



Numerical Simulation of a Reactivity Controlled Compression Ignition Engine in order to Investigate the Effects of Adding Water to Low Reactivity Fuel

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ABSTRACT

For decreasing the fuel consumption of internal combustion engines, and also reducing the emissions, investigation of the effective parameters on power, emissions, and the combustion phasing is important. In this study, the influence of adding water to a Reactivity Controlled Compression Ignition (RCCI) engine has been numerically investigated. For this purpose, water with different mass fractions was added to the air-fuel mixture. In order to simulate the engine, AVL Fire software was used. The results show that substituting a portion of gasoline fuel with water, up to 10% mass fraction, raises the combustion chamber pressure. In this condition, the production of hydroxyl free radicals, as one of the characteristics for the start of combustion, occurs earlier. Furthermore, Indicated Mean Effective Pressure (IMEP) remains unchanged. By further increasing the water mass the production of hydroxyl radical decreases, and the high-temperature heat release is delayed; also comparing to when water was not added, average temperature of the combustion chamber reduces, while the amount of CO production does not change. Increasing the number of water moles increases the maximum in-cylinder pressures so that compared to pure gasoline mode, by replacing 20% of gasoline mass with water, the indicated mean effective pressure approximately stays the same.

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NOMENCLATURE

Latin Letters		Abbreviation	
$C(kg)$	Mass concentration of species	3D	Three dimensional
$g\left(\frac{kg}{s^2}\right)$	Body force	aBDC	After bottom dead center
$H\left(\frac{J}{kg}\right)$	Specific enthalpy	aTDC	After top dead center
i	Ith species	CAD	Crank angle
$k\left(\frac{m}{s^2}\right)$	Turbulence kinetic energy, equilibrium constant	CFD	Computational fluid dynamics
$L(m)$	Length scale	EVO	Exhaust valve opening
$P(Pa)$	Pressure	HCF	High cetane fuel
$\dot{q}\left(\frac{W}{kg}\right)$	Specific energy source production	HOF	High octane fuel
$\dot{r}\left(\frac{kg}{s}\right)$	Species source production	HTHR	High-temperature heat release
$S_H(J)$	Source of species enthalpy	IMEP	Indicated mean effective pressure
$S_k(mol, kg)$	Source of species mass	ISFC	Indicated specific fuel consumption
$T(s)$	Time scale	IVC	Intake valve closing
$U, u\left(\frac{m}{s}\right)$	Velocity	LHV	Low heating value

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$\bar{u}_i, \bar{u}_j \left(\frac{m}{s}\right)$	Averaged turbulence velocity	LTHR	Low-temperature heat release
$x_i, x_j, x_k (m)$	Spatial variable	PCCI	Premixed charge compression ignition
Greek Letters			
δ_{ij}	Kronecker delta	PFI	Port fuel injection
$\varepsilon \left(\frac{kg}{m \cdot s^3}\right)$	Weighted turbulence dissipation rate	RCCI	Reaction control compression ignition
$\lambda \left(\frac{W}{m \cdot K}\right)$	Conduction coefficient	RoHR	Rate of heat release
$\mu \left(\frac{kg}{m \cdot s}\right)$	Viscosity	rpm	Revolution per minute
$\mu_t \left(\frac{kg}{m \cdot s}\right)$	Turbulence viscosity	SoHTHR	Start of high-temperature heat release
$\rho \left(\frac{kg}{m^3}\right)$	Density	TDC	Top dead center

INTRODUCTION

Considering the development of internal combustion engines and their various applications, increasing their efficiency as well as reducing the combustion emissions and fuel consumption, from them are the main purposes of research in this field [1, 2]. The Compression-Ignition (CI) engines present higher thermal efficiencies compared to the Spark-Ignition (SI) engines due to their higher compression ratio; as regards the air-fuel mixture in these types of engines is not homogenous; they produced a high amount of emissions. For this reason, some efforts are made to design these engines in a way that not only they have higher power and efficiency, but they also produce lower levels of Nitrogen Oxides (NO_x) and soot emissions [3, 4]. On this basis, researchers initially investigated the more advanced Premixed Compression-Ignition (PCI) engines [5–7], and then a new technology called Low-Temperature Combustion (LTC) was developed. LTC engines had two major characteristics: high thermal efficiency, even as high as CI engines, and lower emissions [8]. In this kind of engine, the air-fuel mixing procedure and time, as well as their preparation for the combustion are influential parameters.

One of the well-known LTC engines is Homogenous Charge Compression Ignition (HCCI) engine. In the HCCI engines, the combustion starts from several high-temperature points in the combustion chamber; thus the combustion forms without flame propagation [9]. However, controlling the start of combustion timing and duration of the combustion process in these engines are so difficult, makes their practical application challenging so that in most cases the HCCI engines are set on low-load conditions [10]. Another kind of LTC strategy is PCCI. The more homogenous fuel-air mixture in PCCI engines, which is created due to early injection of fuel, increases the combustion performance in these engines. The fuel injection procedure includes the fuel atomization and mixing the fuel with the entering air to the combustion chamber [11, 12]. For years, controlling the combustion duration and ignition delay were serious

challenges for designing LTC engines until Kokjohn et al. [13] and Hanson et al. [14] recommended the usage of two fuels with different specifications for solving the combustion control problems. The idea was to use two fuels in a CI engine simultaneously; a High Reactivity Fuel (HRF) for controlling the start of combustion and a Low Reactivity Fuel (LRF) for using during the combustion process. They called this strategy Reaction Control Compression Ignition (RCCI). In the RCCI strategy, the combustion phasing is controlled using the energy ratio or mass fraction of two fuels and the combustion duration is controlled by the means of fuel reactivity stratification [15–17].

The probability of engine knocking in LTC engines and high levels of unburnt hydrocarbon (HC) emissions are still challenges for the commercial application of these recent combustion strategies [18]. Changing or mixing fuels together is a technique for enhancing the performance and decreasing the emission levels in LTC engines. Fuel property optimization is an effective way to control the reactivity gradient between premixed fuel and direct injection fuel to extend the RCCI operating conditions. Various studies have focused on this issue, and one of the major aims of these investigations was to test different HRFs and LRFs [19–21]. Typical low-reactivity fuels such as natural gas, hydrogen, methanol and ethanol are often applied as premixed fuels in RCCI combustion, while biodiesel, dimethyl ether (DME), and other high reactive fuels considered as diesel alternatives in RCCI have attracted wide attention [22, 23]. However, due to the special characteristics of different fuels, each fuel can have destructive effects on engine performance in addition to its advantages [24]. These effects can be controlled by adding species that do not participate in the combustion process. For overcoming these difficulties, Taghavifar et al. [25] evaluated different percentages of spraying water in a dual fuel diesel CI engine and observed that the engine knocking problem was solved but the soot emission was increased. Also, studies have shown that spraying a specific amount of water can decrease the NO_x emission in a CI engine [26]. It should be noted that species such as hydroxyl (OH) and hydrogen

peroxide (H₂O₂) are considerably influential on controlling the ignition delay and burn duration; thus the water spray can be effective on the efficiency and performance of CI engines [27, 28].

The influence of adding water on the combustion process and the amount and time of producing these species in the combustion chamber led the researchers to investigate how the addition of water can affect the combustion process. In 2019, El Shenawy et al. investigated the effects of adding water as an emulsion with diesel fuel in a premixed charge compression ignition (PPCCI) diesel engines and they show that the water concentration enhancement leads to improvement in the brake specific fuel consumption and an increase in the brake thermal efficiency also it reduces the CO, UHC, smoke opacity and Nox emissions from the engine [29]. Pirola et al. in a numerical study added water mixed with air through the air inlet manifold of a CI engine. they observed that that oxygen-enriched air enhances the thermal efficiency of the engine (up to 13%) and reduces significantly soot emissions; on the other hand, in-cylinder peak pressure and NOx emissions increase. The latter can be significantly reduced by using humidified air maintaining the advantage in terms of thermal efficiency and in soot reduction, nevertheless, the baseline case NOx emissions cannot be restored [30]. But Ayhan in an experimental study on a CI engine with B20 fuel demonstrated that with direct water injection, a distinctive reduction (56%) in NOx emissions and increases in HC, CO, and smoke emissions are observed, compared to B20 blend results [31]. In 2014, Pandey et al. experimentally examined the effects of adding hydrogen fuel as well as different amounts of water through the inlet manifold of a CI engine. The results showed an enormous heat is absorbed with the transformation of water into super-heated steam [11]. Taghavifar et al. [25] numerically investigated the influence of water direct injection through a separate nozzle in a CI engine. They tested various percentages of water with temperatures in the range of 27-60 °C. Their results showed that in the mass fraction of 15% and temperature of 60 °C, the power and torque reach their maximum, but in the mass fraction of 5% and temperature of 27 °C the lowest amount of emissions can be obtained [25]. Christensen et al. [32] experimentally evaluated the possibility of using water injection for controlling the start of combustion in an HCCI engine. In their investigation, they examined various air to fuel ratios, and inlet pressures for three different fuels including isoctane, ethanol, and NG. According to their results, only a certain range of water mass fractions can enhance the ignition time and reduce the combustion rate in these engines. Also increasing the water percentage leads to higher CO emissions, which shows the reduction of combustion quality [32].

Previous studies showed that spraying water with different mass fractions, has various effects on the quality of combustion, efficiency, and power in the ICES; thus in

this study in addition to analyzing the influence of adding water to the LRF in a RCCI engine, the possibility of reducing the LRF fuel and substituting it with water without a significant change in the Indicated Mean Effective Pressure (IMEP) was examined. Despite the changes in the equivalence ratio and the reduction in intake fuel mass, attempts were made to keep the output power characteristics almost constant to ensure the accuracy of the result analysis. Since there are various types of combustion regimes in ICES, simulating the combustion in them is always challenging, so for modeling and numerical simulation of the engine, the AVL Fire software was coupled with detailed chemical kinetics and it was utilized for this purpose. The reason for using chemical kinetics code software was to increase the precision of the combustion process calculations. The important point about this study is to accurately evaluate the effects of some chemical species (such as hydroxyl) on the combustion procedure and controlling the start of combustion. It is noteworthy that even though this issue is important, studies have not focused on the effects of injecting water on the production or consumption of these species so far. Also, due to the selection of gasoline as the LRF, the production and consumption of species such as formaldehyde (CH₂O) and hydroxyl radical as influential parameters on controlling the start and duration of combustion have been examined.

METHODOLOGY

Governing equations and solution method

In this investigation, for analyzing the effects of adding water to the fuel-air mixture, the mass fraction of added water to the fuel-air mixture was calculated using Equation (1), so that the total mass of gasoline and water was constant in all of the cases, but their mass fractions were changed.

$$\text{water mass fraction} = \frac{m_{\text{water}}}{m_{\text{gasolin}} + m_{\text{water}}} \times 100 \quad (1)$$

For simulating the closed cycle of the engine numerically, the AVL Fire software was utilized. The governing equations in this section include the conservation, continuity and turbulence modeling equations. The effects of turbulence were considered using the k- ζ -f turbulence model [33].

$$\frac{\partial \rho}{\partial t} + (\nabla \cdot \rho U) = 0 \quad (2)$$

$$\frac{D(\rho U_i)}{Dt} = \rho g_i - \frac{\partial P}{\partial x_i} + \frac{\partial P}{\partial x_j} \left[\mu \left(\frac{\partial U_i}{\partial x_j} - \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} \right) - \rho \overline{u_i' u_j'} \right] \quad (3)$$

$$\frac{D(\rho H)}{Dt} = \rho \dot{q}_g + \frac{\partial P}{\partial t} + \frac{\partial}{\partial x_i} (U_j \tau_{ij}) + \frac{\partial}{\partial x_j} \left(\lambda \frac{\partial T}{\partial x_j} \right) \quad (4)$$

$$\frac{D(\rho C)}{Dt} = \rho \dot{r} + \frac{\partial}{\partial x_j} \left(D_j \frac{\partial C}{\partial x_j} - \rho \overline{C u_j} \right) \quad (5)$$

$$\rho \frac{Dk}{Dt} = \rho(P - \varepsilon) + \frac{\partial}{\partial x_i} \left(\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right) \quad (6)$$

$$\rho \frac{D\varepsilon}{Dt} = \rho \frac{C_{\varepsilon 1} P - C_{\varepsilon 2} \varepsilon}{T} + \frac{\partial}{\partial x_j} \left(\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right) \quad (7)$$

$$\rho \frac{D\zeta}{Dt} = \rho f - \rho \frac{\zeta}{k} P + \frac{\partial}{\partial x_j} \left(\left(\mu + \frac{\mu_t}{\sigma_\zeta} \right) \frac{\partial \zeta}{\partial x_j} \right) \quad (8)$$

$$f - L^2 \frac{\rho^2 f}{\partial x_j \partial x_j} = \left(C_1 + C_2 \frac{P}{\zeta} \right) \frac{2/3 - \zeta}{T} \quad (9)$$

$$P = -2\mu_t S: S - \frac{2}{3} [\mu_t (trS) + k] (trS) \quad (10)$$

$$\nu_t = C_\mu \zeta \frac{k^2}{\varepsilon} \quad (11)$$

In the analysis of an ICE, solving chemical reactions is vital for the evaluation of fuel oxidation and heat release. During the oxidation process, besides the temperature and pressure of the combustion chamber, recognizing the procedure of production and consumption of some species such as free radicals are important. Some of these species are OH, H₂O₂ and CH₂O. These species have critical effects on the quality, start, and duration of the combustion process. The production of formaldehyde can indicate the start low-temperature heat release as well as the consumption of HRF which is the starter of initial combustion in an RCCI engine; thus in the numerical examinations, the time of formaldehyde production is an important parameter. The hydroxyl radical has been known as a significant species for increasing the quality of combustion because this species is highly effective at the start of combustion timing [27]. Hydrogen peroxide is a species that moves the combustion process forward and can produce free radicals for advancing the combustion process after its decomposition [27, 28]. Equations (12) and (13) show the production of OH [27].



Considering the aims of this study, the accuracy of calculations for examining the effects of adding water to the fuel is important; thus for this purpose, detailed chemical kinetics was employed for solving the chemical reactions and increasing the precision of the results. Figure 1 shows the simulating stages using 3D CFD AVL FIRE code coupled with detailed chemical kinetics. According to this figure, after the execution and analyzing the generated mesh for the geometry, by considering the boundary and thermodynamic conditions in the software, the numerical simulation is done based on the mass conservation and momentum equations. For

simulating the fuel injection the Kelvin–Helmholtz and Rayleigh–Taylor models were utilized. After the completion of the Computational Fluid Dynamics (CFD) calculations, the combustion computations are performed. To calculate the effect of chemistry, a chemistry solver is coupled to FIRE. A DME reduced chemical mechanism consists of 77 species and 457 reactions used for gasoline/diesel combustion chemistry calculations. IF the temperature of the computational cells is higher than 600 K, the chemical kinetics code is used for correcting the data such as the concentration of the species and the heat release. These stages are repeated until the crank angle (CA) reaches the exhaust valve opening moment.

Validation

For validation of the numerical simulation and chemical reactions, the in-cylinder pressure and Rate of Heat Release (RoHR) parameters were compared with the experimental data from the study of Shafaghat et al. [35]. The validation was performed on a light-duty four-stroke single-cylinder compression ignition engine. Table 1 shows the detailed specifications of the engine.

In this engine for the direct injection of the fuel into the combustion chamber, a common rail system was employed. This engine was also equipped with a Port Fuel Injection (PFI) system. Table 2 presents the characteristics of the direct and port fuel injection systems.

After the injection of gasoline fuel through the port, it entered the cylinder mixed with air, and the diesel fuel was directly injected into the combustion chamber. The injected mass of diesel fuel and gasoline in each cycle was 10.5 and 12 mg, respectively. The performance of this engine was set on a fixed speed of 1150 rpm, the diesel start of injection timing of 20° CA before Top Dead

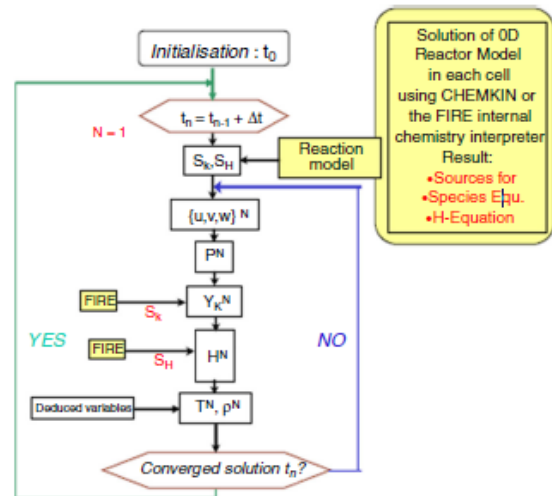


Figure 1. The strategy of coupling AVL fire and detailed chemical kinetics [34]

Table 1. The specifications of the engine [35]

Item	Specification
Type	Single cylinder, water cooled, four-stroke, direct injection
Bore (mm)	92
Stroke (mm)	95.5
Displacement (cc)	630
Compression ratio	17.1
Intake valve opening (CAD bTDC)	20
Intake valve closing (CAD aTDC)	47
Exhaust valve opening (CAD bTDC)	35
Exhaust valve closing (CAD aTDC)	14
Number of valves	2

Table 2. Specifications for the port and common-rail injection system [35]

Items	Common-rail injection system	PFI injection system
Number of holes	8	5
Hole diameter (µm)	120	-
Spray angle	120	-
Injection pressure (bar)	600	3

Center (bTDC), and fuel combustion duration of 2.5° CA. The specifications of the two mentioned fuels have been presented in Table 3.

Based on the data from the experimental study, and by considering nozzle holes and symmetry of the problem, for the numerical simulation in the AVL Fire software, 1/7th of the combustion chamber was selected for modeling and mesh generation. Considering the dimensions and the geometry shape, a mesh consisted of 60000 number of cells, was chosen for the simulations (Figure 2).

Table 3. Diesel and gasoline fuel properties [35]

Fuel type	Natural gas	Diesel
Density (kg/m ³)	-	814.8
Cetane number	-	44
Octane number	130	-
LHV (MJ/kg)	48.4	44.64
Viscosity	-	1.483
H/C ratio	4	1.9
Stoichiometric A/F ratio	17.2	-

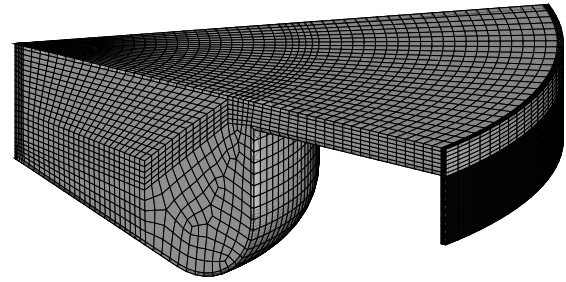


Figure 2. Computational grids at TDC

Figure 3a shows the pressure and heat release rate results based on the crank angle also Figure 3b shows the NOx emission. As can be observed, the pressure results from the numerical and the experimental data are compatible with good accuracy. These results include the maximum in-cylinder pressure and the pressure rise due to combustion in two stages. Furthermore, the numerical results for the time of heat release in both stages have appropriate compatibility with the experimental data and the moment of both high and low-temperature heat release have been well-predicted by the numerical simulation. Since only NOx emission was reported in the experimental study [35], therefore, the calculated NOx emission was compared with the experimental results. Numerical calculation of emission was acceptable with respect to the percentage of reported error.

In the simulated RCCI engine, the combustion process included two subprocesses. The first stage is the Low-Temperature Heat Release (LTHR), which is highly dependent on the HRF, and the second stage is the High-Temperature Heat Release (HTHR), which is based on the combustion of premixed fuel (Figure 4).

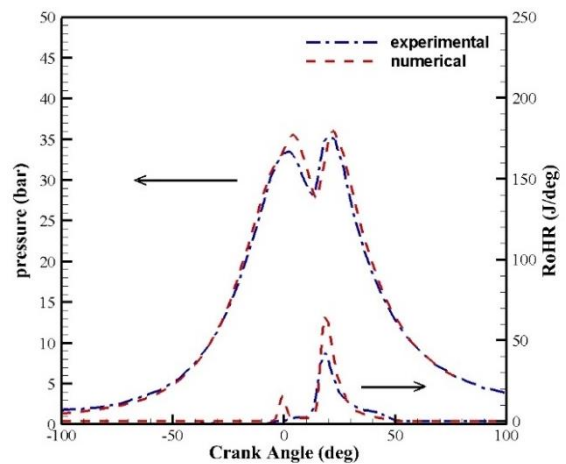


Figure 3a. A comparison of the measured and calculated in cylinder pressure and RoHR [35]

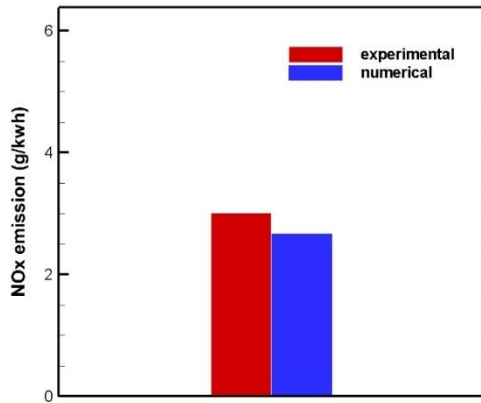


Figure 3b. A comparison of the measured and calculated NOx emission

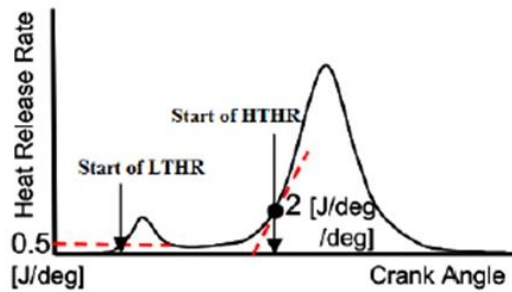


Figure 4. Process of heat release in RCCI mode [36]

The process of water injection

In order to inject the water, various methods can be used, such as simultaneous direct injection of water into the combustion chamber using a separate injector [25], direct injection of emulated water with HRF through the common injector into the combustion chamber [37], the addition of water steam into the fuel-air mixture [38], and spraying the water using a separate injector at in the air inlet manifold [39]. In this study, considering the start of injection (SOI) timing of the experimental model, for injecting the water, it was added to the fuel-air mixture. For this purpose, a portion of gasoline in the fuel-air mixture was substituted with water with different mass fractions, in a way that the amount of gasoline reduction was equal to the amount of water addition.

RESULTS AND DISCUSSIONS

In this investigation, the HRF was directly injected into the combustion chamber at the CA of 20° bTDC, on the other hand, gasoline as the LRF entered the combustion chamber through the inlet manifold.

Figure 5 illustrates the RoHR as well as the combustion rate of gasoline and diesel fuels based on the CA in this special engine. Considering the RoHR plot, the combustion includes two stages which are LTHR and

HTHR. Due to the fact that in this study, chemical kinetics mechanism in AVL Fire software was used to calculate the heat release rate, so it was possible to derive the heat release rate of each chemical species. According to Figure 5, comparing the heat release rate of two types of fuel (gasoline and diesel), it is observed that most of the heat from the combustion of diesel fuel is released in the cold combustion stage. Also, a larger share of gasoline fuel heat is released in hot combustion. In fact, diesel fuel starts the combustion and gasoline fuel continues it. Therefore, to calculate the start of high temperature heat release timing, a graph of gasoline fuel consumption rate was extracted and the moment when 5% of the gasoline total heat was released, was considered as the SoHTHR. Finally, this value was checked with start of production of formaldehyde (indicating the start of HTHR) and the calculated SoHTHR value was validated. This parameter was defined to clarify the analysis of the results for this particular engine according to the fuel combustion process in all cases.

Considering the fact that the total mass of gasoline and water in all studied mass fractions were kept constant, for analyzing the effects of adding water in the fuel-air mixture more precisely, investigation of water to gasoline mole ratio is important; because the molar mass of water is considerably lower than the molar mass of gasoline, thus with addition of a specific mass of water, and reducing the same amount of mass from the gasoline, the total mole number increases. Figure 6 shows the water to gasoline molar ratio. For the water mass fractions lower than 10%, the mole ratio is lower than 1, meaning that the number of available water moles in the fuel-air mixture is lower than the gasoline moles. In the mass fraction of 15%, the number of water and gasoline moles are almost equal, also in the mass fraction of 20%, the water moles are higher than the gasoline moles.

Ignition delay and combustion duration are two of the fundamental characteristics of CI engines. As can be

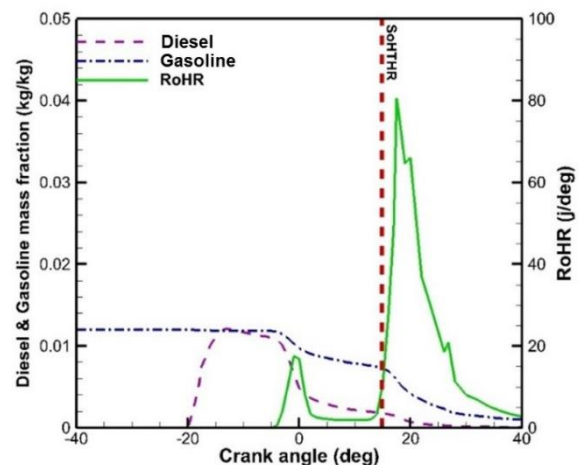


Figure 5. Effect of gasoline and diesel burning on the combustion process

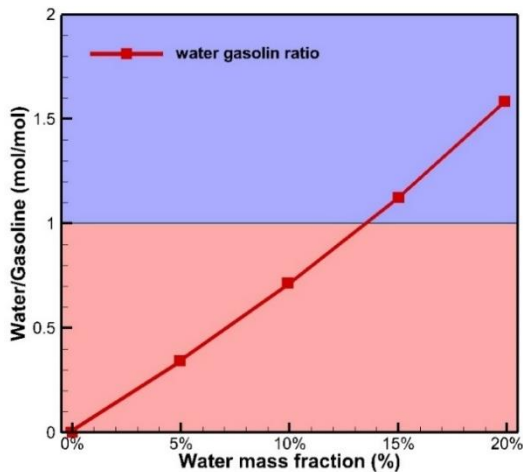


Figure 6. Molar ratio of water to gasoline

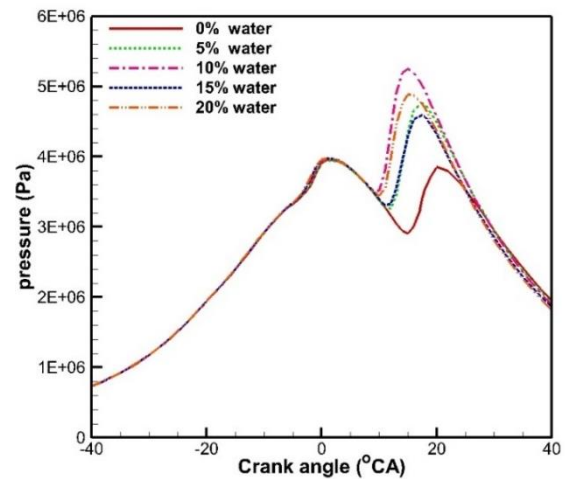


Figure 7. In-cylinder mean pressure

observed, the ignition delay is not changed in different mass fractions of water, because as it was mentioned in Figure 5, the share of initial combustion until reaching 10% of the total heat release due to the combustion of HRF is related to the diesel fuel. Since the amount of injected diesel fuel through direct injection in these cases is not changed, the ignition delays are almost the same. With the mass fraction of water, up to 10%, the combustion duration decreases considerably and the HTHR occurs earlier; because considering the water to gasoline mole ratio, and the dominant effect of gasoline in the combustion process, the higher total moles of the mixture increases the in-cylinder pressure, and the mixture combusts earlier, thus the SoHTHR advances and the combustion duration decreases. According to Figure 7, it can be observed that the advancement of SoHTHR and combustion duration makes the combustion process happen when the piston is located at a higher point in the cylinder. This leads to a higher maximum mean pressure in the combustion chamber. For mass fractions more than 10%, the combustion duration increases again, and the SoHTHR retards; because in the mass fraction of 15%, besides the significant mass percentage reduction in gasoline, according to Figure 6, the mole numbers of water and gasoline are almost the same, so both of them affect the combustion process equally. The high specific heat capacity of water leads to the absorption of the released heat from the combustion and reduction of the combustion product temperature [39]. This reduction in temperature retards the SoHTHR and results in a lower reaction rate, and finally, it increases the combustion duration. The extension of combustion duration reduces the in-cylinder pressure again, as can be seen in Figure 8. In the water mass fraction of 20%, again the combustion duration decreases and the HTHR starts earlier; because as it was shown in Figure 6, in this mass fraction of water, the number of water moles is significantly higher than the gasoline. The

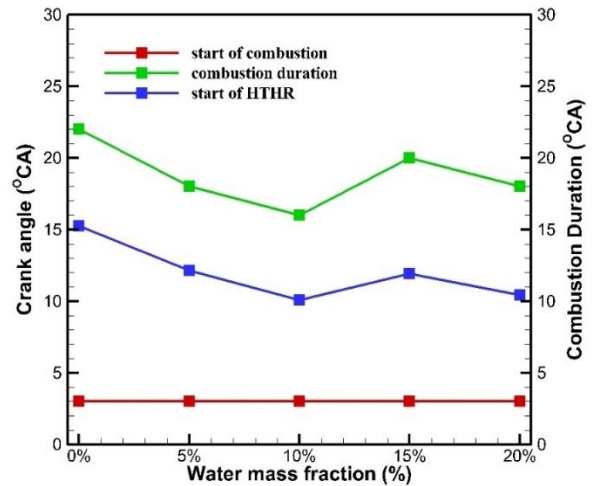


Figure 8. Combustion duration, start of combustion, and SoHTHR

higher number of moles affects the in-cylinder pressure, as it can be observed in Figure 7. This increase in pressure makes the HTHR happen earlier, so the combustion duration decreases again.

Figure 9 shows the procedure of formaldehyde production and consumption based on the CA. Considering Figure 5, Start of Low-Temperature Heat Release (SoLTHR), and also the start moment of formaldehyde species production; at the same time that the combustion starts, the formaldehyde begins as an indication for the LTHR. In fact, formaldehyde is the starter of combustion in dual-fuel LTC engines. Furthermore, it can be observed that in all mass fractions, with the addition of water, the start moment of formaldehyde production does not change, as the ignition delay stayed the same; however, the injection of water affects the start moment and the amount of formaldehyde consumption. Moreover, it can be observed that with

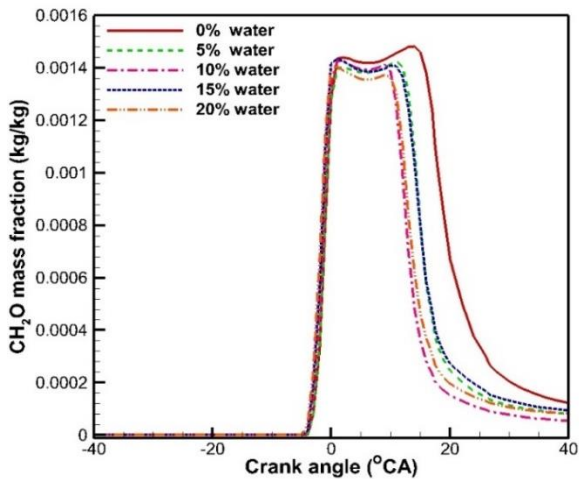


Figure 9. Production and consumption process of CH₂O

increasing the water percentage, due to the reduction of gasoline, the formaldehyde production decreases, and in all water addition percentages, with increasing the water mass fraction, due to the rise of in-cylinder pressure, the formaldehyde consumption starts earlier. For the same reason, the hydroxyl radical production begins earlier as well. Comparing Figures 9 and 10 reveals that at the same time that the CH₂O consumption starts, hydroxyl radical production begins, and the maximum hydroxyl radical production coincides with the SoHTHR moment.

OH-radicals are one of the effective parameters in controlling CI engines [40]. During the combustion process, significant amounts of free hydrogen radicals are produced and consumed. One of the most important free radicals in hydrogen is the hydroxide radical. Most of the OH radicals, react with the remaining fuel molecules and produce water and heat, which leads to higher reaction temperature and accelerates the oxidation process [27]. As it can be noticed in Figure 10, with increasing the

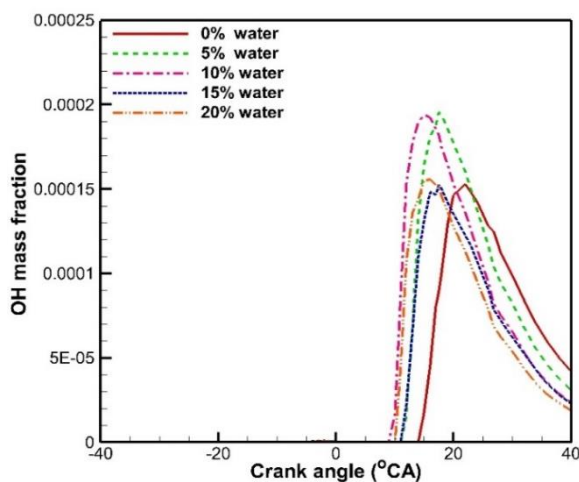


Figure 10. Production and consumption process of OH

water mass fraction up to 10%, and the rise of in-cylinder pressure, the maximum amount of hydroxyl radical production increases, also the production of OH radicals starts earlier. With increasing the water mass fraction to 15%, it can be observed that besides retarding the start of hydroxyl production, which shows a delay in SoHTHR, the amount of hydroxyl production decreases. Because with the equality of water and gasoline mole numbers, the heat absorption by water decreases, and it leads to a reduction of hydroxyl production rate. In the mass fraction of 20%, due to the lower fuel to water mole ratio, the amount of hydroxyl production decreases; because the added water is not consumed in the combustion process and the produced OH is just the product of fuel oxidation.

As it can be observed in Figure 11, the trend of changes in the hydrogen peroxide radicals is like the variations in hydroxyl radicals. The H₂O₂ produces free radicals for the advancement of the combustion process [27, 28]. Due to the instability of H₂O₂ and OH radicals, with higher maximum hydroxyl radical production, the maximum amount of H₂O₂ production decreases. This trend can be clearly seen in the plot of Figure 11.

As it can be observed in Figure 12, with increasing the mass fraction of water up to 10%, the combustion chamber temperature increases. By reviewing Figure 7, it can be found that this temperature rise is due to the increase in combustion chamber pressure. Also, considering Figure 13, it can be observed that by increasing the water mass fraction up to 10%, the maximum value of RoHR increases; because as it can be observed in Figure 8, with increasing the water mass fraction up to 10%, combustion duration decreases, consequently the heat releases in a shorter time, thus the RoHR rises. In the mass fraction of 15%, the combustion chamber temperature decreases (Figure 12). The justification for this phenomenon is as it was shown in Figure 6, the mole numbers of water and gasoline are equal; thus besides the reduction in the gasoline mass and

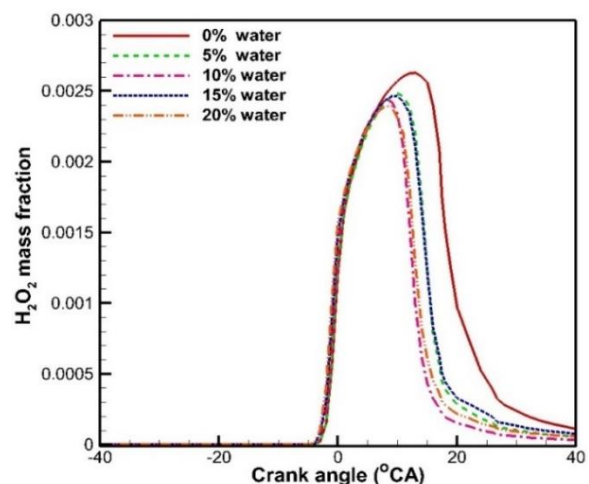


Figure 11. Production and consumption process of H₂O₂

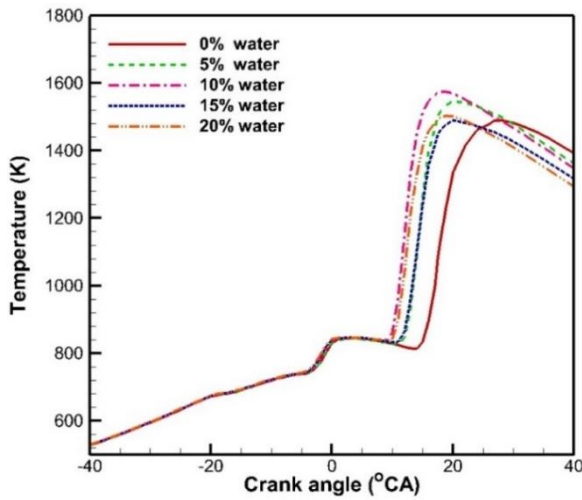


Figure 12. In cylinder mean temperature

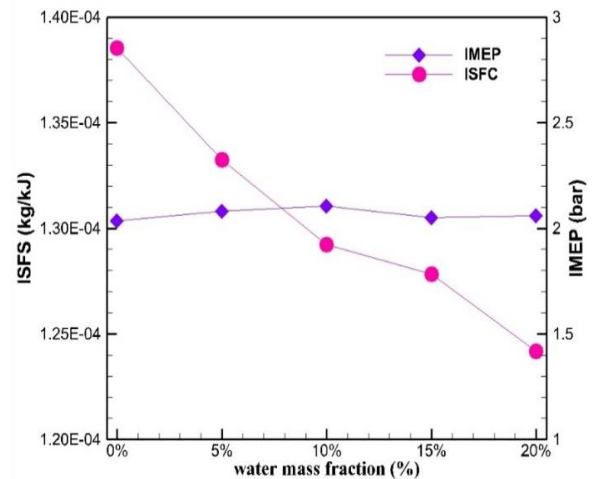


Figure 14. IMEP and ISFC

the heat release, some of this heat is absorbed by water, which results in a lower mean temperature of the combustion chamber. The important point in Figure 12 is for the mass fraction of 20%, which is not much different with the case with the mass fraction of 15% in terms of combustion chamber temperature; while according to Figures 7 and 8, despite another reduction in the combustion duration, the mean combustion chamber pressure is increased. The rise of the combustion chamber pressure in this condition is the result of the increase of water moles and reaching this water to the super-heated circumstances [39].

IMEP, as one of the major characteristics of ICEs, indicates the indicated output power of the engine. Also, the Indicated Specific Fuel Consumption (ISFC) shows the ratio of consumed fuel to the output power. As it can be observed in Figure 14, the IMEP value in different mass fractions of water is not significantly changed which

shows that by adding water against the mass of gasoline fuel that is deducted, despite the lower amount of heat release, changing the start of combustion timing and the in-cylinder pressure prevented the engine from losing power. but the ISFC values have been considerably decreased with the addition of water mass fraction. This shows that replacing a portion of the fuel in the fuel-air mixture with water can reduce fuel consumption by 20% while it keeps the output power constant.

According to Figure 15, and observing the final amount of CO and CO₂ emissions, the quality of combustion can be compared in different water mass fractions. It is noteworthy that the amount of air input in all of the cases with different water mass fractions was kept constant, and the water replaced different portions of the gasoline fuel with the same amount of mass. Considering this point, it can be observed that the addition of water up to the mass fraction of 10%, considerably

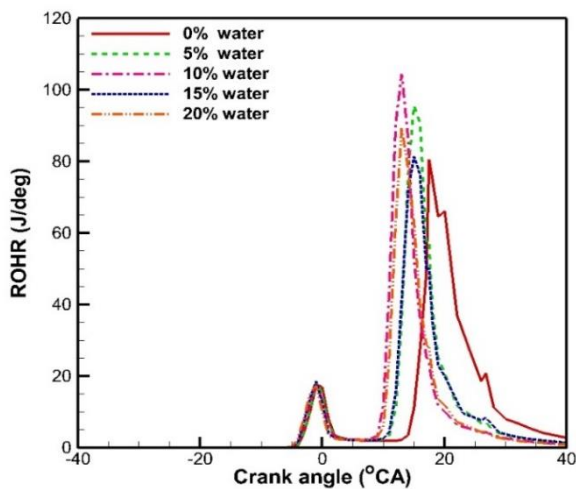


Figure 13. Rate of heat release

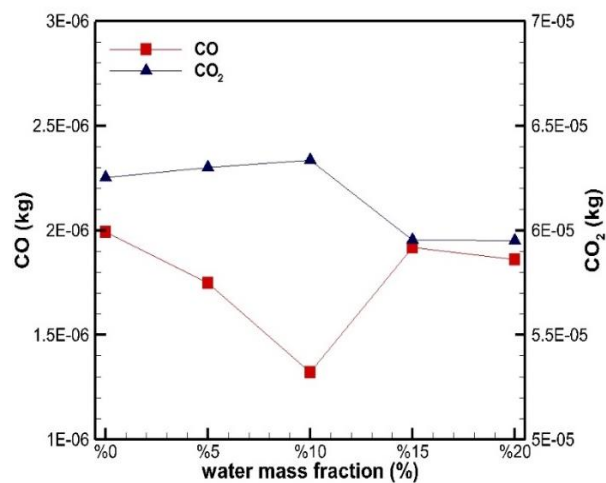


Figure 15. Carbon monoxide emission and carbon dioxide gas

reduces the CO emission and it increases the CO₂ emission level, which indicates the high quality of combustion. Because, besides the 10% reduction of the gasoline fuel, the rise of in-cylinder pressure due to increase of water moles, can also enhance the quality of combustion, and reduce the CO emission level [41, 42]. With increasing the water mass fraction to 15%, the quality of combustion decreases significantly, because the number of water and gasoline moles in this mass fraction, are almost equal, and since both of these materials, affect the combustion process equally, water absorbs some of the combustion heat and it decreases the combustion quality. According to Figures 15 and 7, it can be observed that in the mass fraction of 20%, the pressure rise is not due to the increase of combustion quality because the CO and CO₂ emission levels are not significantly changed; thus as it was indicated before, this pressure rise can be due to the higher number of water moles in the combustion chamber [43].

NO_x emissions generation are strongly dependent on the combustion temperature [44]. By comparing Figures 12 and 16, it can be seen that the decrease in temperature caused by the addition of water to the combustion process reduces the temperature and also reduces NO_x emission. At the 20% ratio of water addition, this emission is drastically reduced, while according to the Figure 14 the value of IMEP is not reduced, because the combustion temperature is low and the increase in pressure inside the cylinder is due to the addition of water to the fuel-air mixture.

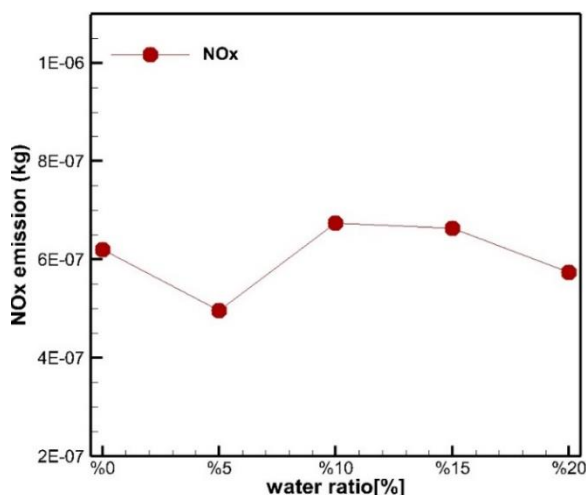


Figure 16. NO_x emission

CONCLUSIONS

In this study, the effects of adding different mass fractions of water to the fuel-air mixture in an RCCI engine was numerically investigated. For the numerical simulation of

the engine, AVL Fire software was used coupled with detailed chemical kinetics. In order to analyze the combustion quality under the engine operating conditions, different topics such as evaluating the combustion procedure, the production and consumption of effective free radicals in the fuel oxidation process, and the influential parameters on the output power and the ISFC were examined. Furthermore, the CO and CO₂ emission levels were investigated. The results show: Fuel collision to piston bowl rim edge changes the fluid flow regime, and it transfers a portion of the high reactivity fuel to the space between the piston head and cylinder. It prevents the mixture from homogenizing, and it causes an increase in the UHC emission.

- The production and consumption procedure of hydroxyl radicals is one of the characteristics of the combustion start. The production of hydroxyl begins with the consumption of formaldehyde.
- With the addition of water to the entering fuel-air mixture, the reduction of fuel consumption is possible without a decrease of indicated power output.
- The effectiveness of water addition in the fuel-air mixture depends on the water to gasoline mole ratio. The species with a higher mole number has a dominant influence on the combustion process.
- Increasing the water mass fraction too much can increase the CO emission level, and reduce the combustion quality; because as water absorbs the released heat from the combustion reaction, it decelerates the combustion procedure.
- The addition of water up to the point that the number of water moles gets higher than the LRF moles, leads to higher in-cylinder pressures, which is due to the increase of water moles. This higher in-cylinder pressure as a result of the higher number of water moles causes the process and combustion product temperatures not to increase.

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**Persian Abstract****چکیده**

برای کاهش مصرف سوخت موتورهای احتراق داخلی و همچنین کاهش انتشار گازهای گلخانه‌ای، بررسی پارامترهای موثر بر توان، انتشار گازهای گلخانه‌ای و فزاینده‌ی احتراق حائز اهمیت است. در این مطالعه، تأثیر افزودن آب به موتور RCCI به صورت عددی بررسی شده است. برای این منظور آب با کسر جرمی متفاوت به مخلوط هوا و سوخت اضافه شد. به منظور شبیه‌سازی موتور از نرم افزار AVL Fire استفاده شد. نتایج نشان می‌دهد که جایگزینی بخشی از سوخت بنزین با آب، تا ۱۰ درصد، فشار محفظه احتراق را افزایش می‌دهد. در این شرایط تولید رادیکال‌های آزاد هیدروکسیل به عنوان یکی از ویژگی‌های شروع احتراق زودتر اتفاق می‌افتد. علاوه بر این، فشار متوسط موثر نشان داده شده (IMEP) بدون تغییر باقی می‌ماند. با افزایش بیشتر توده آب، تولید رادیکال هیدروکسیل کاهش می‌یابد و انتشار حرارت در دمای بالا به تأخیر می‌افتد. همچنین در مقایسه با زمانی که آب اضافه نشده است، دمای متوسط محفظه احتراق کاهش می‌یابد، در حالی که میزان تولید CO تغییر نمی‌کند. افزایش تعداد مول‌های آب، حداکثر فشارهای درون سیلندر را افزایش می‌دهد به طوری که در مقایسه با حالت بنزین خالص، با جایگزینی ۲۰ درصد از جرم بنزین با آب، میانگین فشار موثر نشان داده شده تقریباً ثابت می‌ماند.