EXPERIMENTAL AND NUMERICAL INVESTIGATION OF METHANE COMBUSTION IN A HCCI ENGINE UNDER ENRICHED OXYGEN CONDITIONS

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Abstract
In the context of the energy transition towards renewable energy, it is necessary to exploit any viable technological solution to decrease our footprint on the environment, but also to rethink the way we produce, store and use energy. The conversion of energy stored as e-fuels can be tackled with internal combustion engines. Homogeneous Charge Compression Ignition (HCCI) engines represent an appealing alternative to spark ignition and compression ignition engines due to their high thermal efficiency, high fuel flexibility and low NO_x emissions. However two main technical limitations are associated to this type of technology. The first one is the low control on ignition timing, as combustion is driven by kinetics. The second one is the low power density, because of the high intake temperature needed to achieve combustion and the low values of equivalence ratios used. Having a high intake temperature and a combustion which is happening approximately at the same moment in all the combustion chamber, also leads to low operating ranges. We have experimentally investigated the influence of oxygen enrichment in the oxidiser in methane HCCI combustion, as a way to increase the mixture reactivity and hence, decrease the intake temperature of the mixture. The parameters of interest of combustion are ignition timing and Maximum Pressure Rise Rate. Furthermore, a kinetic analysis has been performed with OpenSMOKE++ to investigate the chemical reactions underlying the combustion behaviour. It has been experimentally found that increasing the oxygen fraction from 21 to 49% allows to decrease the intake temperature of the mixture by 30 K. From the numerical point of view, it has been found that the mixture is less sensitive to intake temperature at higher oxygen percentages. By increasing the oxygen percentage in the oxidiser up to 100% we expect to be able to further decrease the intake temperature, leading to an extension of the operating range and increase of the power density. In future works, the potential of increasing the fuel content in the mixture will be evaluated.

Introduction
The necessity of carrying out the energy transition towards renewable sources, drives the scientific community to investigate new energy production and storage techniques. In this context, the potential of photovoltaic panels and wind turbine has been widely investigated and assessed, but they carry the need of foreseeing an energy storage solution in order to be viable [1]. Indeed, the calculations done to assess the energetic profitability of renewables are done considering that all the energy that is produced is either immediately used or stored for later needs. Due to intermittent renewable production and the need to transport energy under a convenient form, energy storage in the form of a renewable fuel (hydrogen and its derivatives) is considered in many studies on the transition of energy systems [2]. However, energy losses in the production and re-conversion process need to be compensated by using highly efficient technologies. In this context, Homogeneous Charge Compression Ignition (HCCI) engines can be good candidates since they are characterized by high thermal efficiency, high fuel flexibility and low NO_x emissions [3]. The high fuel flexibility has been investigated in several works. For example, in [4, 5],

it has been showed that it is possible to fuel the engine both with low or high octane number fuels varying the operating parameters such as intake temperature and compression ratio. The two main disadvantages are the poor ignition control and the low power density. The first one is due to the fact that the combustion is mainly driven by chemical kinetics. The second one is caused by the high intake temperature needed to achieve combustion and the low values of equivalence ratios used. In order to overcome these issues, several techniques have been investigated throughout the years. As this type of engines has large fuel flexibility, blending fuels with different ignition properties is an option. Indeed, blending ammonia and hydrogen has proved to be able to increase power density up to 50 % and to extend the operating range [6]. Inducing composition and thermal stratification is also a technique which allows to smooth the combustion. It is worthwhile to smooth the combustion as it allows to increase the equivalence ratio of the mixture keeping an acceptable value of Maximum Pressure Rise Rate (MPRR). Water direct injection can induce thermal inhomogeneities in the mixture and it has proved to enhance power density and to expand the load limit by 350% [7]. Another technique to induce thermal stratification in the combustion chamber is adopting a glow plug, as done in [8]. In particular, it allows to broaden the temperature distribution prior to ignition and therefore to control the rate of heat release in HCCI. Partial mixture inhomogeneities have shown to help controlling combustion duration [9].

Oxy-fuel combustion is also an appealing technique which has proved to have a potential in different fields and for numerous applications. The idea laying behind oxy-fuel combustion is to burn a fuel substituting partially or totally the nitrogen in the air with oxygen. The main advantage is that fuel consumption is decreased as heat produced during combustion is not used to increase the temperature of N_2. Higher flame temperatures are also possible. In addition to that, in the context of power to fuel technology, oxy-fuel combustion is also very interesting. Indeed, the excess of electricity coming from renewables is used to perform water electrolysis. For each mole of hydrogen produced, half a mole of oxygen is also generated as a side product. Using the oxygen produced in this process would have a double effect. On the one hand it would enhance the mixture reactivity allowing a decrease of the intake temperature and, hence, an increase of the density of the mixture. This would lead to an increase of the operating range as a higher amount of fuel could be used. On the other hand it would reduce the nominal cost of H_2 produced via electrolysis, as all the products of the process would be effectively used. In terms of emissions, when applied to methane, oxy-fuel combustion produces only CO_2 and H_2O; the volume of the flue gases is hence reduced and this leads to lower heat losses. Moreover, having a more simple composition of flue gases allows for easier and less expensive after-treatment systems, as, for example, it is easier to capture CO_2 [10]. Oxy-fuel combustion has been used for decades in industrial applications and lately it has been extended to different technologies, giving promising results. In the context of power plant for carbon capture and storage, oxy-coal combustion has proved to give good performances and the potential of retrofitting a coal power plant to oxy-firing has been investigated in [11]. Coupled with air humidification [12] and EGR [13], oxy-fuel combustion has proved to reduce soot and NO_x emissions in diesel engines. Oxy-fuel combustion has been investigated in a HCCI engine fueled with n-heptane in [14] and it has been found that it was possible to increase the Heat Release Rate (HRR) in the Low Temperature Combustion region by 5 times. Finally, in [15] oxy-fuel combustion applied to an ammonia HCCI fueled engine has proved to affect positively the adiabatic flame temperature and the laminar flame speed.

This work focuses on investigating the effects of increasing the oxygen percentage in the feeding mixture. An experimental campaign has been performed, investigating an oxygen content up to 49 % in the mixture with methane. In order to be able to investigate conditions which would have been impossible to test on the bench because of safety reasons, a kinetic analysis using OpenSMOKE++ [16] has been performed. The kinetic analysis has also been performed with the goal of obtaining a deeper insight into the chemistry underlying the combustion behaviour.

Experimental set-up

The experiments for this work have been conducted on a test bench at UCLouvain. All the details of the engine and the bench have been explained in [17], and are summarised in Table 1. The engine is a single-cylinder Diesel engine (Yanmar L100V) retrofitted for HCCI conditions.

Table 1: YANMAR L100V, air cooled, single cylinder characteristics.

Displacement Volume, V_c	436 cm^3
Bore / Stroke / Conrod	86/75/145 mm
Geometric Compression Ratio	23.0:1
Effective Compression Ratio	21.9:1
Intake Valve Opening (IVO)	340 CAD ATDC
Intake Valve Closure (IVC)	127 BTDC
Exhaust Valve Opening (EVO)	127 CAD ATDC
Exhaust Valve Closure (EVC)	380 CAD ATDC

The in-cylinder pressure is measured by a high frequency piezoelectrican AVL GH15D pressure sensor placed where the Diesel injector originally was. Its signal is amplified by a AVL FlexIFEM 2P2E. In order to obtain the desired compression ratio of 22:1, the piston bowl has been filled with 4032 aluminum alloy and then machined to obtain a flat piston, which is ideal for HCCI engines as it decreases drastically crevice volume. The feeding lines of oxygen and air are decoupled for high and low mass rates, with different mass flow meters, in order to avoid high values of uncertainty in the mass flow measurement. The gaseous mass flows are measured and controlled by Brooks Mass Flow Controller (MFC) SLA-585X. The intake and exhaust pressures are measured with absolute piezoelectric KISTLER 4260 transducers. The intake, exhaust and cylinder-wall temperature measurements are done with type K thermocouples. A constant velocity of 1500 rpm is provided by an electric motor. The torque sensor is a HBM T40B Torque flange mounted between the HCCI engine and the electric motor and the crank angle is acquired every 0.1 CAD by a Heidenhain ROD 426 rotary encoder. The acquisition of all the data is done by a National Instruments Compact Rio 9022. The two lines of oxygen are fed by an oxygen bottle for low mass flow rates, while higher flow rates of oxygen are provided by a Pressure Swing Absorption (PSA) oxygen generator Noxerior OP - 60 Ecoline. In this machine, the absorption capacity of the zeolite, which is a porous material, is exploited to absorb nitrogen from compressed air, leaving oxygen with a purity that can reach a value of 95%.

Experimental campaign

The main parameters which influence the combustion are the intake pressure, the mixture equivalence ratio and the intake temperature. As far as the intake pressure is concerned, it was decided to keep it close to atmospheric pressure, as investigating a turbocharged engine was not in the scope of this work. In order to be able to make comparison among the different oxygen percentages, the fuel flow, thus the FuelMEP of the mixture, defined as

$$\text{FuelMEP} = \frac{m_f \text{LHV}}{V_d}, \tag{1}$$

was kept constant. In Eq. (1), m_f is the mass of fuel, LHV is the Lower Heating Value of the fuel and V_d is the displacement of the engine. This means that, for each oxygen percentage, the amount of fuel per cycle was kept constant and equal to a reference value, while the composition of the oxidizer was changed according to the percentage of oxygen which had to be investigated. The reference value for the amount of fuel at the different intake temperatures and oxygen percentages, was the one for which the equivalence ratio is equal to 0.4 for combustion with air at an intake temperature of 393 K, which correspond to a value of FuelMEP of 7.88 bar.

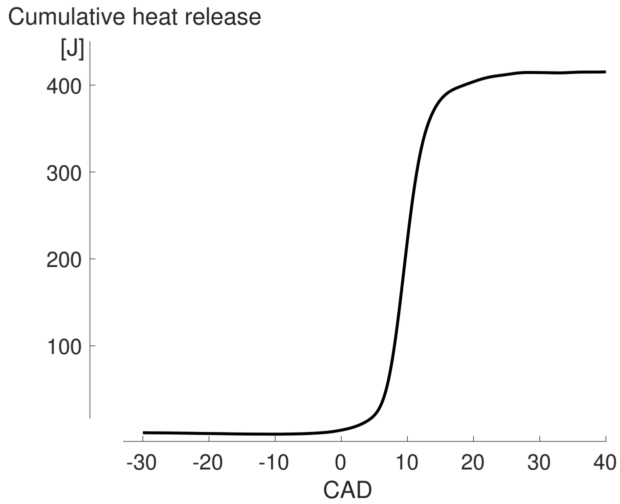


Figure 1: Typical cumulative heat release curve obtained from a pressure trace.

The operating conditions of the experimental campaign are reported in Table 2. Four different oxygen percentage ranges have been investigated at four different intake temperatures. The intake temperatures are the minimum ones allowing combustion with the oxidiser composition in the lower limits of the ranges (21%, 27%, 32% and 41%) while the upper limits of oxygen percentage in each range have been chosen such that the MPRR was kept below the safety threshold of 17 bar/CAD.

Table 2: Operating conditions.

Range	Oxygen percentage range	Intake temperature	ϕ
#1	21% - 25%	425 K	0.300 - 0.252
#2	27% - 31%	408 K	0.233 - 0.203
#3	32% - 40%	402 K	0.197 - 0.158
#4	41% - 49%	389 K	0.154 - 0.129

Post-processing method and uncertainty quantification

The post-processing method adopted has been described in [18]. It will be briefly summarized here. To account for cycle-to-cycle variability, 100 cycles have been acquired for each operating condition. Pressure was the only measurement performed in real time. The pressure signals need to be filtered and pegged in order to remove noise and to obtain the correct absolute pressure. Then, the Top Dead Center (TDC) offset, the effective compression ratio and the blow-by are computed in order to calculate the Heat Release Rate and the combustion timing. The heat losses are calculated in such a way as to obtain a flat cumulative HRR before and after the combustion, as shown in Fig. 1. A pressure trace in motoring conditions has been used to calibrate all the important parameters needed to compute the HRR. Combustion timing and combustion duration are calculated from the cumulative heat release curve. In particular, combustion ignition is estimated as the timing at which 10% of the total heat has been released.

The uncertainty analysis methodology adopted has been extensively explained in [19]. The main steps are reported here. It is important to distinguish between quantifying the uncertainty of quantities which have been directly measured and quantities which are calculated during the post processing phase, as the post processing procedure it-self may induced a certain level of uncertainty. For quantities directly measured it is important to distinguish between Type A and Type B uncertainties. Type A uncertainty comes from the statistical methods used to analyse the data, and it can be interpreted as the stochastic behaviour of the measured quantity. The definition of Type A uncertainty is

$$u_A = \sqrt{\frac{1}{n(n-1)} \sum_{i=1}^{n} (x_i - \bar{x})^2}, \tag{2}$$

where n is the number of measurements performed, x_i is the i-th measurements and $\bar{x}$ is the mean value of the n measurements. The uncertainty given by the inaccuracy of the measurement system is Type B uncertainty, defined as

$$u_B = \sqrt{u_{ref}^2 + u_{LC}^2 + u_{lin}^2 + u_{fit}^2 + u_{repeat}^2 + \sum u_{drift}^2}, \tag{3}$$

accounts for linearity, linearisation, repeatability, temperature or pressure drift, reference, and least count (LC) uncertainties. The total uncertainty of a quantity directly measured is

$$u_{tot} = \sqrt{u_A^2 + u_B^2}. \tag{4}$$

In this work, $U_{95,x}$ are reported on the graphs, which are the uncertainty on the measurement of x with a 95% probability. It is defined as:

$$U_{95,x} = 1.96 \cdot u_{tot} \tag{5}$$

To calculate the uncertainties on non directly measured quantities $Z = f(W_1, ..., W_n)$, they have to be expressed as a function of directly measured quantities only. Then, the uncertainty is calculated as follows:

$$u_z = \sqrt{\sum_{i=1}^{n} \left(\frac{\partial f}{\partial W_i}\right)^2 \cdot u_{Wi}^2} \tag{6}$$

In Table 3 the average uncertainties on the most significant parameters are reported.

Table 3: Average uncertainties of maximum in cylinder pressure, MPRR, ignition timing (CA10), intake temperature and oxygen percentage.

Parameter	U_{95}
P_{max}	1.15%
MPRR	4%
CA10	0.24 CAD
T_{in}	1.76 K
$\%O_2$	$< 0.1\%$

Experimental Results and discussion

The goal of this experimental campaign was to fully characterize the behavior of methane HCCI combustion in oxygen-enriched conditions. The main parameters of interest are the pressure trace, MPRR as it represents an indicator for safety combustion, combustion timing, as it affects efficiency, and the influence of the body temperature on the overall behavior. First it has been found that the potential of extending the operative range of methane HCCI combustion is such that it is not possible to run the engine at a fixed mixture intake temperature varying the oxygen percentage from 21% to 49%.

As shown in Fig. 2, increasing the oxygen percentage from 21% to 49% has allowed to decrease by almost 30 K the minimum intake temperature at which there is methane auto-ignition. Moreover, at higher oxygen contents the oxygen percentage range in which it is possible to have combustion at the same intake temperature is broader.

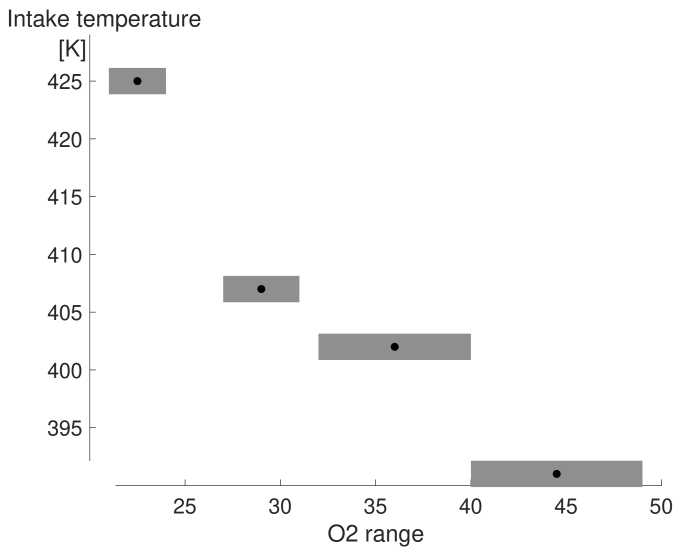


Figure 2: Intake temperature of the mixture as a function of the oxygen percentage. Enriching the mixture with oxygen allows to decrease the intake temperature by almost 30 K

In Fig. 3, the pressure evolution as a function of the crank angle degree is reported for the range 27 to 31% of oxygen. As it is possible to notice, the combustion peak is advanced with the increase of oxygen percentage and, hence, higher, meaning that the combustion timing is earlier. So the effect of oxygen is to decrease the ignition delay.

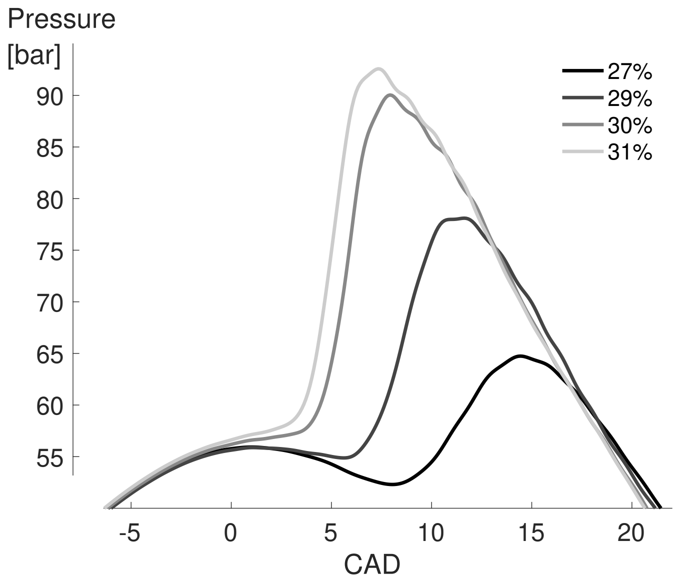
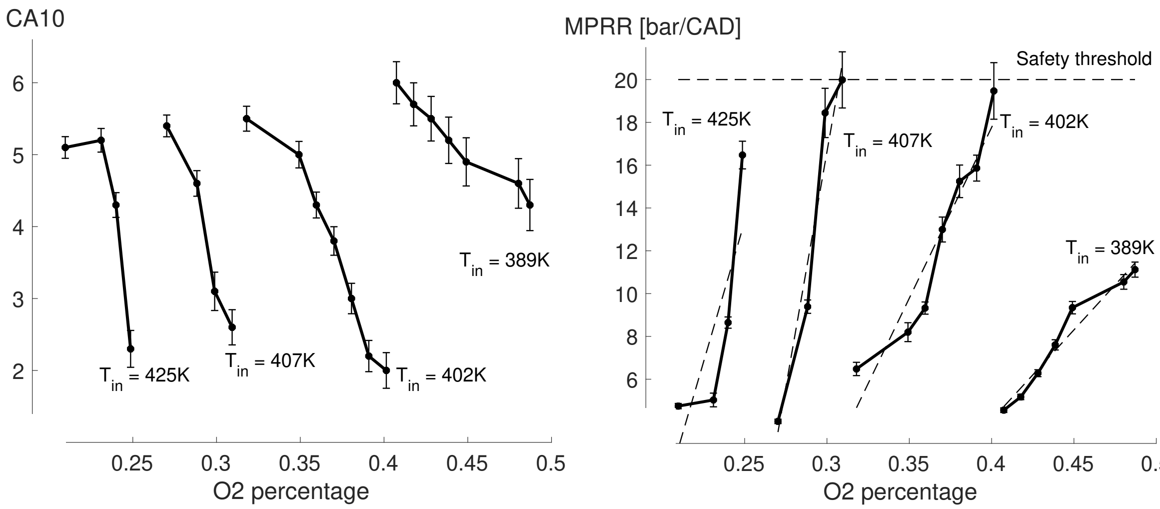


Figure 3: Pressure evolution at different oxygen percentages. The intake temperature of the mixture is $T_{in} = 408$ K.

Figure 4 shows the influence of oxygen percentage on the ignition timing and on the MPRR. The oxygen addition causes an advance in the combustion timing and, therefore, an increase in the MPRR. The decrease of the advance of the combustion timing is non linear and diminishing at higher oxygen percentages. This means that the combustion timing is less sensitive to oxygen addition at higher oxygen concentrations. Similar observations can be done for the MPRR showed in Fig. 4b. Furthermore, it is possible to notice that the MPRR at 49% oxygen, at the end of the last range is 11 bar/CAD, well below the safety threshold of 20 bar/CAD. This means that, at T_{in} = 389 K, it is possible to further increase the oxygen percentage, leading to a broader range with respect to range 32-40 %, which already was broader than the previous ones.



(a) (b)

Figure 4: Influence of oxygen percentage on (a) ignition timing, and (b) on MPRR. The influence of oxygen addition at higher oxygen concentrations is less important. The dashed lines in (b) represent the linear regression of the experimental data.

As previously mentioned, the engine with which the experimental campaign has been performed is an air-cooled engine and hence it is difficult to control the body temperature. This could be the reason why the lines in Fig. 4 are not straight. In Fig. 5 the influence of the body temperature on the MPRR in the range from 23% to 25% oxygen content is shown, at constant intake temperature. The combustion behaviour is extremely sensitive to the body temperature at low oxygen percentages.

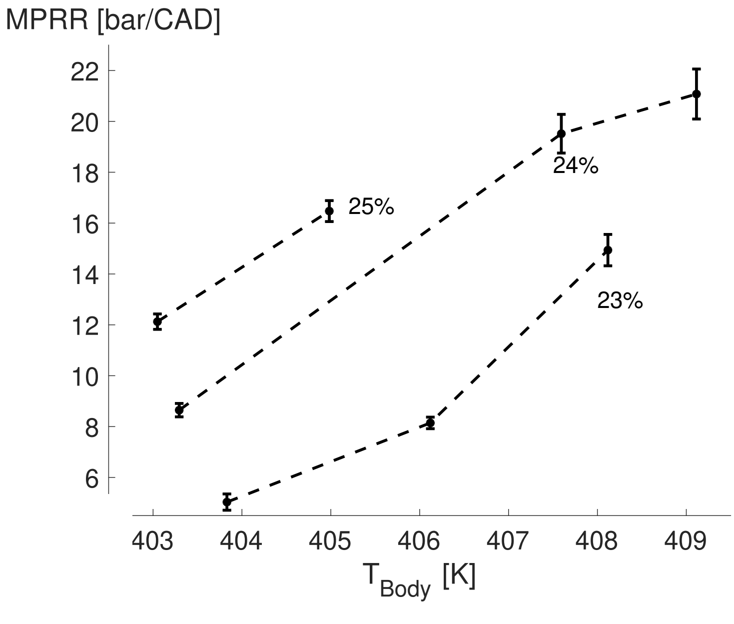


Figure 5: Influence of the body temperature on the MPRR at low oxygen percentages and constant intake temperature. The combustion behaviour is extremely sensitive to small changes in the body temperature.

This can be explained by the fact that at low oxygen percentage the combustion is highly enhanced by a small increase in oxygen content, but the intake temperature needs to be still high in order to have combustion and the ignition timing is still very sensitive to changes in the temperature of the mixture. The high impact on the combustion behaviour of the body temperature and the difficulty to control it, makes the combustion behaviour difficult to govern in these conditions. Moreover, it makes difficult to isolate the oxygen addition contribution at low oxygen percentages. This means that in a real steady-state application, in case of lack of effective ways to control the body temperature it is safer to operate the engine at higher oxygen percentages.

Kinetic analysis
In order to better understand the effect of oxygen enrichment of the oxidizer, kinetic simulations of high temperature, high pressure combustion of oxygen-enriched mixtures were performed. In particular, the kinetic software OpenSMOKE++ [16] was used to carry out simulations on constant-volume, batch reactors with increasing O_2 concentration in the mixtures, from air to pure oxygen as oxidizer. The Aramco 2.0 was used as kinetic mechanism [20]. The initial temperature of the reactants was varied to indirectly evaluate the effect of the intake temperature, as higher intake temperatures will result in higher temperatures at the ignition point. The FuelMEP of the mixture has been kept constant and oxygen percentages from 21 to 100% have been tested. For each condition, the ignition delay time was calculated, since it qualitatively represents the reactivity of the mixture. The trend of ignition delay time as a function of the initial temperature at different oxygen fractions is shown in Fig. 6.

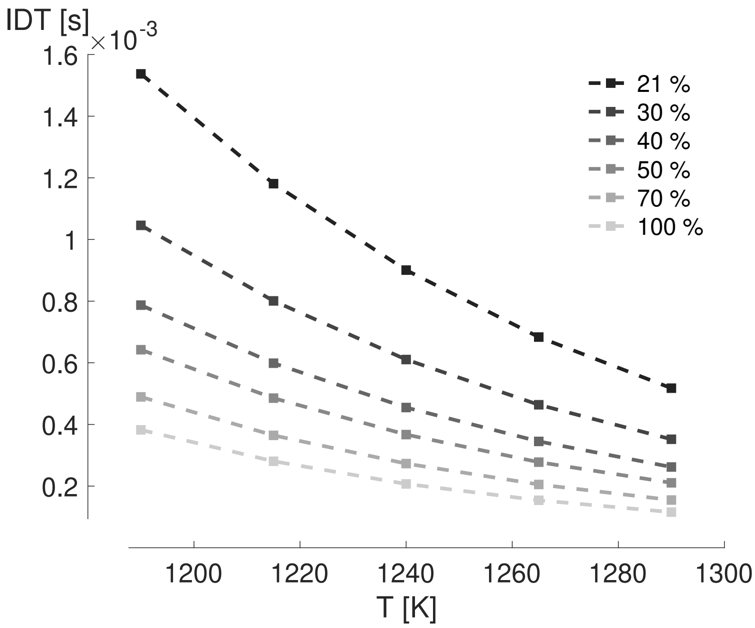
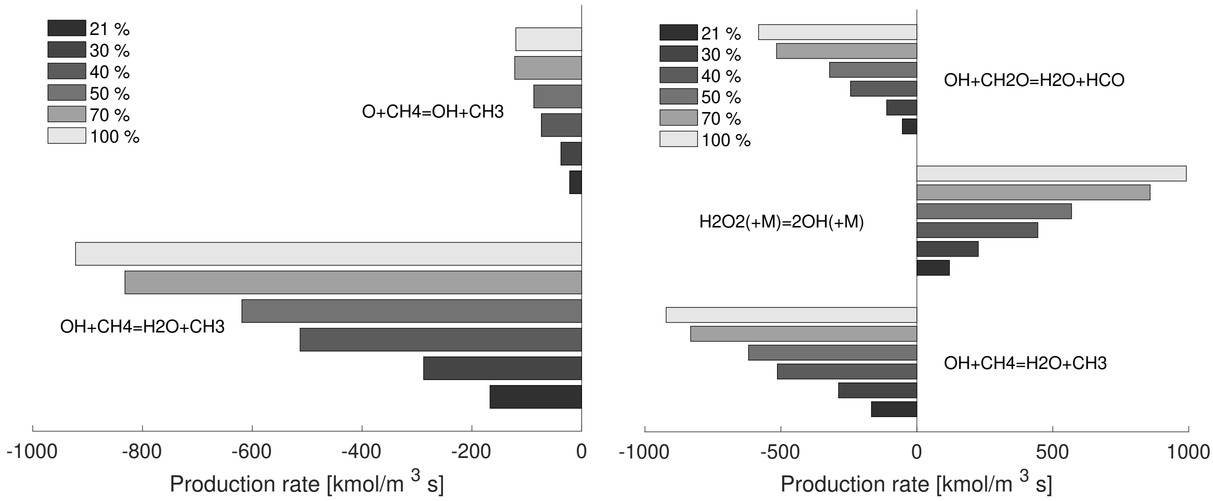


Figure 6: Ignition Delay time as a function of different initial temperature. Variations of temperature at higher oxygen contents have a lower impact.

The ignition delay time decreases non linearly both with the increase of oxygen percentage and with the increase of the initial temperature. At higher oxygen percentages, the curves tend to overlap, meaning that the influence of the oxygen addition in that region is less important. Moreover, at higher O_2 content, the ignition delay time becomes less sensitive to changes in intake temperature. This explains the trend observed during the experiments. In the context of future works, having a mixture that is less sensitive to changes in intake temperature opens the door to the possibility of increasing the fuel content of the mixture, thus extending the operating range and increasing the power density.

The goal of performing the kinetic analysis was to better understand the main chemical reactions of influence on the combustion behaviour, so a Rate Of Production Analysis (ROPA) was carried out to investigate the effect of O_2 addition on the main chemical reactions. Initial conditions of pressure and temperature of the reactor were selected in order to emulate operating conditions encountered during the engine cycle, namely 60 atm and 1190 K, as observed from experiments. In Fig. 7a the ROPA of methane is reported.



(a) (b)

Figure 7: ROPA of (a) CH_4 and (b) OH for different oxidizer compositions at T_{in} = 1190 K and p_{in} = 60 atm. The consumption of methane is faster because of the enhanced production of OH radicals.

The main reactions of consumption of methane are:

$$OH + CH_4 = H_2O + CH_3 \tag{7}$$

$$O + CH_4 = OH + CH_3 \tag{8}$$

As OH radicals are highly involved in the consumption of methane, the three most important reactions for the production/consumption of OH radicals in the low-temperature combustion region are reported in Fig. 7b. As we can observe, OH radicals are mainly consumed by the reaction:

$$OH + CH_4 = H_2O + CH_3 \tag{9}$$

And the absolute rate of reaction increases with the O_2 concentration in the oxidizer. This behaviour can be related to an increased availability of OH radicals. In fact, the reaction:

$$H_2O_2 + M = 2OH + M \tag{10}$$

becomes more and more important at increased O_2 concentrations. This is due to the enhanced third body efficiency for this reaction. Higher concentrations of H_2O_2 are also present and this can be explained by the ROPA of HO_2 reported in Fig. 8. Higher oxygen contents lead to a higher production of HO_2 via the reactions:

$$O_2 + HCO = HO_2 + CO \tag{11}$$

$$H + O_2 + M = HO_2 + M \tag{12}$$

The HO_2 produced is consumed in the reaction

$$2HO_2 = O_2 + H_2O_2 \tag{13}$$

which leads to the production of H_2O_2, involved in the production of OH radicals as seen in Eq. (10). As the availability of OH radicals is higher at higher oxygen percentages, the reaction

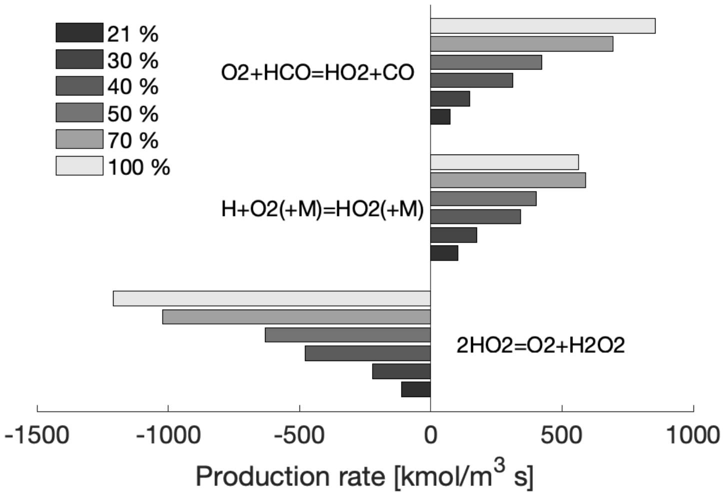


Figure 8: ROPA CH_4. The higher availability of OH radicals at higher oxygen contents leads to a faster consumption of CH_4

in Eq. 7 is also faster, leading to a faster consumption of methane.

The reaction rate of the two main reactions for OH consumption/production were analyzed (Eq. 10 and 9) and results are reported in Fig. 9. As expected, the reactivity of the mixture increases at higher oxygen concentrations and at higher temperatures. What is important to notice is that the increase in the reactivity when oxygen is added to the oxidizer is more pronounced at low O_2 values and it almost reaches a plateau above roughly 75% of O_2. This trend somehow explains the trend observed in the experiments, since lower intake temperatures were necessary to accommodate more O_2-enriched mixtures in the engine, otherwise the combustion would have been too violent. Moreover, it explains why, at higher oxygen percentages, the ignition timing was found to be less sensitive to oxygen addition.

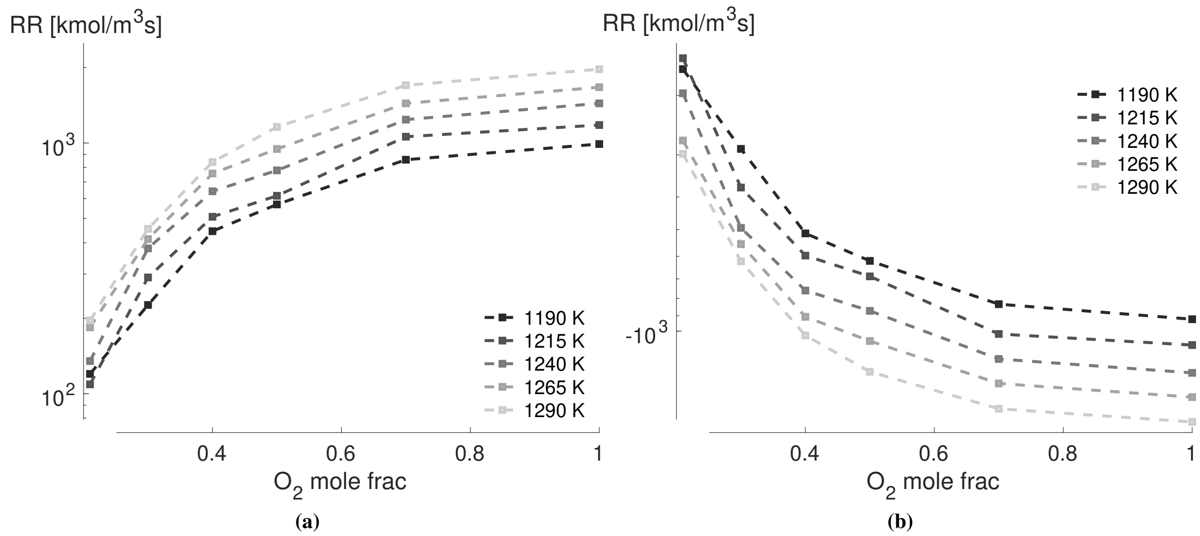


Figure 9: Absolute reaction rates of the two main reaction for OH production H2O2(+M)=2OH(+M) (a) and consumption OH+CH4=H2O+CH3 (b) for different oxidizer compositions and at different temperatures

The competitive effect on the reactivity between lower temperatures and higher O_2 in the oxidizer can potentially allow to find appropriate operating conditions in order to perform full oxy-fuel combustion of methane, and this aspect will be subject of future works.

Conclusions

The aim of this work was to perform an investigation of the influence of oxygen addition to the combustion of methane in HCCI engines. With this goal, an experimental campaign has been performed with a 22:1 effective compression ratio HCCI engine, varying the oxygen percentage from 21 to 49, keeping a constant FuelMEP and varying the intake temperature. Moreover, kinetic analyses were performed in order to better understand the influence of oxygen enrichment and to explore operating conditions outside the safety domain. A qualitative sensitivity analysis of the reactivity of the mixture with the variations of temperature has been performed. The results are the following:

- Oxy-fuel combustion has a great potential in decreasing the necessary intake temperature for which stable combustion is achieved, up to 30 K in the range 21 to 49%. Decreasing the intake temperature would lead both to an increase of the density of the mixture and to the increase of the operative range of the HCCI engine, opening the door to the possibility of increasing the power density.
- The sensitivity of the combustion to oxygen addition is decreased at higher O_2 percentages. This means that in practical application the tuning of the intake temperature at high oxygen percentage is less delicate.
- At fixed intake temperature, the possible O_2 range is broader at high O_2 concentrations.
- Numerical analysis has proved that the mixture at high oxygen concentrations is less sensitive to changes in the intake temperature.
- The mixture has shown to be less sensitive to temperature changes at higher oxygen concentrations, proving the potential of increasing the operating range with oxygen addition.

Acknowledgments

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