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Hydrogen addition to ethanol-fuelled engine in lean operation to improve fuel conversion efficiency and emissions

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HIGHLIGHTS

- Engine performance is reproduced or improved up to 20% air excess, 6% hydrogen.
- Operation with 40% air excess requires 6% hydrogen to ensure adequate performance.
- Up to 2% hydrogen and 20% air excess improves fuel conversion and carbon emissions.
- Oxides of nitrogen emissions unaffected with up to 2% hydrogen and 20% air excess.
- 6% hydrogen with 40% excess air also provides benefits to efficiency and emissions.

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ABSTRACT

This work applies computer simulation to investigate the combined approach of hydrogen (H_2) addition with lean operation to enhance the potential of ethanol as a clean engine fuel for low-carbon transportation. To this end, this research evaluates how this operation regime impacts brake power, fuel conversion efficiency, and exhaust emissions. A dedicated software was used to perform a parametric study with varying amount of hydrogen addition and excess air ratio. The software combustion and performance parameters were calibrated against available experimental data and optimised for engine operation at the tested conditions. The results show that hydrogen addition does not produce noticeable effects on brake power and fuel conversion efficiency for lean operation with up to 20% air excess. However, for operation with 40% air excess, 6% H_2 addition is necessary to keep the power at the same level of the engine baseline condition while simultaneously improving fuel conversion efficiency. Operation in the range of air excess between 10% and 30% together with hydrogen addition up to 2% can simultaneously produce noticeable improvements of fuel conversion efficiency, carbon monoxide (CO) and hydrocarbon (HC) emissions, without compromising brake power and oxides of nitrogen (NO_X) emissions.

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1. Introduction

The adoption of pure electric vehicles is seen as a solid alternative to reduce emissions in the transport sector, but it requires large investments in electricity networks to support the increase in electric power demand [1]. Therefore, a more realistic scenario in the short and medium term for developing countries may be the deployment of hybrid-electric vehicles and the increased adoption of biofuels. In Brazil, for example, biofuels account for 25% of transport fuel but the transport sector is still responsible for 72% of oil energy demand and 59% of carbon dioxide (CO_2) emissions. Bioethanol replaces 46% of gasoline utilization in the country, while biodiesel shares 9.6% of diesel fuel use [2]. As a solution for a transition period, modern engines operating with biofuels in hybrid-electric configurations can be more cost-attractive than pure battery and fuel cell electric cars [3]. Possible configurations may also have the engine as a range extender [4].

Bioethanol is an adequate carbon neutral renewable fuel to replace gasoline, but it has much lower energy density than the fossil fuel. One way to compensate it is to supplement ethanol-operated engines with small quantities of a high energy density fuel, such as hydrogen (H_2) [5] Among H_2 properties to enhance ethanol application as engine fuel are its high lower heating value and flame speed [6], and extended the flammability limit [7], thus combustion can occur in poor or diluted regimes and allow for reduction of carbon emissions. Hydrogen also can improve the potential of gasoline-ethanol mixtures, as hydrogen addition to these blends yielded better combustion, emission, and performance, though with slightly higher oxides of nitrogen (NO_X) emissions [8]. The high flame temperature of H_2 can increase the production of NOx [9], but this can be counterbalanced by lean operation.

Experiments adding small amounts of H_2 to ethanol in a variable compression ratio CFR (Cooperative Fuel Research) engine improved fuel consumption [10]. Although high compression ratio and H_2 content increase flame temperature, its negative effect on NO_X emissions is partially offset by the high heat of vaporization of ethanol. Fuel consumption and engine efficiency can be optimised with ignition timing tunning when operating with ethanol and hydrogen [11].

The addition of H_2 to an engine operating with ethanol at idle and stoichiometric conditions was observed to decrease the cyclic variation of the indicated mean effective pressure (IMEP), hydrocarbons (HC) and carbon monoxide (CO) emissions [12]. The use of H_2 resulted in higher temperature peaks and NO_X production, and, for concentrations higher than 4% v/v H_2 in air, lower volumetric efficiency and reduced flame development and propagation led to loss of power and engine instability. Operation at wide open throttle condition reduce pumping losses at partial loads, keeping improved combustion stability by the addition of H_2 to ethanol-air mixture [13].

Lean-burn operation with hydrogen-enhanced ethanol has been shown to offer promising benefits in terms of engine performance, emissions, and combustion characteristics. The supplementation of hydrogen not only extends the lean limit but also minimizes cycle-by-cycle variations and HC emissions, particularly for leaner mixtures [14]. By injecting hydrogen into the system, the degree of constant volume combustion can be increased, leading to improved cylinder pressure and temperature, and subsequently enhancing the indicated mean effective pressure [15]. Improved combustion stability has also been observed with high hydrogen concentrations in ultra-lean ethanol-air mixture, also decreased NO_X emissions, but it did not oppose the heavy loss of power and torque outputs [16]. Similarly, another investigation of an SI engine operating under lean conditions using hydrous ethanol-gasoline blends enhanced with synthesis gas demonstrated a decrease in NO_X emissions and an increase in fuel consumption with leaner mixtures [17].

The loss in power output and increase in fuel consumption due to lean operation can be compensated by techniques such as turbocharging. The achievement of adequate power output for fuel mixtures and pressure boost in lean engine operation demands substantial optimisation, which often involves extensive investigations to calibrate the engine electronic control unit (ECU) using lookup tables [18,19]. While traditional experimental calibration requires significant resources and infrastructure [20], virtual engine calibration offers a cost-effective alternative, enabling comprehensive parametric engine studies without the physical prerequisites [21]. As Grasreiner suggests [22], virtual calibration employs simulation methods instead of experimental measurements to develop the engine optimal operation map.

Research using GT-Suite modelling for virtual calibration of a stationary engine operating with natural gas and hydrogen blends showed how the control of operating parameters such as equivalence ratio and spark timing can optimize combustion phasing and keep good performance while maintaining NO_X concentration acceptable [23]. A study using a quasi-dimensional (QD) model and a genetic algorithm (GA) demonstrated that optimal fuel composition and operating conditions in a spark ignition engine with $CH_4/H_2/CO$ blends can notably reduce NO_X emissions and improve thermal efficiencies compared to methane-fuelled engines, marking a cost-effective and efficient method for initial fuel blend screening [24].

When it comes to studying ethanol and hydrogen mixtures, simulation methods are very useful to compare them with other fuels and guide experimentation. A computational study demonstrated that adding different liquefied gaseous fuels to primary fuels can impact efficiency and combustion, with benzene-hydrogen mixtures showing the highest efficiency increases, while the use of mixtures of ethanol and liquefied hydrogen resulted in decreases [25]. Research conducted using a commercial engine simulation software found that the addition of up to 10% by volume of hydrogen to ethanol or other fuels can enhance engine performance under lean burn conditions [26]. The addition of 10% hydrogen to ethanol showed an enhancement in engine brake torque [27]. These studies [26,27] indicated that the addition of hydrogen increased ignition delay and combustion duration across all the fuel blends, having as consequence decreased HC, CO, and CO_2 emissions and increased NO_X emissions.

This paper aims to use H_2 and turbocharging to increase fuel conversion efficiency and reduce emissions of an ethanol-fuelled engine operating under lean mixture conditions. A dedicated engine simulation model is applied for the investigation, with the engine operating with lean fuel-air mixtures.

While there is a considerable number of reports in the literature on the use of hydrogen-enhanced ethanol engine, there is a noticeable research gap in the optimisation of performance and emissions of ethanol-fuelled engines, particularly at lean-burn conditions. The main novelty of this research, in comparison with previous works, is to perform the optimisation with the supply of hydrogen and use of turbocharging to compensate the power losses associated with lean burn. Detailed engine maps demonstrating operation areas of air excess and hydrogen addition under constant engine speed and power output for reduction of carbon and NO_X emissions and increase of fuel conversion efficiency are presented. The outcomes of this research are expected to indicate further improvements that can be achieved for ethanol-fuelled engines assisted by hydrogen addition and turbocharging as a low-to-zero-carbon technology, depending on the H_2 source, whether the engine will be used as main powertrain or range extender in hybrid electric systems.

2. Methodology

The research was carried out using AVL Boost, a dedicated software for thermodynamic simulation of 2- and 4-stroke Otto or Diesel cycle internal combustion engines. The simulation model is based on the application of energy conservation of energy to a control volume on the cylinder content [28]:

$$\frac{d(m_c u_c)}{d\theta} = \sum \frac{dm_i}{d\theta} h_i - \sum \frac{dm_e}{d\theta} h_e - p_c \frac{dV_c}{d\theta} + \frac{dQ_f}{d\theta} - \sum \frac{dQ_w}{d\theta} - h_{bb} \frac{dm_{bb}}{d\theta} \quad (1)$$

Where $\frac{d(m_c u)}{d\theta}$ is the rate of change of internal energy in the cylinder (kJ/°CA), $\frac{dm_i}{d\theta} h_i$ is the enthalpy flow into the cylinder (kJ/°CA), $\frac{dm_e}{d\theta} h_e$ is the enthalpy flow out of the cylinder (kJ/°CA), $p_c \frac{dV}{d\theta}$ is the work done by the piston (kJ/°CA), $\frac{dQ_f}{d\theta}$ is the fuel heat release rate (kJ/°CA), $\frac{dQ_w}{d\theta}$ is the wall heat loss rate (kJ/°CA), and $h_{bb} \frac{dm_{bb}}{d\theta}$ is the enthalpy flow due to blow-by (kJ/°CA). m stands for mass (kg), u is specific internal energy (kJ/kg), h is specific internal enthalpy (kJ/kg), p is pressure (kPa), Q is heat (kJ), and θ is crank angle (°CA). Subscripts c, i and e refer to cylinder, inlet, and exit, respectively.

The simplifications adopted for Eq. (1) consider the mixture is homogeneous at the beginning of combustion, the air-fuel ratio of the unburned mixture is constant during combustion, burnt and unburnt gases have the same pressure and temperature but different compositions, and no fuel evaporation inside the cylinder. The fuel heat release rate is given by Ref. [28]:

$$\frac{dQ_f(\theta)}{d\theta} = m_f Q_{LHV,f} \frac{dx(\theta)}{d\theta} \quad (2)$$

where m_f is the fuel mass (kg), $Q_{LHV,f}$ is the fuel lower heating value (kJ/kg), and $\frac{dx(\theta)}{d\theta}$ is the burn rate (kJ/°CA).

Simulation of the combustion process applies two-zone models, where the control volume is split into two zones and the first law of thermodynamics is applied to the burned and unburned zones separately, considering different temperatures in the burned and unburned gases. This principle is applied when both valves are closed, while Eq. (1) is applied to the open part of the engine operation cycle. The fuel mass fraction burned $x(\theta)$ is calculated by Wiebe equation, which has also been applied to blends of hydrogen and natural gas [29,30]:

$$x(\theta) = 1 - e^{-a\left(\frac{\theta-\theta_i}{\Delta\theta}\right)^{m_{wiebe}+1}} \quad (3)$$

where the four tuning constants are: coefficient a, normally used to model spark plug number and location; coefficient m_{wiebe}, also known as combustion chamber shape factor, used to model the flame front propagation; θ_i, the angle of start of energy release or start of combustion; and $\Delta\theta$, the combustion duration.

The combustion process indicators here used were CA_{50}, the crank angle at which 50% of intake fuel mass is burned and, therefore, half of the process heat is released, and CA_{pp}, the crank angle at which peak cylinder pressure is achieved. CA_{pp} was used as a reference for spark timing and combustion phasing control [31].

The model was used to perform a parametric analysis verifying the influence of hydrogen addition and fuel/air mixture equivalence ratio (φ) on engine performance, defined as [6]:

$$\varphi = \frac{\dot{m}_{H_2}\left(\frac{A}{F}\right)_{s,H_2} + \dot{m}_E\left(\frac{A}{F}\right)_{s,E}}{\dot{m}_A} \quad (4)$$

where $\dot{m}_A$, $\dot{m}_E$ and $\dot{m}_{H_2}$ are the air, ethanol, and hydrogen mass flow rates, respectively (kg/s); $\left(\frac{A}{F}\right)_{s,H_2}$ and $\left(\frac{A}{F}\right)_{s,E}$ are the respective stoichiometric air/fuel ratios of hydrogen and ethanol.

The hydrogen fraction $H_2(\%)$ of the total fuel admitted into the engine is here expressed on energy basis as [6]:

$$H_2(\%) = \left(\frac{\dot{m}_{H_2} Q_{LHV,H_2}}{\dot{m}_{H_2} Q_{LHV,H_2} + \dot{m}_E Q_{LHV,E}}\right) \cdot 100\% \quad (5)$$

where Q_{LHV,H_2} and $Q_{LHV,E}$ are the hydrogen and ethanol lower heating values, respectively (kJ/kg).

The simulation was performed based on a 74 kW ethanol engine operating at 3500 rpm, as a power generator in a series hybrid configuration, which characteristics are shown by Table 1 [6]. A naturally aspirated gasoline engine was modified from its original factory settings to operate with a retrofitted turbocharger and intercooler using ethanol as fuel. The baseline condition of the experimental data [6] here used to calibrate the simulation software was $H_2 = 0$, $\varphi = 1$ and $p_i = 1.36$ bar, for which the modified engine achieves its highest efficiency at the rated power. This condition was established after extensive fine-tuning of the modified engine operating with ethanol, turbocharger, and intercooler, aiming to achieve the highest efficiency. The configurations used in the parametric analysis with varying H_2 energy concentration are shown in Fig. 1. Hydrogen concentrations of 0%, 3% and 6% [6], fuel/air mixture equivalence ratios of 0.7, 0.85 and 1.0, and manifold intake air pressure (p_i) of 1.36 bar, 1.42 bar and 1.48 bar were tested while keeping a constant engine speed and power output. The upper p_i limit was set to assure safe turbocharging operation.

Table 1 – Engine specifications.

DESCRIPTION	SPECIFICATION
Engine type	Ethanol-fuelled spark ignition engine
Bore × Stroke	86 × 86 mm
Total displacement	1998 cm^3
Combustion chamber geometry	Pent roof
Number of cylinders	4
Mechanism and number of valves	DOHC/8 intake and 8 exhaust valves
Compression ratio	10
Max power	113/6000 kW/rpm
Nominal operating power	74/3500 kW/rpm
Maximum torque	198/4250 kW/rpm
Fuel injection system	Port fuel injected
Ignition system type	Electronically controlled ignition
Air intake	Air-cooled turbocharging

The AVL Design Explorer tool was applied to search for an optimal parameter configuration in the AVL Boost by two ways [32]: (1) systematic change of values within an allowable set, and (2) design of experiments (DOE) to learn the dependencies between the design parameters (input) and the response parameters (output). This method minimizes two objective functions representing the mechanical load and combustion phasing parameters. The chosen parameters were mechanical brake power (P_b), fixed at 74 kW, and the crank angle of peak cylinder pressure (CA_{pp}), defined as 14° and restricted to occur after CA_{50}. All used simulation constraints and their boundaries are shown by Table 2. In addition to CA_{pp} and P_b, other output metrics evaluated were cylinder pressure diagram, peak cylinder pressure value (p_{max}), and CA_{50}.

The AVL Impress tool was used for data post-processing and graphics creation [33]. The first step of the data post-processing stage was to filter the resulting dataset to only those that deviated up to ± 1.5% from the target mechanical power. A correlation matrix was developed in which the degree of correlation between two parameters was given by their absolute Pearson coefficient ($|r|$), where a high correlation was achieved if $0.5 < |r| < 1$. All correlations with $|r| < 0.5$ were discarded as insignificant. The experimental data used to calibrate the simulation software parameters were produced under the engine conditions shown by Fig. 2 [6]. Due to concerns with the engine longevity from turbocharging operation the peak cylinder pressure was limited to 80 bar as a target, based on values observed when the engine operated close to its rated range.

Using the optimised parameters, operation maps were generated by the simulation for the fuel conversion efficiency (η_f), defined as [6]:

$$\eta_f = \frac{P_b}{\sum \dot{m}_f Q_{LHV,f}} = \frac{P_b}{\dot{m}_E Q_{LHV,E} + \dot{m}_{H2} Q_{LHV,H_2}} \quad (6)$$

where P_b is the mechanical brake power (kW).

Operation maps were also produced for carbon monoxide (CO), hydrocarbons (HC) and oxides of nitrogen (NO_X) emissions. The emission model used the default calculation in the simulation software to provide results for a qualitative analysis. Measured data of fuel conversion efficiency, CO and HC emissions were included as references to the operation map limits.

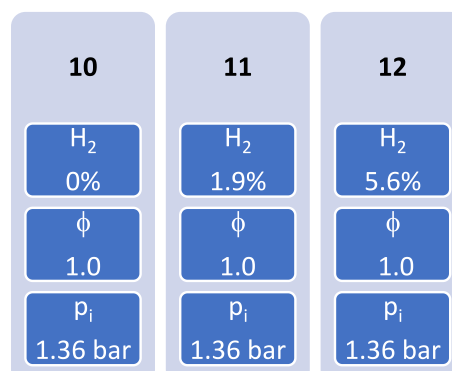

Fig. 2 – Matrix of engine conditions for experimental data at 3500 RPM, 74 kW, full load.

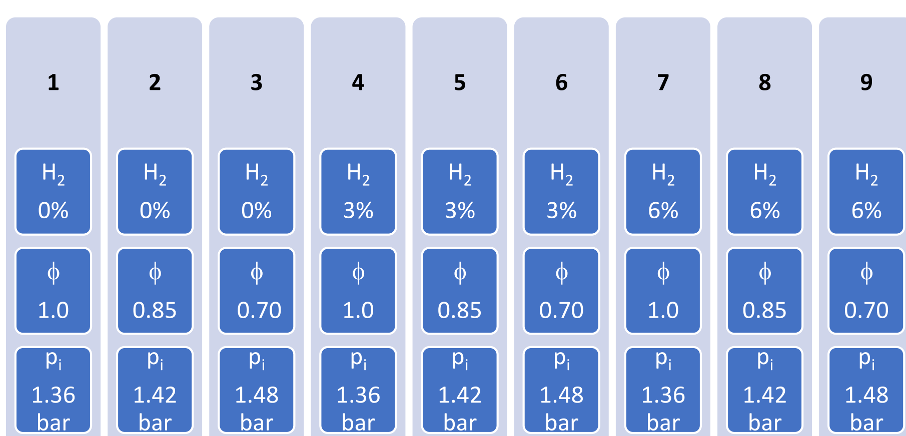

Fig. 1 – Matrix of engine parameters for simulation at 3500 RPM, 74 kW, full load.

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Table 2 – Boundary limits of simulation constraints.

CONSTRAINT	Lower boundary	Upper boundary
Temperature difference between piston crown and cylinder head (°C)	15	-
Temperature difference between piston crown and exhaust (°C)	20	40
Temperature difference between piston crown and cylinder liner at TDC (°C)	20	50
Temperature difference between cylinder head and exhaust (°C)	0	-
Temperature difference between exhaust and cylinder liner at TDC (°C)	0	-
Temperature difference between cylinder liner at TDC and BDC (°C)	0	25
(CA_{pp} – CA_{50}) (°CA)	0	-

3. Results and discussion

Fig. 3 shows the CA_{pp} and peak pressure attained after parametric optimisation for simulation with target values of 14°ATDC and 80 bar, respectively, for the conditions identified in Fig. 1. Also shown in Fig. 3 are the experimental CA_{pp} and peak pressure data at the conditions identified in Fig. 2, used to calibrate the simulation software. The average uncertainties of the experimental CA_{pp} and peak pressure data are ±0.2°ATDC and ±0.4 bar, respectively. The optimisation aims to achieve the specified power output and combustion phasing for each engine operating condition, in a coordinated effort to keep the peak cylinder pressure the closest possible to the baseline condition and, thus, to avoid damage to the engine and increased NO_X production. The figure reveals that simulation of conditions 3 (H_2 = 0%) and 6 (H_2 = 3%), both at φ = 0.7, pi = 1.48 bar, fall far from the target CA_{pp} and peak pressure values. In these cases, the expected decrease of peak cylinder pressure due to lean mixture operation could not be fully compensated by turbocharging or hydrogen addition. The experiments using 5.6% H_2 at stoichiometric condition, pi = 1.48 bar (condition 12) could reach the target peak pressure at a slightly lower CA_{pp} than the target one. Hydrogen concentration effects on the attainment of the target CA_{pp} are clearly seen in Fig. 4, where simulation at condition 3 and experiments at condition 12 show the highest departure from the target value though with deviations of only 2.5% and 1.1%, respectively.

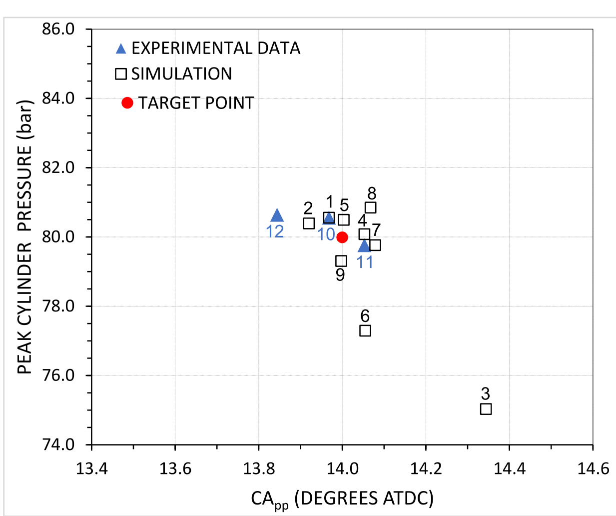

Fig. 3 – Calibration points of peak cylinder pressure and its crankshaft position.

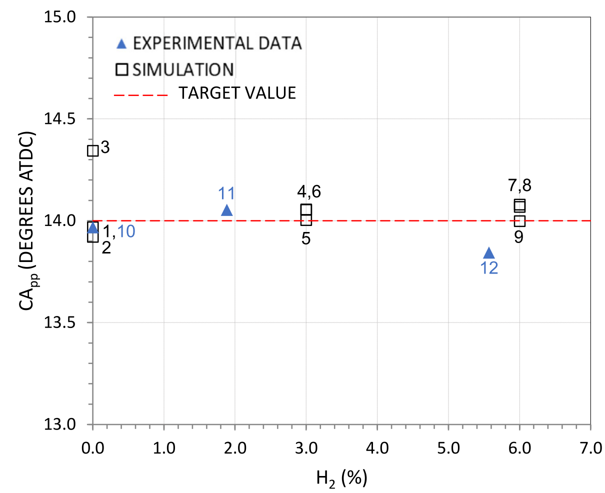

Fig. 4 – Calibration points of crankshaft position of peak cylinder pressure with varying hydrogen concentration.

Fig. 5 directly demonstrates the attainment or lack of the desirable engine performance by the simulated and experimental data conditions through the display of output crankshaft power against H_2 concentration. The average uncertainty of the experimental mechanical power data is ±0.3 kW. These

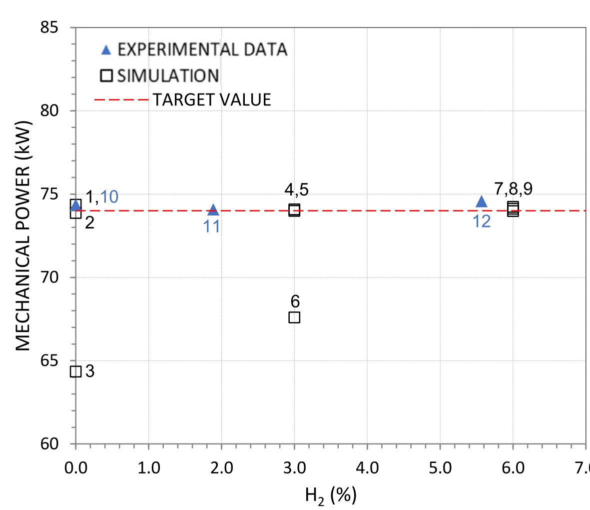

Fig. 5 – Calibration points of crankshaft power with varying hydrogen concentration.

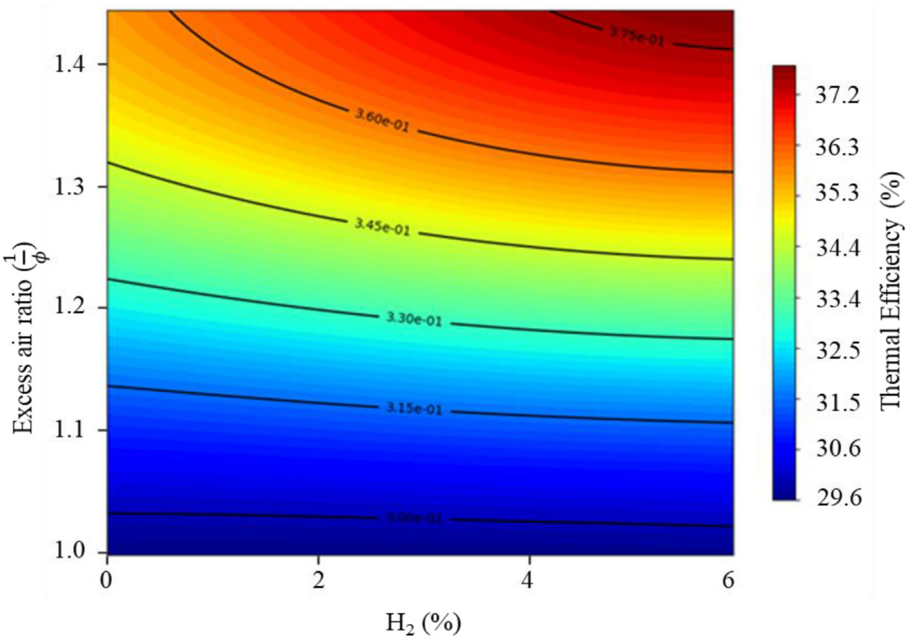

Fig. 6 — Variation of fuel conversion efficiency with excess air ratio and hydrogen concentration.

results confirm that very lean operation with $\varphi = 0.7$ (43% air excess) can only achieve the desired performance with the addition of a minimum of 6% H_2. All other tested conditions attain the rated power, revealing the complementarity of hydrogen content and intake pressure boost to achieve adequate engine performance with lean mixture operation. Hydrogen addition benefits lean engine operation by extending ethanol flammability limit and stabilising the combustion process [16], while turbocharging compensates for the power losses associated with excess air regimes [34].

Hydrogen addition has no noticeable effect on fuel conversion efficiency for stoichiometric mixture and little effect on slightly lean mixtures, as shown by Fig. 6. However, increased hydrogen addition can cause significant enhancement of fuel conversion efficiency for very lean operation. This effect can be related to the condition of 6% H_2 addition being able to make the engine reach its rated power even when operating with 43% air excess (see Fig. 6). Increased fuel conversion efficiency with hydrogen addition has also been found by other authors [13,35], though the extent of the improvement

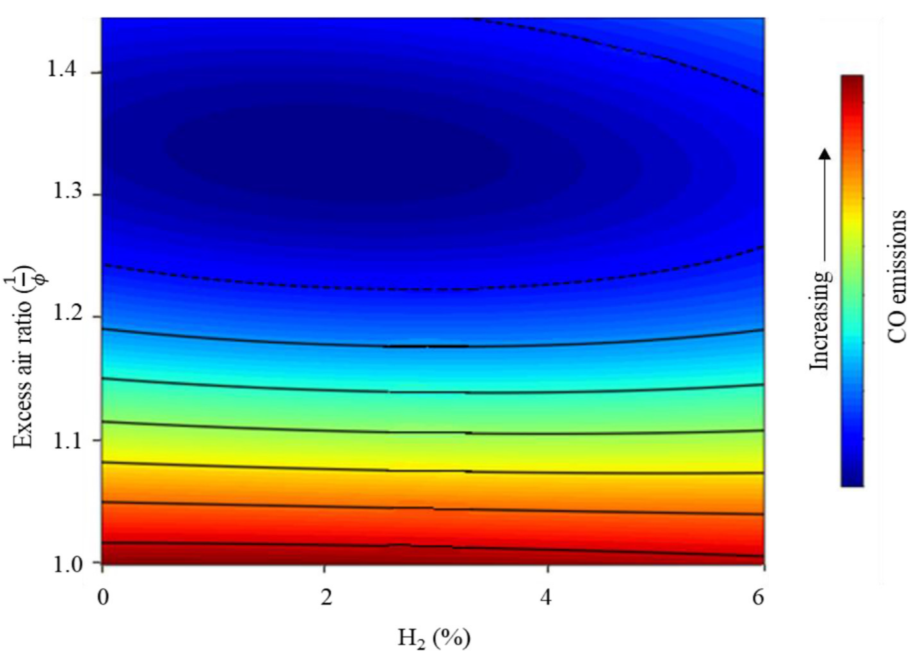

Fig. 7 — Variation of CO emissions with excess air ratio and hydrogen concentration.

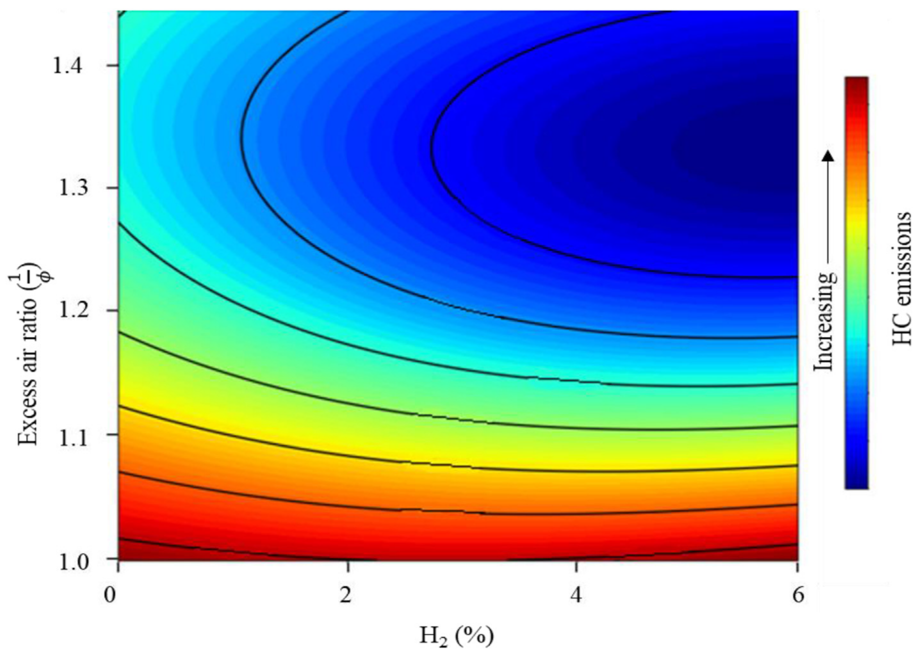

Fig. 8 – Variation of HC emissions with excess air ratio and hydrogen concentration.

obtained is subjected to variation in engine configuration. Reductions of CO_2 emissions from H_2 addition are expected to the same order of fuel consumption reduction as result of lean operation and improved fuel conversion efficiency [5].

Carbon monoxide emissions show low sensitivity to hydrogen addition, but they are deeply decreased as the mixture is made leaner (Fig. 7). CO reduction with increased air excess is a generally well-known trend for engine operation, here being confirmed as a benefit from ethanol lean burn [12,16]. HC emissions are little affected by H_2 addition for stoichiometric and slightly lean mixtures, but for very lean mixtures the addition of hydrogen can be highly beneficial to reduce HC emissions, as shown by Fig. 8. Similar findings have also been reported elsewhere [14]. Very lean mixture can make it difficult for the flame to start and propagate, thus producing HC from the partial burn effect [36]. Hydrogen

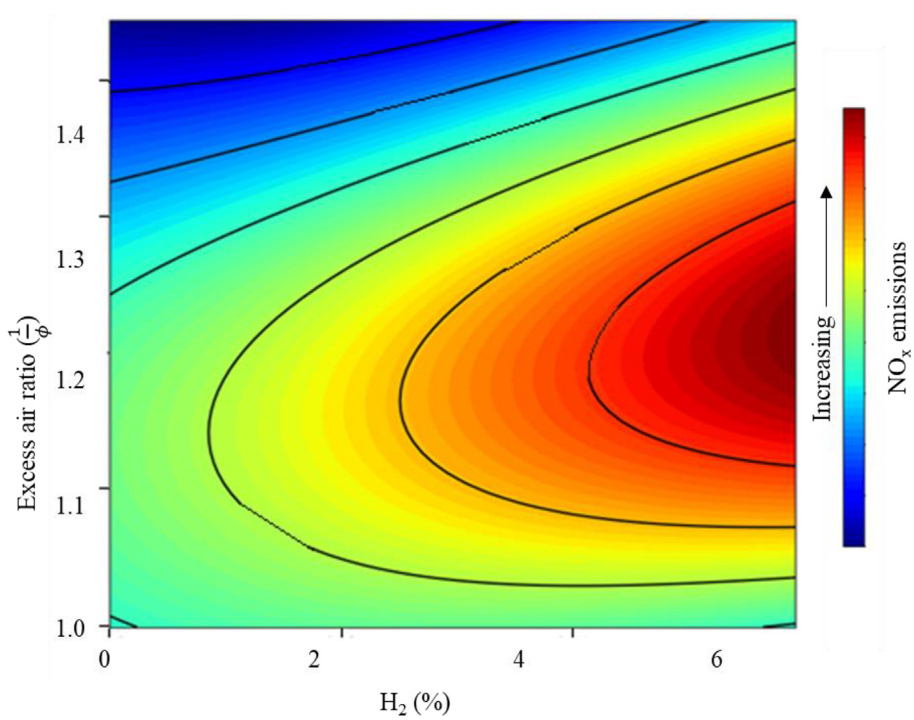

Fig. 9 – Variation of NO_X emissions with excess air ratio and hydrogen concentration.

addition improves the ethanol-air mixture flammability and propagation, therefore reducing HC emissions as the combustion process can be completed.

NO_X production is known to depend on cylinder mixture temperature and oxygen availability, the combination of both producing a peak at slightly lean mixtures [37]. One of the drawbacks of hydrogen addition to engines is the increase of peak combustion temperatures [15,27], resulting in higher production of NO_X [38,39]. Fig. 9 shows that the highest increase of NO_X emissions occurs at around 1.2 air excess ratio and high hydrogen concentration. However, low H_2 addition to very lean mixtures does not seem to cause any harm to NO_X emissions, in agreement with the findings of other authors [16,40].

4. Conclusion

From the results obtained in this research, the following conclusions can be drawn:

- Engine combustion characteristics and performance can be satisfactorily reproduced or improved at various conditions for lean operation up to 20% air excess, hydrogen addition up to 6% and turbocharging
- Lean operation with 40% air excess will require at least 6% H_2 addition to ensure proper combustion and unaffected performance
- Small hydrogen addition of up to 2% of fuel energy content together with intake pressure increase by turbocharging can extend the lean limit of an ethanol-fuelled engine to operate with up to 20% air excess, simultaneously improving fuel conversion efficiency and carbon emissions, and having no awkward effects on NO_X emissions
- Increasing hydrogen addition to 6% of fuel energy content can allow similar benefits on fuel conversion efficiency and emissions for operation with 40% excess air and possibly over.
- With properly calibrated engine maps, the combined use of turbocharging, hydrogen enrichment and lean operation has proved the potential to achieve high efficiency and low emissions without power derating.

These findings can give support to the application of typical amounts of H_2 generation that can be produced on-board [5], as an alternative to the transport and storage challenges associated to the use of compressed hydrogen.

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.

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