NUMERICAL STUDY OF WATER ADDITION ON THE COMBUSTION CHARACTERISTICS IN AN HCCI ETHANOL ENGINE

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ABSTRACT

Low-temperature combustion modes have attracted global attention in recent years, especially the homogeneous charge compression ignition (HCCI) mode. The HCCI combustion produces high-speed combustion, achieving relatively high thermal efficiencies while emitting low NOX and soot. However, due to the lack of direct control to start the combustion, one of the main challenges in this type of engine is to ensure that auto-ignition occurs close to the top dead center for a wide operation range. There are a few combustion phase control techniques to solve this limitation, and one of them is water injection. In this regard, this paper explores the influence of water concentration in an ethanol HCCI engine as a form of combustion phasing control. The work was conducted numerically using a zero-dimensional single-zone model with a chemical kinetic mechanism containing 56 species and 383 reactions. The numerical model results were well agreed with the reported experimental data. The water fraction ranged from 0 to 18% by mass at 3% intervals. The results demonstrate that water injection is an efficient strategy to control the combustion phasing by adjusting the charge reactivity. The increase in water fraction reduced in-cylinder pressure and heat release rates. Furthermore, the combustion phase was advanced, the combustion duration was extended, and thermal efficiency was about 44.3% with the increase in water concentration.

Keywords: Combustion, Controlled Auto-Ignition (CAI), Ethanol, Homogeneous Charge Compression Ignition (HCCI), Single-zone numerical model, Water injection.

NOMENCLATURE

A_w	wall area
B	cylinder bore
CAD	crank angle degrees
CAI	controlled auto-ignition
CDC	conventional diesel combustion
CI	compression ignition
CO	carbon monoxide gas
CO_2	carbon dioxide gas
h_C	heat transfer coefficient
H_2O	water
HC	hydrocarbons
HCCI	homogeneous charge compression ignition
HRR	heat release rate
ICE	internal combustion engines
IMEP	indicated mean effective pressure
L	stroke length
LTC	low temperature combustion
p	instantaneous in-cylinder pressure
NOx	nitrogen oxides
NVO	negative valve overlap
PCCI	premix charge compression ignition
R	ratio of connecting rod length to crank radius
R_C	represents the compression ratio
RCCI	reactivity-controlled compression ignition
SI	spark ignition
SOC	start of combustion
$\overline{S_p}$	mean piston speed (characteristic velocity)
T	temperature, Kelvin
T	instantaneous in-cylinder temperature

TDC	top dead center
TSCI	thermally stratified compression ignition
T_w	wall temperature
V	instantaneous volume

Greek symbols

θ inverse of equivalence ratio,

INTRODUCTION

The rapid socioeconomic growth of the world population results in energy crises and depletion of fossil fuel sources, which are the largest portion of the current energy matrix. Fossil oil is the most used fuel in the world today (32% of all primary energy), and the transport sector was the main fossil oil consuming sector, resulting in 25% of all CO_2 emissions in 2017 (IEA, 2019a and IEA 2019b). Thus, great attention is being given to the transport sector, which uses internal combustion engines (ICE) as the main power source. These engines generate their power through the combustion process, where fuels are mostly of fossil origin, resulting in environmental pollutions. Therefore, the use of ICE in transportation is a major issue in relation to global warming, pollutant emissions and health hazards (Punov et al., 2017; Telli et al., 2018). Another concern is the finite nature of fossil fuel resources, which are diminishing over time. This reality may raise fossil fuel prices as consumption continues to climb due to population growth and improvements in living standards (Mittal et al., 2015; U.S. Energy Information Administration, 2015; Rosa et al., 2021).

In this context, governments have been encouraging the use of renewable fuels, depending on local availability, and also creating stringent emission legislations to reduce our dependence on fossil fuels and the amount of greenhouse and pollutant gases emitted into the atmosphere. In recent years, researchers have focused on advanced combustion modes that are highly efficient, environment friendly and capable of using biofuels. Among these combustion strategies, low temperature combustion (LTC) has received much attention because it can provide higher efficiencies in relation to conventional combustion modes and it is possible to run with flexible fuels (Srivastava et al., 2018; Krishnamoorthi et al., 2019). LTC concepts include several techniques, such as homogeneous charge compression ignition (HCCI), premix charge compression ignition (PCCI) and reactivity-controlled compression ignition (RCCI) (Agarwal et al., 2017; Rosa et al., 2020). One of the LTC concepts is the Homogeneous Charge Compression Ignition (HCCI) combustion, also known as Controlled Auto-ignition (CAI) combustion, which uses the basic elements of compression ignition (CI) and spark ignition (SI) (Agarwal et al., 2017). HCCI combustion operates unthrottled and with a highly diluted homogeneously air-fuel mixture. HCCI combustion process occurs due to the sequential auto-ignition, driven by thermal stratification during the compression stroke, which occurs naturally as a result of the heat transfer phenomena, that cooled the areas near the cylinder wall (Dec and Hwang, 2009; Snyder et al., 2011). These cold areas mix turbulently with the hot core of the cylinder at the end of the compression stroke, resulting in temperature distribution. Consequently, the hot parts ignite first, releasing heat and compressing the cold parts until they ignite (Gainey and Lawler, 2021). In CAI combustion, there is no diffusive flame or flame propagation, resulting in a reduction of nitrogen oxides (NOx) and soot, as their formation is directly associated with the flame temperature and the equivalence ratio (Bendu and Murugan, 2014).

Although the HCCI combustion mode has numerous inherent advantages over traditional SI and CI modes, it still has several limits and technological challenges to overcome in real-world applications. The challenges to overcome are controlled auto-ignition timing, combustion phase, low power output, high levels of CO and HC emissions and homogeneous mixture preparation (Bendu and Murugan, 2014; Saxena and Bedoya, 2013; Telli et al. 2021). Controlling the ignition timing and combustion phasing, on the other hand, are two key challenges that impact the high pressure rise rate, knocking, operation range limitation, and even thermal efficiency. Unlike the conventional combustion modes that have a direct combustion control mechanism (the spark in SI engines and fuel injection in CI engines), HCCI combustion mode has no direct control mechanism to the auto-ignition timing and the subsequent combustion phasing (Hasan and Rahman, 2016; Maurya and Saxena, 2018). In fact, several factors influence the auto-ignition timing and combustion phasing, including intake air temperature and pressure, fuel chemical and physical properties, thermal stratification, engine geometry and other parameters (Dec and Sjoberg, 2004). In this regard, it is difficult to ensure that the controlled auto-ignition occurs close to the top dead center (TDC) for a wide operation range in an HCCI combustion. However, to overcome the difficulties, there are a few ignition timing and combustion phasing control techniques being researched in recent years.

Duan et al. (2021) reviewed different ignition timing and combustion phase control strategies used in the HCCI engines. Among all the strategies, there is one technique that introduces directly or indirectly a reaction suppressor within the charge, especially water. The water injection method has previously been studied in PCCI and HCCI combustion, demonstrating that it allows the combustion control and expansion of the engine operational load (Christensen and Johansson, 1999; Iwashiro et al., 2002). Lawler et al. (2017) defined the use of direct injection of water in HCCI engines, to control the average temperature and the temperature distribution before ignition, as

Thermally Stratified Compression Ignition (TSCI). The authors demonstrated that the direct water injection increases the combustion duration and reduces the heat release rate, resulting in a forced thermal stratification and improved operating range.

Valero-Marco et al. (2018) studied the use of direct water injection in an HCCI gasoline engine operating at 1500 rpm. CAI combustion was achieved using negative valve overlap (NVO) and water was directly injected into the combustion chamber. Results showed that water injection was effective in reducing and controlling the reactivity of the charge during HCCI combustion. It reduced the pressure rise rates and knock occurrence, slowing down the combustion and retarding the combustion phasing. In addition, an increase from an initial load of 3.5 bar indicated mean effective pressure (IMEP) without water injection to a final load of 10 bar IMEP with water addition was observed. Otherwise, water injection can decrease the combustion stability since the reactivity of the charge is decreased.

Ahari and Neshat (2019) investigated the effects of water addition on natural gas HCCI combustion using a thermodynamic multi-zone model coupled to a semi-detailed chemical kinetics mechanism. The authors used five different quantities of water added to the fuel. Water was added to the in-cylinder charge while maintaining the total amount of mass inside the combustion chamber and the overall air-fuel ratio constant. The addition of water retards the start of combustion and decreases peak values of in-cylinder pressure and heat release rate. Furthermore, water injection of up to 3% in mass improves engine thermal efficiency and reduces exhaust pollutant gases. The findings showed that injecting water into an HCCI engine might help control the combustion process.

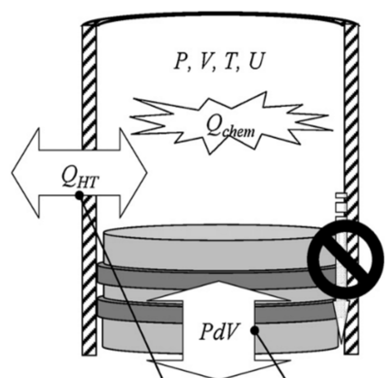
Du et al. (2020) studied the effects of seven different mass water fractions added to a natural gas HCCI combustion. The study was conducted using a multi-zone model coupled with a detailed chemical reaction mechanism (53 species and 325 reactions). Using the artificial inert species method, the thermal, dilution, and chemical effects of water on the start of combustion (SOC) were investigated. The results indicated that heat release rates and in-cylinder pressure decreased, and SOC was delayed with increased of water addition at different loads. At higher loads, water addition controlled the SOC and reduced the ringing intensity. Finally, the authors found that the water's thermal effect was more significant on SOC than dilution or chemical effect.

Following the recent works on the potential of the water injection approach to control the combustion and expand the load of an HCCI engine, this paper employs a single zone model using chemical kinetics to study the auto-ignition of ethanol HCCI combustion operating with water injection, as mean of combustion phasing control. This study uses a numerical model for ethanol HCCI combustion with different water concentrations to observe the performance and combustion characteristics. In addition, this paper deals with the combustion of ethanol, which is a low carbon and renewable fuel, influencing the reduction of fossil fuel dependence and pollutant emissions.

METHODOLOGY

Numerical model

The study was conducted in a model of a four-stroke HCCI single-cylinder engine using the single-zone model, also known as the zero-dimensional model, from ANSYS CHEMKIN software. In the zero-dimensional model, the engine's completely thermodynamic properties are considered, modeling the engine cycle by the differential form of thermodynamics first law, and considering the work absorbed/produced by the piston. Chemical and thermal analyses were modeled on a homogenous closed-volume engine cycle system, neglecting any mass input or output during the combustion process. The only dimension of the problem is the time, considering the combustion chamber as a uniform reactor with uniform temperature, pressure, and composition. Therefore, the volume of the combustion chamber is considered a transparent thermodynamic system. Figure 1 illustrates the scheme of the first law of thermodynamics for a single-zone model from (Komninos and Rakopoulos, 2012).



$$dU = \delta Q_{HT} - P_{cyl}dV_{cyl}$$

Change in U *Heat transfer to the wall* *Work*

Figure 1 - Scheme of the first law of thermodynamics for single-zone models (Komninos and Rakopoulos, 2012)

Variations in reactor volume are determined by the interaction between the slider and the crank, which is used to determine piston motion in the engine cylinder. In addition, the model only deals with the closed part of the cycle, disregarding the intake and exhaust cycle. This type of model aims to simulate the auto-ignition process of the air-fuel mixture and allows the use of detailed chemical kinetic models, enabling the investigation of chemical reactions that contribute to the temperature and pressure inside the cylinder. The single-zone model is widely used in HCCI engine simulations works, such as Shahsavan and Mack, 2018; Hasan et al., 2018; Hasan et al., 2021.

The numerical model uses the geometry of the reciprocating engine to calculate the engine volume over the combustion cycle. The cylinder volume serves to find the piston work in the energy equation. Equation (1) describes the instantaneous cylinder volume at any crank angle (θ).

$$V = V_C\left[1 + \frac{R_C - 1}{2}\left(R + 1 - \cos\theta - \sqrt{R - \sin^2\theta}\right)\right] \quad (1)$$

Where V represents the instantaneous volume, V_C is the clearance volume, R is the ratio of connecting rod length to crank radius and R_C represents the compression ratio. Equation (2) shows the rate of volume change.

$$\frac{dV}{d\theta} = V_C\left[\frac{R_C - 1}{2}(\sin\theta)\left(\frac{1 + \cos\theta}{\sqrt{R^2 - \sin^2\theta}}\right)\right] \quad (2)$$

Inside the engine cylinder, convection and radiation heat transfer occurred to the cylinder wall. However, in the numerical model, the radiation is neglected because of the low in-cylinder temperature and soot, which are characteristics observed in HCCI engines. Therefore, the convective heat transfer in the combustion chamber to the cylinder wall was modeled as described in Eq. (3) based on (Stiesch, 2013):

$$\frac{dQ_{HT}}{dt} = h_c A_w (T - T_w) \quad (3)$$

The heat transfer coefficient is represented by h_C, A_w is the wall area and T_w is the wall temperature. The wall area is calculated by Eq. (4), which is the sum of the piston, cylinder head and cylinder wall area.

$$A_w = \frac{\pi B^2}{4} + \left(\frac{\pi B^2}{4} + \frac{4V_C}{B}\right) + \left[\left(\frac{\pi B L}{2}\right)\left(R + 1 - \cos\theta - \sqrt{R - \sin^2\theta}\right)\right] \quad (4)$$

Where B is the cylinder bore and L is the stroke length.

In this study, the heat transfer coefficient is modeled using the Woschni correlation as described in Eq. (5). This correlation was adjusted to a gasoline HCCI engine, as reported in Hasan et al. (2021).

$$h_c = 129.8 B^{-0.2} p^{0.8} T^{-0.55} (2.228\overline{S_P})^{0.8} \quad (5)$$

Where $\overline{S_p}$ is the mean piston speed, as the characteristic velocity, T as instantaneous in-cylinder temperature and p as the instantaneous in-cylinder pressure.

Chemical kinetic mechanism

Ethanol was used as a test fuel, and the main chemical properties can be seen in Table 1. The chemical reaction during the combustion process was solved using a specific ethanol chemical kinetic mechanism. This work uses the Marinov (1999) detailed chemical kinetic model for ethanol oxidation. The mechanism comprises 56 species and 383 reactions and considered spans the temperature range of 1000–1700 K, a pressure range of 1.0–4.5 atm, and an equivalence ratio range of 0.5–2.0. According to Marinov (1999), the mechanism was validated with experimental data sets, such as laminar flame speed data from a constant volume bomb and counter flow twin-flame, and ignition delay data behind a reflected shock wave.

Table 1. Ethanol physicochemical properties (Kumar et al., 2013; Telli, 2018)

Properties	**Ethanol**
Density at 20°C (g/ml)	0.7851
Cetane number	5 – 8
Research octane number	109
Lower Heating Value (MJ/kg)	26.9
Boiling point (°C)	78.37
Molar mass (g/mol)	46.06
Auto-ignition temperature (°C)	423
Latent heat of vaporization (MJ/kg)	0.92
Viscosity (10e-3 Pa.s)	1.078

Operating conditions and model validation

Table 2 presents the engine's geometric configurations used in the numerical analysis with the single-zone model. The numerical model was verified using Telli et al. (2020) experimental data from an ethanol HCCI cylinder with the same configurations shown in Table 2. In the experiments, the three-cylinder engine was coupled to an electric generator, operating at a constant speed of 1800 rpm and with 10 kW of electric power. The modified engine operated with cylinder #1 running on ethanol HCCI combustion, attained via total recirculation of exhaust gas from cylinder #3, which runs on conventional diesel combustion (CDC). Cylinder #2 was also run on diesel combustion and it was used to motor the setup. The cylinder #3 exhaust gas recirculation was the major heat source for the auto-ignition of the ethanol cylinder (#1). In addition, the combustion phasing was controlled using the water injection technique.

Figure 2 presents the in-cylinder pressure of the single-zone zero-dimensional model in relation to the experimental data reported by Telli et al. (2020). The modelling verification was carried out for IMEP = 4 bar, CA50 = 4 CAD ATDC, CR = 14:1, N = 1800 rpm, Tin = 406 K, Pin = 1.4 bar, λ = 1.4 and H_2O injected = 7% mass basis. As can be seen in Figure 2, the peak in-cylinder pressure is adequately reproduced, demonstrating that the important reaction pathways are very well represented.

Following the numerical model analysis, simulation runs were carried out to evaluate the potential of water injection to control ethanol HCCI combustion. To verify the water injection effect on combustion and performance, the same inlet temperature and pressure, lambda (the inverse of equivalence ratio, ϕ) and speed of the experimental tests were used. Water addition to the charge leads to the decrease of intake of air and ethanol because they are replaced by water. Water mass fraction in the charge composition was varied from 0 to 18%. The total mass in cylinder is constant during the water addition process.

Table 2. Detailed engine specifications used in the numerical model

Specification	Value
Type of engine	Single-cylinder, four-stroke
Compression ratio (CR)	14:1
Bore (mm)	102
Stroke (mm)	120
Connecting rod length (mm)	207
Swept volume (cm³)	980.3
Intake valve close (CAD)	-162 ATDC
Exhaust vale open (CAD)	113 ATDC
Engine Speed (rpm)	1800

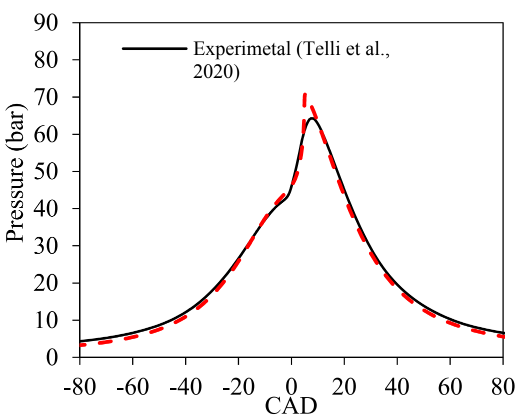
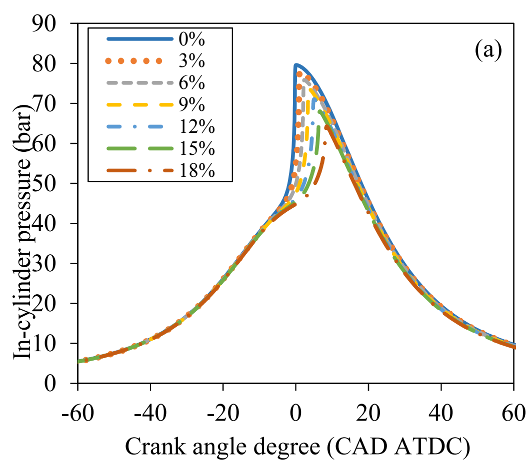


Figure 1 - Comparison of the present numerical model with experimental data from Telli et al., (2020). CR = 14:1, N = 1800 rpm, Tin = 406 K, Pin = 1.4 bar, and λ = 1.4, H_2O injected = 7% mass basis.

RESULTS AND DISCUSSION

In this section, the main results obtained in the zero-dimensional numerical model are presented. Figure 3 shows in-cylinder pressure curves (a) and the net heat release rate (HRR) (b) in relation to the water mass fraction in HCCI combustion. The highest peak in-cylinder pressure and heat release rate were for 0% of water mass fraction, reaching the maximum pressure value of 79.6 bar. It is observed that as water concentration increases, the in-cylinder pressure and heat release rate tend to decrease. For 18% of water mass fraction in HCCI combustion, the peak in-cylinder pressure was 64.3 bar, representing a reduction of about 19.2% compared to 0% of water fraction, and in the case of HRR, this difference was even higher. In Figure 3 it is also possible to notice that the combustion was delayed with the increase of the water concentration, getting further away from the TDC. The in-cylinder pressure curve and heat release rate were substantially reduced with 18% of water mass fraction, and if the water mass fraction is increased further, the combustion will be severely degraded, and misfire may occur. The maximum in-cylinder pressure and HRR correspond to 0% of water fraction because HCCI combustion is very close to TDC. Thus, the volume of the cylinder is small and, as the pressure has an opposite effect, the HRR and peak in-cylinder pressure are high. On the other hand, when combustion is delayed due to an increase in water, the volume increases while the pressure decreases. Furthermore, some of the energy released during combustion was lost to water vaporization due to the water high latent heat of vaporization, which helps reduce heat release rates.



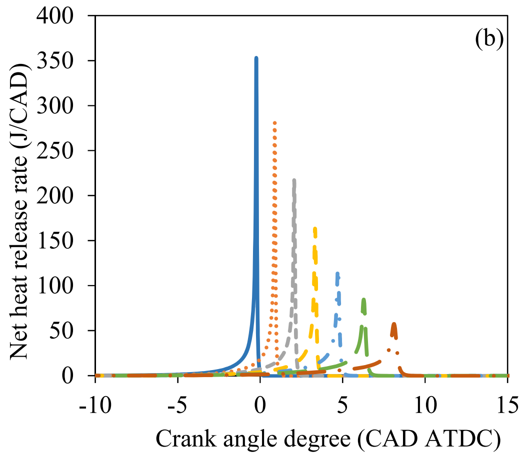


Figure 3 – In-cylinder pressure (a) and net heat release rate (b) in relation to water fraction (% in mass basis)

Figure 4 shows the in-cylinder temperature curve in relation to the percentage of the water mass fraction in the HCCI combustion. Note that the temperature curves tend to decrease at higher water concentrations. It can also be attributed to the high latent heat of vaporization of water, which causes some of the energy released during the combustion process to be lost, reducing combustion temperatures. The highest in-cylinder temperature was 1916 K for 0% of water mass fraction, while the lowest was 1697.7 K for 18% of water fraction, thus having a maximum peak temperature difference of 11.4%. It is interesting to note that water mass fractions above 6% result in maximum in-cylinder temperatures close to or below 1800 K, which could result in lower NO_X production by the thermal mechanism as described by (Agarwal et al., 2017).

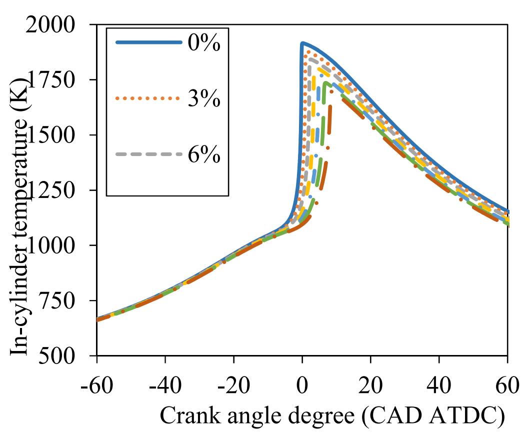
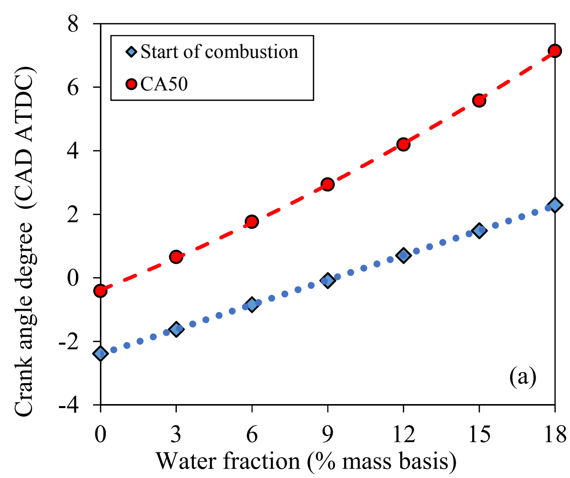


Figure 4 - In-cylinder temperature in relation to water fraction (% in mass basis)

Figure 5 shows the variation of the crank angle position at the start of combustion, CA50 and the parameter CA10-90 (b) in relation to water fraction in HCCI combustion. The start of combustion is defined as the crank angle degree where 10% of the fuel mass has been burned and depends on pressure, temperature, and charge composition during the compression stroke. The CA50 represents the crank angle degree where 50% of the fuel mass has been burned and is known as combustion phasing. CA10-90 is defined as the combustion duration and is the difference between the crank angle degree where 10 and 90% of the fuel mass have been burned, respectively.

In Figure 5 (a), the start of combustion is advanced to higher values of water mass fraction. The CA10 ranged from -2.4 to 2.3 CAD ATDC for 0 to 18% water fraction, respectively. The higher the water fraction, the more the combustion will be delayed, as more energy will be used to vaporize the water, reducing in-cylinder temperatures. Therefore, as the concentration increases, the chemical reaction rate slows down, taking a long time to reach the charge auto-ignition conditions, so the start of combustion is delayed. In this context, as the start of combustion can be changed by controlling the air-fuel mixture reactivity with the water addition, the combustion phasing (CA50) can be adjusted to better position the combustion to avoid knock occurrences and expand the HCCI operational load. The CA50 followed the same trend results of the start of combustion and ranged between -0.4 and 7.2 CAD ATDC.



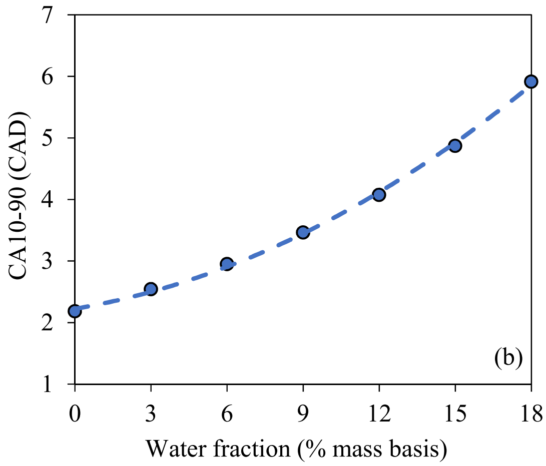


Figure 5 – Start of combustion, CA50 (a) and CA10 90 (b) in relation to water fraction (% in mass basis)

In figure 5(b), the shortest combustion duration was 2.2 CAD at 0% of water fraction and the longest combustion durations was 5.9 CAD at 18% of water mass fraction, representing a difference of about 68%. The heat release rate is lower for higher water concentration values and, consequently, the in-cylinder temperatures. Then, the combustion tends to be slower at these conditions, resulting in longer combustion durations. It is important to highlight that at 0% of water fraction, the HCCI combustion is extremely fast, which means that all the fuel energy is released in a very short period, causing knock, and limiting the operation at high loads. Thus, the addition of water to HCCI combustion plays a significant role in controlling the combustion phase, reducing heat release rates, and increasing the combustion duration.

Figure 6 presents the results of IMEP (a) and thermal efficiency (b) in relation to water mass fraction in HCCI combustion. IMEP tends to be reduced with increasing water concentration. IMEP values ranged from 3.9 to 4.6 for 0 to 18% of water fractions, respectively, representing a reduction of 15.2%. With the addition of water, combustion is increasingly advanced in relation to TDC, producing less work per cycle and reducing the IMEP. Also, when water is added to the combustion, part of the air and ethanol are replaced by water to keep the amount of mass and lambda constant. The thermal efficiency for all water fractions was very similar, ranging from 44.1 to 44.4%. The thermal efficiency of HCCI combustion with water fractions of between 6 to 12% was slightly higher. It is believed that this is due to the CA50 being better positioned since for 0 to 3%, it is before or very close to TDC, and for 15 and 18% of water fractions, the combustion is very advanced, which could have reduced thermal efficiency.

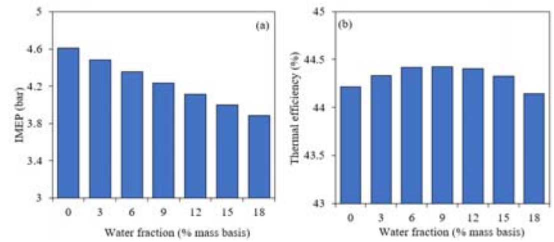


Figure 6 – IMEP and thermal efficiency in relation to water fraction (% in mass basis)

CONCLUSIONS

This paper studied numerically the HCCI combustion of ethanol using a single-zone zero-dimensional model. The model was verified with experimental data. It was explored the use of water injection as a means of HCCI combustion control. Seven water mass fraction values were simulated, and parameters related to performance and combustion characteristics were evaluated.

It was noticed a decreasing trend in in-cylinder pressure, in-cylinder temperature and net heat release rate, whereas the water fraction increased. The maximum in-cylinder pressure and temperature were 79.6 bar and 1916 K for 0% water fraction, respectively. However, with 18% of water fraction, these values decreased to 64.3 bar and 1697.7 K. The main reasons for this reduction were that the CA50 was delayed and the water high latent heat of vaporization, which reduces the heat release rate and in-cylinder temperature.

The start of combustion and CA50 were delayed with the increase in water fraction. As the water addition increase, the chemical reaction rate slows down, taking more time to achieve the charge auto-ignition conditions, retarding the SOC and consequently the CA50. It was clear that the water injection technique is able to control the charge reactivity and adjust the combustion phasing between 0.4 and 7.2 CAD ATDC from 0 to 18% of water concentration. In addition, since the heat release rate is lower for higher values of water addition, the combustion tends to be slower at these conditions, resulting in longer combustion durations. The combustion duration varied from 2.2 to 5.9 CAD for 0 and 18% of water fraction, representing a difference of about 68%.

Finally, IMEP decreased with the increase of water fraction, from 4.6 to 3.9 bar, due to the later combustion phase and the replacement of part of the ethanol and air by water. Thermal efficiency did not change significantly with increased of water concentration and ranged from 44.1 to 44.4%. Overall, the results were satisfactory, showing the potential for water injection to control the combustion in HCCI engines. With the water injection, the heat release rate can be reduced, and the combustion phasing can be adjusted to better position the combustion to avoid knock and expand the maximum load in HCCI engines.

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RESPONSIBILITY NOTICE

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