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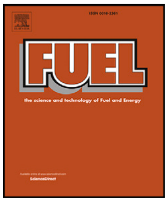

Full length article

Numerical analysis of zero-carbon HCCI engine fuelled with steam diluted H_2/H_2O_2 blends

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ABSTRACT

The addition of hydrogen peroxide and steam to a hydrogen-fuelled HCCI engine was investigated at various fuel lean conditions (ϕ_{eff} = 0.2–0.6) and compression ratios (15–20) using a 0-dimensional numerical model. The use of hydrogen peroxide as an ignition promoter demonstrated increased IMEP (16%–39%), thermal efficiency (up to 2%), and reduced NOx (50%–76%) when compared to the conventional method of intake charge heating. When hydrogen peroxide was used as an ignition promoter, a 15% addition of steam was sufficient to reduce NOx by 93%–97%, though this reduced IMEP and thermal efficiency slightly. When heat transfer was considered and steam addition was increased from 0%–10%, no increase in intake air heating was able to match the IMEP of 5% hydrogen peroxide addition without an increase in the equivalence ratio (up to 40%). The parametric space of hydrogen peroxide (0%–25%) and steam (0%–40%) addition was explored in view of engine performance metrics, showing the complete range of conditions possible through control of both inputs. A three-order reduction in NOx was possible through steam addition. An optimal balance of performance and emissions occurred at 5%–10% hydrogen peroxide and 10%–15% steam addition. In a study of compression ratio, very little hydrogen peroxide addition (<5%) was required to achieve 98% of the maximum efficiency at higher compression ratios (19–20), though at lower compression ratios (<17) impractical quantities of hydrogen peroxide were required. The 10% steam addition present at these conditions led to extremely low NOx levels for ϕ_{eff} of 0.3 and 0.4, though at ϕ_{eff} of 0.5 NOx levels would require some after-treatment. Maintaining constant a high or low load across steam additions was possible through reasonable adjustment of hydrogen peroxide addition.

1. Introduction

Advances in alternative propulsion technologies are needed to reduce the carbon footprint of heavy duty transport applications, such as marine vessels for shipping which contribute to around 3% of global emissions annually [1]. The use of batteries is a common approach, however issues remain surrounding batteries as a replacement for fossil fuels in these settings with challenges of safety and recyclability which have yet to be solved [2,3]. It is also well documented in the literature that the zero-emissions feature of electric cars only applies at the exhaust pipe and not on a life cycle basis, while at the same time non-exhaust particulate matter (PM) becomes a significant problem that needs to be tackled [4,5]. Also, converting any heavy-duty vehicle from internal combustion engine to an entirely different method of power generation such as a battery or fuel cell will no doubt entail financial costs, therefore an ideal solution would rely on retrofitting of the existing internal combustion engines widely used in heavy-duty applications to minimise cost and maximise speed of implementation.

Hydrogen has long been considered as a replacement for fossil fuels, being a main candidate for carbon-free propulsion with its only emissions upon combustion with oxygen being water, NOx as well as particle number (PN) emissions, the latter being favoured with hydrogen's increase in the in-cylinder charge [6,7]. Most research involving hydrogen as a primary fuel has been performed in the context of spark ignition (SI) engines [8–10]. The use of hydrogen in compression ignition (CI) mode has not been particularly attractive, mainly because of hydrogen's high autoignition temperature; the thermodynamic conditions achieved at the top dead centre (TDC) of a conventional CI engine cylinder are not sufficient to initiate ignition. To tackle this, three strategies have been proposed. Firstly, the increase of the compression ratio to achieve the appropriate thermodynamic conditions, suitable to enable ignition of the charge [11]. The literature relevant to this approach is quite scarce, but there is a consensus that compression ratios above 29 would be required to enable smooth

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operation [12,13]. Such compression ratios are significantly higher than those used in conventional CI engines (15–20). Therefore, such an approach in essence implies engine redesign that will significantly reinforce the engine's mechanical strength. The second approach that has been proposed is the use of a glow plug to preheat the inlet air or charge at temperatures sufficiently high to enable the charge's ignition close to the TDC [14–19]. This approach is conceptually simple and has been tested for both conventional CI and homogeneous charge compression ignition (HCCI) engines. Despite it simplicity this is also not very attractive because the preheating of the charge/air leads to the decrease of the engine performance (indicated mean effective pressure, indicated/brake thermal efficiency) due to the decrease of the volumetric efficiency [19–23]. Plus, issues associated with abnormal combustion and reduced operational range have also been reported, particularly in HCCI mode [20,19]. The third approach entails the use of a dual fuel strategy, where a second more reactive fuel (sometimes called pilot fuel) initiates ignition through direct injection [11]. This approach has been the most popular of all three because of the many advantages that it offers; operational flexibility, reduced NOx and good engine performance, to name a few. However, the role of the pilot fuel has been mainly played by carbon-based fuels (particularly diesel [24–26]), thereby not favouring the drastic reduction to greenhouse gases. Recently an alternative approach has been proposed by the authors of the current work; the use of hydrogen peroxide as an ignition promoter [27–29].

The idea of using hydrogen peroxide for propulsion purposes is not actually new and dates back to the 1930s when it was first used as a rocket fuel [30]. Since then its use as a fuel has mainly been limited to aerospace and military applications. In academic research hydrogen peroxide has been used as an ignition promoter in engine experiments (i.e., for the same purpose as in the current study) with fuels like diesel [31–34], jatropha oil [35] and butanol [36]. Apart from the fact that it can be produced from renewable sources [37], hydrogen peroxide has also the advantage that there is an existing logistics mechanism available to support its production, storage and distribution. The reason for this is because it is a substance used for other purposes besides as a fuel: medical use as an antiseptic, domestic use as a cleanser and disinfectant, and in the food sector for processing and bleaching certain foods, to name only few applications.

In the earlier work of [27] the effect of hydrogen peroxide addition to hydrogen/air mixtures on the ignition delay time and NOx emissions were investigated numerically in the context of a homogeneous and adiabatic batch reactor. It was reported that a mere 10% (per hydrogen volume) addition of H_2O_2 to H_2/air mixtures can lead to ignition delay times relevant to CI engines. Later, it was reported that the H_2O_2 addition to H_2/air mixtures in the context of premixed laminar flames leads to a significant increase of the laminar flame speed, the heat release and NOx emissions, while also reducing the thermo-diffusive instability of the flame and inducing a broadening of the reaction zone [28]. The work of [29] was the first numerical investigation reported in the literature that explored the H_2O_2 addition to H_2/air mixtures in the context of engine simulations. The engine model used was the single zone homogeneous adiabatic HCCI model from the Chemkin Pro suite. The investigation focused on the engine performance characteristics, the combustion phasing and NOx emissions. It was showcased that the use of hydrogen peroxide as an ignition promoter results in significantly improved engine performance and lower NOx at lean conditions when compared to the case of preheating the charge to sufficiently high inlet temperatures. The latter aimed to simulate the use of a glow plug. In fact it was demonstrated that the ignition promotion achieved by the hydrogen peroxide addition was sufficient to enable the effective use of mixture with equivalence ratio as lean as 0.1. It was also demonstrated that with the proper adjustment of the equivalence ratio between 0.1 and 0.4, the required amount of hydrogen peroxide to achieve the desired ignition did not exceed 10% of the hydrogen volume at a wide range of engine speeds (1000–3000 rpm). Finally, it was shown that the increase of the initial content of hydrogen peroxide leads to the enhancement of the engine performance and the reduction of NOx. In some cases (at extremely lean conditions) NOx emissions decreased to such low values that would enable the operation of the engine without the use of any after-treatment.

The current study aims to build further on the earlier work of [29]. Here, the effect of steam dilution of H_2/H_2O_2/air mixtures is numerically explored in view of the engine performance, combustion phasing and NOx emissions. The motivation for the use of steam dilution is twofold. Firstly, in a real engine demonstration hydrogen peroxide would need to be injected into the cylinder diluted in water because hydrogen peroxide becomes unstable in pure form. Besides, hydrogen peroxide is sold in the market in diluted in water form. The concentration of the hydrogen peroxide readily available in the market ranges between 3 and 35%, depending the grade (typically food grade hydrogen peroxide has the highest concentration). Secondly, steam dilution is a well-established method for reducing NOx emissions and mitigating (or eliminating) the occurrence of engine ringing, the latter being a known issue in HCCI engines, particularly at high loads [38–44].

The workbench for the numerical investigation herein will be Chemkin's single zone HCCI model, following the same practice as in [29]. Despite its inherent weaknesses due to the underlying assumptions made to reach a simple mathematical formulation, the single zone HCCI model can still provide some valuable insight if carefully used, which justifies its wide use by the research community [45–47]. As a result, the results produced by such a simplified model will need to be treated with care. For example, the emphasis will be placed on exploring the qualitative aspects rather than the quantitative ones. In addition, the results will be used to identify trends in the effect of the steam dilution of the H_2/air mixtures with the various H_2O_2 content. Consequently, the current work may serve as a feasibility study that can credibly inform subsequent analyses of the fuel blend in either high-fidelity simulations or real-world engine testing.

2. Material and methods

In the current work, the single-zone zero-dimensional HCCI model from the Chemkin Pro suite was used for the computational investigation. For a detailed description of the model the reader is referred to Chemkin's manual [48]. Here, only a brief description will be provided. The model integrates in a closed system (hence no mass exchange) the species mass fractions and energy equations along with one equation for the volume change to account for the piston movement. To maintain consistency with the earlier works of [27–29] the employed chemical mechanism was *Aramco 3* (for the hydrogen chemistry) [49], coupled with the nitrogen sub-mechanism of *Glarborg et al.* [50], both well-established reaction schemes. The model takes inputs of engine parameters (summarised in Table 1), such as compression ratio, engine speed, cylinder bore, piston stroke, and starting conditions of pressure and temperature. Unless otherwise stated, the compression ratio was maintained at 17 and the inlet temperature and pressure were maintained at 320 K and 1 bar, respectively. Simulations were mostly performed using the adiabatic model, however heat losses were also considered in some cases. For the latter cases, the heat loss Q from the gas to the solid walls was calculated from Eq. (1):

$$Q = hA(T - T_{wall}) \tag{1}$$

where h the heat transfer coefficient, A the internal surface area of the cylinder, T the temperature of the gas and T_{wall} the wall temperature, maintained at 430 K. The heat transfer coefficient h was calculated from Eq. (2) [51]:

$$h = \lambda \alpha Re^{b} Pr^{c} D^{-1} \tag{2}$$

where λ the gas conductivity, Re and Pr the Reynolds and Prandtl numbers, respectively, and α, b and c constants that were assigned the default values of 0.035, 0.71 and 0, respectively. The velocity

Table 1
The parameters used in the single-zone HCCI engine model employed in the current study.

Engine configuration	Single cylinder
Bore (mm)	100
Stroke (mm)	105
Connecting rod to crank radius ratio	3.714286
P_{in} (atm)	1
T_{in} (K)	320
Simulation start (CAD)	−180
Simulation end (CAD)	180
Compression ratio	15–20
Engine speed (RPM)	1000, 2000, 3000

in Reynolds number was calculated on the basis of the average gas velocity, given by the Woschni correlation. In the latter, the modelling parameters C_{11}, C_{12} and C_2 were given their default values of 2.28, 0.308 and 3.24, respectively.

Hydrogen peroxide (H_2O_2) addition was defined on the basis of the mole fraction of H_2; for example 10% addition of H_2O_2 indicates 10% of the mole fraction of H_2. It is also assumed that the decomposition of H_2O_2 leads to the formation of one mole of water (H_2O) and half mole of oxygen (O_2). This affects the total amount of O_2, altering the actual equivalence ratio from the desired value, thereby constituting problematic the use of the conventional definition of the equivalence ratio. Therefore, in line with previous works that considered the addition of H_2O_2 [28,29], an effective equivalence ratio (ϕ_{eff}) was used instead:

$$\phi_{eff} = \frac{X_{H_2}/(0.5X_{H_2O_2} + X_{O_2})}{(X_{H_2}/X_{O_2})_{st}} \tag{3}$$

where X_{H_2}, $X_{H_2O_2}$ and X_{O_2} the mole fractions of H_2, H_2O_2 and O_2, respectively and the subscript *st* denotes stoichiometric conditions.

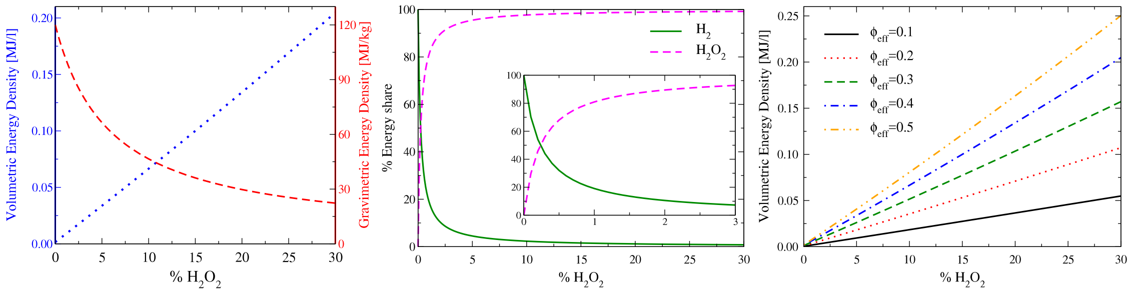
On mass basis, the energy density of hydrogen is much higher (40 times) than hydrogen peroxide's respective one; in particular hydrogen has a gravitational energy density of 120 MJ/kg while for hydrogen peroxide it is 3 MJ/kg. However, on a volume basis hydrogen peroxide has an energy density equal to 4.428 MJ/l which is more than 400 times larger than the energy density of hydrogen (0.0104 MJ/l) [52]. Since the addition of hydrogen peroxide is performed on the basis of the hydrogen mole fraction (hence volume) and considering that the initial volume and the effective equivalence ratio are maintained constant, it is reasonable to expect that the addition of hydrogen peroxide will lead to the increase of the volumetric energy density of the mixture. At the same time, it is expected that the gravimetric energy density of the mixture will drop with the addition of hydrogen peroxide, since hydrogen peroxide has significantly lower gravimetric energy than hydrogen. The results presented in Fig. 1(a) confirm indeed these expected trends. It is worth noting that although the increase of the volumetric energy density of the mixture due to the addition of hydrogen peroxide is linear, the gravitational energy density decrease is non-linear (logarithmic). Fig. 1(b) also underlines the strong influence of the hydrogen peroxide addition on the volumetric energy density; at merely 2% of H_2O_2 addition, 90% of the volumetric energy density is due to hydrogen peroxide, which is not surprising given the significantly higher volumetric energy density of hydrogen peroxide. Finally, Fig. 1(c) also highlights that as the mixture becomes richer, the addition of hydrogen peroxide results in larger energy increase. This finding will be discussed next but for now it suffices to say that as the mixture becomes richer we expect that the heat release will increase more due to the addition of hydrogen peroxide.

3. Results and discussion

We start the investigation with a comparison between the use of hydrogen peroxide as an ignition promoter to enable the ignition of the H_2/air mixture against the case of preheating sufficiently the H_2/air mixture, with the same level of steam dilution in both cases and while also maintaining constant the effective equivalence ratio. The increased inlet temperature in the latter scenario aims to simulate the case of the use of a glow plug which has been one of the proposed strategies to enable hydrogen use in CI engines. The earlier work of [29] did not consider any steam dilution and highlighted that the use of hydrogen peroxide is more advantageous than the preheating of the charge not only in terms of engine performance but also on NOx emissions. The improved engine performance was the result of the increased volumetric energy density achieved by the addition of hydrogen peroxide, as highlighted in Fig. 1, while the reduced NOx emissions were the outcome of the significantly lower reached temperatures. Here we will examine how this advantageous features are maintained or altered due to the addition of steam dilution.

In the first part of this comparison, the system is adiabatic. Following the same practice as in [29], the comparison between the two approaches is performed for fixed (effective) equivalence ratio, engine speed and ignition CAD, the latter being determined on the basis of the maximum temperature rate of change. The latter is selected because the crank angle where the temperature's maximum rate of change occurs is typically correlated with the crank angle where the maximum heat release rate takes place. Hence, in the current study CAD_{ign} is used as an indicator of the ignition delay time. For all examined cases in this comparison, the ignition CAD is maintained at 5 CAD aTDC. The results of this comparison are summarised in Table 2. For example, Table 2 shows that at $\phi_{eff} = 0.3$, engine speed of 1000 rpm and no steam dilution (0% H_2O) we need to add 1.8% of H_2O_2 to achieve ignition at +5 CAD aTDC. In order to achieve the same ignition CAD without any hydrogen peroxide, we would need to increase the inlet temperature by 44 K, i.e., to 364 K.

At $\phi_{eff} = 0.3$ and engine speed of 1000 rpm, Table 2 shows that the hydrogen peroxide content varies between 1.8% and 5.3% for the range of steam dilution 0%–15%. In the case where no hydrogen peroxide is added and ignition is achieved through the increase of the inlet temperature, T_{in} increases by 44–63 K compared to the hydrogen peroxide case (with T_{in} = 320 K), which indicates an increase in the range of 13.75%–19.69%, with this increase being more pronounced for high steam dilution. In all cases of steam dilution enhanced engine performance is achieved by the addition of hydrogen peroxide rather than the increased inlet temperature case. In particular, IMEP torque and power all increase by 16%–26% in the hydrogen peroxide case, with this increase becoming more prominent as steam dilution increases. This can be explained on the basis of the mixture's energy density; while steam dilution increases the difference in the energy density of the mixture between the two cases also increases (at 0% H_2O the energy density increases 8.6 times with the addition of H_2O_2, while at 15% H_2O this increase becomes 23.8 times larger). On the other hand, the effect of hydrogen peroxide addition on the thermal efficiency appears to have a negligibly small positive influence ($\sim$ 2%) at all steam dilution cases, in consistence with the earlier work of [29]. NOx emissions are generally very low and become extremely low (for both cases) when steam dilution increases to 15%. However, the case of hydrogen peroxide leads to consistently significantly lower NOx emission values compared to the case of the inlet preheating. This is most probably due to the reduced maximum temperatures reached in the cylinder (around 5%), as a result of the significantly lower inlet temperature used in the case of hydrogen peroxide (320 K). The only caveat with the use of hydrogen peroxide is the increase of the maximum pressure. Maximum pressure decrease with steam dilution but this decrease is larger in the case of the inlet preheating, therefore, when comparing the hydrogen peroxide case against the inlet preheating we observe that their difference in maximum pressures increases (from 8.5% to 13.6%) with the increase of the steam dilution (from 0% to 15%). This finding is the result of the higher energy density difference achieved at the high steam dilution cases as previously explained.



(a)

(b)

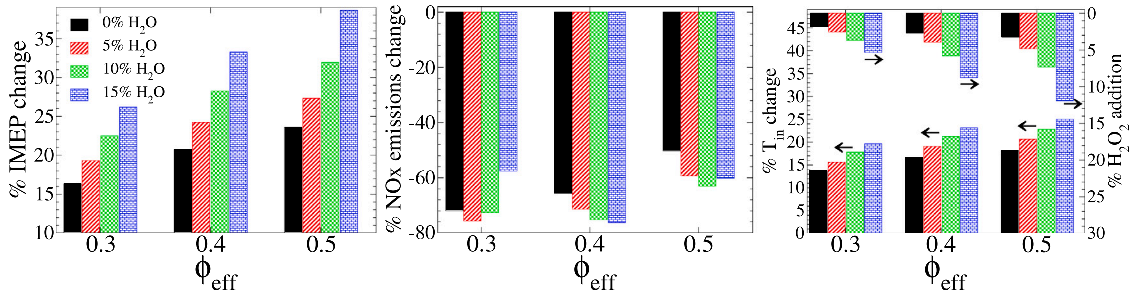
(c)

Fig. 1. The variation of the volumetric/gravimetric energy density (a) and the energy share (b) of the initial mixtures at ϕ_{eff} = 0.4 as a function of the initial percentage of hydrogen peroxide Also, in (c) the variation of the initial mixture's volumetric energy density at various effective equivalence ratios is shown, as a function of the initial percentage of hydrogen peroxide.

Table 2
Comparative investigation of the case where H_2O_2 is used for the ignition promotion of the H_2/air mixture against the case where the H_2/air mixture is ignited by sufficiently increasing the inlet temperature. A meaningful comparison is achieved by maintaining the ignition delay time constant at +5 CAD aTDC for all cases. Steam dilution varies between 0 and 15% in increments of 5, at ϕ_{eff} = 0.3, 0.4 and 0.5 and engine speed of 1000, 2000, and 3000 rpm. The displayed results include: the percentage of steam (H_2O) dilution, the percentage of the initial quantity of H_2O_2, the inlet temperature and maximum temperatures in Kelvin, the maximum pressure in bars, NOx emissions in parts per million by volume, dry (ppmvd), IMEP in bars, torque in N · m, power in J/s and the thermal efficiency (n_{th}).

ϕ_{eff}	Speed rpm	% H_2O	% H_2O_2	T_{in} K	T_{max} K	P_{max} bar	NO_x ppmvd	IMEP bar	Torque N · m	Power J/s	η_{th}
ϕ_{eff} = 0.3	1000	0	1.8	320	1962	102	11.67	6.93	45.5	4770	0.588
		0	0.0	364	2046	94	41.64	5.96	39.1	4100	0.581
		5	2.6	320	1886	99	3.39	6.58	43.2	4528	0.585
		5	0.0	370	1979	89	13.92	5.51	36.2	3795	0.576
		10	3.7	320	1815	95	1.31	6.24	41.0	4297	0.582
		10	0.0	377	1916	85	4.79	5.10	33.5	3508	0.572
		15	5.3	320	1749	92	0.79	5.93	38.9	4081	0.580
		15	0.0	383	1855	81	1.86	4.70	30.8	3234	0.568
ϕ_{eff} = 0.4	2000	0	2.7	320	2238	115	341.4	8.76	57.5	12061	0.575
		0	0.0	373	2329	102	994.0	7.26	47.6	9990	0.565
		5	4.0	320	2148	111	98.60	8.35	54.8	11491	0.572
		5	0.0	381	2247	97	345.0	6.72	44.1	9249	0.561
		10	5.8	320	2066	107	28.29	7.97	52.3	10963	0.569
		10	0.0	388	2168	92	114.0	6.21	40.8	8548	0.558
		15	8.8	320	1991	104	8.65	7.63	50.1	10503	0.567
		15	0.0	394	2092	88	36.40	5.73	37.6	7881	0.554
ϕ_{eff} = 0.5	3000	0	3.3	320	2479	125	3615.0	10.34	67.9	21352	0.559
		0	0.0	378	2567	110	7256.4	8.37	54.9	17275	0.547
		5	4.8	320	2380	121	1250.4	9.91	65.1	20465	0.558
		5	0.0	386	2472	104	3073.8	7.79	51.1	16074	0.547
		10	7.3	320	2289	117	413.3	9.52	62.5	19647	0.557
		10	0.0	393	2380	99	1119.0	7.21	47.3	14893	0.544
		15	11.9	320	2213	114	148.8	9.23	60.6	19052	0.554
		15	0.0	400	2293	94	374.0	6.66	43.7	13743	0.542

As the effective equivalence ratio and engine speed increase to 0.4 and 2000 rpm, respectively, the same trends between the two cases (hydrogen peroxide use versus inlet preheating) in engine performance and NOx emissions with steam dilution are maintained, with few noticeable differences. Firstly, the hydrogen peroxide strategy now exhibits a more notable increase of IMEP, torque and power compared to the inlet preheating case, varying between 21% and 33% (higher than the range of 16%–26% at ϕ_{eff} = 0.3) as steam dilution increases from 0% to 15%. This can be explained on the basis of the mixture's energy density, which for the hydrogen peroxide case addition it now becomes 12.6–38.8 times higher than the respective case of inlet preheating (depending the steam dilution level). Secondly, the thermal efficiency is still favoured negligibly (∼2%) by the addition of hydrogen peroxide, with the difference between the two strategies (hydrogen peroxide versus inlet preheating) having a trend to increase as steam dilution increases. Thirdly, the absolute values of NOx emissions of all cases increase by an order of magnitude compared to the respective cases at ϕ_{eff} = 0.3, yet they are still considered acceptably low (particularly in the hydrogen peroxide approach), suggesting that an after-treatment would probably still not be required. The hydrogen peroxide strategy has consistently ∼70% lower NOx emissions than the inlet charge preheating approach. The difference between the two approaches becomes more pronounced as the steam dilution increases. The reason for this finding is because as steam dilution increases the difference of the in-cylinder maximum temperatures between the two strategies becomes more pronounced. For instance, at 5% steam dilution, T_{max} is equal to 2148 K and 2247 K for the hydrogen peroxide and inlet preheating strategies, respectively, i.e., a 4.41% decrease in favour of the hydrogen peroxide strategy. However, at 15% this difference increases to 4.8%. This phenomenon (i.e., the increase in the difference of T_{max} between the two strategies as steam dilution increases) is believed to be due to the increase of the inlet temperature that is required to achieve ignition as steam dilution increases, in the inlet preheating charge strategy. T_{in} increases from 373 K to 394 K, for the 0% and 15% steam dilution cases, respectively. Finally, the hydrogen peroxide strategy is still consistently exhibiting higher maximum pressures than the inlet preheating strategy, but the difference between the two strategies



(a) (b) (c)

Fig. 2. The change in IMEP (a) and NOx (b) from the addition of H_2O_2 compared to the approach of inlet preheating, for the cases considered in Table 2. In (c) the required initial amount of H_2O_2 (upper and left axes) is compared against the required increase of the inlet temperature to achieve the same ignition delay time, for the cases examined in Table 2.

becomes more pronounced at $\phi_{eff} = 0.4$ than 0.3, which is due to the higher obtained energy density.

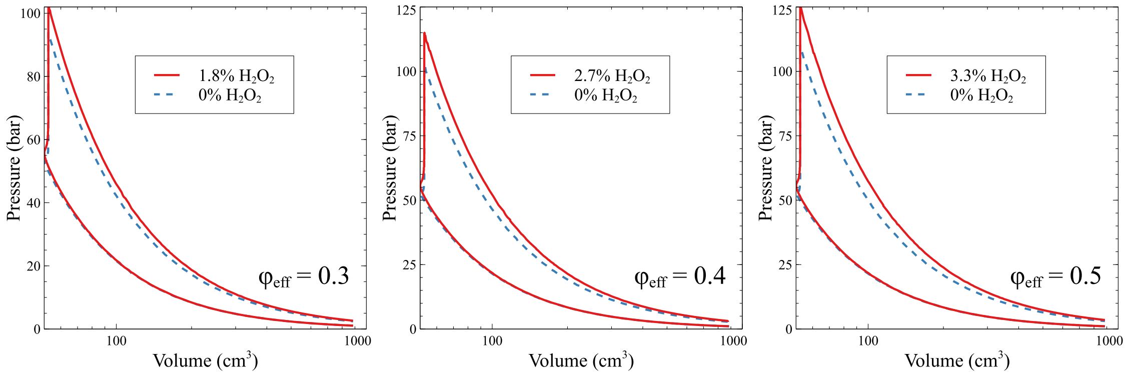
When the effective equivalence ratio increases further to 0.5 and the engine speed increases to 3000 rpm, the difference between the two strategies in view of engine performance becomes more pronounced; the increase of IMEP, power, torque achieved by the addition of hydrogen peroxide ranges between 24% and 39% against the case of inlet charge preheating, with the difference increasing as steam dilution increases. The increase of the thermal efficiency achieved by the hydrogen peroxide approach is still negligibly small, in the neighbourhood of ~2%. However, unlike the previous equivalence ratios, NOx emissions are now becoming considerably high, particularly at the low steam dilution cases. In agreement with the earlier findings though, the hydrogen peroxide case achieves a considerable decrease in NOx emissions compared to the inlet charge preheating approach, with this decrease becoming slightly less pronounced and ranging between −50% and -60% for steam dilution 0%–15%. The fact that the difference of the maximum obtained temperatures between the two strategies decreases at $\phi_{eff} = 0.5$ (in the range of 3.43%–3.82%) compared to the respective values at $\phi_{eff} = 0.4$ (in the range of 3.91%–4.83%) has a direct effect on the aforementioned decrease in the difference of produced NOx emissions between the two strategies. Finally, the maximum in-cylinder pressure drops with steam dilution but the hydrogen peroxide approach results in higher values compared to the respective cases of inlet charge preheating. These increases range between 14%–21%, depending the steam dilution level, but they are higher than those reported for the previous effective equivalence ratio cases.

In summary, the hydrogen peroxide addition strategy, when compared to the inlet charge preheating approach:

- results in notably higher (16%–39%) engine performance (IMEP, power and torque) values, as displayed in Fig. 2a. The difference between the two approaches in view of these metrics is favoured as steam dilution or effective equivalence ratio increase. In either case, the achieved enhancement is the result of the higher mixture's energy density.
- leads to mixtures with significantly higher (9–53 times larger) energy density with the difference being favoured with the increase of the effective equivalence ratio or the steam dilution.
- produces a negligible improvement (~2%) of the thermal efficiency, which is generally favoured as the effective equivalence ratio or the steam dilution increase. The marginal improvement of the thermal efficiency is due to the competition between the specific fuel consumption and the lower heating value (LHV), both being the two components used to calculate the thermal efficiency. With the addition of hydrogen peroxide the specific fuel consumption increases due to H_2O_2's higher molecular weight, while the H_2O_2's LHV (3 kJ/g) is significantly lower than the respective value of H_2 (120 kJ/g). The outcome of this competition results in the marginal increase of the thermal efficiency.
- induces a remarkable decrease (50%–76%) of NOx emissions, as displayed in Fig. 2b, reaching values of less than 150 ppmvd while also maintaining high load (9.2 bar of IMEP). This decrease is generally inversely proportional to the steam dilution level and the effective equivalence ratio.
- causes an increase to the maximum obtained pressure, this being the outcome of the increased energy density. The increase of the maximum pressure becomes more pronounced as the steam dilution or the effective equivalence ratio increase.
- generally requires less than 10% H_2O_2, with the worst case being at $\phi_{eff} = 0.5$ (3000 rpm) and 15% H_2O where 11.9% H_2O_2 is required, as illustrated in Fig. 2c. At the same time, to achieve the same ignition CAD without any H_2O_2, a considerable increase of the inlet temperature is required, increasing as the effective equivalence ratio or the steam dilution increase. In the worst case, a 25% increase of the inlet temperature is required ($\phi_{eff} = 0.5$, 3000 rpm, 15% H_2O).

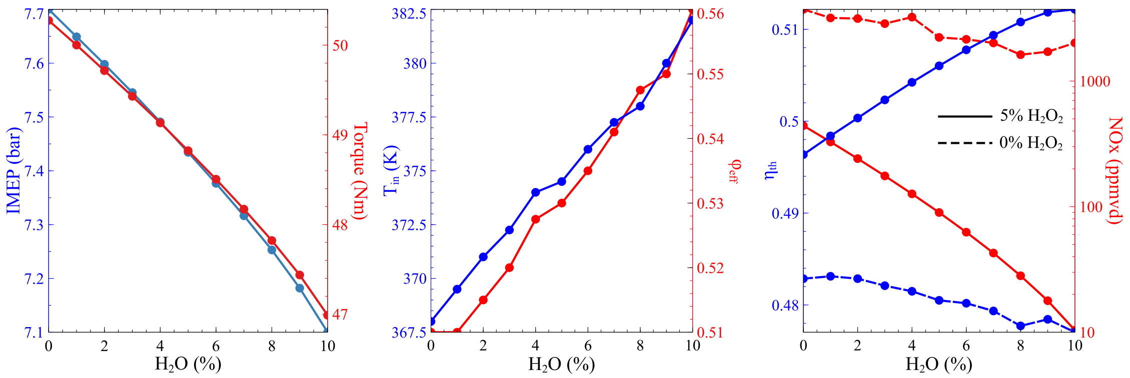
To explore further the effect of the hydrogen peroxide addition on the engine cycle, the P–V diagrams for three of the cases in Table 2 are illustrated in Fig. 3. These P–V diagrams display the compression stroke, followed by the combustion process (which practically occurs under constant volume) and finally the power stroke. At the selected conditions the hydrogen peroxide strategy achieves enhanced engine performance (IMEP, power and torque) ranging between 16% and 24% (proportional to the increase of the effective equivalence ratio). Since IMEP, power and torque are all functions of the indicated work (which is determined based on the enclosed area in the P–V diagram), it is intuitive that the enclosed area with the hydrogen-peroxide strategy is larger than the inlet charge preheating approach, for all three examined cases. Fig. 3 also clearly illustrates that the increased work achieved by the hydrogen peroxide strategy is the result of the higher pressure reached at the start of the power stroke.

The computational campaign exploring the comparison between the hydrogen peroxide strategy against the inlet charge preheating approach while increasing the steam dilution level is next extended to include heat losses. In this part of the investigation, we keep the engine speed constant at 2000 rpm for all cases. In the hydrogen peroxide approach, the effective equivalence ratio is maintained fixed at 0.4 and the hydrogen peroxide content is kept constant at 5%. By running different steam dilution scenarios from 0% to 10% H_2O the results displayed in blue in Fig. 4 were obtained. The obtained IMEP and torque curves shown in Fig. 4(a) were used as a reference for the inlet charge preheating approach, i.e., the same IMEP and torque values were obtained by properly adjusting the inlet temperature. In most occasions, the adjustment of the inlet temperature was not sufficient to achieve the same output in terms of IMEP and torque, hence the equivalence ratio was also properly adjusted to the minimum possible value. These results are reported in Fig. 4(b) where it is shown that with the only exception of 0% and 1% H_2O, in all other cases the



(a)
(b)
(c)

Fig. 3. Pressure–Volume diagrams of the two strategies (hydrogen peroxide strategy versus inlet charge preheating) for three of the cases displayed in Table 2. (a) ϕ_{eff} = 0.3, 1000 rpm and 0% H_2O with the hydrogen peroxide strategy using 1.8% H_2O_2 (red solid line) and the inlet charge preheating approach having T_{in} = 364 K (blue-dashed line). (b) ϕ_{eff} = 0.4, 2000 rpm and 0% H_2O with the hydrogen peroxide strategy using 2.7% H_2O_2 (red solid line) and the inlet charge preheating approach having T_{in} = 373 K (blue-dashed line). (c) ϕ_{eff} = 0.5, 3000 rpm and 0% H_2O with the hydrogen peroxide strategy using 3.3% H_2O_2 (red solid line) and the inlet charge preheating approach having T_{in} = 378 K (blue-dashed line).

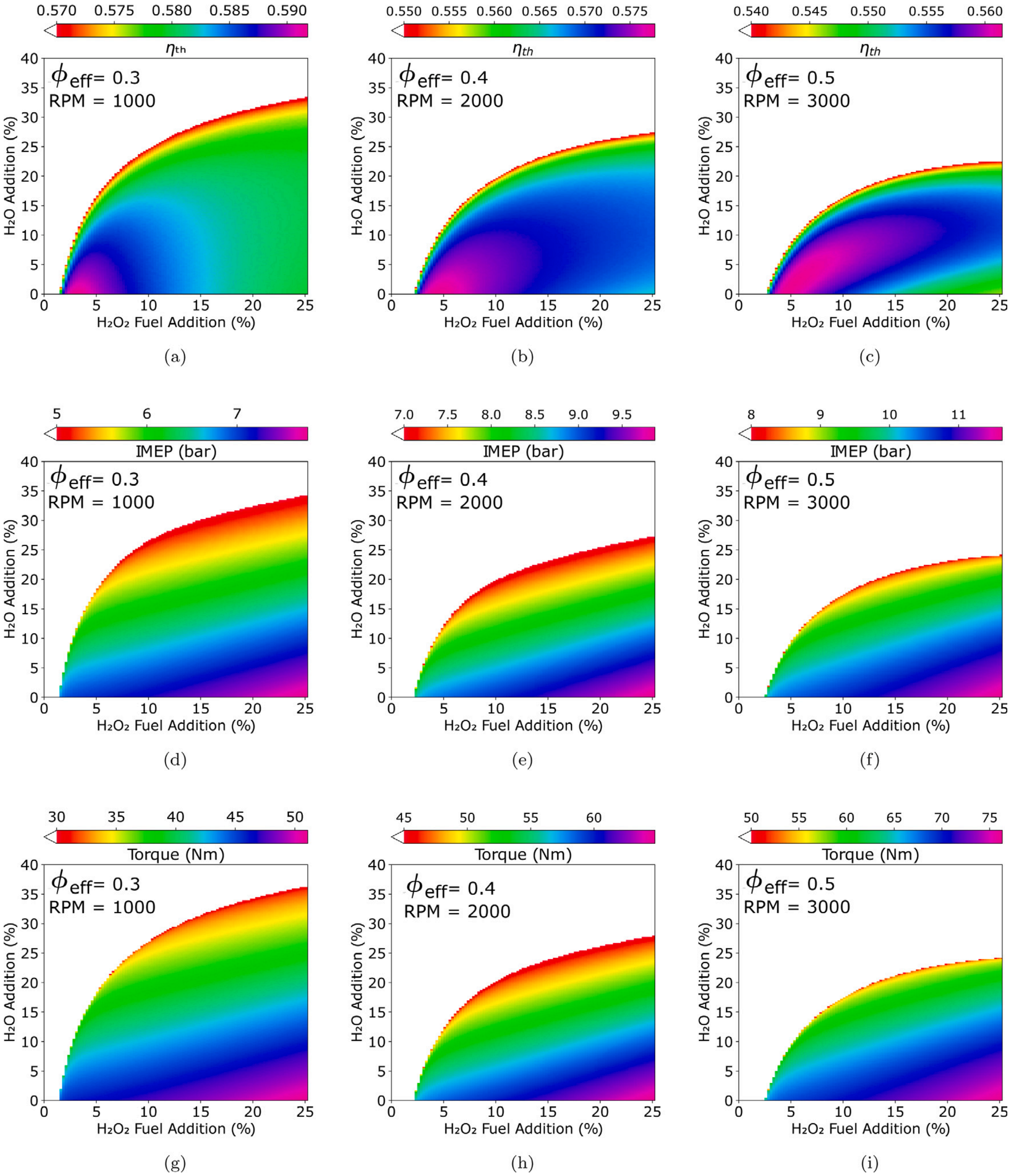


(a)
(b)
(c)

Fig. 4. Numerical campaign at 2000 rpm and steam dilution ranging between 0 and 10%. For the hydrogen peroxide strategy the H_2O_2 content was maintained fixed at 5% (T_{in} = 320 K, ϕ_{eff} = 0.4). The IMEP and torque results for the hydrogen peroxide strategy are shown in (a). These engine outputs were used as a reference for the inlet charge preheating approach, i.e., the same IMEP and torque values for each steam dilution level were reproduced by the proper increasing of the inlet temperature. In most cases, the increase of the inlet temperature was not sufficient, therefore the equivalence ratio had to also be increased to the minimum required value. The results of the required increased inlet temperatures and equivalence ratios to achieve the same IMEP and torque output in the inlet charge preheating approach are shown in (b). The variation of the thermal efficiency and NOx emissions as a function of steam dilution for the two considered strategies is shown in (c). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

equivalence ratio was also increased to allow for reaching the same IMEP and torque values as in the hydrogen peroxide strategy at the same steam dilution level. These results demonstrate that at 10% of steam dilution, with the hydrogen peroxide strategy we would need 5% H_2O_2 to achieve an IMEP of 7.1 bar. In order to achieve the same IMEP value at the same steam dilution level with the inlet charge preheating strategy, increasing the inlet temperature by 62.5 K to 382.5 K (19.5% increase) would not be sufficient, therefore an additional remarkable increase of the equivalence ratio would be required, in the neighbourhood of 40%. This required (practically linear) increase of the equivalence ratio is in fact proportional to the steam dilution level and corroborates the strong impact of hydrogen peroxide on the enhancement of the engine performance characteristics. Partly, this enhancement is also manifested in Fig. 4(c) which depicts the variation of the thermal efficiency between the two strategies as a function of the steam dilution. The hydrogen peroxide strategy has consistently higher thermal efficiency ranging between 2.8% and 7.3%, i.e., slightly higher than what was reported in Table 2. Probably most important though is the tremendous decrease of NOx emissions achieved through the hydrogen peroxide strategy, with the difference against the inlet charge preheating approach being even more than two orders of magnitude. For instance, at 10% H_2O the hydrogen peroxide approach leads to the production of 10 ppmvd in NOx while the respective value in the case of the inlet charge preheating exceeds 1000 ppmvd. In fact, in the inlet charge preheating approach, NOx emissions appear to always remain higher than 1000 ppmvd and steam dilution has small effect on their reduction. This is probably due to the fact that both the inlet temperature and the equivalence ratio needed to be adjusted (to achieve the desired IMEP/torque output) which largely cancelled the effect of steam dilution for in-cylinder temperature reduction, hence leading to high NOx emissions.

With H_2O_2 addition being established as an advantageous method of ignition control against the more conventional inlet charge preheating, in view of engine performance and NOx emissions, the next step is to investigate the incremental increase of the steam dilution level as a function of H_2O_2 content. The focus of the analysis will be on the engine performance outputs (IMEP, torque), NOx emissions as well as combustion phasing under adiabatic conditions. Sweeps were performed for 0%–25% and 0%–40% H_2O_2 and H_2O respectively, in increments of 0.25%. The simulations took place at ϕ_{eff} and engine speeds of 0.3/1000 rpm, 0.4/2000 rpm, and 0.5/3000 rpm. The results from this parametric study are shown in Figs. 5–7. This approach was intended to visually represent the range of engine performance possible across every practical combination of H_2O_2 and H_2O, and to determine the overall sweet spots for each performance metric in order to narrow down the theoretical ideal combination of H_2O_2 and



(a) (b) (c)

(d) (e) (f)

(g) (h) (i)

Fig. 5. Contour plots of the thermal efficiency η_{th} (a, b, c), IMEP (d, e, f), and torque (g, h, i) as a function of the hydrogen peroxide initial content ranging between 0 and 25% and the steam dilution level ranging between 0 and 40%, at ϕ_{eff} and engine speed of 0.3–1000 rpm (a, d, g), 0.4–2000 rpm (b, e, h), and 0.5–3000 rpm (c, f, i), respectively.

H_2O. The ideal conditions would be chosen based on a balance of maximisation of performance and efficiency and the minimisation of NOx emissions. The colourmaps are presented in three sections, the first being engine performance metrics of η_{th}, IMEP, and torque, the second being combustion phasing metrics of CAD_{ign} and rapid burn angle (RBA), and the third being NOx and T_{max}.

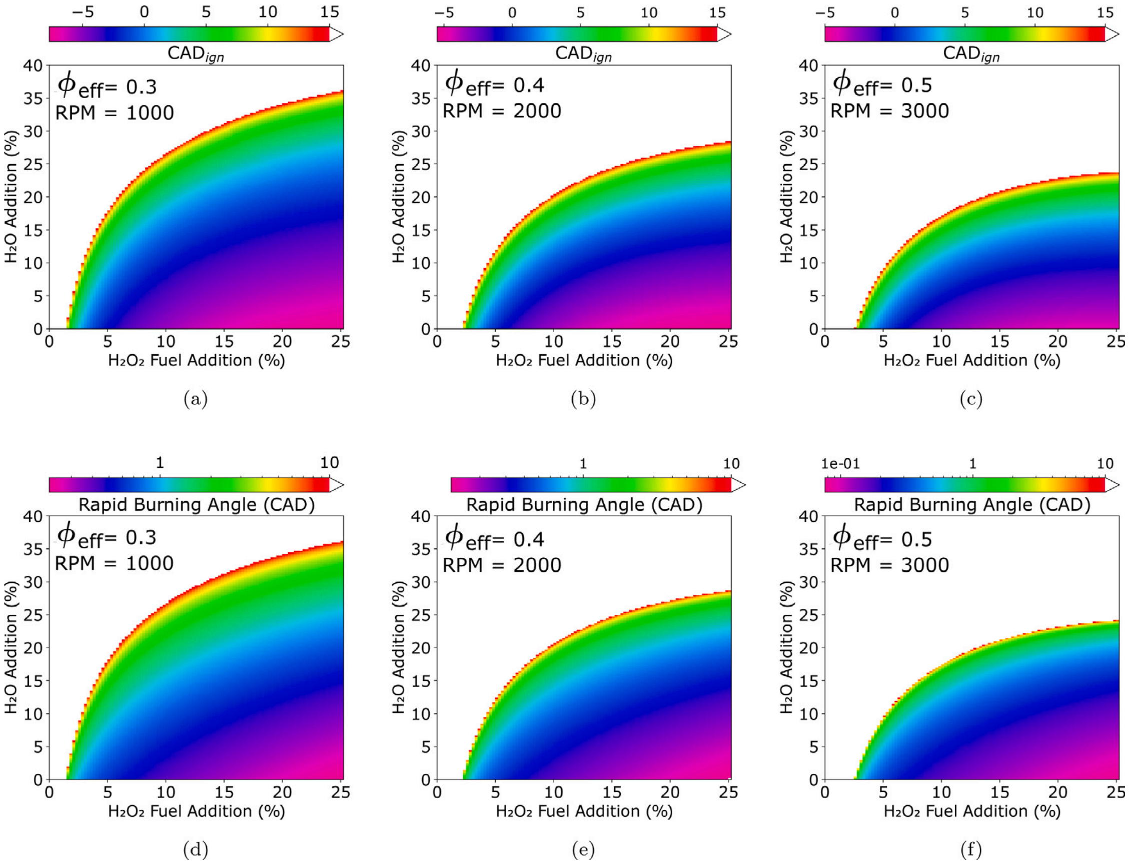
Figs. 5(a)–(c) show that increasing H_2O_2 addition initially increases the thermal efficiency reaching a maximum and later decreases, creating a non-monotonic response. At ϕ_{eff} = 0.3 the shift in the response of η_{th} occurs at 3% H_2O_2 at 0% H_2O, and at 4.5% at ϕ_{eff} = 0.4 and 0.5. At ϕ_{eff} = 0.3, 0.4, and 0.5, thermal efficiency peaked at values of 59.2%, 57.8%, and 56.1% respectively. The decrease in thermal efficiency upon further introduction of H_2O_2 past these points was due to the advancement of CAD_{ign} into negative values (i.e., CAD before TDC) which led to an increase of the negative work on the piston. This resulted in a drop in thermal efficiency of 1.2–1.5% from the peak value at 3–4.5% H_2O_2 to 25% H_2O_2, in the case of no steam dilution present. Increasing H_2O addition generally has a negative effect on the thermal efficiency. This trend becomes less pronounced as H_2O_2 addition increases and as ϕ_{eff} decreases. For instance, at 25% H_2O_2 and ϕ_{eff} = 0.3 η_{th} remains relatively unchanged due to steam dilution up until the threshold of non-ignition where η_{th} decreases rapidly upon further H_2O introduction. It appears to be possible to slightly offset some of the losses in thermal efficiency caused by H_2O addition to η_{th} with further introduction of H_2O_2. This effect becomes particularly evident at ϕ_{eff} = 0.5. For instance, in the case of 5% addition of H_2O_2 and no steam dilution the thermal efficiency is 56.1%. If the steam dilution is increased to 5% the thermal efficiency will drop to 55.9%. To achieve the same thermal efficiency at 5% of steam dilution we would need to increase the initial H_2O_2 from 5% to 7.5%. Another way to view the non-monotonic response of η_{th} is that the loss in thermal efficiency from the advance of ignition prior to TDC due to increased H_2O_2 addition could be offset by sufficient steam addition. In general, when sufficiently far from the threshold of no-ignition, the thermal efficiency does not vary significantly, exhibiting a maximum variation of 1.5%.

Another observation that can be made on Figs. 5(a)–(c) is that the steam dilution range that allows the ignition of the mixture increases with the addition of H_2O_2 and decreases with the increase of engine speed. Both are intuitive findings since the more the hydrogen peroxide in the mixture the more energy dense the mixture while the higher the engine speed the less time available to ignite. It is worth probably to note that the decrease in the steam dilution range that allows the ignition of the mixture as the engine speed and the equivalence ratio increase is only due to the increase of the engine speed and not the increase of the equivalence ratio. In fact these two parameters have competitive outcomes, i.e., the increase of the equivalence ratio tends to increase the operational range while the increase of the engine speed tends to decrease it, but it seems that the increase in the engine speed is much stronger for the conditions under examination.

In terms of power and torque, Figs. 5(d)–(i) display that increasing H_2O_2 addition enhances IMEP and torque, with these trends continuing linearly up until the maximum values of both IMEP and torque at 25% H_2O_2 addition, regardless the ϕ_{eff}. The increase of IMEP and torque due to the increase of H_2O_2 is, as already explained, the result of the higher obtained energy density of the mixture (as shown in Fig. 1) which leads to higher produced work (as shown in Fig. 3). The maximum values for IMEP and torque at ϕ_{eff} of 0.3, 0.4, and 0.5 are 7.8 bar/51.2 Nm, 9.9 bar/65 Nm and 11.6 bar/76.5 Nm, respectively. These results suggest that low to medium loads (4.9–7.2 bar/32.2–47.5 Nm of IMEP and torque, respectively) can very well be achieved with very lean mixtures ($\phi_{eff} = 0.3$) and 10% hydrogen peroxide addition, allowing the steam dilution level to go up to 27%. Increasing the effective equivalence ratio to $\phi_{eff} = 0.4$ while maintaining the hydrogen peroxide addition to 10% results in medium to high loads of 6.7–9.2 bar/43.7–60.1 Nm of IMEP and torque, respectively, while also the steam dilution can go up to 20.75%. Finally, increasing further the effective equivalence ratio to $\phi_{eff} = 0.5$ and maintaining the hydrogen peroxide content to 10% leads to loads of 8.3–10.8 bar/54.5–70.6 Nm (IMEP and torque, respectively) with the maximum steam dilution at 17.5%. Hence, by increasing the effective equivalence ratio from 0.3 to 0.4 the range of available load depending the steam dilution, at 10% H_2O_2, slightly increases to 2.5 bars/16.4 Nm (for IMEP and torque, respectively) and the minimum and maximum IMEP/torque values increase by 37% (e.g., from 4.9/7.2 to 6.7/9.2 bar for IMEP). However, increasing further the effective equivalence ratio from 0.4 to 0.5 induces a less pronounced increase (24%) on the minimum and maximum IMEP and torque values. So, from a load output perspective, the engine could operate at very lean conditions while also maintaining sufficiently high IMEP and torque outputs with only 10% hydrogen peroxide addition. Increasing the H_2O dilution has a negative effect on IMEP and torque, greater in magnitude than the positive effects of increasing H_2O_2 addition which indicates a trade-off in performance when steam dilution is used to counter NO_x emissions that will be discussed next. For example, at $\phi_{eff} = 0.3$, 10% H_2O_2 and 0% H_2O the IMEP value is 7.24 bar. Increasing the steam dilution by 5% results in an IMEP value of 6.87 bar, i.e., 5.06% decrease. Further increase of the steam dilution by another 5% (i.e., 10% H_2O in total) results in an IMEP value of 6.5 bar, i.e., 5.71% further decrease. On the other hand, if the hydrogen peroxide is increased by 5%, i.e., total of 15% H_2O_2, the IMEP values at 0%, 5% and 10% H_2O would be 7.42, 7.05 and 6.67 bar, respectively; compared to the IMEP values at 10% H_2O_2 for the same steam dilution contents, we can observe increases in the order of 2.41%, 2.48% and 2.51%, respectively. Of course this has largely to do with the way that the additions of H_2O_2 and H_2O are defined. The first is defined on the basis of the hydrogen mole fraction which generally varies between 0.1 and 0.2 for the conditions under study. Hence in the case of 1% H_2O_2, the mole fraction of H_2O_2 will in theory vary between 0.001 and 0.002. On the other hand, 1% steam dilution means that the mole fraction of H_2O will be 0.01, i.e., five to ten times larger than the mole fraction of H_2O_2.

The strong effect of H_2O_2 addition on the ignition CAD (CAD_{ign}) is evidenced by the results displayed in Figs. 6(a)–(c). At $\phi_{eff} = 0.3$ (1000 rpm) and 0% H_2O, the minimum amount of H_2O_2 to achieve ignition is 1.5%, with $CAD_{ign} = +8.03$. Increasing H_2O_2 to 3.25% is sufficient to result in ignition CAD before the TDC, i.e., $CAD_{ign} = -0.38$. At 5% steam dilution the critical H_2O_2 quantity to achieve negative CAD_{ign} increases to 4.5%, while at 10%, 15% and 20% of steam dilution the critical H_2O_2 quantities become 6.5%, 9.75% and 15% respectively. Increasing the effective equivalence ratio and the engine speed to 0.4 and 2000 rpm, respectively, has an adverse effect on the minimum required quantity to achieve ignition CAD before the TDC. In particular, at 0%, 5%, 10% and 15% of steam dilution the critical H_2O_2 quantities become 4.75%, 7.25%, 11.0% and 19.25% respectively. Similarly, at $\phi_{eff} = 0.5$ (3000 rpm) and 0%, 5% and 10% of steam dilution the critical H_2O_2 quantities become 6.0%, 9.25% and 16.5% respectively. These results indicate that as either the steam dilution or the engine speed increase the critical H_2O_2 to achieve CAD before the TDC increases. This is intuitive because in the former case (i.e., by increasing the steam dilution) the mixture becomes less reactive while in the latter case the available time to ignite decreases. Another aspect related to the effect of steam dilution on the ignition CAD is that when starting from a negative CAD (i.e., CAD_{ign} before the TDC) the relative change of CAD_{ign} due to the addition of H_2O_2 initially increases up to some point close to the TDC and then decreases, regardless the ϕ_{eff} and the engine speed. This is indicative of the reinforcement that the ignition CAD experiences due to the pressure rise as a result of the compression of the mixture during the compression stroke: the closer CAD_{ign} occurs to the TDC the larger the effect it experiences by the mere compression of the mixture. Another interesting finding is that steam dilution tends to increase the range of H_2O_2 addition that has practical application. For instance, at $\phi_{eff} = 0.3$ and 5% H_2O, the range of H_2O_2 addition that has value in terms of CAD_{ign} (in essence, the range of H_2O_2 addition values that give CAD_{ign} after or equal to the TDC) ranges between 2% and 4.5% while at 15% H_2O this range becomes 4%-9.75%. Finally, Figs. 6(a)–(c) also demonstrate that the H_2O_2 addition required to achieve ignition increases logarithmically with the increase of H_2O addition.

The investigation of the response of the rapid burning angle (RBA) as a function of the steam dilution level and the hydrogen peroxide initial quantity, can also be insightful although the results should be interpreted with care since mixture/thermal inhomogeneities and turbulence (which are not taken into account in the employed model) can play key role to the increase of the heat release rate. It is noted that the rapid burning angle (RBA) is defined as the difference between CAD90 and CAD10, i.e., the crank angle degrees where the 90 and 10% of the heat release occur. Figs. 6(d)–(f) show that all cases that have CAD_{ign} before the TDC are also characterised by extremely low RBA, which is generally an undesired feature in HCCI engine operation since it can lead to very high pressure rise rates and knock. However, it is also shown that steam dilution can be an effective tool in managing the very low RBAs. For instance, at $\phi_{eff} = 0.3$ and 10% H_2O_2 where $CAD_{ign} = +0.751$, increasing the steam dilution from 17% to 27.5% can increase the RBA from 1.13 CAD to 9.46, i.e., an 8-fold increase. It has to be highlighted though that as the effective equivalence ratio and the engine speed increase it becomes more challenging to control the RBA even with the use of steam dilution and high RBA values are harder to achieve. In that case, in a conventional CI setup alternative approaches should then be explored for the control of the high pressure rise rates, such as the injection strategy (injection duration/timing, multi-injection etc.).



(a) (b) (c)

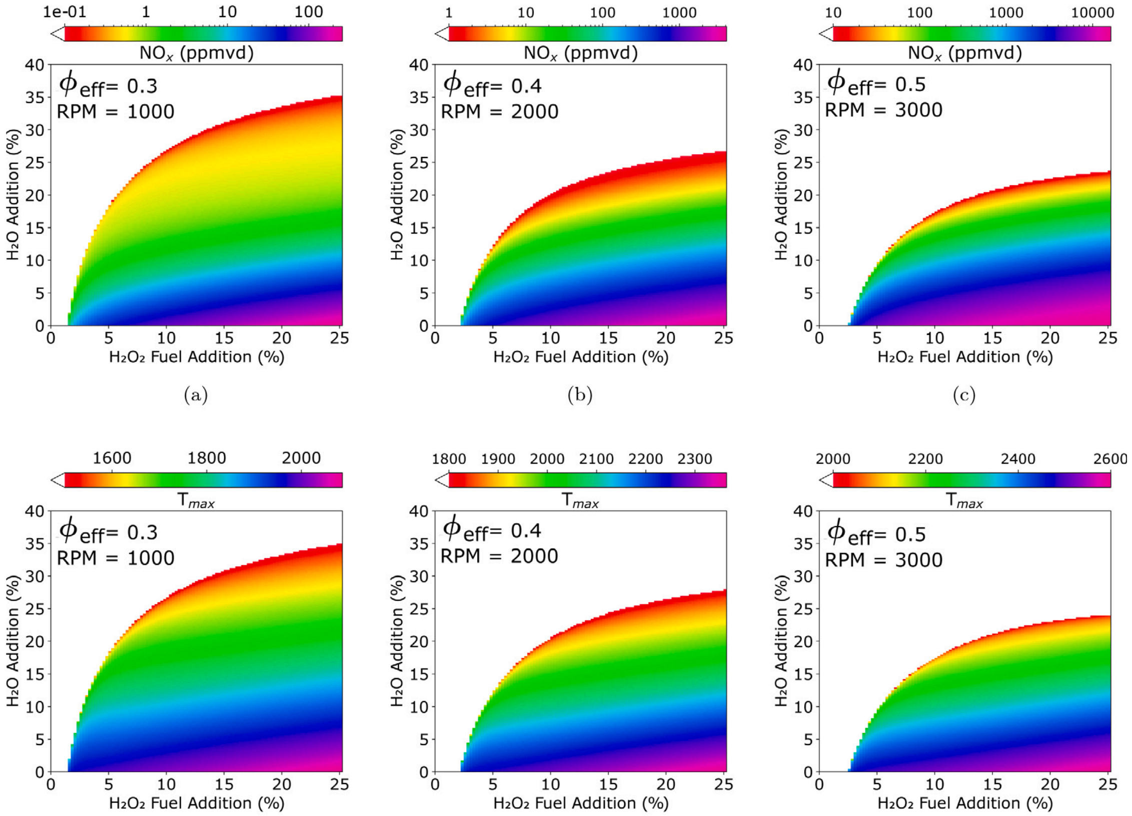
(d) (e) (f)

Fig. 6. Contour plots of CAD$_{ign}$ (a, b, c), and Rapid Burning Angle (d, e, f) as a function of the hydrogen peroxide initial content ranging between 0 and 25% and the steam dilution level ranging between 0 and 40%, at ϕ_{eff} and engine speed of 0.3–1000 rpm (a, d), 0.4–2000 rpm (b, e), and 0.5–3000 rpm (c, f), respectively.

NOx emissions is the third important aspect that needs to be investigated since the motivation of using steam dilution in the first place was mainly to control NOx emissions. Firstly, Fig. 7 shows that there is an almost perfect correlation between temperature and NOx emissions which is not surprising since the main pathway for the production of NOx is the thermal which largely depends on the temperature. Secondly, from the NOx perspective steam dilution would probably only be required at ϕ_{eff} = 0.5 (3000 rpm) and potentially partly to ϕ_{eff} = 0.4 (2000 rpm) while for ϕ_{eff} = 0.3 (1000 rpm) it would not be necessary at all due to the extremely low obtained NOx emissions values. In general, regardless the ϕ_{eff}, the introduction of steam dilution appears to have a strong effect on both the maximum temperatures and NOx emissions, enabling a three-order reduction in the production of NOx and more than 500 K reduction of the maximum temperatures. For instance, at ϕ_{eff} = 0.5 (3000 rpm), 10% H_2O_2 and 0% H_2O NOx emissions rise up to 9750 ppmvd while the maximum reached temperature becomes 2526 K. By increasing the steam dilution to 15%, the maximum temperature drops to 2193 K (i.e., 13.2% decrease) while NOx emissions drop to 97 ppmvd, i.e., two orders of magnitude. Most important, the predicted NOx emissions can be so low with the use of steam dilution (at sufficiently high effective equivalence ratios, e.g., ϕ_{eff} = 0.5) or without even the use of any steam dilution (at sufficiently low equivalence ratios, e.g., ϕ_{eff} = 0.3) that no after-treatment would be required. Two additional observations can be made. Firstly, as steam dilution increases the relative decrease of NOx production increases. For instance, at ϕ_{eff} = 0.5 (3000 rpm) and 5% H_2O_2, the drop of NOx emissions from 0% to 1% H_2O is 22.2%, from 1% to 2% H_2O the decrease becomes 24%, from 5% to 6% H_2O it becomes 31.4 and so on. This phenomenon is due to the fact that when maintaining constant the effective equivalence ratio and the hydrogen peroxide percentage (which is determined on the basis of the hydrogen mole fraction), the introduction of steam dilution leads to the decrease of the mole fractions of hydrogen and hydrogen peroxide. The relative change of this decrease becomes more pronounced as the steam dilution increases. For instance, at ϕ_{eff} = 0.5 (3000 rpm) and 5% H_2O_2, the decrease in the initial mole fraction of H_2 due to the increase of steam dilution from 0 to 5% is 5%, while increasing the steam dilution from 5% to 10% yields a 5.3% decrease in the hydrogen mole fraction which grows to 5.6% when increasing the steam dilution from 10 to 15%. Secondly, the aforementioned phenomenon becomes less pronounced as the initial hydrogen peroxide quantity increases. In other words, as the initial hydrogen peroxide increases the mixture becomes less sensitive on the decrease of NOx emissions due to the introduction of steam dilution. This occurs because by maintaining constant the effective equivalence ratio, the introduction of hydrogen peroxide leads to the increase of both the hydrogen peroxide and (most important) the hydrogen mole fractions. The higher hydrogen mole fraction allows for the creation of a richer radical pool that eventually leads to higher NOx emissions for the same dilution level (or smaller relative decrease when compared against the same dilution levels).

In summary, the parametric exploration of H_2O_2 addition with steam dilution demonstrated H_2O_2 as an effective method of increasing the engine cylinder output in terms of IMEP, torque and thermal efficiency, while also not having (to some extent) an adverse effect on NOx emissions.

- At ϕ_{eff} = 0.3 and 1000 rpm, the thermal efficiency has average maximum and minimum values of 58.48% and 53.41%, respectively. These averages are obtained on the basis of the minimum and maximum values throughout the steam dilution range (0%–40%) per hydrogen peroxide addition case. In overall, the variation of η_{th} due to steam dilution is not significant and the actual thermal efficiency values are maintained relatively high for



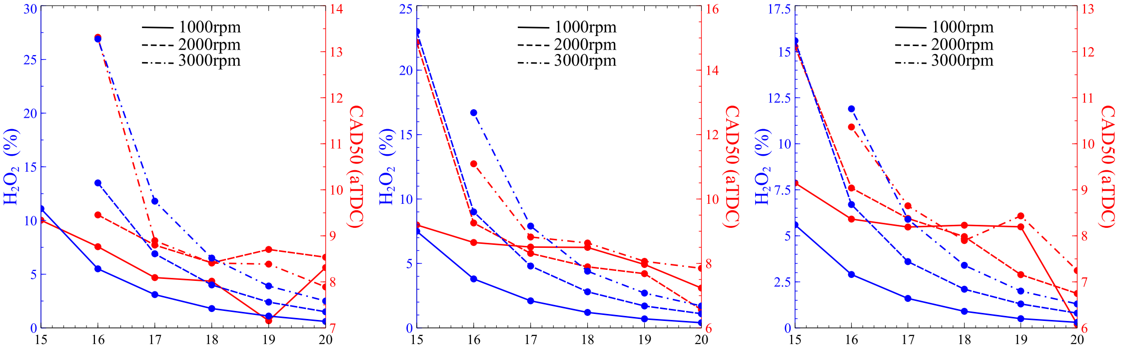
(a) (b) (c)

(d) (e) (f)

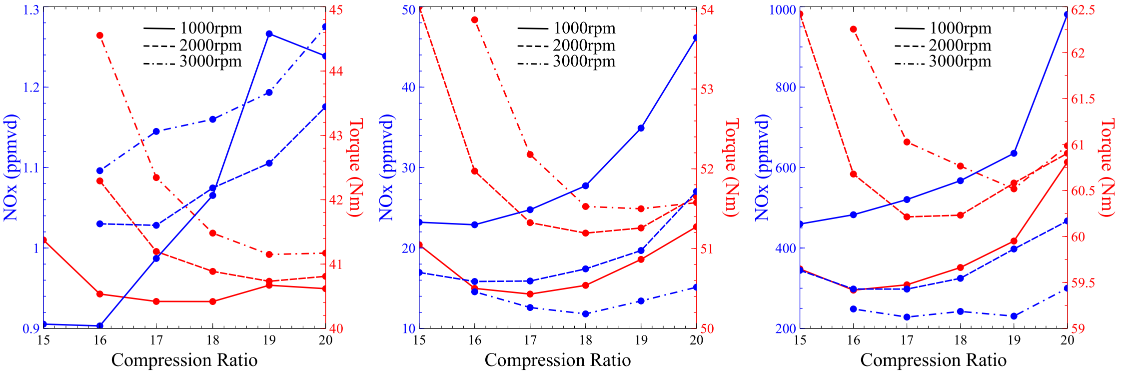
Fig. 7. Contour plots of NOx (a, b, c), and maximum temperature (d, e, f) as a function of the hydrogen peroxide initial content ranging between 0 and 25% and the steam dilution level ranging between 0 and 40%, at ϕ_{eff} and engine speed of 0.3–1000 rpm (a, d), 0.4–2000 rpm (b, e), and 0.5–3000 rpm (c, f), respectively.

all examined conditions. At 10% H_2O_2 and 20% H_2O the thermal efficiency becomes 58% which is a merely 0.6% drop from the respective value when no steam dilution is included. IMEP and torque also exhibit average maximum and minimum values of 7.37 bar/48.33 Nm and 4.99 bar/32.37 Nm, respectively. At 10% H_2O_2 and 20% H_2O the respective IMEP and torque values are 5.7 bar and 37.65 Nm. In terms of NOx emissions, the average maximum and minimum values are 126.1 and 0.175 ppmvd, respectively, while at 10% H_2O_2 and 20% H_2O the respective NOx value is 0.68 ppmvd, indicating that no after-treatment would be required. As for the CAD_{ign} and RBA at 10% H_2O_2 and 20% H_2O they reach values of 2.6 CAD aTDC and 1.6 CAD, respectively. All the aforementioned results showcase the feasibility of using H_2O_2 and H_2O for reasonably low loads while also maintaining NOx emissions to low values. Of all the examined sets of H_2O_2 and H_2O combinations probably the most interesting ones are in the neighbourhood of 10% H_2O_2 and 20% H_2O since they lead to good engine performance output, extremely low NOx and acceptable RBA. For the latter though it is noted that additional strategies should be considered for its further improvement. It is noted that in the case of 10% H_2O_2 and 20% H_2O the initial quantity of H_2O_2 against the aggregate quantity of H_2O_2 and H_2O on a volume basis is 4.35%, which is significantly lower than the hydrogen peroxide solutions available freely in the market (30% for food grade hydrogen peroxide).

- At ϕ_{eff} = 0.4 and 2000 rpm, the thermal efficiency has average maximum and minimum values of 57.25% and 52.43%, respectively. At 9% H_2O_2 and 15% H_2O η_{th} becomes 56.73% which is very close to the average maximum efficiency across all different steam dilution scenarios. In view of engine outputs, the average maximum and minimum values of IMEP/torque are 9.32 bar/61.2 Nm and 6.58 bar/44.6 Nm, respectively. In the special case of 9% H_2O_2 and 15% H_2O the respective values become 7.65 bar/50.2 Nm. In terms of NOx emissions, the average maximum and minimum values are 2185.7 ppmvd and 1.9 ppmvd, respectively, while in the special case of 9% H_2O_2 and 15% H_2O NOx emissions become 9.19 ppmvd. For the latter case, the CAD_{ign} and RBA reach the values of 4.69 CAD aTDC and 1.06 CAD, respectively. These results are important for two reasons. Firstly, because they demonstrate that with the combined use of H_2O_2 and H_2O we can increase the equivalence ratio and obtain higher loads than those at ϕ_{eff} = 0.3 with no adverse effect on the efficiency or NOx emissions. Secondly, these results corroborate that a mere 9% of H_2O_2 (along with 15% H_2O) would be sufficient to deliver very good results in terms of performance and NOx. On a volume basis, 9% of H_2O_2 is 6.95% of the initial aggregate quantity of H_2O_2 and H_2O.
- At ϕ_{eff} = 0.5 and 3000 rpm, the thermal efficiency has average maximum and minimum values of 55.85% and 51.85%, respectively, i.e., lower than those obtained at ϕ_{eff} = 0.4. Similarly, the average maximum and minimum values for IMEP/torque/NOx emissions are 10.97 bar/72.0 Nm/11,221 ppmvd and 8.17 bar /53.7 Nm/31 ppmvd, respectively. Notice that the average maximum value for NOx emissions is particularly high but apart from that these results look promising. At 10% H_2O_2 and 8.5% H_2O IMEP/torque reach the values of 9.9 bar/65.0 Nm, respectively, NOx emissions reach 1140 ppmvd and η_{th} becomes 55.98%. At this set of conditions (i.e., 10% H_2O_2 and 8.5% H_2O), the ratio of the hydrogen peroxide against the sum of steam and hydrogen peroxide on a volume basis is 18.22%. All these are acceptable values but for higher torque/IMEP values it is becoming challenging to identify a set of conditions that can satisfy simultaneously



(a) ϕ_{eff} = 0.3 (b) ϕ_{eff} = 0.4 (c) ϕ_{eff} = 0.5



(d) ϕ_{eff} = 0.3 (e) ϕ_{eff} = 0.4 (f) ϕ_{eff} = 0.5

Fig. 8. (a, b, c): The minimum required H_2O_2% to achieve 98% of the maximum thermal efficiency, along with CAD50. (d, e, f): NO_x emissions and engine cylinder torque. All figures: H_2O addition is maintained constant at 10%, compression ratios vary between 15 and 20 (in increments of 1), ϕ_{eff} = 0.3, 0.4, and 0.5, and engine speeds of 1000, 2000, and 3000 rpm.

high torque (> 67 Nm), low NOx emissions (<1000 ppmvd) and reasonable RBA (> 1 CAD). This is an inherent feature of HCCI engines, hence not surprising. High torque can be reached but only with the caveat of high NOx and very small RBA and vice versa. This challenge could (at least in principle) be addressed in the context of an RCCI type of engine, which, unlike the current HCCI type, would allow for (among other things) the full control of the injection strategy.

In the next part of the study, we explore on the influence of the compression ratio on the engine performance characteristics, while maintaining constant to all cases the steam dilution at 10%. In particular, we identify the minimum H_2O_2 quantity required to achieve 98% of the maximum possible η_{th} for a given effective equivalence ratio, compression ratio and engine speed. For the determined H_2O_2 quantity we then monitor CAD50 (i.e., the CAD aTDC where the heat release rate reaches 50% of its maximum value), NOx emissions and torque. Compression ratios are varied between 15 and 20 in increments of 1, at ϕ_{eff} of 0.3, 0.4, and 0.5, and at engine speeds of 1000, 2000, and 3000 rpm for each ϕ_{eff}. The results are displayed in Fig. 8.

Firstly, increasing the compression ratio dramatically decreases the required quantity of H_2O_2 addition needed to maintain 98% η_{th}, with this trend levelling off towards an asymptotic limit at higher compression ratios of 19–20. This limit was ~1% H_2O_2 addition across ϕ_{eff} 0.3–0.5. Considering that in the absence of any ignition promoter and/or inlet preheating (glow plug) hydrogen ignition requires compression ratios above 29:1 [12,13], the results presented in Fig. 8 showcase the strong effect that hydrogen peroxide can have on hydrogen's ignition process. As the compression ratio increases to high values of 19 and 20 the increased in-cylinder temperatures also increase, yet, hydrogen peroxide still plays key role in enabling the ignition of the system which could only be achieved otherwise with the preheating of the charge. However, the advantages of the proposed use of hydrogen peroxide against the approach of inlet preheating have already been established in [29] as well as in the first part of the current study. With increasing ϕ_{eff}, the amount of H_2O_2 addition required at lower compression ratios is reduced which is expected since the increase of ϕ_{eff} suggests enhancement of the mixture's reactivity. Increasing the engine speed increased the required H_2O_2 addition as expected. At very low compression ratio (15), engine speed of 3000 rpm and regardless the effective equivalence ratio, the required H_2O_2 addition was beyond practical limit (>50%). This phenomenon becomes more pronounced at ϕ = 0.3 where the required H_2O_2 addition being beyond practical limit is also observed at the engine speed of 2000 rpm. In general, we observe that the required hydrogen peroxide quantity remains below 15% at all engine speeds throughout the compression ratio range, with the exceptions of:

- compression ratio of 15, engine speed of 2000 and 3000 rpm and ϕ_{eff} = 0.3, 0.4 and 0.5
- compression ratio of 16, engine speed of 3000 rpm and ϕ_{eff} = 0.3 and 0.4

These results are consistent with those reported in [29] and suggest that the proposed strategy of using hydrogen peroxide to promote the ignition of steam diluted hydrogen/air mixtures would only be a practically valuable option for compression ratios equal to or larger than 17.

The results of CAD50 are largely correlated with the variation of the minimum required H_2O_2 quantity to maintain the thermal efficiency at 98% of its maximum value. It is observed that CAD50 generally advances with the increase of compression ratio or the engine speed or the effective equivalence ratio. For the compression ratios that have more practical interest, i.e., CR ≥ 17, CAD50 varies in the range of 6 to 9 CAD aTDC for all equivalence ratios and engine speeds, which are considered acceptable values.

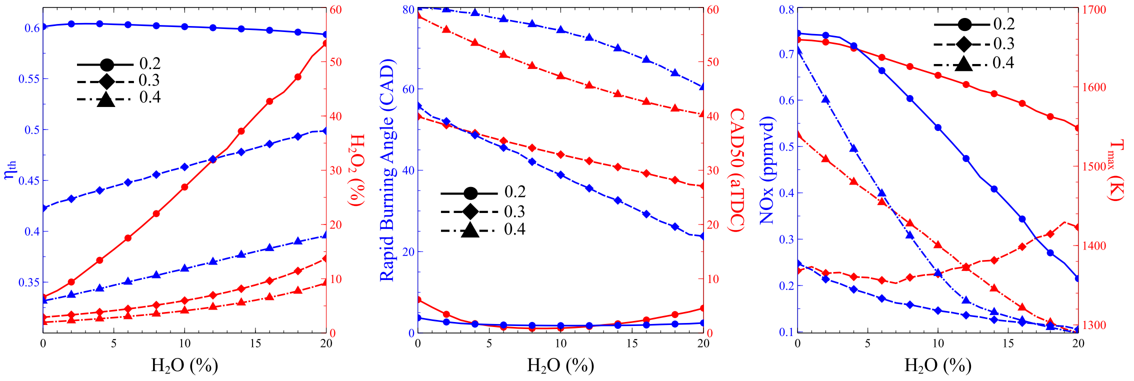
Of particular interest are the results on NOx emissions and torque. At ϕ_{eff} = 0.3 NOx emissions generally increase with the increase of the compression ratio but are extremely low (1–1.3 ppmvd) for all engine speeds, suggesting that no after-treatment would be required regardless the engine speed. Increasing the effective equivalence ratio to 0.4 we observe that NOx emissions increase by an order of magnitude (ranging between 10 and 50 ppmvd) but are still considered very low. Their values appear to decrease with increasing engine speed and this trend is maintained at ϕ_{eff} = 0.5. The reason for this trend relates to the fact that the timescale for the formation of NOx is considered slow and mainly acts after the ignition occurrence [27,53]. When the engine speed is increased the available post-ignition time (which is when NOx are formed) decreases, hence the available time for the formation of NOx also decreases. At ϕ_{eff} = 0.5 NOx emissions increase one to two orders of magnitude further, now ranging between 200 and 1000 ppmvd. Their increase becomes generally more pronounced with the increase of the compression ratio which is reasonable because an increase of the compression ratio results in an increase of the maximum temperature, thereby, NOx formation. Therefore, for CR ≥ 17 and ϕ_{eff} = 0.5 an after-treatment for NOx emissions would probably be required, in consistence with the findings reported earlier.

With regard to the produced torque, it generally increases with the increase of the effective equivalence ratio and the engine speed but (mostly) not the compression ratio. What is probably more interesting and has practical values is the fact that the range of variation of the torque for the different compression ratios is generally small and becomes significantly narrow when focusing on compression ratios equal to or greater than 17. For instance, at ϕ_{eff} = 0.3 torque varies between 40.5 Nm and 42.5 Nm, i.e., 2 Nm range. Increasing further the effective equivalence ratio to 0.4 and 0.5 results in ranges of 50.5–52.2 Nm and 59.5–61.2 Nm, respectively. Hence, from an engine performance point of view there is no significant benefit in increasing the compression ratio to above 17, since it results in less than 5% increase of torque. In any case, the torque results presented in Fig. 8 corroborate the findings reported earlier on the basis of Fig. 5; an effective equivalence ratio of 0.3 can be sufficient to maintain low torque values and low NOx while for higher torque values higher effective equivalence ratios should be sought, regardless the compression ratio.

Finally, to further investigate the effect of H_2O addition on engine performance a sweep of H_2O addition was performed from 0 to 20%, while the torque was maintained constant through adjustment of H_2O_2 addition, while the effective equivalence ratio was maintained constant. This was carried out for two scenarios, both at an engine speed of 2000 rpm: one representing a low torque value of 33 Nm, and another representative of high torque values of 65 Nm. The effect on parameters of thermal efficiency, rapid burning angle, CAD50, NO_x, and T_{max} was monitored. For the low torque scenario, ϕ_{eff} of 0.2, 0.3, and 0.4 were tested and for the high torque scenario, ϕ_{eff} of 0.4, 0.5, and 0.6 were investigated. The results for both scenarios are presented in Figs. 9 and 10.

Starting with the low torque scenario, the thermal efficiency presents an opposite trend between ϕ_{eff} = 0.2 versus 0.3 and 0.4, in that in the case of ϕ_{eff} = 0.2 η_{th} slightly decreases with the increase of steam dilution while for the other two cases it decreases. The reason for this opposite trend is because in the former case a well established ignition occurs from the very beginning (i.e., 0% H_2O) and as the initial steam dilution increases it can only decrease the efficiency as showcased also earlier in Fig. 6. However, at ϕ_{eff} = 0.3 and 0.4 the engine operates right on the threshold between ignition and no-ignition. Hence, when H_2O increases, H_2O_2 also increases, the latter having a strong positive effect on the thermal efficiency as discussed earlier, tending to establish a strong ignition event. This phenomenon becomes more obvious when looking at the combustion phasing in Fig. 9(b) where it is shown that in the ϕ_{eff} = 0.2 case the RBA ranges between 1 and 4 CAD and CAD50 varies between 0 and 7 CAD aTDC, i.e., very close to the TDC. On the other hand, at ϕ_{eff} = 0.3/0.4 the RBA is significantly higher ranging between 23–56/60–80 CAD. Similar is the variation of CAD, ranging between 27–40/40–59 CAD aTDC for ϕ_{eff} = 0.3/0.4. The very late ignition occurring at ϕ_{eff} = 0.3/0.4 combined with the slow ignition process result in the very low thermal efficiency values described earlier. Another interesting finding observed from Fig. 9 is that at ϕ_{eff} = 0.2 the results have practical value up to steam dilution of 7% where the required H_2O_2 quantity becomes 19.7%. For higher steam dilution levels the required H_2O_2 quantity increases to high values reaching 53.4% for 20% H_2O. On the other hand, at ϕ_{eff} = 0.3/0.4 the required H_2O_2 quantity always remains in practically valuable levels, below 14%/10%. In terms of NOx emissions, all three effective equivalence ratios lead to extremely low values regardless the steam dilution levels. In particular, at ϕ_{eff} = 0.2/0.3/0.4 NOx emissions range between 0.20–0.75/0.10–0.25/0.10–0.71 ppmvd, respectively. The decrease in NOx emissions due to steam dilution is generally well-correlated with the decrease in the maximum temperature with the exception of ϕ_{eff} = 0.3 above 7% of steam dilution where a small increase of T_{max} is observed.

In the high torque scenario, all three examined effective equivalence ratios have qualitatively different thermal efficiency responses to the steam dilution variation. In particular, at ϕ_{eff} = 0.4 the thermal efficiency is initially maintained constant and later decreases, at ϕ_{eff} = 0.5 the thermal efficiency initially increases up to steam dilution of 6% and then gradually deteriorates while at ϕ_{eff} = 0.6 the thermal efficiency increases up to steam dilution of 19% and then remains practically constant. These results can be explained on the basis of the combustion phasing. At ϕ_{eff} = 0.4 CAD50 is initially negative (i.e., before the TDC) and as steam dilution increases it is retarded and at some point (between 14 and 15% H_2O) it becomes positive. The shift of CAD50 from negative to positive is correlated with the change in the response of the thermal efficiency (from practically constant to gradual decrease). The same reason (the ignition timing as represented by CAD50) causes the change in the response of the thermal efficiency for the case of ϕ_{eff} = 0.5 as well, with the difference that the shift of CAD50 now occurs from positive to negative CAD. In the ϕ_{eff} = 0.5 case this shift occurs between 6 and 7% H_2O. It is noted though that for steam dilution higher than 10% (and 13.15% H_2O_2 addition) in the ϕ_{eff} = 0.5 case, the ignition timing starts to gradually retard, thereby exhibiting a similar CAD50 response to the ϕ_{eff} = 0.4 case. These results indicate that there are well-defined thresholds for the ignition advancement that can be achieved through the addition of H_2O_2 with steam dilution. These thresholds depend on the mixture's effective equivalence ratio, the steam dilution level and the engine speed and are the result of changes in the effect of the chemical pathways introduced by the addition of H_2O_2. Increasing further the effective equivalence ratio to 0.6 indicates that the increase of steam dilution and the subsequent increase of H_2O_2 to maintain the torque constant at 65 Nm leads to a notable decrease of CAD50, from 26.6 to 2.4 CAD aTDC. At the same time the required initial H_2O_2 quantity for the ϕ_{eff} = 0.6 case is always maintained below 12% as opposed to ϕ_{eff} = 0.4 and 0.5 that reaches maximum values of 65% and 32%, respectively, at 20% H_2O. So, from a practical point of view, high load could not be achieved by ϕ_{eff} = 0.4 since it would require more than 28% H_2O_2 while at ϕ_{eff} = 0.5 steam dilution would be meaningful up to 11%–14% where the initial hydrogen peroxide is maintained equal to or below 15%–20%. In terms of NOx emissions, all three examined effective equivalence ratios reach generally to high values, which only drop to less than 1000 ppmvd at H_2O_2/H_2O quantities of 43%/10%, 22%/15% and 2.8%/11% for ϕ_{eff} = 0.4, 0.5 and 0.6, respectively. Hence, as also highlighted earlier, high load engine operation would most probably necessitate the use of after-treatment to decrease them to acceptable levels. The non-monotonic behaviour of NOx at ϕ_{eff} = 0.5 can be explained by the previously discussed trends of combustion phasing, with this having a strong effect on NOx formation.

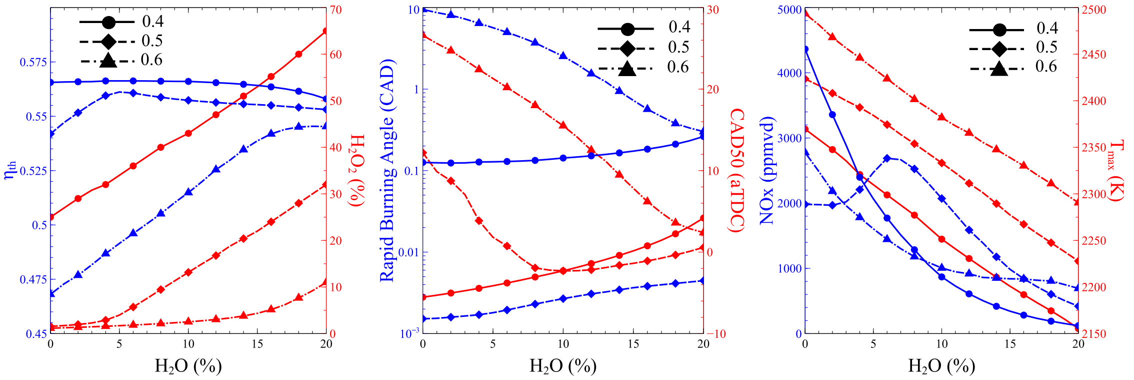


(a)

(b)

(c)

Fig. 9. The variation of η_{th} (a), RBA and CAD50 (b), NOx emissions and T_{max} (c) when varying the steam dilution from 0% to 20% while maintaining constant the torque at 33 Nm (representative of low load) by increasing the initial quantity of H_2O_2 (a), at an engine speed of 2000 rpm. The investigation is performed at three effective equivalence ratios of 0.2, 0.3 and 0.4.



(a)

(b)

(c)

Fig. 10. The variation of η_{th} (a), RBA and CAD50 (b), NOx emissions and T_{max} (c) when varying the steam dilution from 0% to 20% while maintaining constant the torque at 65 Nm (representative of high load) by increasing the initial quantity of H_2O_2 (a), at an engine speed of 2000 rpm. The investigation is performed at three effective equivalence ratios of 0.4, 0.5 and 0.6.

4. Conclusions

The current study aims to provide further numerical proof for the feasibility of a novel technology that relies on hydrogen and hydrogen peroxide as fuels in CI engines. The employed numerical model despite its inherent weaknesses provided valuable insight about the feasibility of the new technology, yet the produced results should be treated with care, due to lack of proper validation with engine experiments. The numerical investigation revealed the following:

- using H_2O_2 as the method of ignition promotion lead to significantly improved (16%–39%) performance (IMEP, power, torque) compared to the increased intake charge temperature approach, with the addition of steam dilution for NO_x reduction increasing the benefits against intake heating.
- the hydrogen peroxide strategy is advantageous against the inlet charge preheating approach not only in terms of performance but also in view of NOx emissions, where a remarkable decrease (50%–76%) were reported reaching in many cases values less than 150 ppmvd.
- the difference between the two approaches in terms of NOx emissions production was reported to become much more pronounced when the comparison is performed on the basis of the same power output, reaching in certain cases a two orders of magnitude difference.
- another striking difference between the aforementioned approaches was the fact that with the inlet charge preheating approach which aims to simulate the use of a glow plug, in order to achieve the same power output a significant increase of the mixture's equivalence ratio was also required, in some cases more than 40%.
- increasing the steam dilution addition generally has a negative effect on the thermal efficiency and this trend becomes less pronounced as H_2O_2 addition increases and as ϕ_{eff} decreases. In general, when sufficiently far from the threshold of no-ignition, the thermal efficiency remains high and does not vary significantly, exhibiting a maximum variation of 1.5%.
- low to medium loads (4.9–7.2 bar/32.2–47.5 Nm of IMEP and torque, respectively) can very well be achieved with very lean mixtures ($\phi_{eff} = 0.3$) and 10% hydrogen peroxide addition, allowing the steam dilution level to go up to 27%. Increasing further the effective equivalence ratio to $\phi_{eff} = 0.5$ and maintaining the hydrogen peroxide content to 10% leads to loads of 8.3–10.8 bar/54.5–70.6 Nm (IMEP and torque, respectively) with the maximum steam dilution at 17.5%.
- in general, regardless the ϕ_{eff}, the introduction of steam dilution has a strong effect on both the maximum temperatures and NOx emissions, enabling a three-order reduction in the production of NOx and more than 500 K reduction of the maximum temperatures. The predicted NOx emissions can be so low with the use of steam dilution that no after-treatment would be required.
- 10% or less of H_2O_2 addition would only be required to achieve low and medium loads with extremely low NOx emissions and high thermal efficiency.

- achieving high loads while also maintaining low NOx was proven to be challenging. Hence, for high loads some after-treatment to tackle with the increased NOx emissions would probably be required.
- compression ratios lower than 17 were reported to be unsuitable for use since they would require significantly higher quantities of hydrogen peroxide.
- maintaining the (high or low) load constant when varying the steam dilution can be readily achieved by properly adjusting the hydrogen peroxide quantity. However, careful consideration must be placed on the selection of the effective equivalence ratio since it can lead to qualitatively different responses as a result of the steam dilution.

The above findings provide numerical evidence for the feasibility of the use of hydrogen in HCCI mode, with steam dilution and hydrogen peroxide as an ignition promoter, and its advantages against the more conventional use of a glow plug. The reported results are promising, yet, despite a reasonable confidence in the model's accuracy in approximating the engine cycle, engine experiments will need to validate the key findings reported herein.

Finally, special attention will need to be paid on the engine operation and performance under high load conditions. The operation of hydrogen engines at high load conditions is typically restricted by engine knock. It is yet to be discovered, through future engine experiments and high-fidelity numerical simulations, how the addition of hydrogen peroxide will affect the onset and development of engine knock. It is envisaged though that the injection strategy along with steam dilution or the use of exhaust gas recirculation (EGR) will be instrumental to this regard.

CRediT authorship contribution statement

Oliver Fernie: Data curation, Formal analysis, Investigation, Resources, Software, Validation, Visualization, Writing – original draft, Writing – review & editing. **Thanos Megaritis:** Formal analysis, Methodology, Writing – original draft, Writing – review & editing. **Lionel Christopher Ganippa:** Formal analysis, Methodology, Writing – original draft, Writing – review & editing. **Efstathios-Al. Tingas:** Conceptualization, Formal analysis, Funding acquisition, Investigation, Methodology, Project administration, Resources, Software, Validation, Visualization, Writing – original draft, Writing – review & editing, Supervision.

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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