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Investigation of the Effects of Diesel Injection Strategies in a Reactivity Controlled Diesel\iso-Butanol Compression Ignition Engine

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Due to very low PM and NOx emissions and considerable engine efficiency, dual-fuel combustion mode such as RCCI strategy attracted lots of attention compared to other combustion modes. In this numerical research work, the impacts of direct injection timing and pressure of diesel fuel on performance and level of engine-out emissions in a diesel-butanol RCCI engine was investigated. To simulate the combustion process, a reduced chemical kinetic mechanism, which consists of 349 reactions 76 species was used. The influence of thirty-six various strategies based on two diesel spraying characteristics such as injection pressure (650, 800, 1000, and 1200 bar) and diesel spray timing (300 to 340 CA with 5 CA steps) have been examined. Results indicated that, under the specific operating conditions like 1000-bar spray pressure by direct injection at 45 CA BTDC and the spray angle of 145 degrees, the level of cylinder-out pollutants such as CO (up to 26%), NOx (about 86%), PM (by nearly 71%) and HC (about 17.25%) have been simultaneously reduced. Also, ISFC decreased by about 2.3%, IP increased by about 2.4%, and also ITE improved by nearly 2% compared to the baseline engine operating conditions.

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1. Introduction

The increment of fuel prices, the reduction of non-renewable resources and the stricter environmental law in connection with the use of compression ignition engines due to the presence of harmful emissions such as PM and NOx, has led the researchers to improving performance simultaneous with emissions reduction in the diesel engines as the primary objective of their researches. For this reason, over the years many approaches such as using various kind of fuel [1-3] or fuel additives [4], and Exhaust Gas Recirculation (EGR) [5, 6] were applied. Furthermore, various combustion strategies such as Homogeneous Charge Compression Ignition (HCCI), Part Premixed Compression Ignition (PPCI), and Premixed Charged Compression Ignition (PCCI) proposed to reduce the amounts of engine-out emissions while the engine performance maintained [7-9].

Reactivity Controlled combustion has led to improve the engine performance level and decrease pollutant emissions simultaneously [10]. Reactivity Controlled Compression Ignition engines offer efficient fuel economy and lower harmful pollutants such as PM and NOx compared to other combustion strategies [11]. Several types of fuels like propanol, ethanol, n-pentanol, iso-butanol, methanol, and the gasoline applied for low reactivity energy source in the RCCI combustion in various experimental and numerical research works to explore the influence of fuels with disparate premixed ratios on cylinder-out pollutants and level of engine performance [12-16]. Zhu et al. [17] experimentally examined the impacts of gasoline-like low reactivity fuels on the characteristics of the combustion process in a RCCI engine. Researchers indicated that by advancing the injection timing, emissions such as PM and CO decreased, but NOx level developed. They observed that at constant injection timing and low reactivity fuel to diesel ratio, ethanol fuel has lower PM and NOx levels compared to gasoline. Other paper numerically explored the effects of diesel to low reactivity fuels ratios on the output emissions and level of performance in a RCCI engine [18]. Researchers found that by increasing the gasoline premixed ratio, homogeneity of combustion process increased, and regions with high temperature inside the combustion chamber decreased. They also indicated that by advancing diesel spray timing or increased in the level of biodiesel fuel, PM emission increased. Finally, they concluded that characteristics of low reactivity fuel like Cetane number and latent heat value have significant impacts on the formation and oxidation processes of pollutant emissions. Qian et al. [19] noted that applying oxygenated fuels as low reactivity fuel has considerable positive effects on pollutant emissions such as PM in reactivity controlled combustion engines. Nonetheless, researchers concluded that at low speed, low engine load operations, injection timing of direct spraying fuel control the combustion phase, and also emissions formation due to a direct relation between combustion characteristics and emissions oxidation and formation processes [20].

Combustion quality in compression ignition engines is significantly influenced by the quality of the air-fuel mixing process. The increase of fuel spray pressure is commonly used in compression ignition engines to improve the combustion quality of air-fuel mixture [21]. In their empirical research, Liu et al. [22]examined the impacts of direct fuel injection pressure on performance level and pollutant emissions of a dual fuel diesel-methanol compression ignition diesel engine. The researcher of this work have concluded that the increment of diesel injection pressure increased the peak of in-cylinder heat release rate point and mean pressure point in the dual fuel diesel-methanol operating conditions. They noted that as higher diesel injection pressure was applied for diesel-methanol dual-fuel engine operating mode, IMEP increased, and BSFC improved simultaneously. They also indicated that increasing diesel spraying pressure led to a reduction of both CO and HC simultaneously. However, NO2 and CO2 slightly increased. Krishnan et al. [23] conducted an empirical research on the effects of injection characteristics and boost pressure on dual fuel diesel-propane compression ignition engine. Their experimental results showed that increasing diesel spraying pressure from 200 to 1300 bar led to the decrement of the maximum in-cylinder pressure, and also, heat release rate peak point noticeably retarded. At the end of their researches, they mentioned that higher diesel spraying pressure led to the increment of both HC and CO pollutants. However, NOx level reduced.

Based on the reviewed papers above, the influences of spray timing and pressure of diesel fuel have been evaluated in many research papers and their positive and adverse impacts on the combustion process of compression ignition engines discussed by many researchers. According to the mentioned results, the combustion timing and the level of cylinder-out pollutants can be controlled by diesel direct spray timing. Besides, fuel spraying pressure has a high and significant impact on air-fuel mixing and the oxidation process. For this reason, this numerical paper focuses on studying the effects of high reactivity fuel (diesel) spray timing and pressure on the specifications of combustion process, engine-out harmful emissions, and performance in a single-cylinder diesel/iso-butanol RCCI engine.

2. Model setup

A commercial software called AVL Fire code was applied for simulating the combustion process of diesel/iso-octane and its tools also were used for the creating of the computational mesh grid [24]. Due to the symmetric geometry of the computational grid and the use of six-hole nozzle, all computations were conducted on sixty-degree segment. Fig. 1 displays the computational mesh.

Figure 2 shows the influence of average cell size on the in-cylinder mean pressure and heat release rate. As illustrated in this figure, by decreasing the cell size from 1.6 to 1.2 mm, maximum combustion pressure and heat release rate peak point negligibly decreased. However, reducing the average size of computational grid from 1.2 to 1.0 mm does not alter the parameters such as heat release rate and in-cylinder mean pressure. For this reason, for all the computation, average cell size was set to 1.2 mm since based on Fig. 2, the numerical achievements are independent of computational grid size. Some of the computational grid specifications are presented in Table 1.

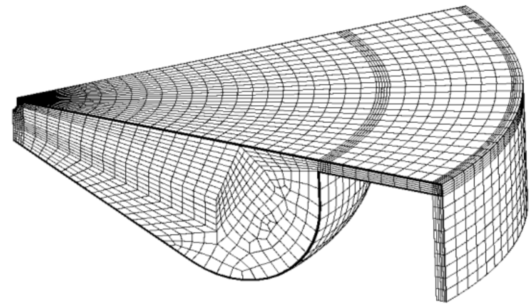

Figure 1: The computational mesh at 360 CA

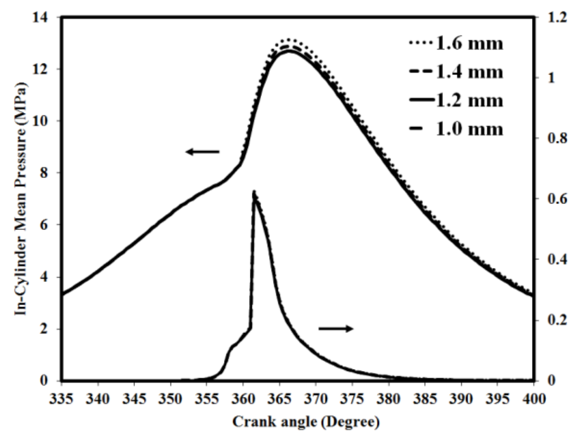

Figure 2: Effects of computational grid size on the in-cylinder mean pressure and heat release rate

Table 1: Specifications of computational mesh

Number of cells @ IVC event (-)	77650
Number of cells @ TDC point (-)	31300
Averaged cell size (mm)	1.2
Number of boundary layers (-)	2
The thickness of the boundary layer (mm)	0.2

The method of detailed kinetic chemistry was applied for dual-fuel diesel/iso-butanol combustion process simulation. For this reason, a mechanism capable of modelling the rates of formation and oxidation of n-heptane, n-butanol, and PAH, developed by [25], was used. The mentioned chemical kinetic mechanism consists of 349 reactions 76 species. Also, the multi-zone

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chemistry solver was used in order to reduce the total calculations time by considering the cells with similar thermochemical characteristics into a single zone [26]. For simulating the break-up process of fuel injected parcels, the Kelvin-Helmholtz and Riley-Taylor models were employed which described in Nordin and Niklar work [27] in detail. Besides, to take parcel-wall interactions into account, Naber and Reitz model was used [28]. This model assumes that the behavior (rebound or reflection) of the injected parcels with the wall is based on the Weber number. The evaporation and heat-up of the injected fuel parcels were calculated by applying Dukowicz model [29]. Finally, to simulate the turbulence flow inside the engine cylinder, the k-zeta-f model was employed [30].

3. Model verification

A direct injection RCCI engine was used for this numerical study [31]. Table 2 shows the engine and fuel injection system specifications.

Table 2: Fuel injection system and engine specifications [31]

Type of engine aspiration	Turbocharger
Bore (mm)	137.2
Stroke (mm)	165.1
Length of connecting rod (mm)	261.6
Compression ratio (-)	16.1:1
Piston bowl volume (L)	0.11
IVC (CA)	217
EVO (CA)	490
Fuel injection system	Common rail direct injection
Injection pressure (bar)	800
Number of injection holes	6
Injection hole diameter (mm)	0.25

The results of the in-cylinder mean pressure and rate of heat release of this numerical research and Wang et al. [32] experimental work are compared in Fig. 3. As illustrated in Fig. 3, obtained results for predicting the in-cylinder trends are reasonably close to experimental results. However, some differences could be due to uncertainties of some parameters such as precise injection duration, the in-cylinder temperature at the start of calculations, and the start of the injection of diesel and port fuel. It must be mentioned that the numerical achievements of the simulation of baseline engine operating conditions and other calculations which will be discussed in detail in the next section, all are based on the in-cylinder uniform air flow swirl ratio of 0.7, piston top surface temperature of 520 K, cylinder walls temperature of 420 K, and cylinder head temperature of 520 K.

Results achieved from pollutant emissions formation for both numerical and experimental researches of baseline operating conditions are compared in Table 3 [32]. Based on compared results in Table 3, pollutant emissions formation is reasonably simulated by CFD Fire code compared with experimental results.

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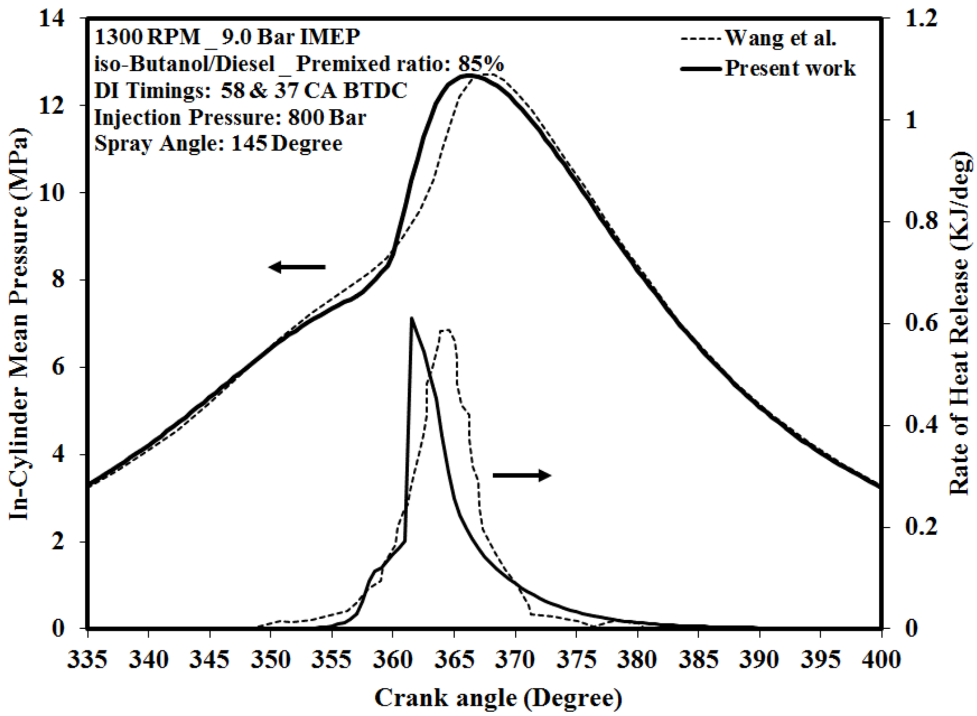

Figure 3: Comparison of numerical and experimental results of in-cylinder rate of heat release and mean pressure for baseline operating conditions [32]

Table 3: Comparison of numerical and experimental results of pollutants for the baseline operating conditions [32]

Pollutants (g/kg. fuel)	NOx	CO	HC	PM
Numerical	0.02	75.9	16.2	0.008
Experimental	0.015	79	17.3	0.01

4. Modelling methodology

Based on the success achieved in verifying the baseline operating conditions with the experimental [32] research results in the previous section, this study aims to evaluate the influences of diesel spraying characteristics on the diesel/iso-butanol combustion process of heavy-duty RCCI engine. Direct injection timing and pressure of diesel fuel are the two variables that change their amounts and explore their effects, is the primary purpose of this numerical study. For this reason, the EGR rate, diesel/butanol ratio, total fuel per cycle, and pressure and temperature of intake air at IVC were constant during all calculations. Totally, in addition to baseline operating mode, 36 study cases based on two diesel injection characteristics such as, spray timing (300 to 340 CA with 5 CA step), and pressure of diesel fuel (650, 800, 1000, and 1200 bar) have been considered and their impacts on the dual-fuel burning specifications (maximum combustion pressure, maximum combustion temperature, and heat release rate peak point), pollutants formation (CO, PM, HC, and NOx) and performance parameters (ISFC, IP, and ITE) were studied. The numerical achievements of this research are gathered in three parts: characteristics of dual-fuel combustion process, engine-out pollutants, and performance parameters, which are analyzed in detail in different sections.

It should be made clear that, in the baseline operating case, diesel fuel is sprayed in two stages, but the goal of this paper is to investigate

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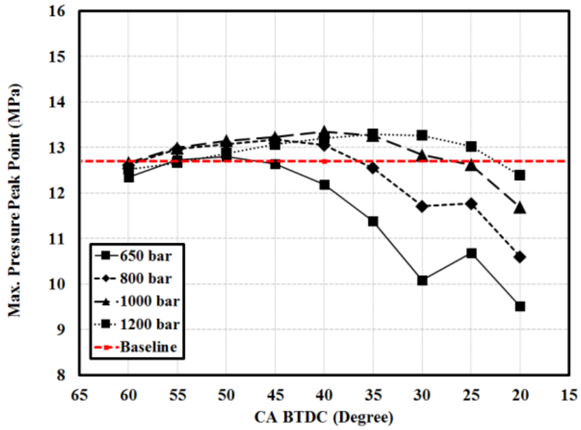
the impacts of single direct injection of diesel fuel on the functional parameters of the engine.



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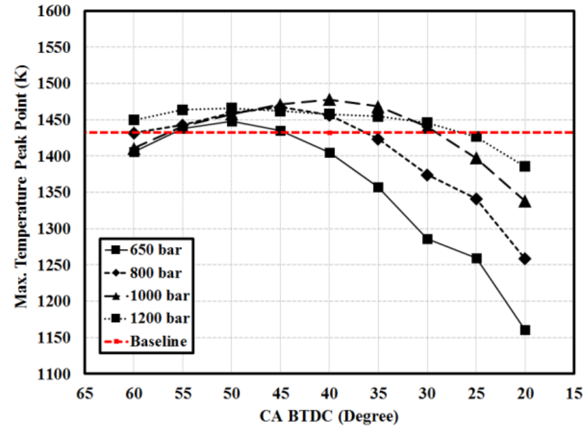

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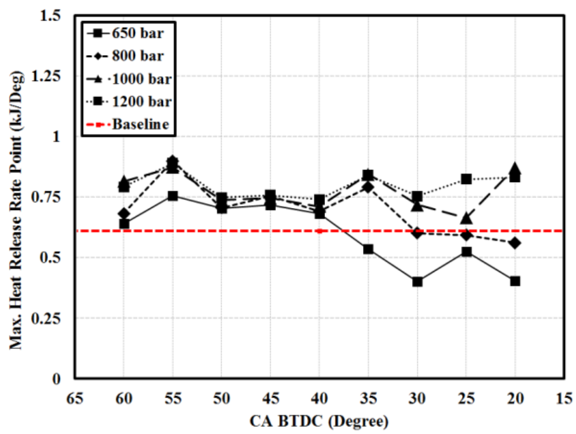

(c)

Figure 4: Effects of study strategies on combustion characteristics

5. Numerical achievements

5.1. Dual-fuel combustion characteristics

Figs. 4(a) and 4(b) reported the impacts of diesel spray timing and pressure on maximum combustion pressure and temperature, respectively.

In compression ignition DI diesel engines, combustion includes two separate stages: the periods of ignition delay and heat release. At the beginning of the combustion, ignition delay takes place and then, the heat release period occurs. From start of fuel spray to start of the burning process is the period of ignition delay. Specifications such as fuel characteristics, pressure inside combustion chamber, and temperature have significant impacts on ignition delay period. Premixed and diffusive combustion are the two burning modes which occur in heat release period. At the beginning of the heat release period, pre-mixed combustion occurs which just air-fuel mixing process happens. After that diffusive combustion will take place and carry on till the end of the burning process. As

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illustrated in Fig. 4(a) and 4(b), by postponing diesel injection timing from 300 to 340 CA, the maximum combustion pressure and temperature first increased and then decreased. For early injection timings due to low in-cylinder pressure and temperature, evaporated fuel accumulated at a low rate, and most portion of air-fuel mixture burns in premixed stage. Because of compression movement of the piston during the compression phase, the pressure and temperature of combustion chamber increased and by spraying fuel with the intermediate timing due to favorable conditions such as in-cylinder pressure and temperature, evaporated air-fuel mixture accumulated with a higher rate and as a result, more evaporated mixture accumulated during the period of ignition delay. Therefore, more evaporated mixture burns in premixed mode and maximum combustion pressure and temperature increased compared to early injection timings for every injection pressure. For late spray timings because of high combustion chamber pressure and temperature, the period of ignition delay is short, and less portion of evaporated mixture could be accumulated, and most portion of the air-fuel mixture burns in diffusive mode. Diffusive combustion led to low pressure and temperature rise rate, and compared with early and intermediate injection timings, maximum combustion pressure and temperature considerably decreased.

Direct diesel fuel spray pressure is the critical characteristic which has a considerable influence on the atomization of fuel droplets and mixing process, and hence, determines the amount of cylinder-out pollutants and engine performance. As displayed in Figs. 4(a) and 4(b), for early spray timings, increasing the pressure of diesel injection has an insignificant influence on maximum combustion pressure and temperature. Due to low temperature and pressure of combustion chamber for early spray timings, increasing injection pressure has little effect on combustion characteristics such as combustion duration because of the long ignition delay period. More extended ID leads to longer combustion duration, and as a result, pressure and temperature rise rates are low. However, for intermediate and late injection timings increasing injection pressure has considerable effects on maximum combustion pressure and temperature. Increasing injection pressure with suitable conditions such as in-cylinder temperature and pressure leads to an increase in temperature and pressure rise rate, and thus, combustion duration could be shortened. In addition, increasing injection pressure leads to improve evaporation process due to smaller droplets that sprayed during the injection. Smaller particles lead to the more rapid mixing process, and following that, the rate of pressure and temperature rise of combustion are high.

Fig. 4(c) shows the effects of diesel spray timing and pressure on heat release rate peak point. As illustrated in Fig. 4(c), for spray pressure of 650 bar, by retarding the spray timing, HRRPP decreased. Low injection pressure leads to longer combustion duration as result of lean air-fuel mixing process and also retarding the injection timing accompanied by more evaporated fuel, which burns in diffusive mode. For this reason, as displayed in Fig. 4, postponing the injection timing simultaneous with low injection pressure led to decrease in the maximum combustion pressure, temperature and HRRPP. As indicated in Fig. 3, for spray pressure of 800, 1000, and 1200 bar, varying injection timing has an insignificant effect on HRRPP. However, increment of spraying pressure resulted in higher HRRPP since the mixing process enhanced and combustion duration became shorter compared to baseline operating conditions.

5.2. Engine-out pollutants

Fig. 5 shows the effect of diesel spray timing and pressure on NOx and PM pollutants, respectively.

As indicated in Fig. 5(a), by postponing the spray timing, the level of NOx first reduced, then increased and again reduced for spray pressures of 650 and 800 bar injection pressure. As indicated earlier, for early injection timings because of low in-cylinder temperature and pressure, the ID period is more extended, and more evaporated air-fuel mixture can be accumulated, and then NOx emissions have increased. As indicated in Fig. 5(a), for intermediate injection timings NOx emissions considerably have increased. Because of the

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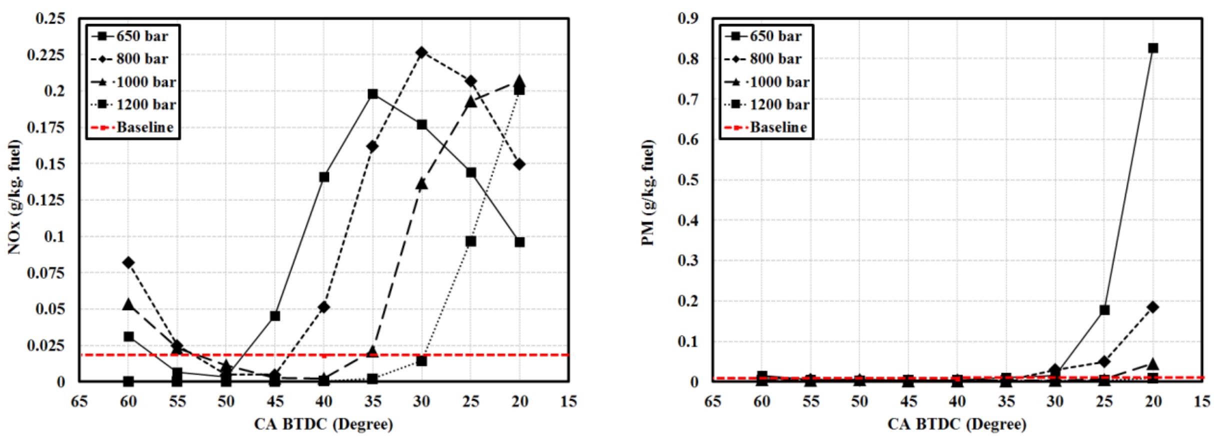
compression movement of the piston, in-cylinder temperature and pressure increased, and due to favorable conditions like pressure and temperature, more evaporated fuel accumulated with a higher rate, which led to higher NOx emissions compared with early injection timings. By late injection timing, for 650 and 800 bar injection pressure, NOx emission has decreased. Late injection timing leads to shorter ID period and diffusive combustion, and as a result due to less accumulated evaporated fuel, NOx emissions have decreased. However, as illustrated in Fig. 5(a), for 1000 and 1200 bar injection pressure, late injection timings led to high NOx compared to 650 and 800 bar fuel spraying pressure. Increasing injection pressure leads to a more rapid mixing process and shorter burning duration that accompanied by higher pressure and temperature rise rate that could increase the NOx emissions for late injection timings. However, for early and intermediate injection timings, increasing injection pressure because of shorter ID period led to lower NOx emissions.



(a) (b)

Figure 5: Effects of study strategies on (a) NOx and (b) PM pollutants

Fig. 5(b) indicates the impacts of spray timing and pressure on PM emission. As illustrated in Fig. 5(b), by retarding the spray timing from 300 to 340 CA, PM level increased. As indicated earlier by late injection timing, less portion of evaporated mixture accumulated during the ignition delay period, and most portion of the air-fuel mixture burns in diffusive burning mode. Diffusive combustion leads to low temperature and pressure rise rate, and therefore, the mixing process can be deteriorated, and PM can be increased. As reported in Fig. 5(b), increasing spray pressure led to a considerable reduction of PM emission. Increasing the pressure of diesel spray led to an improvement of the vaporization of fuel sprayed droplets and air-fuel mixing process. Improvement of the fuel vaporization process led to high pressure and temperature rise rate and as a result, higher flame temperature. This leads to a higher burning rate and reduces the time for more PAH growth.

Figs. 6(a) and 6(b) shows the influence of spray timing and pressure on CO and HC pollutants, respectively.

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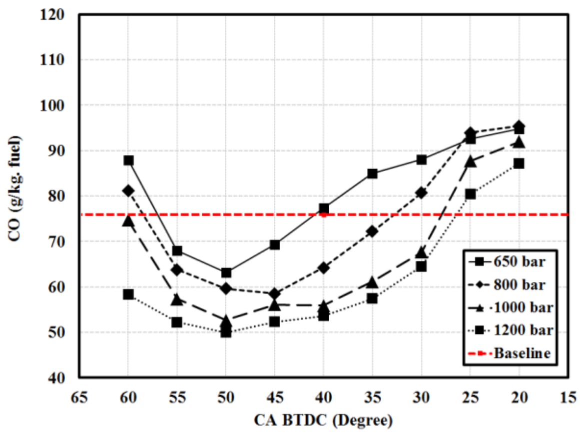

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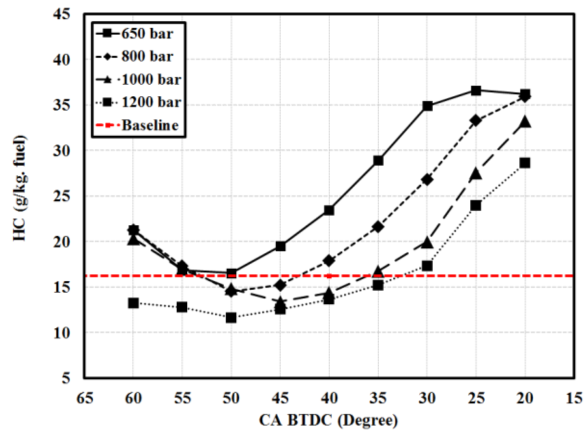

(b)

Figure 6: Effects of study strategies on CO and HC emissions

As indicated in Figs. 6(a) and 6(b), the observed trends for CO and HC are the same. By postponing the spray timing, the amount of CO and HC first decreased and then increased. For early injection timing because of low in-cylinder pressure and temperature, the rate of evaporated air-fuel mixture accumulation is low and less fuel accumulated during the ID period. Lower accumulation rate during ID period led to lower pressure and temperature rise rate and also lower maximum combustion pressure and temperature. The reduction of pressure and temperature of combustion follows by deteriorated mixing process that led to higher CO and HC pollutants. For intermediate injection timings because of suitable conditions such as in-cylinder temperature and pressure rate of evaporated fuel accumulation is high and as a result pressure and temperature rise rate of combustion is higher compared with early injection timings. The higher rate of in-cylinder temperature and pressure change leads to the improved mixing process that results in lower CO and HC pollutants. Also, late spray timing led to diffusive combustion that could weaken the combustion process, and as a result, higher CO and HC have emitted. As illustrated in Figs. 6(a) and 6(b), Increasing the diesel spraying pressure due to an improvement of fuel droplets vaporization and better mixing with air inside the engine cylinder could decrease the CO and HC emissions, simultaneously. Also, increasing the fuel spraying pressure could decrease the length of spray penetration that could wet the cylinder wall and or trapped in an existing gap inside the combustion chamber, which leads to more HC emissions.

5.3. Performance parameters

Figs. 7(a), 7(b), and 7(c) shows the effect of spray timing and pressure on IP, ISFC, and ITE, respectively.

As indicated in Figs. 7(a), 7(b), and 7(c), engine performance first improved then weakened. For early injection timings because of low pressure and temperature of combustion chamber, the rate of evaporated fuel accumulation is lower than intermediate injection timings, which result in less premixed combustion compared to intermediate injection timings. Premixed burnings leads to higher pressure and temperature rise rate, which accompanied by higher maximum combustion pressure and temperature. The increase in temperature and pressure of combustion leads to improving engine performance. However, late injection timings lead to more diffusive combustion. Diffusive combustion accompanied by lower pressure and temperature rise rate compared to premixed combustion, which results in higher ISFC and lowers IP and ITE.

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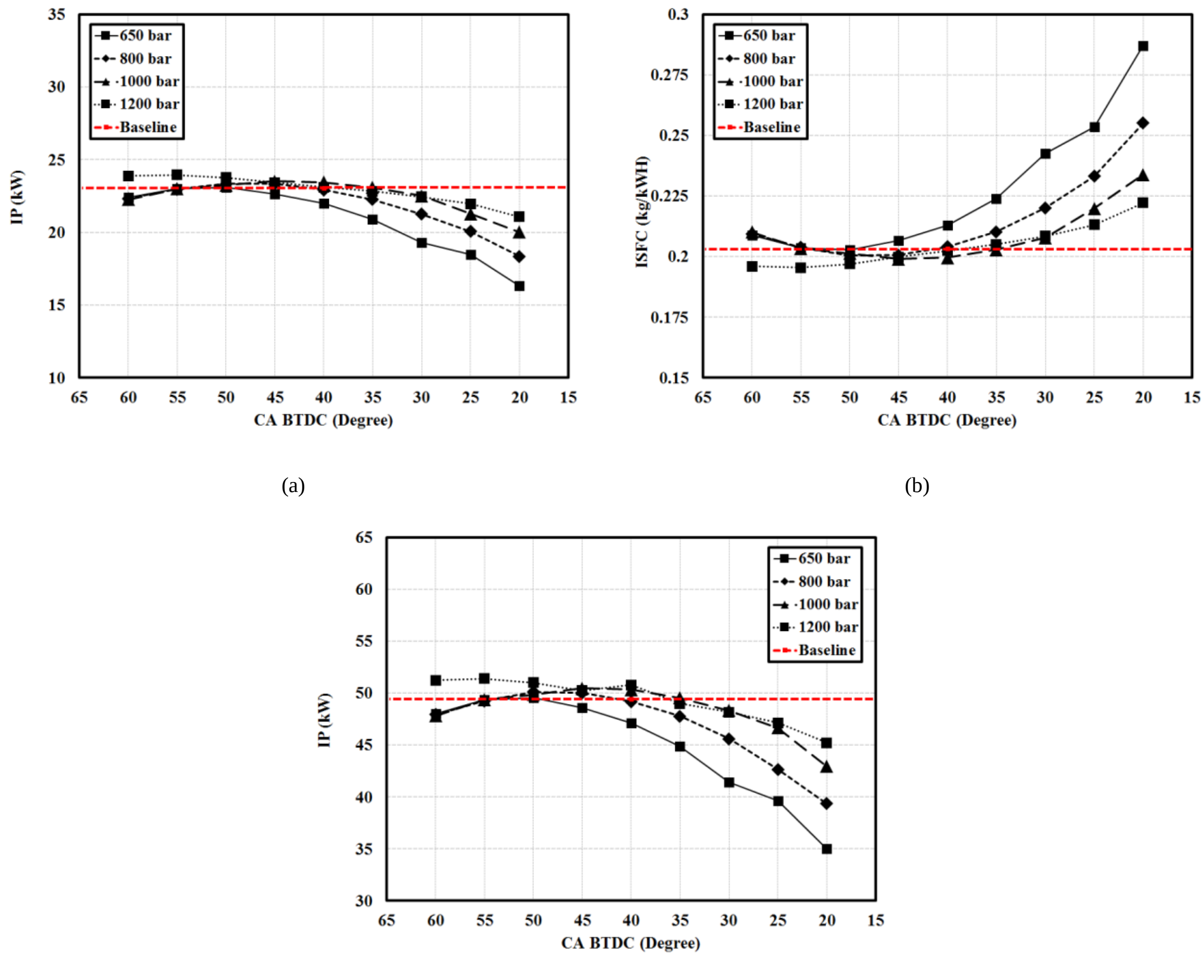

(a) (b)

(c)

Figure 7: Effects of study strategies on engine performance

Based on the results of 36 studied cases, it was observed that spraying fuel under 1000 bar injection pressure at 315 CA as spray timing, engine performance improved and amounts of output emissions reduced simultaneously. For this reason, this fuel spraying method was chosen as an optimum strategy. Table 6 compared the results of the baseline operation case and the optimum case of this research. As reported in Table 4, amounts of engine-out emissions such as CO (26%), HC (17.25%), NOx (86%), and PM (71%) reduced. In terms of performance and efficiency, IP (2.4%), ITE (2%), and ISFC (2.3%) enhanced compared to the baseline case.

Table 4. Comparison of baseline operating conditions and optimal mode of this numerical research

Case study	Baseline	Optimal mode

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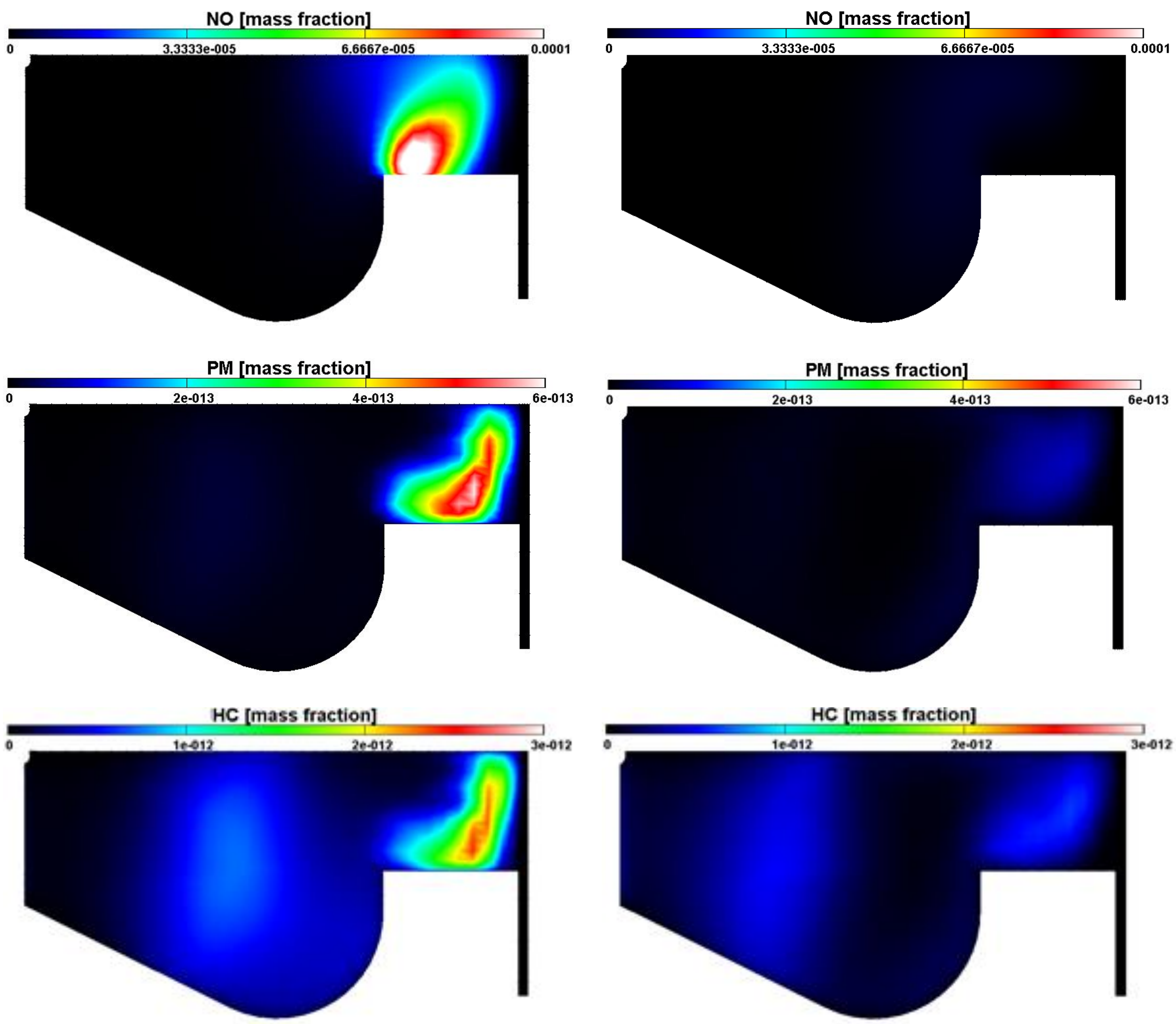
NOx [g/kg. fuel]	0.02	0.0023
PM [g/kg. fuel]	0.008	0.0025
CO [g/kg. fuel]	75.9	56.1
HC [g/kg. fuel]	16.2	13.42
ISFC [kg/kWh]	0.2032	0.1984
IP [kW]	23.04	23.6
ITE	49.42%	50.47%

Fig. 8 presents the emissions contours (NO, PM, CO, and HC) for baseline operating conditions and optimum case. As illustrated in Fig. 8, by injecting diesel fuel at 315 CA under 1000 bar spraying pressure, the amounts of pollutants considerably reduced, and the level of engine performance slightly enhanced compared to baseline operating conditions.



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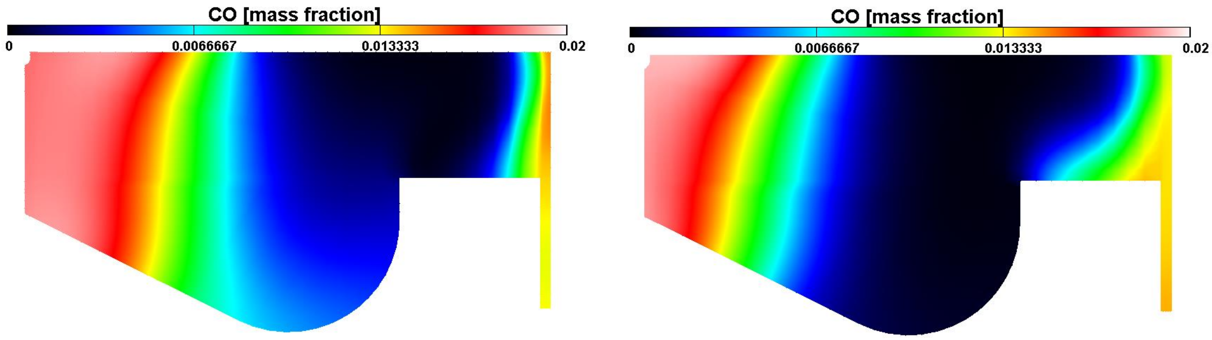

Baseline

Optimal mode

Figure 8: The impacts of single spray timing and pressure on pollutants at 390 CA

6. Conclusion

In this numerical research, the influence of diesel spray timing and pressure on the cylinder-out pollutants and performance in a single-cylinder diesel/iso-butanol RCCI engine were explored. The numerical achievements indicated that for late injection timings, the maximum combustion pressure and temperature decreased, the emissions level such as PM, CO, and HC increased, and also, because of lean air-fuel oxidation, engine performance has weakened. By using early injection timings compared to intermediate ITs, due to more extended ID period and lower evaporated fuel accumulation rate, emissions such as HC, CO, NOx, and PM have increased simultaneously, and moreover, the level of engine performance has decreased compared to intermediate ITs. Also, increasing injection pressure coupled with intermediate ITs (e.g., 315 CA) could decrease the ID period and increase the fuel evaporated accumulation rate that accompanied by lower emissions formation and improved engine performance.

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Abbreviations

BDC	Bottom Dead Center
BSFC	Brake Specific Fuel Consumption
BTDC	Before Top Dead Center
CA	Crank Angle
CFD	Computational Fluid Dynamic
CO	Carbon Monoxide
DI	Direct Injection
EVO	Exhaust Valve Opening
HRRPP	Heat Release Rate Peak Point
ICE	Internal Combustion Engine
ID	Ignition Delay
IMEP	Indicated Mean Effective Pressure
IP	Indicated Power
ISFC	Indicated Specific Fuel Consumption
IT	Injection Timing
IVC	Intake Valve Closing
NOx	Nitrogen Oxides
PAH	Polycyclic Aromatic Hydrocarbon

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PM	Particle Matter
TDC	Top Dead Center
HC	Hydro-Carbons

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