame stability and structure. To obtain more accurate and realistic simulation results, advanced computational methods such as LES (large eddy simulation) are increasingly being used. The article [29] presents a modern approach to modelling hydrogen combustion, taking into account this phenomenon, which plays a key role in hydrogen combustion processes. Based on the results of one- and three-dimensional simulations, LES conducted for a low-vortex, lean H_2/air mixture, the authors demonstrated that the traditional FGM (Flamelet-Generated Manifold) method has limited ability to reproduce the essential properties of the combustion field. The use of an extended version of FGM-PD (taking into account preferential diffusion) not only allows for more accurate representation of temperature distributions, mixture fractions, and main chemical species but also enables the reproduction of characteristic flame structures, such as the "finger-shaped" distributions of the OH radical mass fraction, observed experimentally.

Figure 8 shows how the classic FGM method (left) differs from the extended FGM-PD method (right). As shown in Fig. 8, the classic FGM and its advanced variant, FGM-PD, reveal notably different flame behaviours. The OH radical mass fraction patterns demonstrate how FGM-PD captures a far more complex and uneven structure. From experience, this irregularity makes perfect sense, flames are rarely steady, twist, and fluctuate in reality. The root cause lies in unequal diffusion rates, especially hydrogen's, because its low Lewis number disrupts the local balance and alters how reactions evolve at the flame front [29].

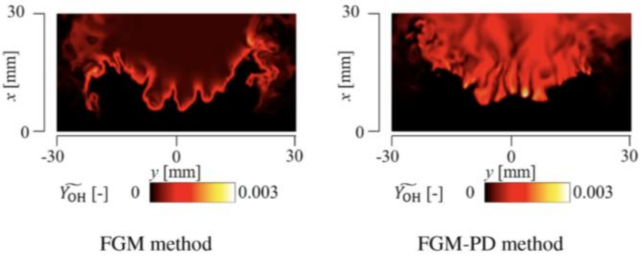

Fig. 8. Comparison of the OH radical mass fraction distribution ($\tilde{Y}_{oh}$) obtained using the classical FGM approach and the modified FGM-PD method accounting for preferential diffusion effects for an H_2/air mixture (cross-section in the plane z = 0 mm) [29]

Mixing hydrogen and air efficiently in direct-injection systems remains one of the hardest nuts to crack for engineers seeking clean, powerful combustion. The intake port's shape and airflow dynamics determine whether the mixture burns evenly. In article [71], simulations with CONVERGE were used to explore how different intake geometries affect mixture uniformity. The numerical predictions closely matched the experimental results. The authors also discovered that an optimized tumble plate increased the tumble ratio – in simple terms, it improved air swirl – leading to improved mixing before ignition. Figure 9 shows this vividly, with higher flow velocities observed in the modified design in both CFD and experiments. Such an agreement demonstrates the value of good modelling in developing efficient hydrogen engines. On top of that, the study identified how the pre-chamber couples with the main combustion chamber – insights that would be nearly impossible to pinpoint through experimental work alone.

In HCCI engines, where the mixture ignites spontaneously, the use of hydrogen as a fuel requires very careful analysis. The combustion process is exceptionally complex and strongly dependent on initial conditions. Therefore, research employs detailed chemical reaction models and three-dimensional CFD simulations, which allow for precise analysis of how the mixture composition and the reaction course change over time. Article [32] provides an example of the application of three-dimensional CFD modelling with an extended chemical kinetics mechanism to analyse hydrogen combustion in a homogeneously charged compression ignition (HCCI) engine. The main goal of this work was to investigate the influence of parameters such as swirl intensity, intake temperature and pressure, compression ratio, and equivalence factor on ignition characteristics and combustion behaviour. The model, developed using the KIVA3 code, enabled precise real-time analysis of the spatial distributions of temperature, pressure, velocity, and turbulence kinetic energy. The detailed kinetics of the hydrogen oxidation reaction enabled consideration of local phenomena, such as elevated-temperature zones that initiate ignition.

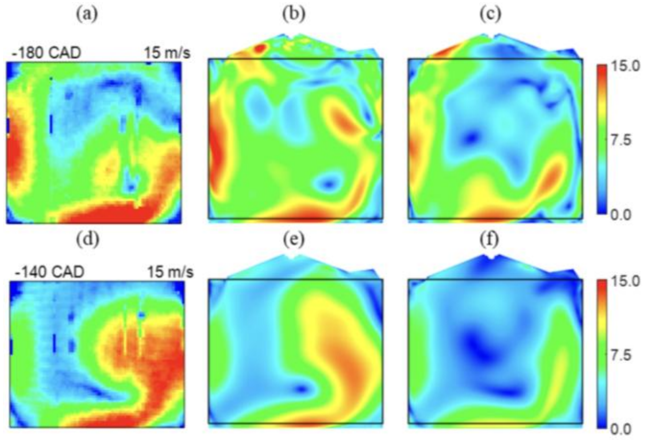

Fig. 9. Comparison of in-plane velocity magnitude (m/s) during the intake stroke under high-tumble conditions without fuel injection. The distributions are shown for two crank angle positions: −180 CAD (a–c) and −140 CAD (d–f). Experimental results are presented in (a) and (d), CFD results obtained with the modified geometry in (b) and (e), and CFD results using the baseline (original) geometry in (c) and (f). The color scale represents the velocity magnitude range from 0 to 15 m/s [71]

Studies have shown that increasing swirl intensity delays autoignition, extends combustion duration, and reduces NO_x emissions, while simultaneously lowering maximum cylinder temperatures and pressures, which may reduce the risk of combustion knock [32]. Figure 10 shows the turbulence kinetic energy (TKE) distribution in the X-Z plane of the combustion chamber of a hydrogen-fueled HCCI engine for various swirl ratio values at −1.971° crank angle (CA). The analysis showed that the intensification of swirl motion leads to a distinct differentiation of the turbulence field throughout the cylinder volume, which directly affects the rate of hydrogen-air mixing and the location of ignition initiation zones. The noticeable differences in the flow structure demonstrate that a properly selected swirl ratio can be an effective tool for controlling combustion, especially under autoignition conditions typical of HCCI engines. This figure provides a valuable complement to the numerical analysis, emphasizing the importance of three-dimensional modelling in predicting local phenomena crucial to the stability and efficiency of hydrogen combustion.

Article [60] focuses on the design and numerical validation of a modern hydrogen combustion chamber for gas microturbines. Due to limited space and extreme thermal conditions, the main goal was to develop a compact, safe, and efficient geometry enabling stable combustion of pure hydrogen. The authors presented, among other things, the concept of the Inverse Micromix injector, which operates based on axial hydrogen injection through a porous material and lateral air supply, which promotes effective mixing of the components and reduces the risk of flashback. A schematic diagram of this design is shown in Fig. 11. CFD analysis allowed for a detailed look at the hydrogen combustion process in the engine chamber. The study examined, among other things, temperature distributions, reactivity levels, and recirculation zones responsible for flame stabilization. Calculations were performed based on the EDC model and simplified chemical kinetics, allowing for optimization of the chamber geometry and verification of the effectiveness of the fuel-air mixing strategy. The obtained results demonstrate that CFD modeling is an effective tool in the design of modern hydrogen combustion systems.

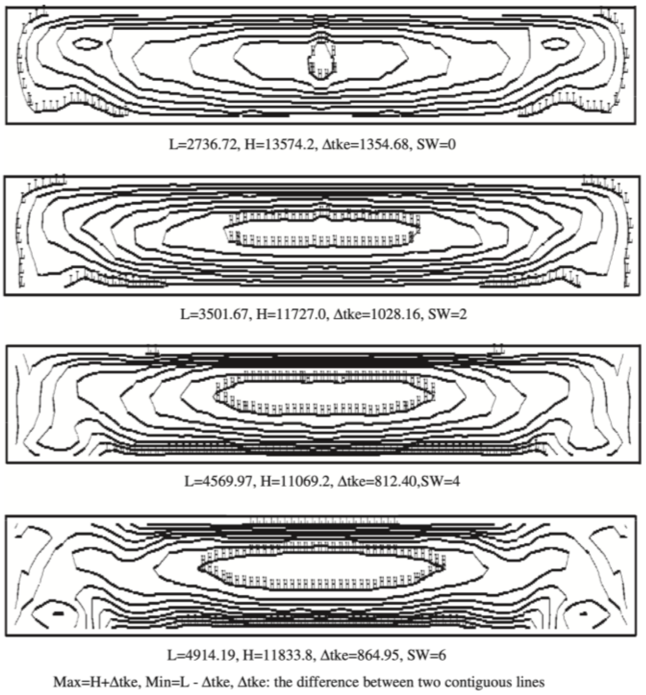

Fig. 10. Distribution of turbulent kinetic energy (TKE) in the X–Z plane of the combustion chamber of a hydrogen-fueled HCCI engine for different swirl ratio values at a crank angle of−1.971° CA [32]

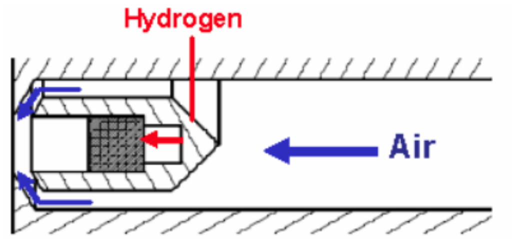

Fig. 11. "Inverse Micronix" injector: working principle [60]

Article [44] illustrates the application of numerical modeling to the analysis of hydrogen combustion processes in hypersonic conditions. The paper analyzes the influence of strut-injector geometry on the hydrogen-air mixing process and combustion characteristics in the scramjet chamber at an air velocity of 2.47 Mach and combustion at 1.5

Mach. A two-dimensional RANS model with a classical k–ε turbulence model and simplified chemical kinetics for hydrogen was used, enabling evaluation of the effectiveness of two injection configurations: a cylindrical strut end and an alternative wedge-shaped end (alternating wedge).

The calculation results showed that the use of a wedge-shaped injector leads to more intense hydrogen-air mixing and a more uniform reaction field, which directly results in an increased share of water vapor in the combustion products and higher maximum temperatures in the chamber. This setup effectively minimizes the distance needed for full reactant mixing, which is especially important in hypersonic propulsion systems, where interaction space and mixing time are severely restricted. The CFD-based study investigates how injector geometry and flow parameters influence hydrogen combustion performance under extreme flow regimes. The comparison of H_2O mass fraction contours in Fig. 12 confirms that the wedge-shaped injector enhances hydrogen conversion efficiency, demonstrating the value of computational modeling in optimizing high-speed hydrogen combustion systems [44].

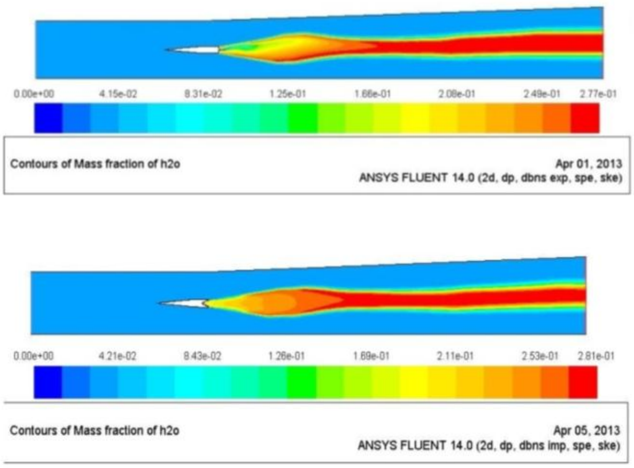

Fig. 12. Comparison of water vapor (H_2O) mass fraction contours in a hydrogen-fueled scramjet combustion chamber: top configuration with a cylindrical strut-injector; bottom configuration with an alternating wedge-shaped strut-injector [44]

The configuration used allows for a significant reduction in the path required to fully mix the reaction components, which is crucial in hypersonic systems, where the time and space for gas contact are strictly limited. CFD simulations were used to practically evaluate the impact of injection geometry and flow parameters on the stability and efficiency of hydrogen combustion under extreme conditions. Figure 12 presents the contours of the water vapor (H_2O) mass fraction for two strut geometries, visually confirming the more efficient hydrogen conversion with the wedge-shaped tip. These results demonstrate that numerical modeling can significantly support the development of modern, high-performance hydrogen-fueled hypersonic systems [44].

CFD modeling provides a powerful tool for examining how hydrogen affects combustion characteristics, even at an industrial scale in oxy-fuel systems. A study by Daurer et al. serves as a representative example, comparing hydrogen and methane combustion in a 180 kW semi-industrial furnace [12]. Their research provides a thorough investigation of hydrogen combustion under oxy-fuel conditions, where pure oxygen serves as the oxidizer. The authors concentrated on validating numerical combustion models and analyzing flame dynamics in realistic high-impulse burner operation. The simulations were performed using 3D RANS models with several turbulence and reaction schemes, covering both simplified and detailed hydrogen kinetics, including the ÓConaire mechanism.

Comparison of simulation results with experimental data for CH_4 combustion confirmed the high accuracy of the approach used. One of the key conclusions was that the turbulence modeling parameters (including modifications to the k–ε model) had the greatest impact on the quality of flame reproduction, while the influence of the combustion and radiation model selection was relatively small. Hydrogen combustion led to a significant increase in maximum flame temperatures (by approximately 400 K relative to CH_4) and a shortening of the flame length, despite the higher fuel jet velocity. This indicates greater heat transfer efficiency in the zone close to the burner and the need for precise calibration of turbulent mixing parameters [12].

Figure 13 illustrates how changes in the turbulence model parameters within the modified version of the k–ε model (P_2–H_2 variants) affect the characteristics of hydrogen combustion in a semi-industrial furnace. The visible differences in the temperature distribution and OH radical concentration intensity demonstrate that even small changes in the diffusion coefficients and turbulent energy production parameters can significantly shift the reaction zone and alter the flame length and stability. This figure provides significant support for the thesis that precise calibration of turbulence models is a key element in modeling hydrogen combustion under industrial conditions.

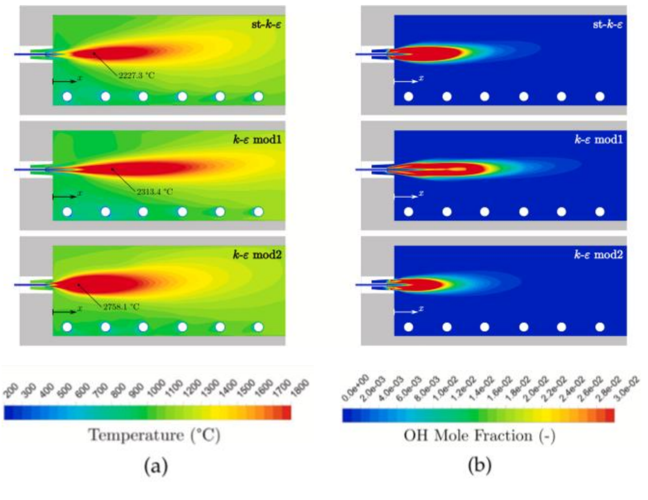

Fig. 13. Effect of parameter modification in the k–ε model on (a) temperature distribution and (b) molar fraction of the OH radical in the main reaction zone for the case of P_2–H_2 combustion in the oxy-fuel configuretion [12]

In their work [48, 49], the authors conducted a 3D numerical analysis of premixed H_2/air combustion in a microscale chamber to examine how geometry, wall heat losses, injection design, and flow conditions affect flame characteristics, temperature distribution, and combustion efficiency. Simulations performed in ANSYS Fluent with a detailed chemical kinetics model (9 species, 19 reactions) captured the essential thermal and reactive behavior of hydrogen combustion at small scales. The findings revealed that high wall thermal conductivity leads to significant heat losses and local flame extinction. On the other hand, introducing multi-step fuel injection effectively minimizes temperature peaks and improves temperature field uniformity. This leads to greater flame stability and improved efficiency – an important consideration for advanced hydrogen microcombustion systems.

Figure 14 shows the temperature distribution along the combustion chamber using different hydrogen injection strategies (single-, two-, and three-stage). The effect of injection staging is clearly visible, which allows not only to reduce peak temperatures in the reaction zone but also to achieve a more uniform thermal distribution throughout the volume, which translates into better operating conditions and lower thermal load on the chamber components [49].

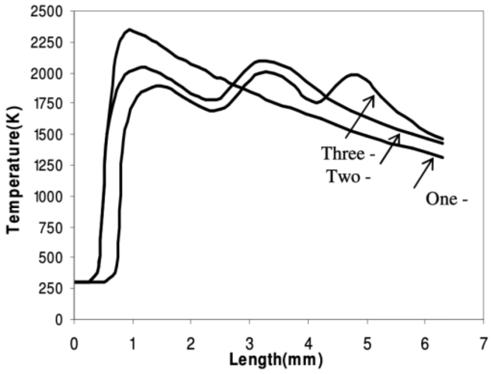

Fig. 14. Temperature distribution in a microscale hydrogen combustion chamber for different fuel supply strategies: single-, two-, and three-stage injection [49]

A significant contribution to the development of hydrogen combustion modeling is made by analyzing processes in compression ignition (CI) engines using non-standard operating atmospheres. Article [24] presents the results of numerical modeling of hydrogen combustion in a compression ignition (CI) engine in which the standard air mixture was replaced with an argon-oxygen atmosphere. The authors' primary goal was to determine the influence of parameters such as injector location, compression ratio, injection start (SOI), and initial temperature on the combustion process and emissions. The simulations were conducted using CONVERGE software and validated with experimental data from a YANMAR NF19SK engine. The findings revealed that replacing nitrogen with argon increased the combustion chamber temperature, shortened the ignition delay, and improved thermal efficiency, while simultaneously reducing NO_x emissions. Relocating the injector from the cylinder head side to its center resulted in higher in-cylinder pressure, temperature, and heat release rate (HRR), which indicates the dominance of mixture-controlled combustion. Additionally, as the compression ratio increased, both pressure and temperature rose, while the maximum HRR decreased, suggesting a more prolonged combustion process [24]. Figure 15 clearly shows how the shape and position of the hydrogen injector affect combustion. When the injector is in the center of the cylinder (G1 setup), the mixing of hydrogen with oxygen and argon becomes more efficient, leading to stronger combustion and a more balanced heat distribution.

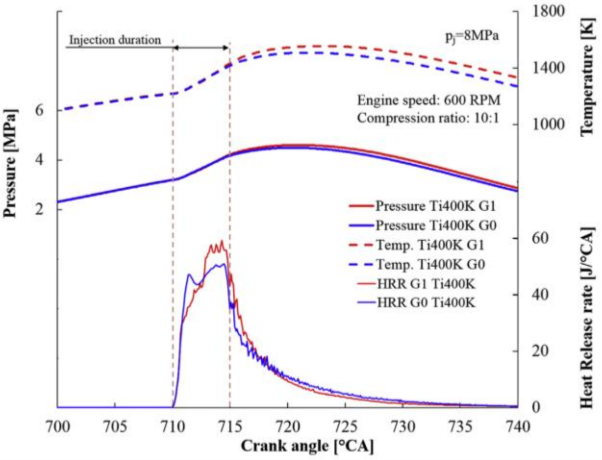

Fig. 15. Variations in pressure (p), average temperature (T_{ave}), and heat release rate (HRR) as a function of injector location [24]

In recent years, an increasing number of modeling studies have focused on local combustion phenomena, such as flame-wall contact (FWI), especially in situations involving thermal diffusion instabilities. Schneider et al. [53, 54] conducted a two-part numerical study analyzing the quenching of a hydrogen-air flame in a head-on quenching configuration, taking into account the variable parameters: equivalence factor, unburned gas temperature, and pressure. These articles provide a comprehensive analysis of the impact of thermal diffusion instabilities on the interaction of the hydrogen-air flame with the combustion chamber walls. These studies, conducted as direct numerical simulations (DNS), focus on the head-on quenching (HOQ) phenomenon – the process of flame quenching as a result of its direct contact with the wall.

In the first part of the work by Schneider et al. [53], high-resolution DNS modeling of the hydrogen–air flame interaction with a wall in a head-on quenching (HOQ) configuration was performed, taking into account thermodiffusion instabilities. The analysis revealed that local mixture fluctuations resulting from differences in hydrogen diffusion lead to a significant increase in local flame reactivity and, consequently, to higher heat fluxes to the wall and shorter quenching distances. This phenomenon is illustrated in Fig. 16, which presents profiles of the normalized heat flux Φ, the local equivalence factor φ/φ_u, the hydrogen mass fraction YH_2, and the heat release rate HRR within a single "flame finger" impinging on the wall [53].

The second part of the analysis covers a broader range of operating conditions relevant to industrial applications, including piston engines and gas turbines. The equivalence factor (φ = 0.4–1.0), pre-ignition mixture temperature (T_u = 298–700 K), and pressure were varied over 1–20 bar. The results show that the intensity of instabilities and their effect on the wall heat flux increase with decreasing φ and

Tu, and with increasing pressure, which increases local reactivity and thermal loads. Based on the obtained data, a predictive model is proposed to estimate the maximum heat flux to the wall as a function of the one-dimensional flame's characteristics. The effects of increased instability on quenching behaviour and wall thermal loads are examined. Figure 17 presents how variations in the equivalence ratio (φ), the unburned mixture temperature (T_u), and the operating pressure (p) affect selected combustion and heat transfer characteristics in the H_{OQ} configuration. The analysis covers the maximum and normalized wall heat flux ($φ_q$, $φ_{q*}$), the extinction distance (x_q), and the Péclet number (P_{eq}), indicating a clear dependence of near-wall heat transfer and flame quenching behavior on the imposed thermodynamic conditions. [54].

To improve the accuracy and efficiency of hydrogen combustion modeling under turbulent conditions, Malé, Lapeyre, and Noir ay developed a new method based on deep learning in their paper "Hydrogen reaction rate modeling based on a convolutional neural network for large eddy simulation" [36]. A deep learning model based on CNN architecture was trained with filtered high-fidelity DNS results to determine local reaction rate distributions in LES calculations. This methodology enables a more realistic representation of preferential diffusion mechanisms and turbulence–chemistry coupling, which are particularly significant in lean hydrogen combustion modeling.

The effectiveness of the method is illustrated in Fig. 18, which presents planar cross-sections of the computational domain for φ = 0.4. The actual reaction rates from the DNS simulation were compared with those from the CNN model at different LES filtering levels (σ = 4, 8, 16). The apparent consistency in the distribution and intensity of the reaction zones demonstrates that the neural network maintains high precision even at lower computational resolution, confirming its suitability for industrial applications involving hydrogen combustion [36].

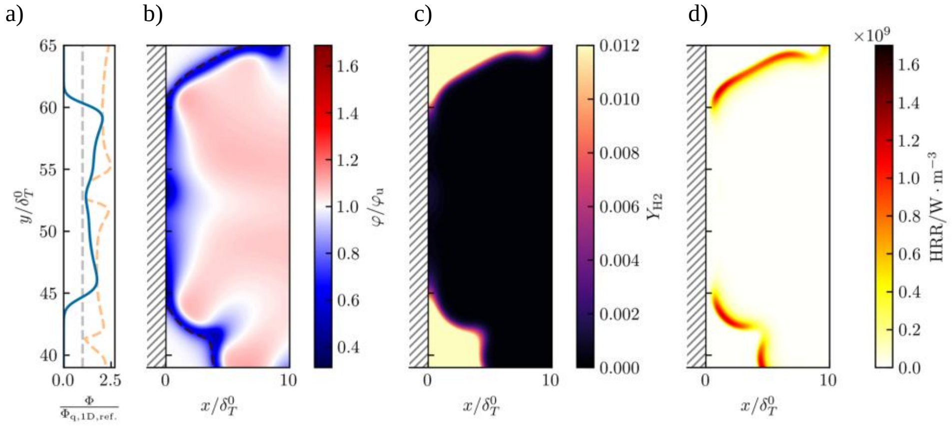

Fig. 16. Normalized heat flux ($\Phi/\Phi_{q,1D,ref}$) – a), equivalence factor (φ/φ_u) – b), hydrogen mass fraction (Y_{H2}) – c), and heat release rate (HRR) – d) along the symmetry axis of a single flame finger at the moment of its contact with the wall. Results obtained for an unstable H_2/air flame (φ = 0.4, 1 bar) in the HOQ configuration [53]

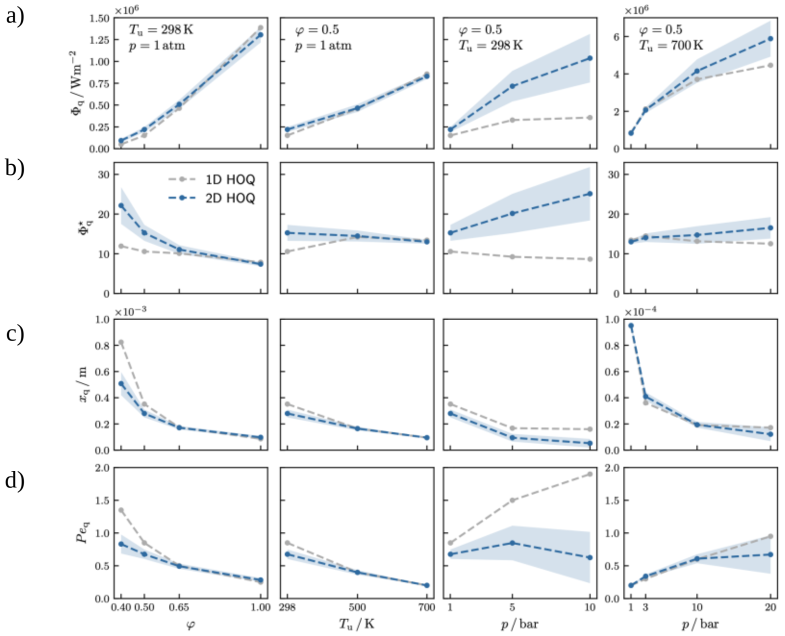

Fig. 17. Influence of changes in the equivalence factor (φ), unburned mixture temperature (T_u) and pressure (p) on: a) maximum heat flux to the wall (Φ_q); b) normalized heat flux ($\Phi_{\star q}$); c) extinction distance (x_q) and d) Péclet number (P_{eq}) in the HOQ configuration [54]

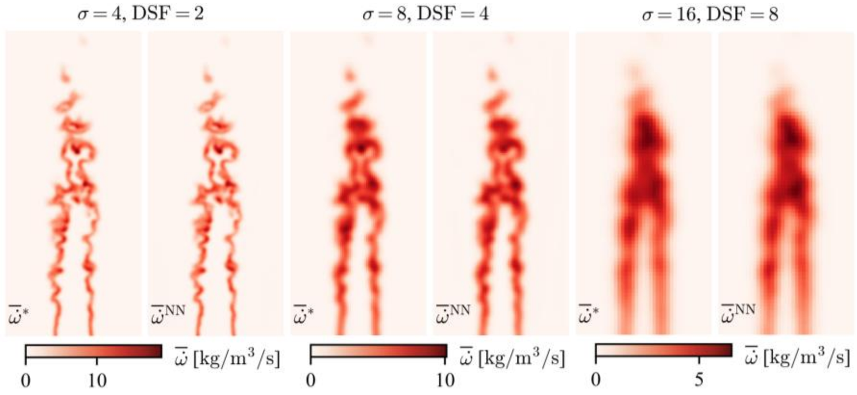

Fig. 18. Comparison of the actual (DNS) and convolutional neural network (CNN) – predicted hydrogen combustion reaction rates in a transverse cross-sectional plane for φ = 0.4 and different LES filter widths (σ = 4, 8, 16) [36]

To better understand the self-ignition and flame stabilization processes at high temperatures, Gruber et al. conducted direct numerical simulations (DNS) of hydrogen combustion in reheat mode [23]. This mode, typical of second-stage combustion in gas turbines, is characterized by the absence of classical spark ignition; ignition is initiated solely by autoignition, placing high demands on modeling reaction kinetics and turbulent phenomena. The analysis considered a wide range of inlet conditions – from laminar to highly turbulent – as well as the influence of heat losses and inlet mixture temperature. Of particular importance were observations of the cyclic appearance and extinction of ignition fronts near the so-called crossover temperature, as well as the identification of self-excited flame instabilities arising from the coupling between the reaction zone and pressure waves [23]. The results of the study are illustrated in Fig. 19, which shows the variation of the reaction front velocity (S_t) over time for different turbulence levels (u′ = 3, 6, 12, and 25 m/s). It is clearly visible that an increase in the intensity of turbulent fluctuations leads to an acceleration of the reaction front and, at the same time, to an increase in the amplitude of its oscillations. This figure provides significant evidence that strong turbulence not only affects combustion acceleration but also the dynamics and stability of the entire self-ignition process.

In the context of developing hydrogen combustion systems in non-overmixed configurations, three-dimensional CFD modeling of the combustion of a hydrogen-methane mixture in a combustion chamber with a variable number of nozzles was performed using the RNG k–ε turbulence model and a simplified non-overmixed combustion model [42]. The study examined how variations in mixture composition, injection geometry, and methane jet velocity influence thermal distribution, combustion efficiency, and possible NO_x emissions. According to the simulation results, enriching the mixture with hydrogen elevates the maximum temperature in the combustion chamber, while shortening the flame and advancing the reaction zone toward the inlet. At the same time, it was found that hydrogen content above 40% increases the risk of excessive NO_x emissions, which requires appropriate calibration of the system geometry. Among the analyzed variants, the best results in terms of combustion stability and temperature uniformity were obtained for the configuration with 16 injection nozzles [42].

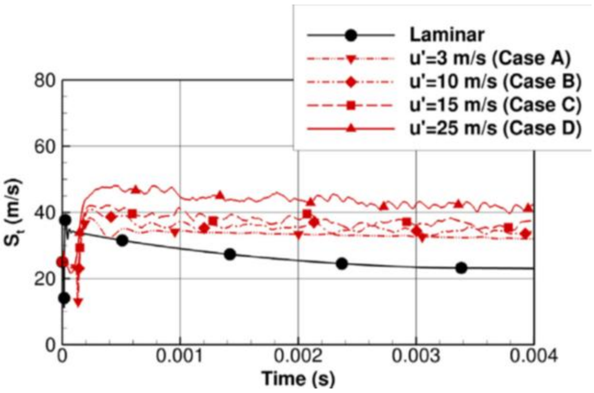

Fig. 19. Temporal evolution of the reaction front propagation speed (S_t) for turbulent hydrogen combustion under autoignition (reheat combustion) conditions, at different turbulence intensities (u′ = 3, 6, 12, 25 m/s); based on DNS data [23]

The characteristic effect of hydrogen content in the fuel on the temperature distribution is shown in Fig. 20, which compares the axial temperature cross-sections in the combustion chamber for mixtures containing 10% to 60% H_2. The noticeable changes in the flame structure and the location of high-temperature zones confirm the importance of selecting the appropriate fuel composition in the design of low-emission, highly efficient hydrogen combustion systems.

The studies described in [10] utilized direct numerical simulations (DNS) to accurately model hydrogen combustion under real-world piston engine operating conditions. The simulations were performed for a full-scale combustion chamber, making this one of the first studies to combine full-resolution flame-scale phenomena with the actual operating parameters of a spark-ignition engine (φ = 0.4237, 800 rpm). The nekCRF solver, based on the spectral-element method and optimized for GPU architecture, was used for the calculations. This approach enabled highly accurate modeling of flow, transport, and chemical reactions. Analysis of the results showed that flame development is strongly dependent on the flow structures generated by the tumble effect, which deform the ignition front and influence its velocity and direction of propagation. Particular attention was paid to flame-wall interactions – both head-on quenching and side-wall quenching – which lead to

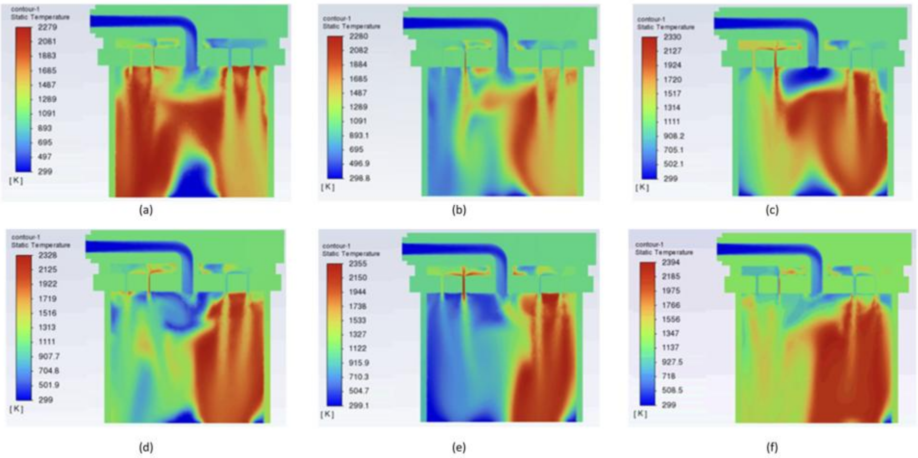

Fig. 20. Temperature distribution in the axial cross-section of the combustion chamber for different hydrogen shares in the H_2/CH_4 mixture (10%, 20%, 40%, 60%) – the influence of the fuel composition on the flame structure and the location of high-temperature zones [42]

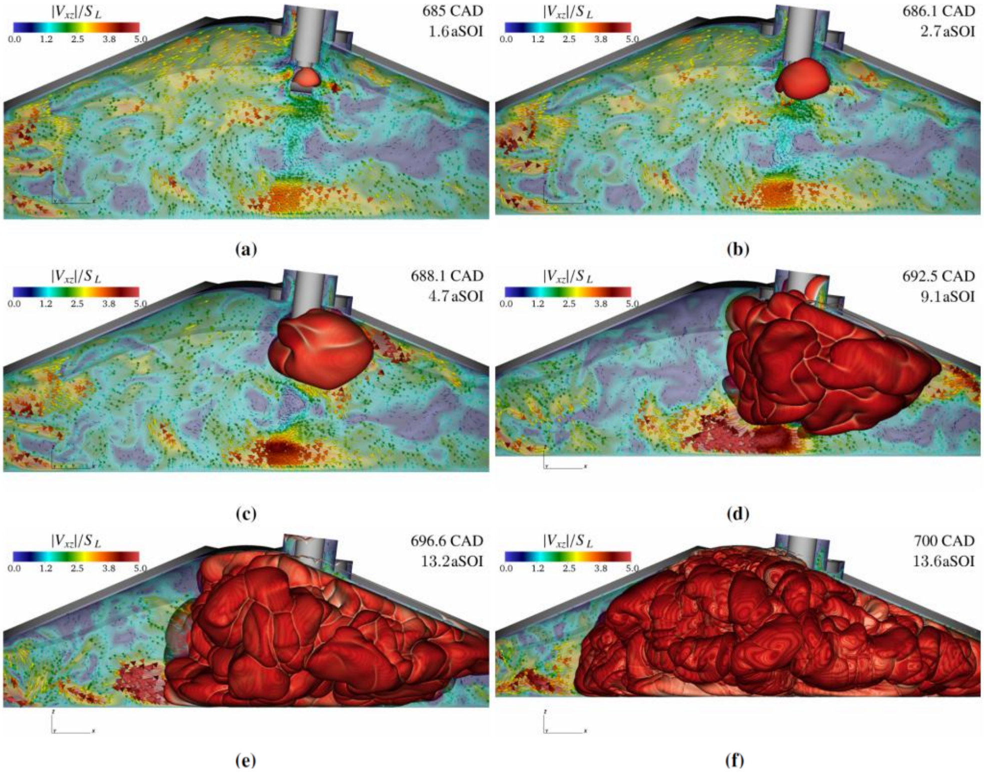

Fig. 21. Temporal development of the flame kernel identified by the $Y_{H2} = 0.0048$ iso-surface, overlaid on the velocity magnitude field in the mid-plane (y = 0), normalized by the local laminar flame speed S_L. Snapshots correspond to: a) 685 CAD; 1.6 aSOI; b) 686.1 CAD; 2.7 aSOI; c) 688.1 CAD; 4.7 aSOI; d) 692.5 CAD; 9.1 aSOI; e) 696.6 CAD; 13.2 aSOI, and f) 700 CAD; 13.6 aSOI. The flame structure is colored according to the heat release rate [10]

a local increase in heat flux, which is crucial for the durability of engine components [10]. The flame front's evolution over time is illustrated in Fig. 21, which shows successive hydrogen isosurfaces ($Y_{H_2} = 0.0048$) in the combustion chamber's symmetry plane. The sequence of images clearly shows the three-dimensional evolution of ignition and its deformation as a result of interaction with the variable flow field and chamber geometry, up to the point of collision with the piston. This figure provides an important complement to the qualitative analysis, showing the dynamics of hydrogen combustion on a real scale with full DNS resolution.

4. Critical comparison of modeling approaches and author-driven selection framework

Although a wide range of numerical techniques has been applied to hydrogen combustion in piston engines, the literature often discusses them separately, without clearly positioning them relative to one another. When these approaches are viewed side by side, certain patterns become apparent. RANS-based simulations continue to dominate engine-scale studies, mainly because they allow full-cycle calculations at an acceptable computational cost. In many practical optimization studies, this trade-off is understandable [50]. At the same time, their averaged formulation can obscure transient flame–turbulence interactions, which are far from negligible in hydrogen-fueled engines where flame propagation is rapid and mixture inhomogeneities strongly influence combustion development.

LES offers a different perspective. Resolving the larger turbulent structures provides a more detailed description of unsteady combustion behavior and is particularly useful when abnormal combustion events or cycle-to-cycle variations are of interest [29]. The improvement in physical representation, however, comes at a substantial computational expense, which makes large parametric campaigns difficult to justify. A similar balance must be considered when selecting combustion models. Flamelet-based approaches provide an efficient compromise for premixed and partially premixed hydrogen operation, whereas detailed chemical mechanisms enhance predictive capability for ignition and NO_x formation but introduce additional numerical stiffness [65].

Taken together, these observations suggest that model selection should not be driven by convention alone. Instead, it should follow a clearly defined logic that links the research objective, the combustion regime, and the available computational resources. On this basis, the present study proposes a structured selection approach intended to make future CFD investigations of hydrogen-fueled internal combustion engines more transparent, consistent, and methodologically grounded.

5. Critical synthesis and positioning of the reviewed studies

The reviewed studies collectively demonstrate that hydrogen combustion in piston engines cannot be treated as a simple fuel substitution problem. Instead, it represents a systemic transformation of combustion physics, engine calibration strategies, and modelling requirements. Experimental studies conducted over the past years leave little doubt that introducing hydrogen into the combustion process profoundly alters flame behaviour. In practical terms, the flame front tends to travel faster, ignition occurs earlier, and engines can operate at much leaner conditions than with conventional fuels. These effects are frequently highlighted as major advantages of hydrogen-based systems. The very features that enhance reactivity and combustion speed also promote higher combustion temperatures, which in turn favor NO_x formation. Moreover, the high reactivity of hydrogen increases the likelihood of phenomena such as pre-ignition or flashback, especially if mixture preparation and ignition timing are not carefully controlled [20].

Second, studies on hydrogen blends (HCNG, H_2–gasoline, H_2–diesel) show that moderate hydrogen fractions (typically 10–30% by volume) yield the most balanced improvements in efficiency and emissions. Beyond this range, diminishing returns or increased instability are frequently observed. This suggests that transitional blend strategies may be technologically more robust in the short term than full hydrogen conversion [6, 30].

Third, numerical modelling has evolved from a supporting tool to a fundamental research driver. Classical FGM and RANS approaches often fail to fully capture preferential diffusion and thermo-diffusive instabilities characteristic of hydrogen flames. The reviewed works clearly show that advanced approaches – LES, DNS, and machine-learning-assisted reaction modelling – are required to accurately predict flame structure, quenching behavior, and turbulence–chemistry interactions.

Viewed as a whole, the body of research does not point to a single universal solution but rather outlines several key paths that appear particularly promising for the continued development of hydrogen combustion systems.

One noticeable shift concerns the way combustion is modelled. Traditional steady-state approaches, although still useful, appear insufficient for hydrogen flames. Because hydrogen combustion is highly sensitive to thermodynamic and diffusive imbalances and preferential diffusion effects, local instabilities often govern flame structure and propagation [29]. Capturing these phenomena reliably requires modelling frameworks capable of resolving fine-scale interactions rather than relying solely on equilibrium-based or averaged descriptions.

A closer reading of the available studies also challenges a fairly intuitive assumption that adding more hydrogen will automatically translate into better engine performance. In reality, the relationship is far more nuanced. Modest hydrogen additions often improve flame responsiveness and allow operation under leaner conditions, but pushing the hydrogen fraction too far does not necessarily bring proportional benefits [46]. In some cases, it can even compromise combustion stability or deliver only marginal efficiency improvements. What appears to matter most is not the absolute hydrogen content but how well the mixture composition aligns with the combustion concept, engine architecture, and control settings. In that sense, precise tuning and system-level optimization outweigh the simple strategy of maximizing hydrogen share.

At the same time, numerical studies consistently point to another critical aspect: combustion outcomes are tightly linked to physical design choices inside the cylinder. The injector location, the generation of swirl and tumble motions, and the distribution of the mixture before ignition all shape the subsequent flame evolution and emission profile [71, 72]. Ignition timing and pollutant formation cannot be understood without considering these flow structures. In other words, combustion chemistry does not operate in isolation, but it unfolds within a geometrically defined, highly dynamic environment. Effective engine development, therefore, requires simultaneous attention to both in-cylinder aerodynamics and reaction kinetics from the earliest design stages [5].

When considered collectively, the reviewed studies suggest three major directions for future hydrogen combustion research:

1. Shift from steady-state modelling to instability-focused modelling

Hydrogen combustion is dominated by thermodynamic and diffusive effects, including preferential diffusion, which require high-resolution modelling beyond classical equilibrium-based methods.

2. Optimization rather than maximization of hydrogen fraction

The literature does not support the assumption that higher hydrogen content always yields better performance.

Instead, optimal fractions depend on combustion regime, engine type, and control strategy.

3. Coupled design of combustion chamber geometry and injection strategy

Numerical studies repeatedly demonstrate that injector placement, swirl intensity, and tumble enhancement significantly alter ignition behaviour and emissions, highlighting the importance of geometry–chemistry coupling.

The body of work discussed here shows that hydrogen combustion research now occupies a space between traditional combustion theory and the rapidly evolving field of advanced numerical simulation. Earlier investigations focused on fairly direct questions about how hydrogen affects emissions, how quickly the flame propagates, and how stable combustion is under different conditions. Today, the scope has broadened. Researchers are increasingly examining interactions spanning multiple scales, from microscopic reaction pathways to large-scale flow structures, while also exploring turbulence-chemistry coupling and data-driven modelling techniques that were previously rarely considered.

At this stage, the key challenges no longer lie in proving that hydrogen can burn efficiently in piston engines. What seems to limit wider industrial adoption is something more complex: integrating hydrogen combustion into complete engine systems, ensuring stable operation across load ranges, and adapting existing infrastructure to accommodate hydrogen's specific fuel requirements. The obstacles are now largely systemic rather than purely scientific.

This review presents a descriptive compilation of existing studies by integrating findings from experimental combustion research, numerical modelling, and engine system optimization. The collected evidence demonstrates that hydrogen combustion in piston engines represents not only a fuel substitution strategy but a distinct combustion regime characterized by strong thermo–diffusive effects, high reactivity, and sensitivity to flow structures.

A key contribution of this review is the identification of three overarching trends:

- the transition from steady-state modelling approaches toward instability-resolving frameworks (LES, DNS)
- the recognition that optimal hydrogen fraction depends on engine architecture and combustion mode rather than simple maximization strategies
- the growing importance of geometry–chemistry coupling in combustion chamber and injector design.

Furthermore, several research gaps remain insufficiently addressed in the literature:

- limited long-term durability analyses under hydrogen combustion conditions
- insufficient validation of high-fidelity models under transient engine loads
- lack of standardized modelling methodologies for preferential diffusion effects
- incomplete integration of combustion modelling with full powertrain system optimization.

By synthesizing these aspects, this review provides a structured research roadmap for future development of hydrogen combustion.

6. Summary and conclusions

The use of hydrogen as an admixture to conventional fuels in piston engines is one of the most promising transitional solutions towards decarbonizing transport and energy. Simulation and experimental studies clearly confirm that even a small proportion of hydrogen in the fuel mixture can significantly improve combustion parameters, such as ignition speed, heat release intensity, and indicated efficiency.

Hydrogen, due to its high octane rating and low ignition energy, facilitates stable combustion while reducing carbon monoxide and unburned hydrocarbon emissions. However, without proper optimization of operating parameters, for instance, if ignition timing is too advanced, issues such as knocking or elevated NO_x formation may arise. Therefore, precise calibration of the ignition timing, injection method, and hydrogen quantity in the mixture is necessary.

Technologies that blend hydrogen with traditional fuels in GDI and TJI systems demonstrate that it is possible to combine high energy efficiency with engine operational safety. The final result depends on many factors, including the level of hydrogen enrichment, initial conditions, mixture characteristics, and combustion chamber geometry. The inherent complexity of hydrogen combustion phenomena highlights the need for sophisticated CFD modeling tools and systematic optimization of engine operating conditions to guide further technological advancements.

Beyond summarizing prior work, this review identifies several structural trends in hydrogen combustion research. A noticeable shift is observed from steady, globally averaged models toward approaches capable of resolving thermo-diffusive instabilities and turbulence–chemistry interactions. The literature also confirms that combustion chamber geometry, in-cylinder flow structures, and chemical kinetics form a coupled system, while the optimal hydrogen fraction depends on engine configuration and control strategy rather than simple maximization. Further progress will require tighter integration of high-fidelity CFD modelling with experimental validation, particularly under transient operating conditions relevant to automotive applications. In addition to summarizing the available literature, this review examines how current modeling approaches perform when confronted with combustion phenomena characteristic of hydrogen. These include its exceptionally high laminar flame speed, increased susceptibility to abnormal combustion events, and the strong sensitivity of NO_x formation under lean operating conditions. Rather than merely listing existing methods, the paper identifies where current modeling strategies remain insufficient or inconsistent, especially in engine-relevant configurations. On this basis, a structured approach to selecting numerical methods is proposed to support more reliable, physically consistent CFD studies of hydrogen-fueled internal combustion engines in future research.

Future research should focus on multi-scale modelling approaches that bridge detailed chemical kinetics with system-level engine simulations. Particular attention should be paid to the interactions among turbulence, preferential diffusion, and ignition control in highly diluted and ultra-lean regimes. The integration of data-driven methods with physics-based CFD models is a promising approach to reduce computational costs while maintaining predictive accuracy. Ultimately, advancing hydrogen combustion in piston engines requires coordinated progress in combustion science, digital modelling, materials engineering, and regulatory harmonization to ensure both technical reliability and environmental effectiveness.

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Nomenclature

AVL FIRE	commercial CFD software for engine combustion modelling (brand name)
CFD	computational fluid dynamics
CJ	Chapman-Jouguet (detonation condition)
CNG	compressed natural gas
DNS	direct numerical simulation
EGR	exhaust gas recirculation
FGM	flamelet generated manifold
FGM-PV	flamelet generated manifold-progress variable
Fluent (ANSYS Fluent)	commercial CFD software by ANSYS (brand name)
GT-Power	engine system simulation software (brand name)
H_2-ICEs	hydrogen internal combustion engines
H_2/NG blend	mixture of hydrogen and natural gas
HCCI	homogeneous charge compression ignition
HCNG	hydrogen-enriched compressed natural gas
HPC	high-performance computing
ITE	indicated thermal efficiency
IMEP	indicated mean effective pressure
LES	large eddy simulation
LHV	lower heating value
LPG	liquefied petroleum gas
MBT	minimum spark advance for best torque
MCCI	mixed-controlled compression ignition
MILD	moderate or intense low-oxygen dilution combustion
MVF	mixture volume fraction
NG_2	methane-dominant composition
OH	hydroxyl radical
PDF	probability density function
RANS	Reynolds-Averaged Navier-Stokes
SCR	selective catalytic reduction
TJI	turbulent jet ignition
TKE	turbulent kinetic energy
ZND	Zeldovich-von Neumann-Döring (detonation model)

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