Results in Engineering 17 (2023) 100799

Contents lists available at ScienceDirect

Results in Engineering

journal homepage: www.sciencedirect.com/journal/results-in-engineering

Impact of hydrogen substitution for stable lean operation on spark ignition engines fueled by compressed natural gas

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ARTICLE INFO

Keywords:
Hydrogen
Methane
Internal combustion engines
Thermal efficiency
Pollutant emissions

ABSTRACT

Compressed Natural Gas (CNG) appears as a midterm solution to conventional fuels, such as gasoline and diesel. The low carbon content and the possibility of being obtained from renewable sources (animal or agriculture waste, landfills, waste of the industry food or aquatic biomass) make CNG an attractive option to reduce Greenhouse Gases (GHG) emission. Applying lean combustion strategies on CNG improves efficiency levels while reducing pollutant emissions. In these conditions, heat transfer losses are reduced, and the thermal efficiency increased, especially at partial loads where increasing air dilution is one of the main strategies to reduce pumping losses. Hydrogen (H_2) addition helps to enhance combustion in these diluted conditions and to reduce the combustion instability. This combustion concept has been widely studied over the last years, however further research is still needed. This investigation focuses on how hydrogen substitution affects the performance and emissions (both CO_2 and pollutant) of a port fuel injection (PFI) spark ignition (SI) engine fueled by CNG. Thus, the main objective of this investigation is to contribute to the existent knowledge about dual-fuel combustion strategies based on CNG and H_2 blends. Results demonstrated that hydrogen substitution helps to reduce the CO_2 emissions by two ways: improving the engine efficiency and substituting part of the main carbon-based fuel. Despite of this advantage, NO_x emissions are not reduced, and they will require after-treatment systems to deal with current pollutant regulations.

1. Introduction and objectives

As a result of the reduction in emissions that contribute to the greenhouse effect, carbon dioxide (CO_2) emissions are expected to be severely limited in the coming decades. Mid and long-term changes in humidity, precipitation, and temperature levels will lead to climate disruption, the consequences of which are unpredictable [1]. The withdrawal of this element from the atmosphere by enhancing biological sinks and by using chemical engineering -to achieve storage and long-term removal is expected to counterattack the devastating predictions. As internal combustion engines (ICEs) are highly dependent on carbon-based fuels, improving thermal efficiency while reducing pollutant emissions is required to achieve worldwide CO_2 emission targets [2]. As an example of these restrictions, European light-duty vehicles must reduce the CO_2 emitted down to 95 CO_2 g/km, and lower values are expected to be reached in the following years.

Conventional carbon-based fuels used in ICEs are not only damaging the environment from a global point of view but also human health is compromised by degrading the air quality [3]. While CO_2, water (H_2O), and nitrogen (N_2) are the combustion products for a complete combustion process of a hydrocarbon, other elements are generated in real conditions (CO, NO_x, unburned HC, PM). These elements are noxious for human health as many medical investigations proved. Air pollution from the tailpipe of transport vehicles causes serious health issues like allergic respiratory diseases (rhino-sinusitis and bronchial asthma), cardiovascular and neurobehavioral effects, and cardiopulmonary mortality. In addition, there is a proven strong relationship between exposure to fine particle-rich environments (PM) and cardiopulmonary mortality [3–5].

The use of alternative fuels such as biodiesel, bioalcohol (methanol, propanol, ethanol, butanol), biogas, natural gas, dimethyl ether (DME), or hydrogen (H_2) could help to achieve the emission targets for the transportation. In particular, Compressed Natural Gas (CNG), which is accomplished by compressing the conventional natural gas at high pressure, arises as a potential solution due to its lower carbon content per molecule if compared with conventional fuels such as gasoline or diesel [6] (i.e. between 20 and 25% of CO_2 reduction is achieved in comparison with traditional fuels). The absence of C–C bonds on the fuel and lean combustion strategies reduces the particulate matter by about

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https://doi.org/10.1016/j.rineng.2022.100799
Received 22 September 2022; Received in revised form 17 November 2022; Accepted 24 November 2022
Available online 16 December 2022
2590-1230/

75% [7]. In addition, CNG could be obtained from renewable sources (animal waste, landfills, waste of the food industry, aquatic biomass, or agricultural waste). Additionally, in European countries, the existing infrastructure for natural gas reduces the cost of implementing this technology for fueling transport purposes.

Applying lean combustion strategies to spark ignition engines (SI) improves efficiency levels while reducing pollutant emissions [8]. In these conditions, heat transfer losses [9] are reduced, and the thermal efficiency increases [10], especially at partial loads where increasing air dilution is one of the main strategies to reduce pumping losses. Moreover, hydrogen addition helps to enhance combustion in these diluted conditions, where the combustion of pure CNG evinces clear stability issues. H_2 is a carbon-free fuel that can also be produced in a sustainable way [11]. In addition, it can be a synergic solution with the use of CNG since current hydrogen production is mostly based on methane reforming from natural gas and the cost for H_2 coming from electrolysis is still too high [12]. The high production cost, the difficulty of storing and the lack of extensive distribution infrastructure are some of the limitations for enabling an economy system based on H_2.

As the green hydrogen economy is being deployed, the use of CNG and H_2 mixtures (HCNG) for fueling ICEs is a realistic mid-term solution with reduced cost and scalable impact. This combustion concept has been widely studied over the last years [13]. For instance, Molina et al. [14] predicted the HCNG combustion using low-order modelling and Artificial Neural Network (ANN). Ma et al. [15] studied the effects of hydrogen enrichment on cycle-to-cycle variation in a spark-ignition engine. A mixture of HCNG was compared to the conventional CNG combustion in a 6-cylinder engine. Results showed a reduction in CCV when hydrogen was added to the fuel blend, demonstrating the capacity of H_2 addition for extending the operating range. In Wang et al. work [16] these CCV reductions are also found. The high flame speed of H_2 [17,18] helps to reduce the instabilities by shortening the flame development duration and favoring the flame propagation, reducing the overall combustion duration. Due to these combustion properties of hydrogen, safety concerns were also studied by Salzano et al. [19], analyzing the explosion behavior of the methane H_2-enriched. This combustion enhancement also evinced the possibility of operating the engine in more diluted conditions [20–22], extending the operation limits. Larsen and Wallace [23] analyzed pollutant emissions and thermal efficiency in a turbocharged SI engine on lean combustion conditions. In this investigation, a blend of 85% natural gas and 15% hydrogen (in volume) was considered. Results suggested the implementation of an after-treatment system to control both unburdened HC and NO_x emissions. Shudo et al. [24] explored the options to avoid the implementation of an after-treatment system in a similar engine. In addition, NO_x emissions were deeply studied and some prediction models reach a relatively accurate prediction ($\varepsilon = 15\%$) [25]. Bell et al. [26] found that blending CNG with hydrogen helps to reduce unburned HC, in particular CH_4.

Following this research line, this investigation experimentally evaluates the effect of H_2 substitution on CNG fuel under lean combustion conditions. The main objective is to contribute to the existent knowledge about dual-fuel combustion strategies using CNG and H_2 blends. Particularly, it is focused on evaluating the impact of hydrogen substitution (with respect to the reference CNG fuel) on engine efficiency and emissions (CO_2 and NO_x) as a first scenario of a fully-developed hydrogen economy transition. These activities are performed in a single-cylinder spark ignition research engine using a port fuel injection (PFI) system.

2. Material and methods

A single-cylinder research SI engine was used to perform the experimental campaign. The gaseous fuels (CNG and H_2) were injected separately through two different port injection systems (PFI). The main specifications and engine layout are presented in Refs. [27,28]. The main engine specifications are presented in Table 1.

The original layout of the test bench, which was intended to use gasoline as fuel, was adapted for dual gaseous fuel strategies as shown in Fig. 1. Some parameters such as the cylinder compression ratio are inherited from this original layout and are not optimized for the different fuel blends used in this experimental campaign.

Regarding fuels, they come from different sources. CNG is extracted directly from the natural gas network and then compressed and stored in tanks. Most of the natural gas used in the experimental tests consists of methane (89.95%), a small part of ethane (6.27%), and other impurities, and hydrogen was supplied directly from pressurized tanks. Impurities values on the H_2 used are low ($H_2O \leq 40$ ppm, $O_2 \leq 10$ ppm) with 99.9% of the gases being pure hydrogen. The main features of each fuel used in the experimental campaign are summarized in Table 2. The energy per mass unit is almost 3 times higher for hydrogen in comparison with CNG. The RON number, which is a parameter for quantifying the auto-ignition resistance of a given fuel, is similar in both fuels. However, there are other phenomena that could generate knocking combustion in the hydrogen [29].

Using an in-house 0D combustion diagnosis tool, combustion parameters such as combustion phasing (CA50), combustion onset (CA10), and combustion duration (CA90-CA10) are obtained. The Heat Release Rate (HRR) is estimated by resolving the energy equation with the measured in-cylinder pressure and assuming several simplifications. For instance, it considers uniform pressure and temperature fields through the whole combustion chamber and several simplifications for estimating the heat transferred to the cylinder walls among others. The model originally considered three different species: air, fuel, and combustion products. The fuel is now adapted as a homogeneous mixture between the two selected fuels (CNG and H_2). The properties of this mixture are weighted by the fuel proportions used in each test, resulting in an equivalent fuel with an average LHV, chemical composition and thermodynamics properties. A detailed model description is found in the work of Payri et al. [30] and Benajes et al. [31].

The experimental facility is fully monitored. This allows an exhaustive control of each relevant parameter, for instance: the water and oil cooling circuit temperatures, the intake boost pressure, and the temperature of the intake air. The fuel mass flow was measured and controlled by different flowmeters installed on each fuel-supply line. CNG was measured by BRONKHORST F-113AC-M50-AAD-55-V flowmeter and hydrogen was measured by F-113AC-1M0-AAD-55-V flowmeter with 0.5% of accuracy. A piezoelectric sensor was used to measure the instantaneous in-cylinder pressure whereas piezoresistive sensors were used to measure the intake and exhaust pressures with 0.2% of accuracy. All the signals were recorded at a sampling frequency of 0.2 CAD. HORIBA MEZA 7100 DEGR measures exhaust gas composition with 3% of accuracy. A sample of the gases coming from the exhaust settling chamber is conducted to the gas analyzer using a 192 °C preheated pipe. Type K thermocouples with an accuracy of 1.5 °C were used.

The methodology used in this investigation aimed at evaluating the impact of increasing the amount of hydrogen in the fuel blend on

Table 1
Main engine specifications.

Number of cylinders (–)	1
Number of strokes (–)	4
Displaced volume (cc)	454.2 cc
Stroke (mm)	86.0
Injection systems	PFI (up to 8 bar)
Ignition system	Spark (spark plug)
Cylinder diameter (mm)	82.0
Compression ratio (–)	10.7
Connecting rod length (mm)	144.0
Valves per cylinder	2 intake, 2 exhaust
Engine management system	AVL Puma Open
Combustion system	4-valve pent roof GDI

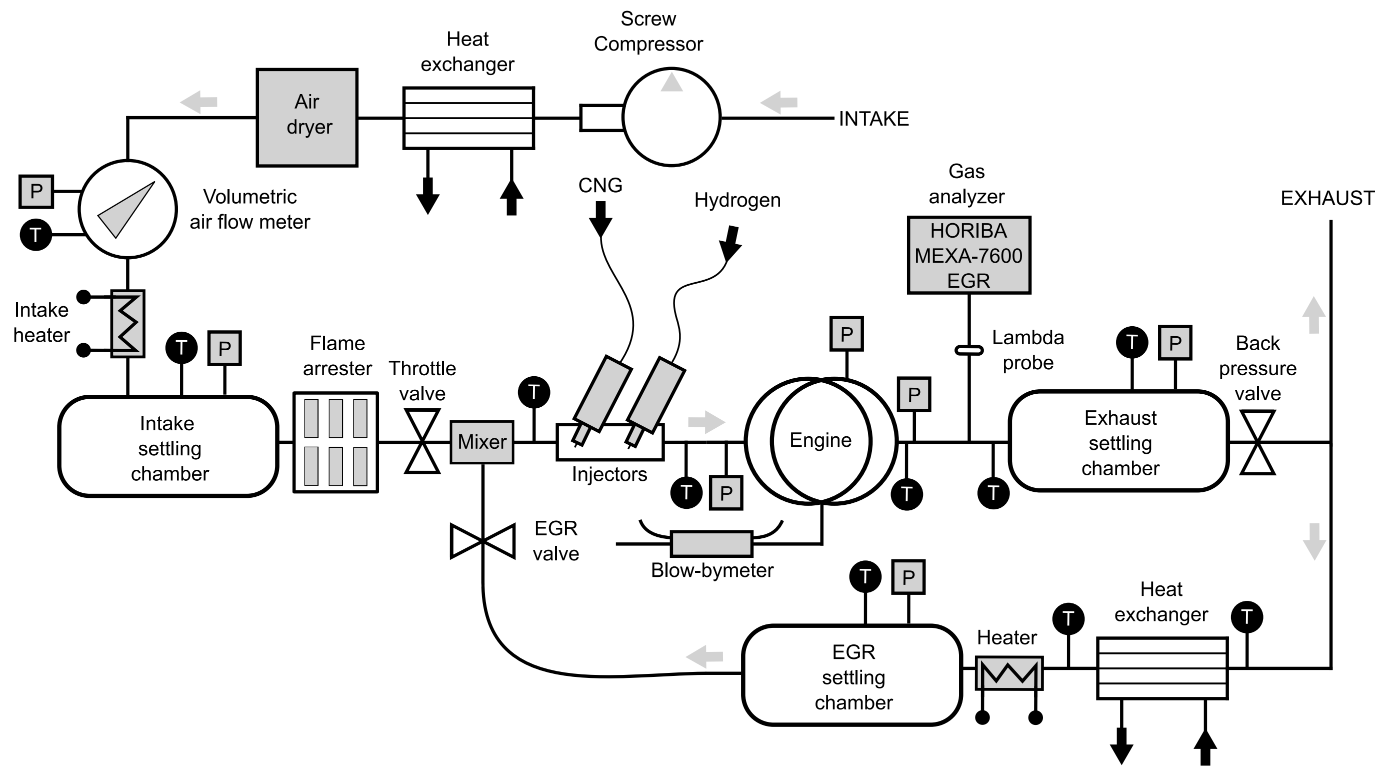

Fig. 1. Test cell layout.

Table 2
Main fuel specifications.

Properties	H_2	CNG
RON	>130	120
LHV	120 MJ/kg	46.87 MJ/kg
Molar mass	2.01 g/mol	17.77 g/mol
Stoichiometric Air-fuel ratio	34.3	16

combustion stability operating at high diluted conditions.

The experimental campaign included three operating points which gather the most relevant conditions within the operating map. The first point corresponds to a medium load and low engine speed (1500 rpm and 7 bar of IMEP). The second one keeps the same engine speed (1500 rpm) and increases the load up to 10 bar of IMEP. Finally, the last point focuses on maximum power requirements, increasing the engine speed up to 3000 rpm while maintaining the load at 10 bar of IMEP. The energy introduced per cylinder and engine cycle is defined by the amount of CNG needed to obtain the load reference values at stoichiometric conditions. Combustion stability was defined as the parameter to determine the maximum air dilution value from each operating point ($COV_{IMEP} < 2\%$). Once the operating points were defined, the fuel composition was changed by increasing the percentage of hydrogen in the mixture. Hydrogen was increased from 0 to 3% mass-based percentage of the total amount of fuel always maintaining the air-to-fuel ratio. The 3% hydrogen mass-based substitution on the fuel corresponds to: 7.5% of the energy injected each cycle, which is approximately 21% of volume fuel fraction. In this investigation, 3% of hydrogen substitution was considered as the upper limit to avoid high volumetric losses [32] and abnormal combustion phenomena due to hydrogen flame instabilities [33]. The idea was to keep a reasonable boost pressure increase when switching to HCNG combustion mode (note that the boosting pressure has to be increased due to the low density of hydrogen [32]) while maintaining the flammability limits under control to avoid back-fire. In addition, 20–25% of hydrogen in volume is traditionally considered as the limit for low hydrogen HCNG blends, which represents a feasible fuel definition for a short-term scenario with low hydrogen availability on the market. A summary of the tests performed for this investigation is shown in Table 3.

3. Results and discussion

The experimental results of the different operating points are organized according to the amount of hydrogen in the fuel, performing a spark timing sweep of each fuel blend. To analyze the hydrogen substitution effect on combustion, instantaneous in-cylinder pressures and heat release rate profiles obtained from non-stoichiometric tests are shown in Fig. 2. In this figure, only the spark timing sweep that was performed at 1500@7 operating point running at maximum air dilution conditions is shown. Four different fuel compositions are included: CNG, CNG +1% of H_2 (HCNG 1%), CNG + 2% of H_2 (HCNG 2%), and CNG + 3% of H_2 (HCNG 3%). These profiles correspond to the most representative cycle [34] to avoid masking effects. This cycle represents the most characteristic engine cycle in terms of combustion without any signal treatment modification.

As it can be seen in Fig. 2, the maximum pressure value is shifted toward TDC, the heat release rate shows a similar trend. The maximum HRR and pressure values are advanced, and they reach higher values as the spark timing is advanced. The combustion phasing is represented by a dashed line, and it can be seen how combustion moves towards the

Table 3
Operating conditions.

Engine speed (rpm)	Engine load (bar)	λ (–)	H_2 (mass %)
1500	7	1 1.5	0
			0-1-2-3
1500	10	1	0
		1.2	0-1-2-3
3000	10	1	0
		1.4	0-1-2-3

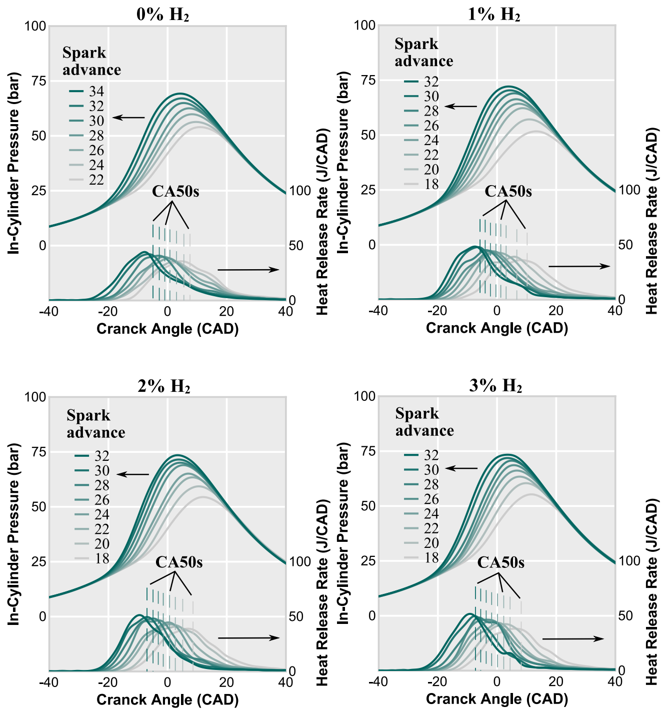

Fig. 2. In-Cylinder Pressure and HRR profiles for different hydrogen substitution percentages at the operating point 1500@7 for different spark advances values.

compression stroke as the spark is advanced. This parameter is critical for achieving an efficient combustion process. Comparing the different fuel compositions, it is easy to observe that hydrogen inclusion increments the maximum pressure and HRR values. For evaluating how hydrogen affects the combustion process in a more concise way, the combustion phasing (CA50) and duration (CA90-CA10) are shown in Fig. 3.

Here, the combustion phasing and the combustion duration are compared for different mixtures and different spark timing values for the three different operation points. As the hydrogen percentage increases in the fuel blend, the combustion has two main effects: the combustion phasing is moved towards TDC and the combustion duration is reduced. Hydrogen substitution shifted combustion approximately 5 CAD when CNG and HCNG 3% are compared at 3000@10 operating point. This difference is reduced in the other two operating points (1500@7 and 1500@10). The Maximum Brake Torque (MBT) point is reached at delayed spark timings as the hydrogen percentage increases. The different combustion behavior of the fuel blends affects the combustion duration, reducing the combustion duration when hydrogen is added.

In general, higher differences on combustion are observed between CNG and HCNG1 when comparing al fuel formulations. This trend is also found on the literature [15,35]. The authors shown that one of the root causes of this behavior is the increase of the laminar flame speed, which has been extensively studied for HCNG mixtures in the following research works [18,36,37]. In addition, the turbulence intensity and S_T/S_L is slightly affected by hydrogen fraction. The higher hydrogen percentage, the higher the turbulent intensity [38], thereby accelerating just combustion. Other investigations pointed out the significant role of the increased amount of H, O and OH radical, as the main reason for combustion acceleration due to hydrogen. The optical measurements of Di Iorio et al. [39] revealed how combustion acceleration and stability as a result of hydrogen addition arise as promoting the reaction rate of some key species during the methane combustion. These findings are corroborated by Schefer in his seminal work [40], in which the addition of hydrogen increased the peak OH mole fractions widening the lean

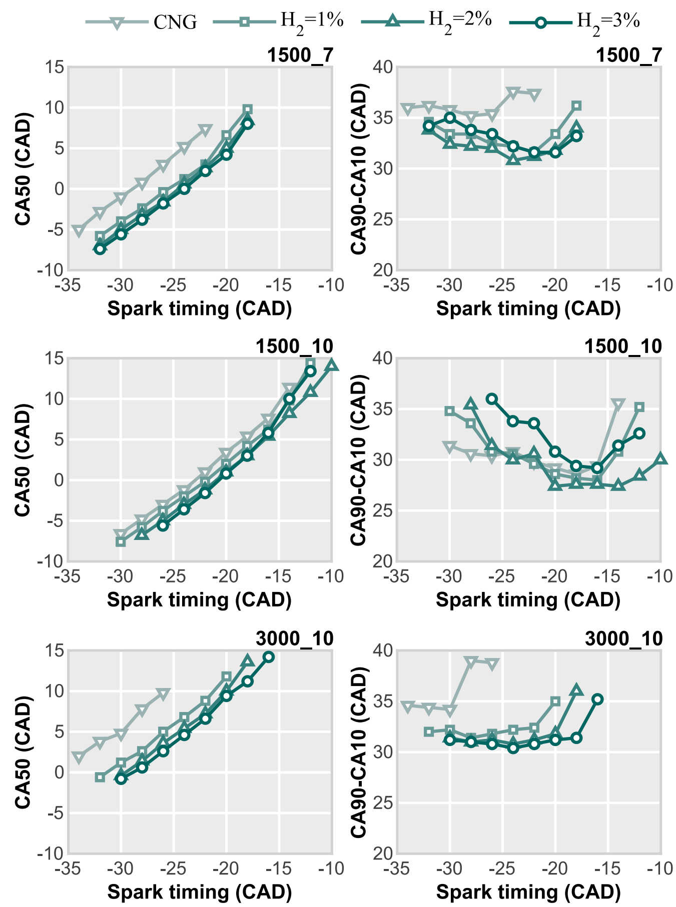

Fig. 3. Combustion phasing (CA50) and Combustion duration (CA90-CA10) for different hydrogen substitution percentages for different spark timing values.

stability range.

To measure the effect of hydrogen on engine performance, the net indicated efficiency (NIE) and indicated specific fuel consumption (ISFC) are selected. In Fig. 4, it can be observed how the indicated efficiency is affected. Analyzing the spark timing sweep results, a maximum performance peak is seen as the ignition timing is delayed towards TDC. Then, the increase of cycle-to-cycle variation (CCV) due to combustion instabilities cause an engine performance lowering for delayed ignition timings. The impact of hydrogen on engine performance varies depending on the operating point, the changes in the combustion process depend on the initial fuel blend composition or the spark timing at which the comparison is establishes. However, in general terms the addition of hydrogen produces an increase in performance, if CNG fuel is compared with HCNG blends. The maximum difference oscillates depending on the considered HCNG blend and the operating point.

Regarding fuel consumption, increasing the hydrogen substitution percentage helps to reduce ISFC. As shown in Table 2, the properties of the fuels are substantially different. Hydrogen LHV is about 120 MJ/kg, more than twice that of CNG LHV. As hydrogen percentage is increased with less fuel total mass is possible to introduce the same energy when hydrogen percentage is increased. Because of this, ISFC is affected by the fuel composition without any impact on the efficiency. Therefore, this must be considered when comparing points of the different fuel compositions. ISFC results are shown in Fig. 4. The optimum fuel composition coincides with the maximum efficiency values and the lower combustion duration.

CO_2 and NO_x emissions on the engine exhaust tailpipe are analyzed in Fig. 5 when hydrogen substitution is increased. While CO_2 are the most relevant GHG emissions, NO_x emissions are critical from the point

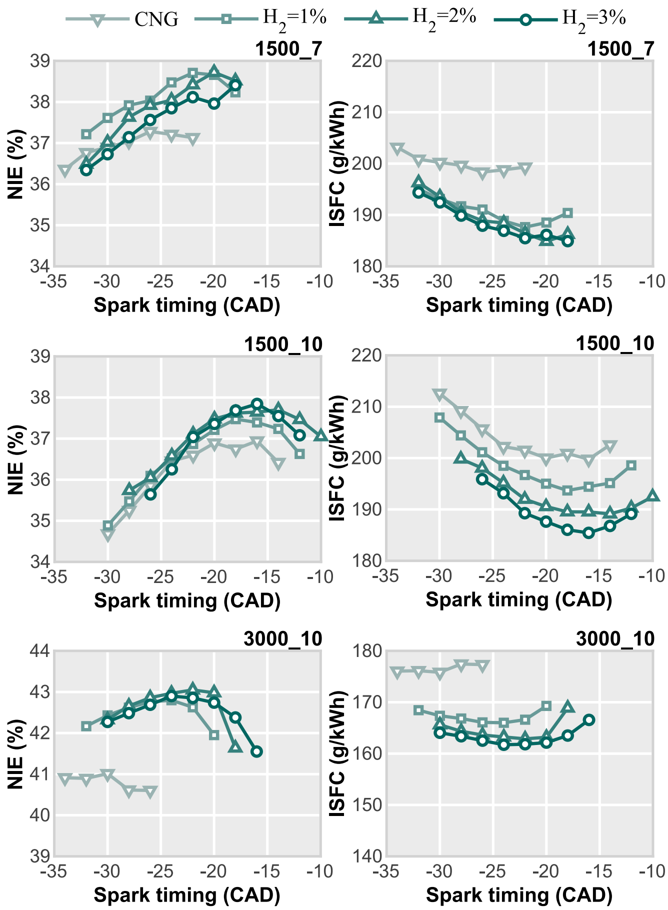

Fig. 4. NIE and ISFC for different hydrogen substitution percentages for different spark timing values.

of view of pollutant regulations.

As expected, increasing the hydrogen in the fuel composition reduces the production of carbon dioxide. In general, the spark timing has almost no effect on carbon dioxide emissions. However, a slight decrease can be observed for extremely delayed spark timings when operating at 3000@10 with CNG probably due to combustion instability issues.

NO_x emissions increase as the percentage of hydrogen substitution is increased due to two main reasons. Hydrogen substitution shifts the combustion to the TDC. This new combustion phasing increases NO_x emissions because higher temperature conditions are reached, promoting its formation by the thermal mechanism. Similarly, the higher adiabatic flame temperature of hydrogen also favour NO_x formation. Moreover, NO_x emissions are significantly affected by spark timing. It can be observed that advancing ignition timing, lower emission levels are obtained, displaying an almost linear relationship.

Finally, the MBT points for each of the operating points are compared, obtaining a big picture on the application of this technology in a vehicle. The main results obtained are presented in Fig. 6. A CO_2 reduction is observed as the hydrogen percentage is increased in the fuel composition. Regarding NO_x emissions, results remain approximately constant when increasing the H_2 percentage. Therefore, an after-treatment system is required to deal with current and future pollutant regulations. Higher air dilution or Exhaust Gas Recirculation (EGR) seems to be the way to deal with pollutant standards without any after-treatment system. Further research is still needed to elucidate which dilution strategy could match better with the use of HCNG fuel blends.

In Fig. 6, the most relevant performance parameters are analyzed as well. The net indicated efficiency tends to increase as the percentage of H_2 is increased in the fuel blend. However, this trend can be inverted for

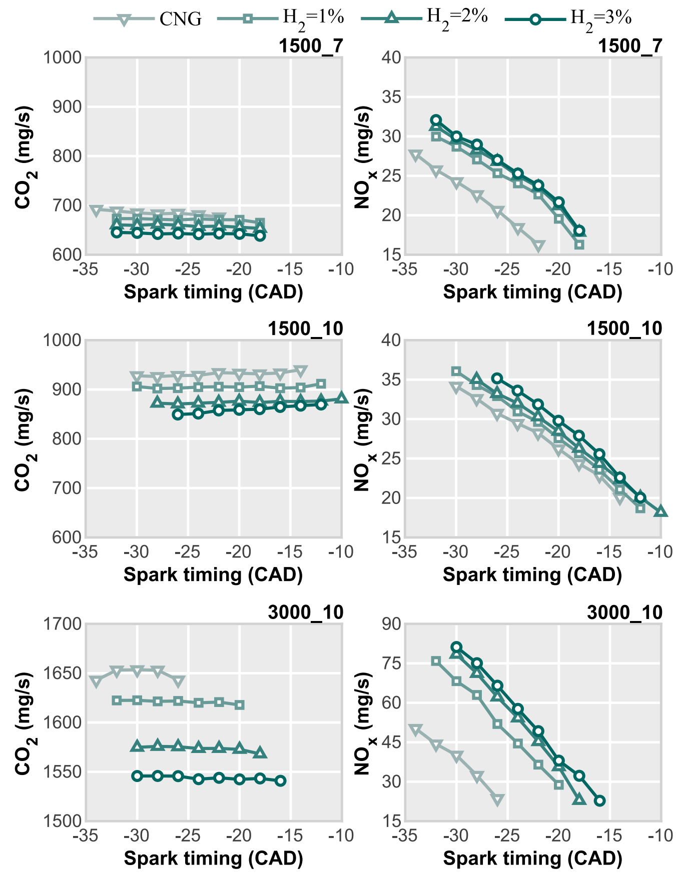

Fig. 5. NO_x and CO_2 exhaust mass flow measurements.

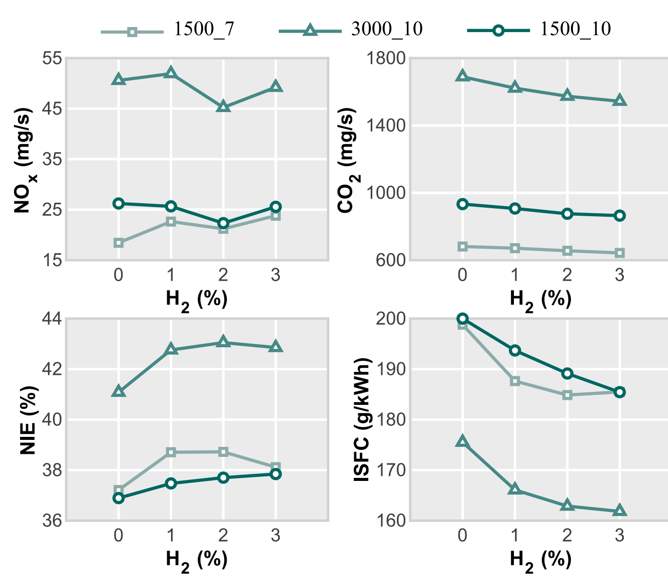

Fig. 6. Emissions (CO_2 and NO_x) and performance (NIE and ISFC) for different operating points and fuel compositions.

higher hydrogen amounts depending on the operating point. The optimum hydrogen substitution percentage is reached at 1%–2% H_2 for 1500@7, 3% H_2 at 1500@10 and 2%–3% H_2 at 3000@10 operating point.

These results have been obtained using a compression ratio (CR) of 10.7, which may not be the optimum value taking into account the anti-knocking properties of both CNG and hydrogen. Different studies [41, 42] point out that CR values close to 12 offer the highest levels of performance. Other authors, such as Park et al. [32] demonstrated how knocking combustion conditions the engine performance under HCNG lean conditions ($\lambda > 1.6$) and high CR. Therefore, further research on how increasing CR affect combustion, engine performance and emissions is still needed.

4. Conclusions

The impact of hydrogen substitution has been experimentally evaluated in a single-cylinder spark-ignition engine. This research work is performed to determine the effects of using HCNG fuel blends on combustion performance and pollutant emissions. The CNG fuel operated in lean condition is compared to three HCNG fuel compositions. The main conclusions obtained from the results can be summarized as:

- The in-cylinder pressure and HRR profiles are affected by hydrogen substitution.
- Hydrogen stabilizes combustion, allowing further delays in combustion phasing. The spark timing control is more relevant in the search for higher thermal efficiency.
- Delaying the combustion could reduce NO_x emissions. However, the minimum levels obtained are still far from avoiding the use of after-treatment systems.
- H_2 substitution helps to reduce the CO_2 emissions in two different, but closely related ways. First, improving the engine efficiency: higher efficiencies reduce the mass of fuel needed to obtain a given amount of useful energy. And secondly, reducing the carbon content of the fuel by hydrogen substitution, resulting in less CO_2 produced.

Funding

This research has been partially funded by FEDER, Spain and the Spanish Government through project RTI2018-102025-B-I00 (CLEAN-FUEL).

M. Olcina-Girona is partly supported by an FPI contract (FPI–S2-22-37816) of the “Programa de Apoyo para la Investigación y Desarrollo (PAID 01–22)” of the Universitat Politècnica de València.

Credit

S. Molina: Project administration, Conceptualization, Supervision, Methodology. **S. Ruiz:** Supervision, Methodology. **J. Gomez-Soriano:** Supervision, Formal analysis, Investigation, Writing - review & editing. **M. Olcina-Girona:** Investigation, Formal analysis, Writing – original draft.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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5. List of acronyms

ANN: Artificial Neural Network
C: Carbon atom
CA10: Combustion after 10% of fuel burnt
CA50: Combustion after 50% of fuel burnt
CA90: Combustion after 90% of fuel burnt
CAD: Crank Angle Degree
CCV: Cycle-to-cycle Variation
CH_4: Methane
CNG: Compressed Natural Gas
CO: Carbon Monoxide
CO_2: Carbon Dioxide
COV: Coefficient of Variation
CR: Compression Ratio DME - Dimethyl ether
GDI: Gasoline Direct Injection
GHG: Greenhouse Gas
H_2: Hydrogen
HC: Hydrocarbons
HCNG: Hydrogen-CNG mixtures
HRR: Heat Release Rate
IMEP: Indicated Mean Effective Pressure
ISFC: Indicated Specific Fuel Consumption
λ: Air-Fuel ratio
LHV: Lower Heating Value
MBT: Maximum Brake Torque
NIE: Net Indicated Efficiency
NO_x: Nitrogen Oxide
O_2: Oxygen
PFI: Port Fuel Injection
RON: Research Octane Number
S_l: Laminar Flame Speed
S_T: Turbulence Flame Speed
SI: Spark Ignition
TDC: Top Dead Centre