

e-ISSN:2757-9077

ENGINEERING PERSPECTIVE

https://sciperspective.com

Research Paper

Multi-Dimensional 3D-CFD/Chemical-Kinetics Modeling of Natural Gas–Diesel RCCI Engines: Combustion Phasing, Efficiency and Emissions

Kamran Poorghasemi[1*], R. Khoshbakhti Saray[2], Hamit Solmaz[3*], Seyed Mohammad Mousavi[4], Alborz Zehni[2]

[1] *Mechanical Engineering Department, Shab.C., Islamic Azad University, Shabestar, Iran.*
[2] *Mechanical Engineering Department, Sahand University of Technology, Tabriz, 51335-1996, Iran*
[3] *Automotive Engineering Department, Faculty of Technology, Gazi University, Ankara, 06500, Türkiye*
[4] *Department of Mechanical Engineering, University of Bath, Claverton Down, Bath, BA2 7AY, United Kingdom*

ABSTRACT

Nowadays, low temperature combustion is a promising concept to implement in conventional internal combustion engines, as it provides lower emissions and higher thermal efficiency. In the current work, the combustion process of an NG/diesel Reactivity Controlled Combustion Ignition (RCCI) engine was investigated using a coupled 3D-CFD/chemical kinetics framework. The reduced chemical kinetics mechanism containing 57 species and 190 reactions was utilized to simulate the combustion of blended fuels. The results show that increasing premixed ratio (PR) (from 75% to 97%), while keeping constant the total input energy in RCCI engine, delays start of combustion (SOC) and CA50 and causes extended burning duration of diesel. In addition, the duration of methane combustion reduces in lower PRs in comparison with higher PRs. When dealing with injection timing, advancing the diesel injection (SOI) until specific value advances the SOC, but afterward retards the SOC. In fact, burning duration for early injection of diesel increases (from 4.2 crank angle degree to 7.4 crank angle degree) while burning duration of methane decreases (from 10.3 crank angle degree to 5.2 crank angle degree). By further advancing SOI timing, combustion efficiency decreases (from 87.5% to 82.8%) while gross indicated efficiency increases (from 40% to 43%). However, HC and CO emissions increase by earlier SOI timing while NOx emissions decrease.

Keywords: 3D-CFD; Chemical Kinetics Mechanism; Combustion Phasing; Natural Gas; Premixed Ratio; RCCI Engine

History
Received: 13.10.2025
Revised : 17.11.2025
Accepted: 11.12.2025

Author Contacts:: Kamran.poorghasemi@iau.ac.ir , khoshbakhti@sut.ac.ir, hsolmaz@gazi.edu.tr, Sm4096@bath.ac.uk, alborz.zehni@gmail.com

Cite this paper: Poorghasemi, K., Saray, R. K., Solmaz, H., Mousavi, S. M., Zehni, A. (2026). Multi-Dimensional 3D-CFD/Chemical-Kinetics Modeling of Natural Gas–Diesel RCCI Engines: Combustion Phasing, Efficiency and Emissions. Engineering Perspective, 6 (1), 69-82. http://dx.doi.org/10.64808/engineeringperspective.1802746

*Corresponding Authors

1. Introduction

Conventional internal combustion (IC) engines including compression ignition (CI) and spark ignition (SI) engines play a significant role in different applications such as transportation and industrial stationary power generation units. CI engines are more attractive duel to the higher thermal efficiency, torque, and power. However, the problem associated with CI engines are the high emission level of nitrogen oxides (NOx) and particulate matter (PM). Consequently, recent research studies have been carried out on the developing of new technologies to improve CI engines' performance and emissions characteristics [1-3]. Recently, low temperature combustion (LTC) concept achieved more attention to replace conventional CI engines by utilizing lean premixed mixture [4,5]. Reactivity controlled compression ignition (RCCI) engine is considered as a popular LTC engine, which has a great potential to improve combustion, performance and emission characteristics. Employing RCCI strategy leads to three main benefits, namely; higher gross indicated efficiency, enhancement of efficiency related to fuel conversion because of decreased heat losses and very low soot and NOx emissions as a result of lean and low temperature combustion [2]. Conversely, the amount of carbon monoxide (CO)

and hydrocarbons (HC) emissions is high enough mainly owing to the presence of low temperature zones near the walls and crevice volumes [3].

Inagaki et al. [6] and Bessonette et al. [7] represented the benefits of dual fuel engines in comparison with diesel engines, but they introduced the high-pressure rise rate as a challenging problem in dual fuel engines. Reitz et al. [8-10], in their research on a Caterpillar single-cylinder engine, found out that the high pressure rise rates could be avoided by using optimized injections [11]. Therefore, they presented a gasoline/diesel in-cylinder fuel blending plan by which emissions were reduced under emission standards levels and net cycle efficiency was over 50% from lower IMEP 4 bar to higher IMEP 14 bar. Kokjohn et al. [12] showed that, by means of the optimized reactivity gradients established in the combustion chamber, the maximum pressure rise rate could be controlled effectively better than the single fuel premixed combustion. Conversely, achievement of engine operating over 14.5 bar IMEP was very challenging for the reason that maximum pressure rise rate increases dramatically and higher level of exhaust gas recirculation (EGR) is required.

RCCI engines use two fuels with different relativities, and a low reactivity fuel (high octane number) like gasoline or natural gas, which introduced in a fully premixed condition supplies the main parts of energy. The second fuel with high reactivity (low octane number) like diesel is injected directly inside the cylinder during compression stroke to provide the proper reactivity stratification. Recently, many research studies on various fuel pairs for RCCI engines have been carried out [13-18], but natural gas/diesel RCCI engines need more studies. Natural gas is a suitable fuel for RCCI engines, given the fact that it has low carbon to hydrogen ratio and consequently low greenhouse gas emissions. Higher reactivity gradient inside the combustion chamber extends the burning duration, and thus reduces the peak pressure rise rate at high-loads [19].

Neiman et al. [19] have worked on the optimization of RCCI engine factors such as mass fraction of fuels, diesel injection timing, diesel fuel quantity in each injection pulses, diesel injection pressure, and ratio of EGR. They used KIVA-3V CFD code coupled with CHEMKIN chemistry and genetic algorithm (NSGA II). The results illustrated the advantageous of double injection strategy of diesel fuel for RCCI engine to achieve high efficiency and low emission levels from low load (4 bar IMEP) to high load (23 bar IMEP) conditions. Doosje et al. [20] investigated RCCI combustion using natural gas and diesel fuel by using a 6-cylinder engine. The engine was capable to satisfy Euro IV soot and NOx emissions standard between 2 and 9 bar IMEP without EGR, but HC emissions was high enough. Walker et al. [21] made a comparison between NG/diesel and gasoline/diesel RCCI combustion with single diesel injection strategy. They found out that methane/diesel RCCI has better capability to increase the load range in comparison with the gasoline/diesel RCCI without using EGR. Zoldak et al. [22] studied an RCCI engine fuelled with NG and diesel to investigate engine emissions, fuel consumption, peak cylinder pressure, and cylinder pressure rise rate by KIVA-CHEMKIN code. The results indicated that an RCCI combustion strategy has a great capability to moderate NOx and soot emissions simultaneously, and decreases fuel consumption compared to a conventional diesel combustion mode at the same air-fuel ratio (AFR) and EGR rate. In addition, they studied the effect of natural gas direct injection method in an RCCI engine, and expressed that the direct injection natural gas strategy provides fuel stratification in combustion chamber and reduces the premixing level. Therefore, the mentioned strategy controls the pressure rise rate, and allows higher operating load range [23]. Min et al. [24] studied the effects of pre-injection factors on combustion of a pilot diesel/NG engine with a modified six-cylinder turbocharged diesel engine. They showed that early pre-injection of compression stroke can be a beneficial way to moderate in-cylinder pressure and heat release rate, and decrease NOx emissions, but late pre-injection timing caused strong combustion with increased NOx emissions. Moreover, high pre-injection quantity causes unstable ignition and combustion. Increasing fuel injection pressure causes higher cylinder pressure, HRR, and NOx production but lower HC emissions. Dahodwala et al. [25] considered diesel and natural gas combustion process in a RCCI combustion by an experimental approach. It was deduced that RCCI combustion with higher NG proportion at partial loads emits lower emissions. They also [26] studied the effect of diesel injection timing and injection duration on combustion phasing of a single cylinder engine using diesel and natural gas fuels. Furthermore, they examined the role of compression ratios at varied loads and speeds. They showed that decreasing the compression ratio retards CA50 and keeps unburned hydrocarbon emissions at standard level. Peykani et al. [27] studied the impact of diesel injection strategies on the combustion of RCCI engine fuelled with natural gas and diesel. They showed that the SOI1 timing, the SOI2 and the diesel fuel injection fuel mass fractions are the main effective elements that affect RCCI engine combustion. In addition, advanced first and second injection timing as well as increasing diesel fuel mass fraction in SOI1 timing are necessary for moderated NOx and soot emissions. Mousavi et al. [28,29] studied the combustion and emission characteristics of NG/diesel dual-fuel engines at part loads, and they investigated the impacts of single and split injection timing on the combustion process. They represented that due to the lean methane/air mixture at low loads, advancing the diesel injection timing provides better diesel/methane/air mixing due to the additional time, which in turn can be streamlined into having a richer and more reactive total mixture. Accordingly, the strong combustion promotes engine performance and decrease CO and UC emissions significantly. In fact, advanced SOI not only can be a useful strategy for extending engine's upper load range, but also it extends lower load range.

In spite of the numerous research works on RCCI combustion, many unclear features of RCCI need to be studied more comprehensively. Appropriate operation of RCCI engines requires a detailed understanding of the interactions between fluid flows, turbulent mixing and chemical kinetics. Combustion process of NG/diesel RCCI is complex, given the fact that two low and high reactivity fuels interact with each other. Combustion phasing is mainly controlled by the relative ratios of two fuels and the combustion duration is affected by the local equivalence ratio stratification between the two fuels. Among all effective parameters, diesel injection timing and natural gas premixed ratio are the most important factors to control the RCCI combustion. The present work is an attempt to study the effects of premixed ratio (PR) of methane and SOI of diesel on combustion phasing of RCCI through 3D-CFD

modelling combined with reduced chemical kinetics. In this way, combustion phasing of each fuel was investigated separately to find out the effects of diesel and methane combustion as well as their interaction on RCCI combustion. To the best of the authors' knowledge there is no comprehensive simulation study to investigate the effects RCCI combustion phasing. The results of this study reveal the optimum premixed ratio and fuel injection timing of RCCI combustion.

2. Model Description

In order to perform a proper simulation of RCCI combustion process, selection of chemical kinetics mechanism and spray model are important. In the current research, a reduced CH_4 mechanism [30,31] was utilized. In addition, the reduced NO mechanism [32] consists of 4 additional species and 12 reactions, was considered. For diesel fuel oxidation, the optimized Valeri mechanism [33] including 23 species and 139 reactions was applied. Therefore, the overall mechanism RCCI combustion modelling has 57 species and 190 reactions.

To ensure accuracy and stability in the CFD model, the simulation employs both temporal and spatial discretization techniques suitable for reactive flow modelling. The time discretization is managed with a constant time-step size aligned with the Courant-Friedrichs-Lewy (CFL) number, ensuring numerical stability throughout the combustion simulation. The CFL number governs the relationship between time step size, spatial grid size, and flow velocity, playing a crucial role in maintaining a stable and converged solution during high-speed flow changes associated with combustion events. Spatial discretization is achieved using the finite-volume approach integrated with the Arbitrary Lagrangian-Eulerian (ALE) method to solve 3D conservation equations. The ALE approach is particularly beneficial for modelling the complex dynamics in the cylinder because it allows control over mesh motion, which helps accommodate large deformations during the compression and expansion strokes [34]. By balancing the CFL number with optimized time-step intervals and the finite-volume approach, the model provides accurate representations of fuel-air mixing, and heat release profiles.

The gas phase kinetics of CHEMKIN-II [35] was coupled with KIVA-3V code in order to calculate chemical species production rate in the mechanism. To be precise, the chemistry subroutine of the KIVA-3V code adapted with DVODE chemistry solver [35]. For each cell, KIVA-3V calculates thermodynamic information such as mass fraction of species, temperature and pressure at each time step and then transfer them to CHEMKIN sub-model. Then CHEMKIN sub-model arranges a group of ODEs system, which is solved by DVODE solver [36]. RNG k-ε model was utilized as a turbulence model [37], Kelvin-Helmholtz Jet stability model was used to simulate atomization and breakup of fuel spray [38], and Han and Reitz model was used as wall heat transfer model [37].

3. Experimental Setup and Engine Specifications

3.1 Engine setup

In this research, all engine tests were carried out in the engine laboratory of University of Alberta [39]. A single cylinder Waukesha CFR engine has been improved to involve a direct injection system for diesel like fuel injection, external EGR and heated intake, and a port fuel injector for natural gas. The engine setup was described in previous studies [40,41] and was presented in Table 1. n-heptane as representative of diesel fuel was injected directly into the cylinder during compression stroke. In addition, natural gas (NG) was introduced to intake air using an injector located upstream of the intake valve. Injection specification is shown in Table 2. EGR is calculated by Eq. (1) as below [39]:

$$EGR = 100x\frac{CO_{2\ ;up}}{CO_{2\ ;\ down}} \quad (1)$$

Table 1. Engine specifications

Parameter	Specification
Engine	Waukesha CFR
Engine type	Water cooled, single cylinder
Combustion chamber	Disk cylinder head, flat- top piston
Throttle	Fully open- Turbocharged
Bore	82.55 mm
Compression ratio	16.9:1
Stroke	114.3 mm
Displacement	612 cc
IVC	146 CAD BTDC
EVO	140 CAD ATDC

Table 2. Diesel injection specifications

Parameter	Specification
Injector type	FSI- GDI
Spray type	Hollow cone
Spray angle	70 degrees
Injection pressure	68.5 bar
Number of nozzles	1

The experimental setup scheme is shown in Figure 1. A pressure transducer (Kistler 6043) was utilized to measure the in-cylinder pressure with 0.1 CAD resolution. In order to avoid cyclic variations errors, the in-cylinder pressure traces measurement were done and averaged over 100 consecutive cycles [42]. Table 3 shows operating conditions for all cases of engine.

In this study, combustion efficiency is calculated as follow [43]:

$$\eta_c = \frac{\int_{-180}^{+180} HRR}{m_{diesel}xLHV_{diesel} + m_{methane}xLHV_{methane}}x100 \quad (2)$$

Where $\sum HRR$ is integrated heat release rate and Lower Heating Value (LHV) for methane and diesel are 50 MJ/kg and 42.3 MJ/kg, respectively [19,38].

PR is the ratio of energy provided by methane to the total energy of combined methane and diesel fuels:

$$PR = \frac{m_{methane}xLHV_{methane}}{m_{diesel}xLHV_{diesel} + m_{methane}xLHV_{methane}}x100 \quad (3)$$

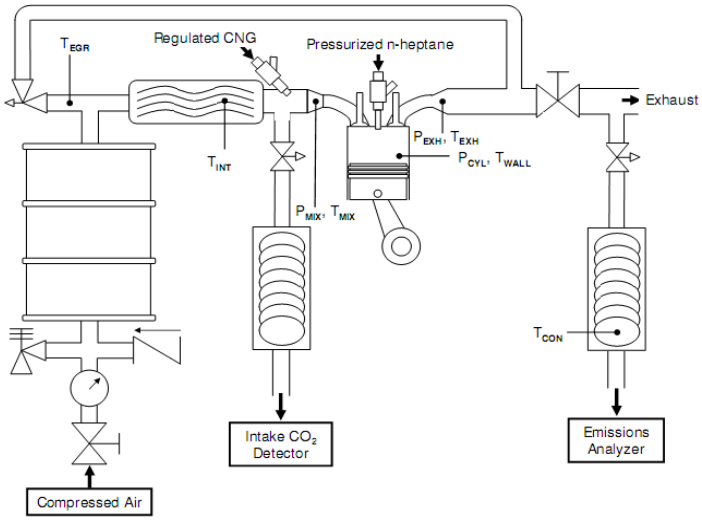


Figure 1. Test setup of the CFR engine [38]

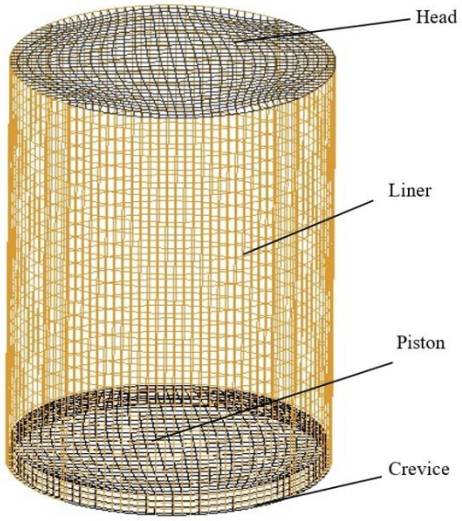


Figure 2. Computational mesh region of the cylinder at BDC

Table 3. Operating conditions of natural gas-diesel RCCI engine

Case	1	2	3
Equivalence ratio (Φ)	0.54	0.37	0.54
NG mass rate (mg/s)	94.4	87.7	94.4
Air mass rate (g/s)	2.9	4.0	2.9
n-heptane mass rate (mg/s)	2.2	4.8	2.2
SOI (aTDC)	-25	-20	-25
% EGR	23.0	0.0	23.0
Premixed ratio (%)	97	96	97
Injection pressure (bar)	69.16	68.09	69.16
IMEP (bar)	3.8	3.9	3.8
Engine speed (rpm)	700	700	700
Geometric compression ratio	16.9	16.9	16.9

3.2 Computational cells and model validation

As shown in Figure 2, a 360 degrees computational meshing of in-cylinder geometry using the ANSYS ICEM-CFD software [44] is considered for simulation. Three different cell sizes verified for case 1 of Table 3. To find the proper mesh resolution for main calculations, the maximum in-cylinder pressure and computational time were considered as a main selection criterion. It can be seen from Figure 3, for the computational grid with 15678 cells, the maximum in-cylinder pressure is in good agreement with the experimental data and it has reasonable time consumption compared to other grids. Thus, the computational grid with 15678 cells was chosen for simulation process.

The simulation considers the time period from the intake valve closing to the exhaust valve opening and the initial in-cylinder mixture at IVC was supposed to be uniform with the turbulence kinetic energy of 1.55 m^2/s^2 and swirl ratio of 0.5 at the start of computation process. The simulated in-cylinder pressure, heat release histories, and emissions with experiments are compared in Figure 4 and Figure 5, respectively. According to what explained above, the simulation results are in good agreement with experiments. Because of the well prediction of in-cylinder pressure, combustion phasing, and emissions, case 1 is preferred for study of the next section.

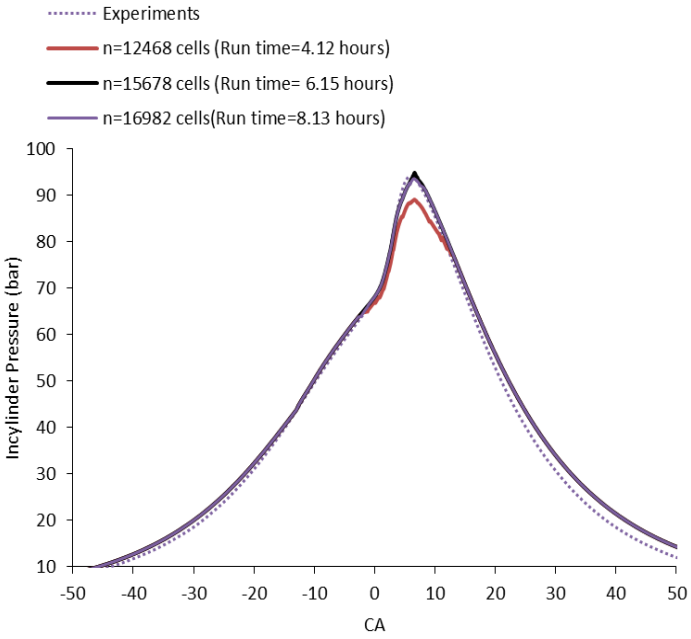


Figure 3. Mesh independency for case 1

4. Results and Discussions

4.1 Methodology

In order to generate the HRR for diesel and methane, at the first step, the code was run with the combined mechanism (introduced in the previous section) including n-heptane and methane oxidation reactions. Then from the results for n-heptane concentration histories, rate of n-heptane consumption was multiplied by LHV of n-heptane to achieve the HRR of the n-heptane, separately. The same method was done for methane. In order to evaluate accuracy of the method, comparison between the total HRR for case 1 resulted from simulation, and divided HRR for n-heptane (Diesel) and methane (NG) are illustrated in Figure 6. It can be seen that the total calculated HRR (which is the sum of n-heptane and methane HRRs) is very close to the total HRR which is resulted from the simulation. There is maximum 1.5° crank angle difference between the total calculated HRR and simulated one. Accordingly, the separation method for HRR of diesel and methane was selected in this study.

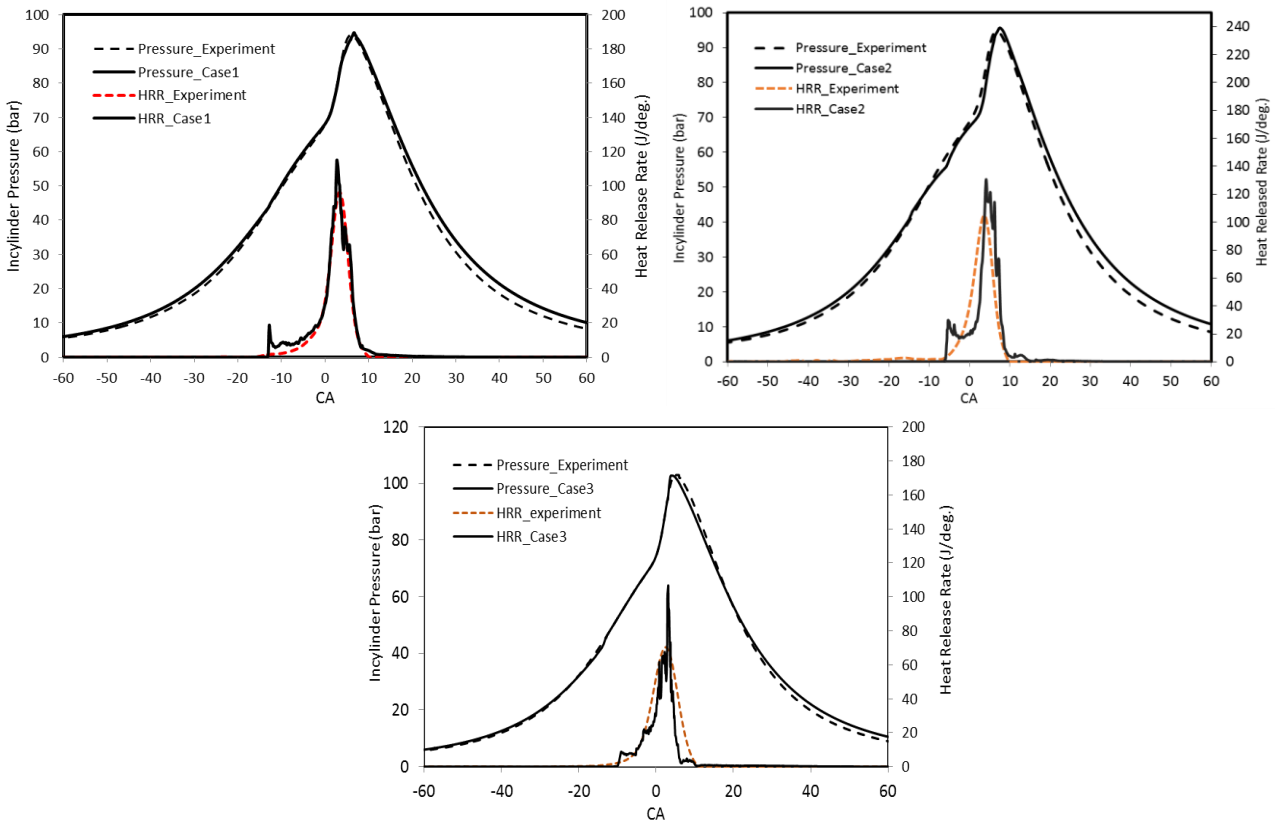


Figure 4. Pressure trace and net HRR validation for the examined engine operating conditions

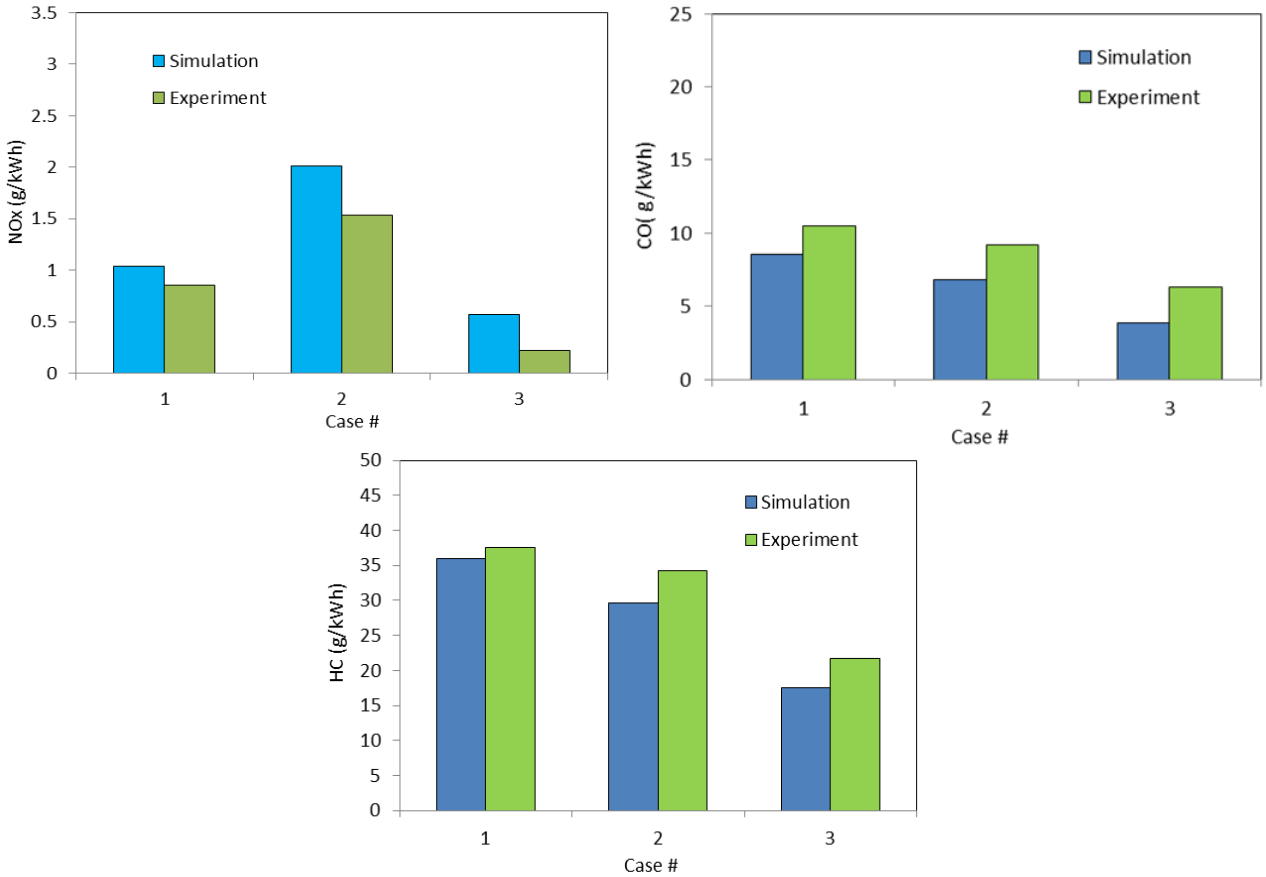


Figure 5. Comparison of numerical and experimental results for engine exhaust emissions

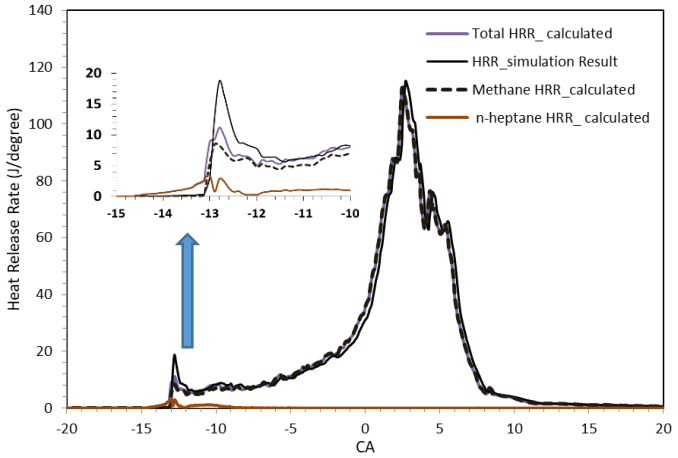


Figure 6. Comparison of total HRR with diesel and methane fuels HRR for the engine operating condition case 1

4.2 Effect of premixed ratio

Figure 7 shows the effect of PR of in-cylinder mixture on HRR. As can be seen, combustion starts earlier and the heat release rate is increased by decreasing the PR, while keeping the total input energy constant. In order to deep understanding of the RCCI combustion and how the PR affects the combustion, it is useful to consider HRR of diesel and methane, distinctively.

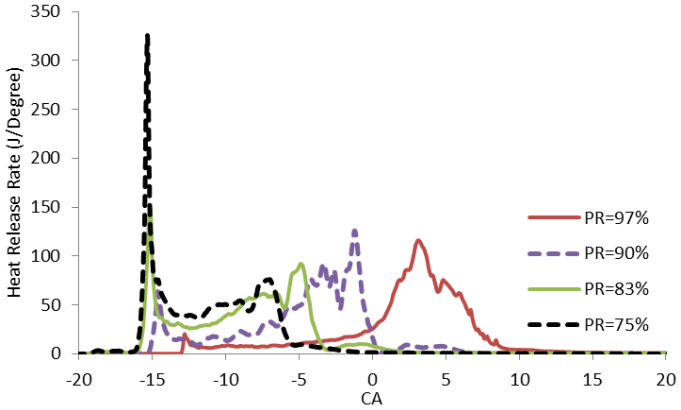


Figure 7. Effects of PR of in-cylinder mixture on HRR for the engine operating condition case 1

Figure 8 illustrates variations of HRR of diesel and methane fuels versus CAD at different PRs. Peak value of HRR of diesel fuel increases from 3.5 J/deg. at 97% PR to 120 J/deg. at 75% PR. Meanwhile, SOC of diesel is advanced from 15 CAD bTDC to 17 CAD bTDC when PR is changed from 97% to 75%. In addition, it can be observed from Figure 8b that decreasing PR advances methane combustion from 13 CAD bTDC in base case to 16 CAD bTDC. HRR of methane is higher in lower PRs compared to higher PRs.

Premixed methane percentage is one of the reliable tools to control combustion phasing [45]. As presented in Table 4, increasing PR from 75% to 97% retards SOC, CA50 and extends BD of diesel. The similar trend can be seen for methane combustion, SOC and CA50 are retarded, and BD is extended. SOC are defined as the crank angle degrees at which 10% of the cumulative heat is released. Moreover, BD is burning duration and was calculated from CA10 (crank angles of 10% of the max accumulated heat release) to CA90 (the crank angles of 90% of the max accumulated heat release). The dependence of combustion phasing on the PR offers a useful way to control the RCCI combustion. Thus, the amounts of the fuels supplied by each of the two fuel systems must be controlled accurately for an engine to be operated at RCCI mode [46]. IDdiesel, is ignition delay of injected diesel fuel which is considered as the time from start of injection to the start of combustion of diesel. In addition, IDmethane is ignition delay of methane fuel that is introduced as a time period from the SOC of diesel to the start of combustion of methane. The results show that Increasing PR from 75% to 97% increases IDdiesel and IDmethane.

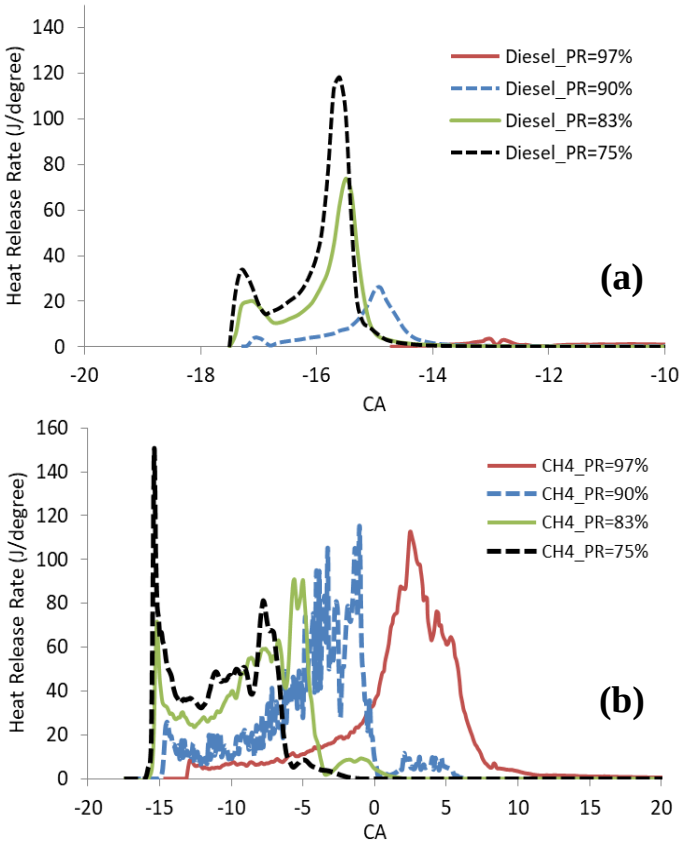


Figure 8. Effect of PR on (a) diesel and (b) methane HRR for the engine operating condition case 1

Figure 9 demonstrates the in-cylinder pressure at different PRs. Increasing PR decreases peak cylinder pressure and retards the combustion phasing due to the decreased reactivity of the mixture by increasing methane fuel portion. Furthermore, diesel fuel acts as a high reactivity initiator of combustion and ignites the methane fuel. Consequently, by increasing PR, the mixture ignites weakly compared to the cases with lower PR. Regarding the symmetry observed in the in-cylinder pressure profiles in Fig. 9, this phenomenon is primarily noted at lower premixed ratios (PR). At these lower PR levels, the diesel fuel injection plays a more significant role in driving the combustion process, resulting in a balanced ignition and combustion pattern. The higher diesel proportion increases the reactivity within the chamber, leading to a more controlled and uniform combustion front that minimizes pressure fluctuations. Consequently, this higher reactivity contributes to a symmetric pressure profile across the cylinder during combustion. In contrast, at higher PR levels, the mixture's reduced reactivity results in less controlled combustion, which can introduce asymmetries in the pressure profiles.

Table 4. Combustion phasing for different premixed ratios for the engine operating condition, case 1

Premixed ratio (%)	97		90		83		75	
	Diesel	Methane	Diesel	Methane	Diesel	Methane	Diesel	Methane
SOC (degree aTDC)	-13.6	-4.5	-16.1	-11.1	-17	-14.5	-17.2	-15.1
CA50 (degree aTDC)	-12.1	2.4	-15	-3.8	-16	-8	-16.4	-10.5
BD (degrees)	4.2	10.3	2.4	10.3	2	10	1.9	8.2
ID_{diesel}(degree)	6.4	-	3.9	-	3	-	2.8	-
$ID_{methane}$(degree)	-	9.1	-	5	-	3.1	-	2.1

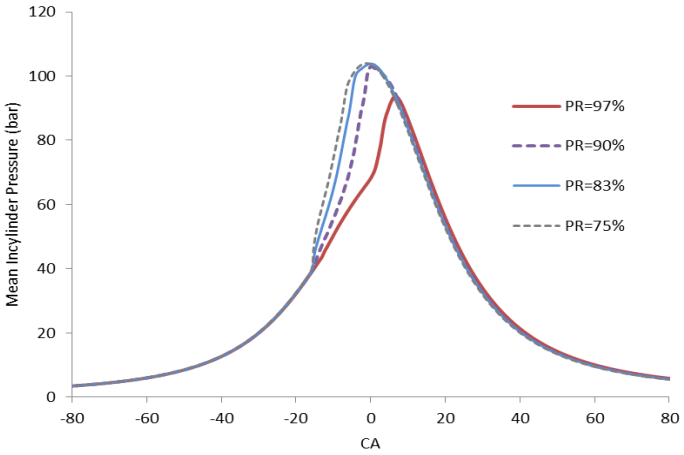


Figure 9. Variations of in-cylinder pressure versus CADs at different premixed ratios for the engine operating condition case 1

Figure 10 shows the effect of PR on combustion efficiency and gross indicated efficiency. It is shown that while gross Indicated efficiency increases by shifting the PR from 75% to 97%, the combustion efficiency decreases. Increasing PR while keeping the SOI constant shifts the combustion phasing after TDC. Thus indicated mean effective pressure increases. As a result of this fact gross indicated efficiency increases even a slight decrease in combustion efficiency.

Figure 11 illustrates the effect of PR on engine exhaust emissions. The general trend shows that HC and CO are increased, but NO is decreased by increasing PR. Increasing PR results in reduction of in-cylinder peak pressure while more retarding the combustion phasing; consequently, the in-cylinder charge temperature is decreased [46]. It is notable that the diesel fuel parcels, impinging the walls, stay unburned and produce HC due to lower temperatures of wall and crevice volume. On the other hand, the low combustion temperature is another parameter, which causes incomplete combustion and consequent formation of higher HC emission that result in the drop of combustion efficiency [27]. In addition, higher in-cylinder charge temperature of lower PRs results in efficient oxidation of CO and consequently, lower CO is produced when ignition occurs near TDC [47].

Figure 12 displays the impact of PR on in-cylinder charge temperature, NO and CH_4 species concentration at 15 and 10 CAD bTDC. Based on the contours, the in-cylinder charge temperature is lower for PR= 90% compared to PR=75%. Hence, the NO concentration is higher in low PRs compared to high PRs. Moreover, at all time steps, the peak values of NO concentration are located near the centerline of cylinder. It is due to high temperature zone of cylinder charge which is caused by richer zones of diesel fuel spray. It could be resulted from in-cylinder mixture temperature and methane contours at 10 CAD bTDC that flame speed is greater in lower PRs because of higher reactivity of in-cylinder mixture caused by higher diesel fuel quantity. However, at all cases the diesel spray is impinged on the piston surface, which is the source of some remained unburned diesel droplets on piston surface.

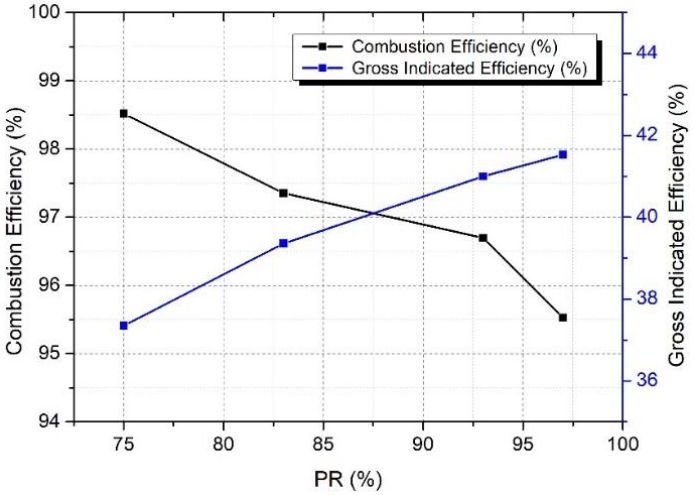


Figure 10. Combustion efficiency and gross indicated efficiency at different PRs for the engine operating condition case 1

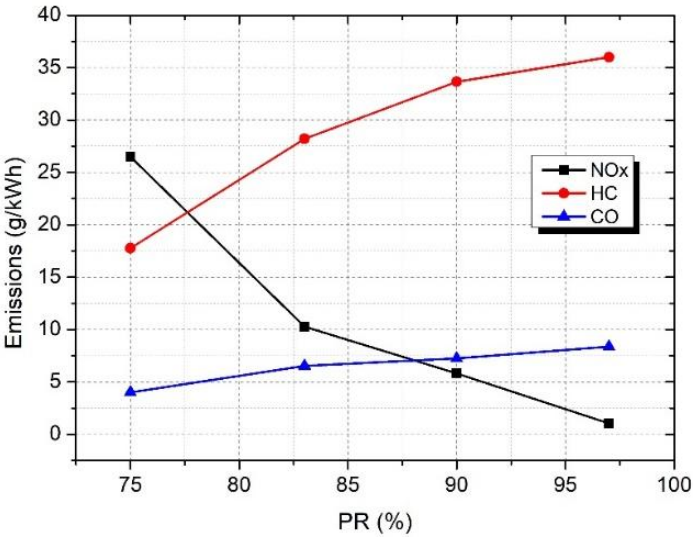


Figure 11. Effects of PR on engine exhaust emissions including HC, CO, and NOx for the engine operating condition case 1

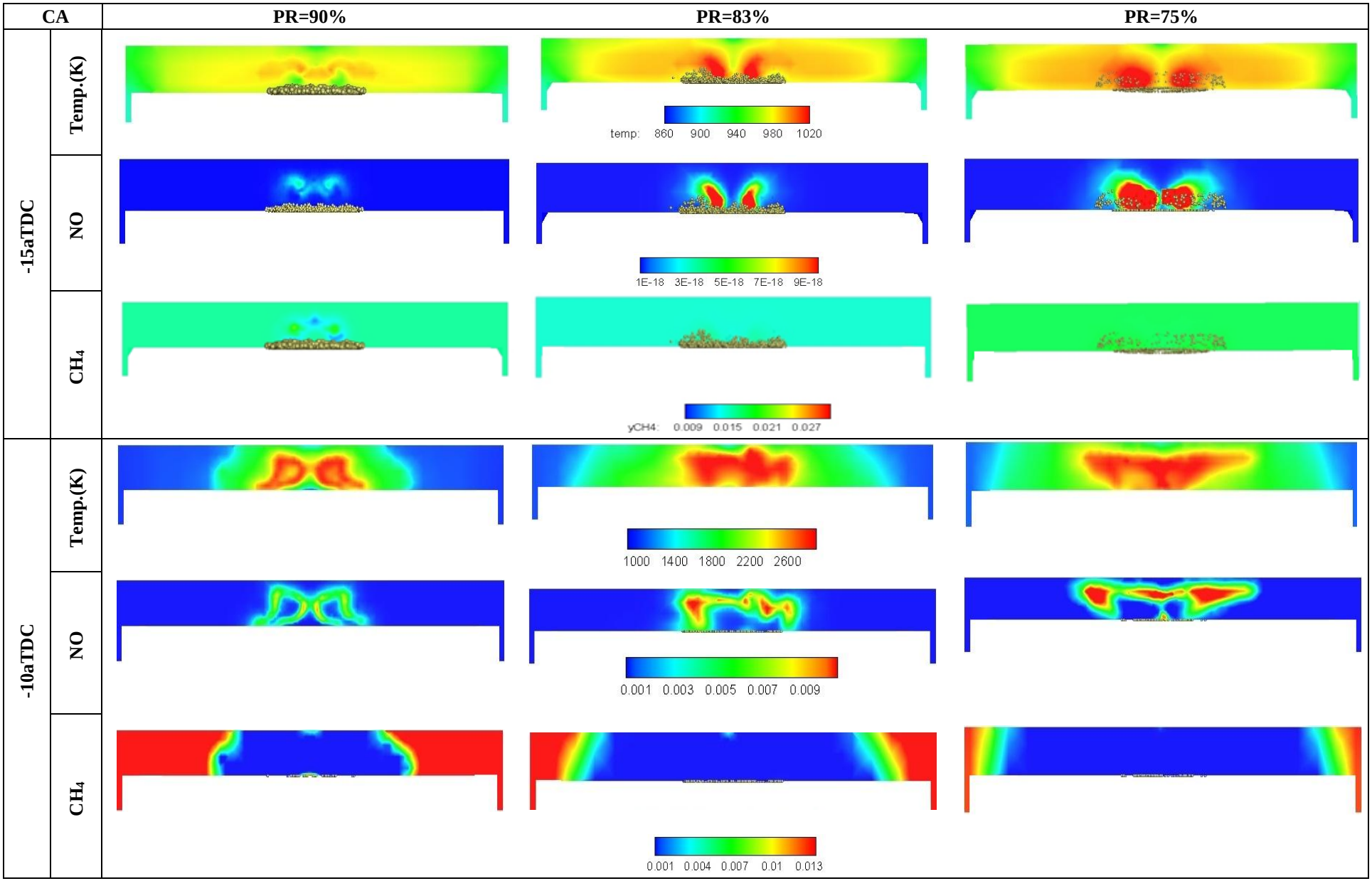


Figure 12. Effect of PR on in-cylinder charge temperature, NO and CH4 concentrations for the engine operating condition case 1

4.3 Effect of diesel injection timing

In RCCI engines, reactivity gradient of in-cylinder mixture is controlled usually by two ways: the ratio of fuels with high and low octane numbers and injection strategy of the fuel with lower octane number [48]. In the injection strategy method, start of injection (SOI) timing is one of the operative methods to control the start of combustion in RCCI engines. However, determining the optimum timing of SOI is a big challenge in dual fuel mode like RCCI engines [2]. In the next section of this study, the effects of various SOIs on the engine performance and emission characteristics are investigated by considering the combustion characteristics of diesel and methane fuels, independently.

Figure 13 shows in-cylinder pressures at different SOI timings for case 1 of Table 2. It is resulted that SOI = -50 CAD aTDC has the maximum peak pressure and SOI = -65 CAD aTDC has the minimum peak pressure. In addition, by increasing mixing time of the diesel and methane-air mixture, equivalence ratio stratification decreases and the in-cylinder mixture becomes more homogenous.

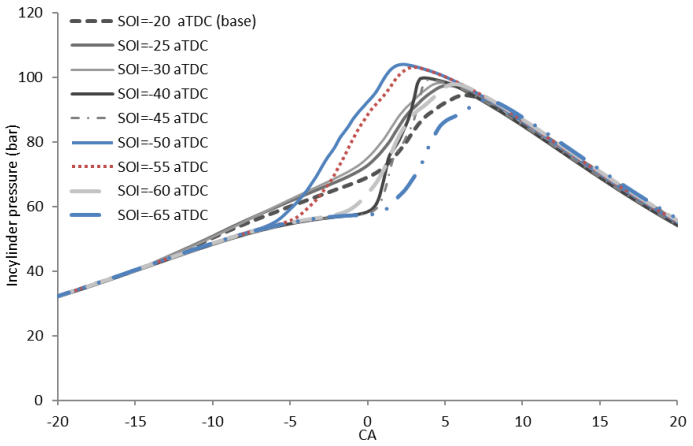
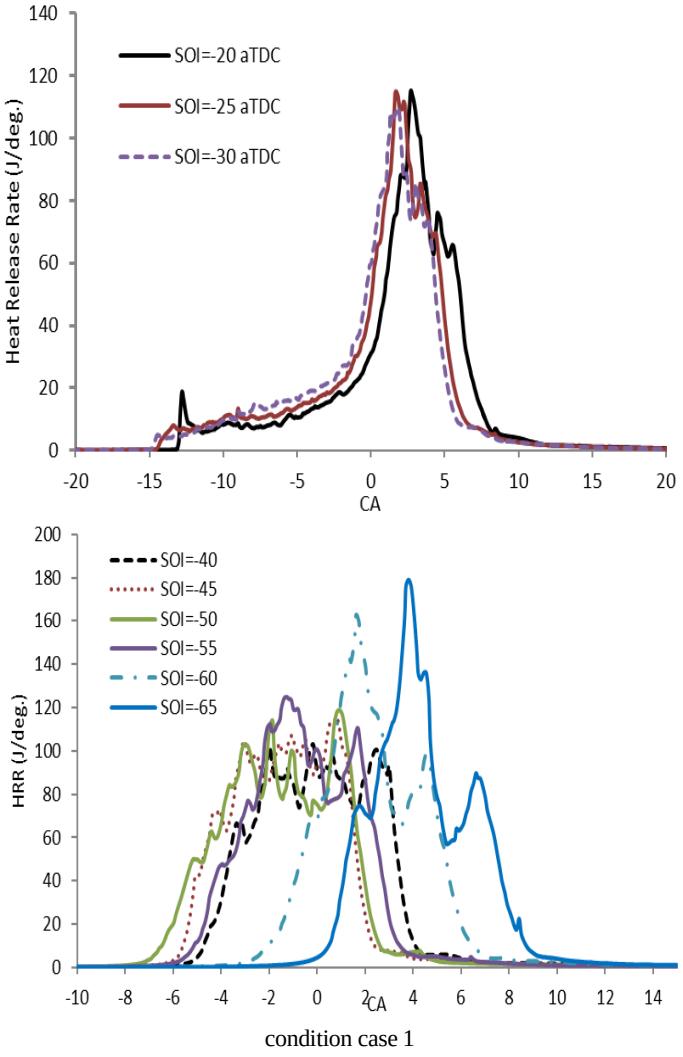


Figure 13. Effects of SOI timing sweep on in-cylinder pressure for the engine operating condition corresponding to case 1

Figure 14 shows variations of the heat release rate history at various SOIs for case 1 in Table 2. As can be seen from this figure, the SOC is advanced by shifting the SOI from -20 CAD aTDC to -30 CAD aTDC. This is because of providing more rich zones within the cylinder at the end of compression stroke which increases the evaporation rate of diesel droplets. Then, by changing the SOI from -30 CAD aTDC to –45 CAD aTDC, the SOC is retarded from about -15 CAD aTDC to -6 CAD aTDC, and the shape of HRR is changed. By considering the spray of diesel fuel and shape of piston crown in this engine (as shown in figure 19), From SOI=-20 CAD aTDC to -45 CAD aTDC the role of wall impingement of diesel spray became more effective due to the lower temperature of cylinder, and the most of injected fuel is accumulated on piston surface. It is obvious that the evaporation rate of diesel fuel affects the formation of ignitable zones.

As it is shown in Figure 15, because of higher temperature of in-cylinder gases near TDC at compression stroke, the rate of evaporation is higher for the cases in which SOI varies in the range of -20 to -35 CAD aTDC compared to the cases in which SOI varies in the range of -40 and -45 CAD aTDC, accordingly less liquid diesel remains on the piston surface at end of combustion. Lower gas temperature and consequently accumulated droplets on the piston crown for the cases with SOI=-40 and -45 CAD aTDC delay the ignition due to the reduction of the mixture reactivity. However, according to Figure 15, by shifting the SOI from -50 CAD aTDC to -65 CAD aTDC, the SOC is retarded due to reduced local reactivity of in-cylinder mixture, which produces less ignitable zones by diesel spray.

Figure 14. Effect of SOI on heat release rate for the engine operating



condition case 1

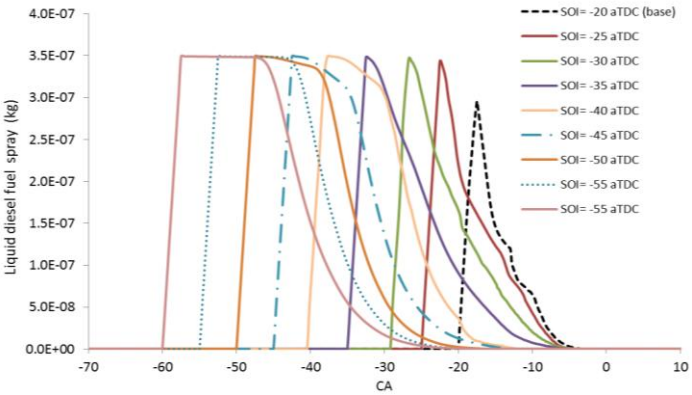


Figure 15. Effect of SOI on the amount of liquid diesel spray for the engine operating condition case 1

Introducing the energy release rate of diesel and methane fuels independently could provide valuable information about the impacts of injection timing on the combustion characteristics. Figure 16 shows the influence of SOI on heat release rate of diesel and methane fuels. It is observed that the combustion will be like dual-fuel process when the injection of diesel fuel starts later in which diesel burning occurs for both premixed and diffusion combustion modes. However, earlier SOI from -20 CAD aTDC to -40 CAD aTDC, shifts the combustion mode from typical dual fuel mode to highly reactivity-controlled combustion mode in which diesel is as a controller of methane combustion, but with more premixed portion compared to the late SOIs. This behaviour is due to the existence of more time for diesel to mix with methane/air mixture. Therefore, there is less rich and ignitable zone, which in turn can be streamlined into the reduced reactivity of mixture, longer mixture delay time. In addition, the methane SOC is shifted from about -15 CAD aTDC to about -8 CAD aTDC. The more advanced SOI leads to the more premixed portion of diesel combustion, and combustion mode is shifting from RCCI mode to HCCI like mode. It means that highly premixed mixture of diesel and methane burns in a HCCI combustion mode.

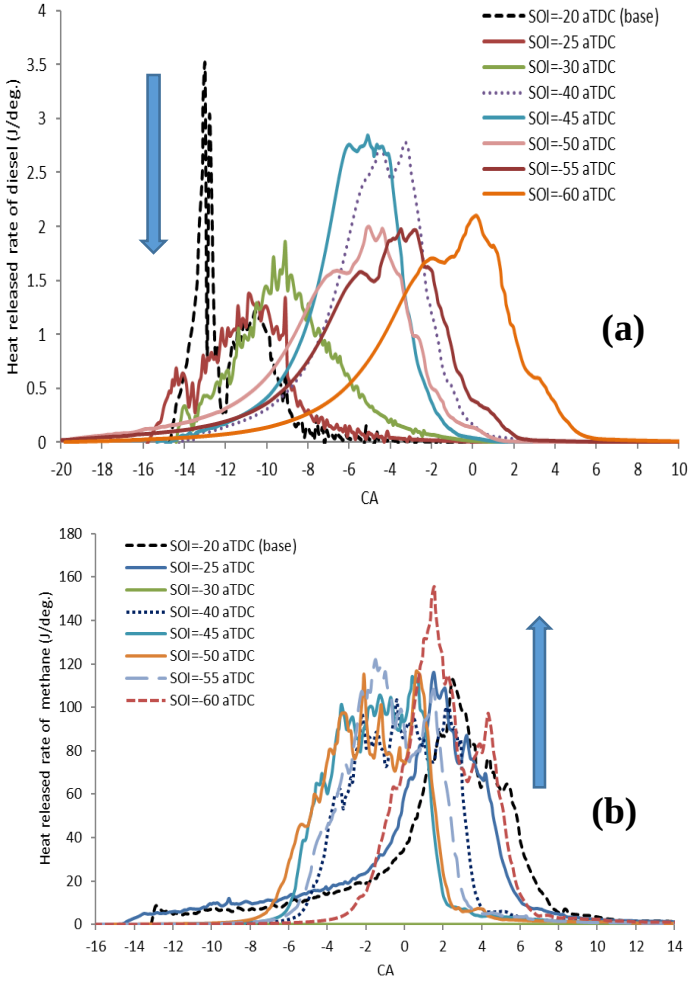


Figure 16. Effect of SOI on (a) diesel and (b) methane fuels heat release rate for the engine operating condition case 1

Table 5 shows the diesel and methane combustion phasing parameters individually including SOC, CA50, BD, IDdiesel and ignition delay of methane (IDmethane) at various SOIs for case 1 in Table 3. It is obvious that the diesel SOC is retarded by advancing the SOI, and results in late combustion of methane. Advancing the diesel injection timing and then penetration of diesel parcels into low temperature gas zones decreases the evaporation rate of diesel fuel. Therefore, possibility of the formation of rich zones with high equivalence ratio reduces remarkably. By advancing the injection timing, burning duration of diesel fuel increases from 4.2 crank angle degree to 7.4 crank angle degree while burning duration of methane decreases from 10.3 crank angle degree to 5.2 crank angle degree. It is due to the nature of HCCI-like combustion in which rapid combustion takes place with shorter burning durations. Ignition delay of diesel fuel increases from 6.4 CAD to 54.9 CAD by advancing SOI from -20 CAD aTDC to -60 CAD aTDC. It is notable that by increasing IDdiesel, Ignition delay of methane (IDmethane) decreases from 9.1 CAD to 3.3 CAD. CA50 is a criterion of combustion timing and it is used to design control systems for stabilizing low temperature combustion mode [49]. Advanced SOI timing retards the CA50 for diesel fuel. It is again expectable that the combustion mode shifts from dual-fuel mode to HCCI-like mode by advancing SOI timing.

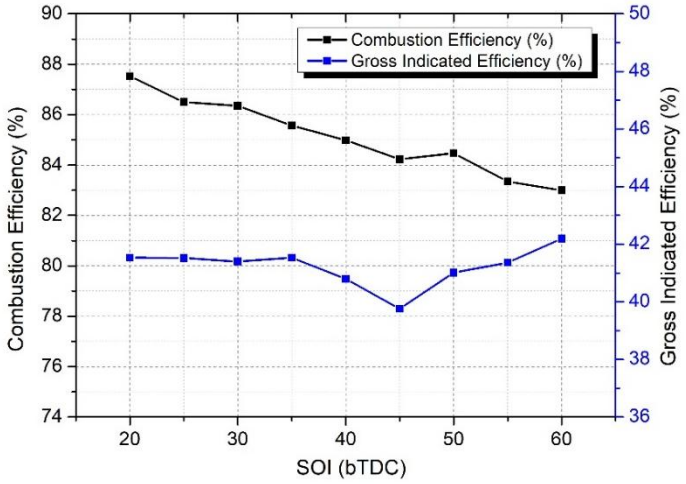


Figure 17. Effects of SOI sweep on Gross indicated efficiency and combustion efficiency for the engine operating condition case 1

Figure 17 illustrates the variation of gross indicated efficiency and combustion efficiency with altering SOI timing. It can be resulted that early injection of diesel increases the gross indicated efficiency from 41.5% to 42.5% with a drop at SOI at -40 aTDC and -45 aTDC due to spray wall impingement as discussed before. In addition, advancing the SOI timing decreases the combustion efficiency owing to the lower combustion temperature at advanced SOIs. The influence of SOI timing is significant on the engine emissions.

Figure 18 shows emission concentrations at different SOI timings for case 1. Trends show that changing SOI timing from the base case (-20 CAD aTDC) to SOI= -65 CAD aTDC reduces NOx emissions, but increases HC and CO emissions. This behaviour comes from the fact that advanced diesel injection decreases in-cylinder temperature because of higher degree of stratification and the lack of rich zones for start of strong combustion by diesel fuel. At -50 CAD, the rise in NOx is primarily due to localized hot spots created by partial diesel combustion, which increases the in-cylinder temperature. These hot spots facilitate a slight NOx increase while reducing HC and CO formation.

Table 5. Effect of SOI timing on combustion phasing of diesel and methane for the engine operating condition case1

SOI (degree a TDC)	-20		-30		-40		-50		-60	
	Diesel	Methane	Diesel	Methane	Diesel	Diesel	Diesel	Methane	Diesel	Methane
SOC (degree aTDC)	-13.6	-4.5	-12	-4.5	-7.0	-3.3	-6.9	-2.8	-5.1	-1.8
CA50 (degree aTDC)	-12.1	2.4	-9.2	1.0	-4.1	-0.2	-3.9	0.0	-0.8	1.78
BD (degrees)	4.2	10.3	6.3	8.7	5.0	6.1	7.3	5.7	7.4	5.2
ID_{diesel}(degree)	6.4	-	17.9	-	33	-	46.5	-	54.9	-
$ID_{methane}$(degree)	-	9.1	-	7.6	-	3.7		3.5	-	3.3

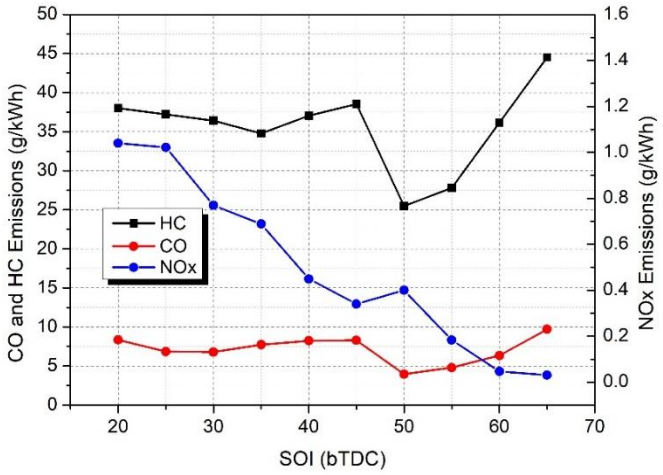


Figure 18. Effect of SOI timing on CO, HC and NOx emissions for the engine operating condition case 1

Figure 19 presents the in-cylinder temperature and equivalence ratio contours for different SOI timings. It can be observed that by advancing the SOI timing, combustion is retarded, but burning rate is increased as shown in Figure 13, 14 and Table 5 because diesel parcels are able to distribute, evaporate, and mix with surrounding air and methane mixture. Hence, the total octane number of whole fuel mixture is lower compared to late SOI timings. In addition, it can be seen that in-cylinder temperature and NOx emissions are low for earlier SOI, but HC and CO emissions are high. Another evidence for higher NOx in the late SOI timing is the local equivalence ratio. This means that the amount of rich zones is high for the cases with late SOI timings, therefore local temperature is increased which will result in more NOx emissions. By considering the combustion efficiency and gross indicated efficiency, the optimum injection strategy for this engine would be SOI=-50 CAD aTDC.

5. Conclusions

In this research, combustion process of an RCCI engine was modelled using KIVA-3V code coupled with CHEMKIN-II at the closed part of the engine cycle. A reduced mechanism, including 57 species and 190 reactions utilized for the combustion simulation. Effects of sweeping of start of injection timing and premixed ratio on diesel and methane combustion and emissions were studied. Hence, the main conclusions are as below:

1. By decreasing PR from 97% to 75%, maximum heat release rate of diesel increases from 3.5 J/deg. in 97% PR to 120 J/deg. in 75% PR. Also, start of combustion of diesel advances. By reducing the PR, methane combustion advances about 10.6 CAD and the average HRR of methane is higher in the cases with lower PRs compared to the cases with higher PRs. By reducing the PR, the ignition points by diesel are increased, and IDdiesel is reduces. Consequently, IDmethane decreases because the higher reactivity gradient inside the mixture provides more energy to ignite the methane.

2. By reducing the PRs from 97% to 75%, in-cylinder temperature increases because of the presence of diesel combustion, which creates local rich regions with high temperatures.

3. From the results trend, increasing methane quantity as the premixed fuel causes higher CO and HC, but lower NO emissions. In addition, increasing PR decreases the in-cylinder peak pressure, and retards the CA50. Consequently, the in-cylinder gas temperature reduces. Moreover, when the PR increases, GIE increases from 37% to 41% while combustion efficiency decreases from 94.5% to 87.5%.

4. The SOI advancing from -20 CAD aTDC to -40 CAD aTDC, changes the combustion from typical pilot dual-fuel to highly reactivity-controlled combustion mode, in which diesel is considered as a controller of methane combustion with more premixed portion compared to late SOIs. This behaviour is due to the better mixing of diesel with methane/air mixture. Hence, advancing the SOI causes less rich and ignitable zones that moderates the role of diesel fuel as an igniter, but creates reactivity stratification of mixture, which increase mixture ignition delay time, and the SOC shifts by about 7 CAD. The more advancing SOI creates premixed diesel/methane/ air mixture, which in turn can be streamlined into the shifting of combustion mode from RCCI mode to HCCI like mode.

5. By advancing the SOI, the SOC of diesel is retarded which results in late combustion of methane. Burning duration of diesel fuel increases 3.2 CAD while burning duration of methane decreases 5.1 CAD by earlier diesel injection. This feature comes from the nature of HCCI-like combustion in which rapid combustion takes place with lower burning durations.

6. Trends shows that SOI advancing from the base case (-20 CAD aTDC) to a case with SOI= -65 CAD aTDC increases HC and CO emissions, but decreases NOx emissions. This behaviour can be attributed to the is the having less in-cylinder temperature and more premixed combustion which leads to low rich zones for start of combustion by diesel.

7. The findings from this study provide a foundation for further exploration of RCCI combustion characteristics in diesel/natural gas engines. Future work should focus on validating the KIVA model and chemical mechanisms against additional experimental data under a range of engine operating conditions Additionally, refining premixed ratio strategies based on these validations could enhance model accuracy and offer deeper insights into optimizing combustion efficiency and emission control in RCCI mode.

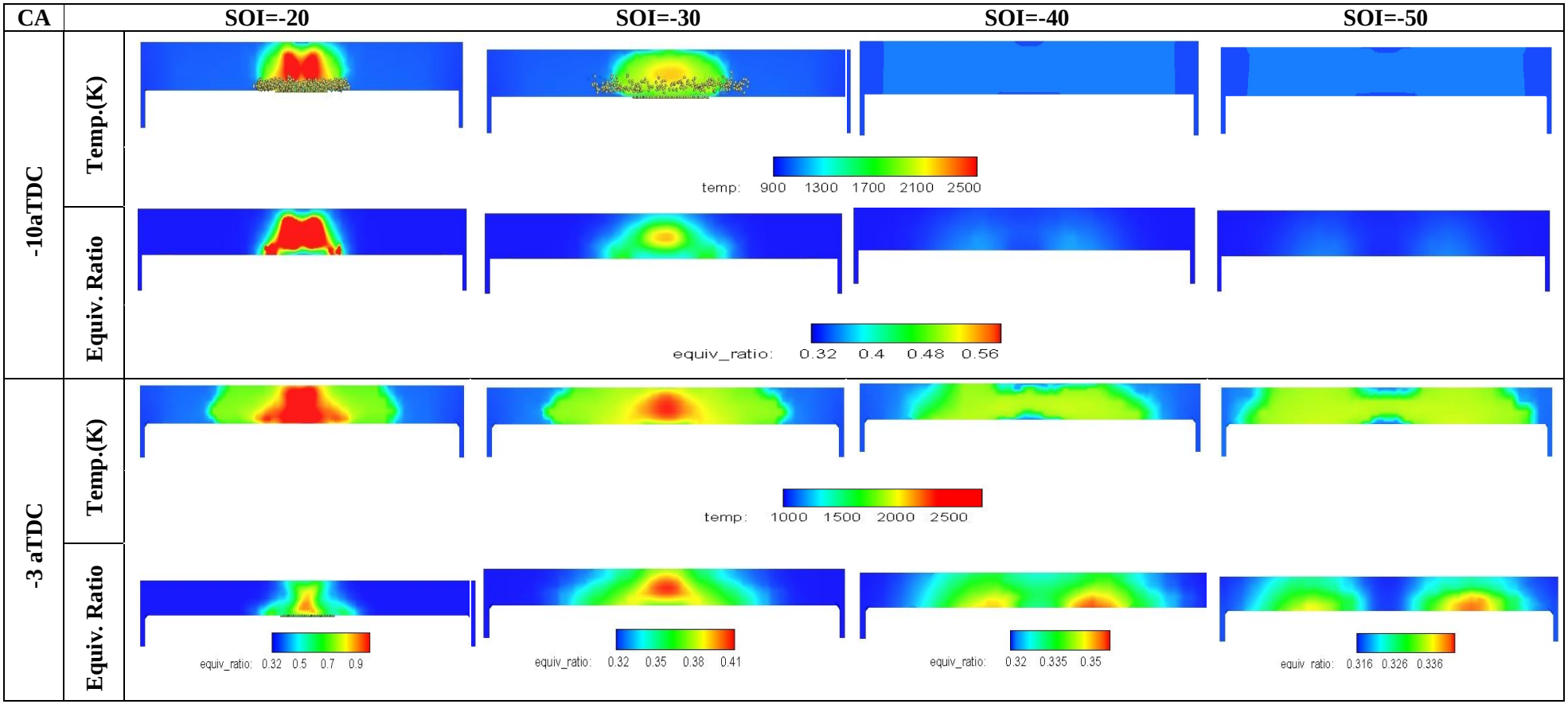


Figure 19. Effect of SOI timing on in-cylinder Temperature and Equivalence ratio for the engine operating condition case 1

Conflict of Interest Statement

The authors declare that there is no conflict of interest in the study.

CRediT Author Statement

Kamran Poorghasemi: Conceptualization, Formal analysis, Methodology, Writing - original draft, Writing - review & editing,. **Khoshbakhti Saray:** Writing - original draft, Writing - review & editing , **Hamit Solmaz:** Formal analysis, Visualization, Methodology, Writing - original draft, Writing - review & editing, **, Seyed Mohammad Mousavi:** Software, Visualization, Writing - original draft, Writing - review & editing , **Alborz Zehni:** Software, Visualization, Validation, Writing - original draft, Writing - review & editing

References

1. Poorghasemi, K., Khoshbakhti Saray, R., Ansari, E., Mousavi, S. M., & Zehni, A. (2022). Statistical analysis on the effect of pre-mixed ratio, EGR, and diesel fuel injection parameters on the performance and emissions of a NG/Diesel RCCI engine using a DOE method. Proceedings of the Institution of Mechanical Engineers, Part D: Journal of Automobile Engineering, 236(2–3), 460–473. https://doi.org/10.1177/09544070211015478
2. Nagareddy, S., Rajeswaran, S. S., Jaganathan, D., Subramanian, V. P. B., & Neelakandan, V. (2025). Turbocharged Six-Cylinder Direct Injection Hydrogen Fueled Spark Ignition Engine Combustion and NOx Control Model. Engineering Perspective, 4(3), 100-110. https://doi.org/10.29228/eng.pers.82203
3. Kethudaoglu, G., Aktaş, F., Karaaslan, S., & Dinler, N. (2024). 0/1 and 3-dimensional cold flow analysis of a diesel engine: A case study. International Journal of Automotive Science and Technology, 8(1), 142–149. https://doi.org/10.30939/ijastech.1384376
4. Türkcan, Ö., & Polat, S. (2025). Combustion and Emission Behaviour of a HCCI Wankel Engine Across Lambda Variations: Insights for Future Aviation-Oriented Rotary Engine Concepts. International Journal of Automotive Science And Technology, 9(4), 626-636. https://doi.org/10.30939/ijastech..1821778
5. Çelik, A., & Kunt, M. A. (2026). A Study on Predicting Engine Performance Outputs by Machine Learning Algorithms in a Single Cylinder HCCI Engine. Engineering Perspective, (1), 57-68. https://doi.org/10.64808/engineeringperspective.1782349
6. Inagaki, K., Fuyuto, T., Nishikawa, K., Nakakita, K., & Sakata, I. (2006). Dual-fuel PCI combustion controlled by in-cylinder stratification of ignitability. SAE Technical Paper No. 2006-01-0028. https://doi.org/10.4271/2006-01-0028
7. Bessonette, P. W., Schleyer, C. H., Duffy, K. P., Hardy, W. L., & Liechty, M. P. (2007). Effects of fuel property changes on heavy-duty HCCI combustion. SAE Technical Paper No. 2007-01-0191. https://doi.org/10.4271/2007-01-0191
8. Kokjohn, S., Hanson, R., Splitter, D., & Reitz, R. D. (2010). Experiments and modeling of dual-fuel HCCI and PCCI combustion using in-cylinder fuel blending. SAE International Journal of Engines, 2(2), 24–39. https://doi.org/10.4271/2009-01-2647
9. Splitter, D., Kokjohn, S., Rein, K., Hanson, R., et al. (2010). An optical investigation of ignition processes in fuel reactivity controlled PCCI combustion. SAE International Journal of Engines, 3(1), 142–162. https://doi.org/10.4271/2010-01-0345
10. Splitter, D., Hanson, R., Kokjohn, S. L., & Reitz, R. D. (2010). Improving engine performance by optimizing fuel reactivity with a dual-fuel PCCI strategy. THIESEL Conference on Thermo and Fluid Dynamic Processes in Diesel Engines.
11. Reitz, R. D., Hanson, R., Splitter, D., & Kokjohn, S. L. (2010). Engine combustion control via fuel reactivity stratification. University of Wisconsin WARF Patent Application, P100054US.
12. Kokjohn, S. L., & Reitz, R. D. (2010). Characterization of dual-fuel PCCI combustion in a light-duty engine. International Multidimensional Engine Modeling User's Group Meeting.
13. Şahin, F., Halis, S., Yıldırım, E., Altın, M., Balaban, F., Solmaz, H., & Yücesu, H. S. (2022). Effects of premixed ratio on engine operation range and emissions of a reactivity controlled compression ignition engine. SAE International Journal of Fuels and Lubricants, 16, 169–179.
14. Halis, S., Solmaz, H., Polat, S., & Yücesu, H. S. (2023). Numerical investigation of a reactivity-controlled compression ignition engine fueled with n-heptane and iso-octane. Sustainability, 15(13), 10406. https://doi.org/10.3390/su151310406
15. Halis, S., Solmaz, H., Polat, S., & Yücesu, H. S. (2022). Numerical study of the effects of lambda and injection timing on RCCI combustion mode. International Journal of Automotive Science and Technology, 6(2), 120–126. https://doi.org/10.30939/ijastech..1105470
16. Bahrami, S., Poorghasemi, K., Solmaz, H., Calam, A., & Ipci, D. (2021). Effect of nitrogen and hydrogen addition on performance and emissions in reactivity controlled compression ignition. Fuel, 292, 120330. https://doi.org/10.1016/j.fuel.2021.120330
17. Curran, S., et al. (2013). Efficiency and emissions mapping of RCCI in a light-duty diesel engine. SAE Technical Paper No. 2013-01-0289. https://doi.org/10.4271/2013-01-0289
18. Yang, B., Yao, M., et al. (2014). Experimental and numerical study on different dual-fuel combustion modes fuelled with gasoline and diesel. Applied Energy, 113, 722–733. https://doi.org/10.1016/j.apenergy.2013.08.074
19. Nieman, D., Dempsey, A., & Reitz, R. (2012). Heavy-duty RCCI operation using natural gas and diesel. SAE International Journal of Engines, 5(2), 270–285. https://doi.org/10.4271/2012-01-0379
20. Doosje, E., Willems, F., & Baert, R. (2014). Experimental demonstration of RCCI in heavy-duty engines using diesel and natural gas. SAE Technical Paper No. 2014-01-1318. https://doi.org/10.4271/2014-01-1318
21. Walker, N. R., et al. (2015). Natural gas for high load dual-fuel reactivity controlled compression ignition in heavy-duty engines. Journal of Energy Resources Technology, 137(4), 042202. https://doi.org/10.1115/1.4030110
22. Zoldak, P., Sobiesiak, A., Bergin, M., & Wickman, D. (2014). Computational study of reactivity controlled compression ignition (RCCI) combustion in a heavy-duty diesel engine using natural gas. SAE Technical Paper No. 2014-01-1321. https://doi.org/10.4271/2014-01-1321
23. Zoldak, P., Sobiesiak, A., Wickman, D., & Bergin, M. (2015). Combustion simulation of dual fuel CNG engine using direct injection of natural gas and diesel. SAE International Journal of Engines, 8(2), 846–858. https://doi.org/10.4271/2015-01-0851

24. Min, X., Cheng, W., Li, Z., Zhang, H., An, T., & Meng, Z. (2016). Pre-injection strategy for pilot diesel compression ignition natural gas engine. Applied Energy, 179, 1185–1193.
25. Dahodwala, M., Joshi, S., Koehler, E., & Franke, M. (2014). Investigation of diesel and CNG combustion in a dual fuel regime and as an enabler to achieve RCCI combustion. SAE Technical Paper No. 2014-01-1308. https://doi.org/10.4271/2014-01-1308
26. Dahodwala, M., Joshi, S., Koehler, E., Franke, M., & Tomazic, D. (2015). Experimental and computational analysis of diesel-natural gas RCCI combustion in heavy-duty engines. SAE Technical Paper No. 2015-01-0849. https://doi.org/10.4271/2015-01-0849
27. Paykani, A., Kakaee, A. H., Rahnama, P., & Reitz, R. D. (2012). Effects of diesel injection strategy on natural gas/diesel reactivity controlled compression ignition combustion. Energy, 90, 814–826.
28. Mousavi, S. M., Khoshbakhti Saray, R., Poorghasemi, K., & Maghbouli, A. (2016). A numerical investigation on combustion and emission characteristics of a dual-fuel engine at part load condition. Fuel, 166, 309–319. https://doi.org/10.1016/j.fuel.2015.10.052
29. Mousavi, S. M., Khoshbakhti Saray, R., Bahlouli, K., Poorghasemi, K., Maghbouli, A., & Sadeghlu, A. (2019). Effects of pilot diesel injection strategies on combustion and emission characteristics of dual-fuel engines at part load conditions. Fuel, 258, 116153. https://doi.org/10.1016/j.fuel.2019.116153
30. Bahlouli, K., Atikol, U., Khoshbakhti Saray, R., & Mohammadi, V. (2014). A reduced mechanism for predicting the ignition timing of a fuel blend of natural gas and n-heptane in HCCI engine. Energy Conversion and Management, 79, 85–96. https://doi.org/10.1016/j.enconman.2013.10.020
31. Poorghasemi, K., Khoshbakhti Saray, R., Bahlouli, K., & Zehni, A. (2016). 3D CFD simulation of a natural gas fuelled HCCI engine with employing a reduced mechanism. Fuel, 182, 816–830.
32. Kokjohn, S. L., & Reitz, R. D. (2013). Reactivity controlled compression ignition and conventional diesel combustion: A comparison of methods to meet light-duty NOx and fuel economy targets. International Journal of Engine Research, 14(5), 452–468. https://doi.org/10.1177/1468087413476032
33. Rahimi, A., Fatehifar, E., & Khoshbakhti Saray, R. (2010). Development of an optimized chemical kinetic mechanism for homogeneous charge compression ignition combustion of a fuel blend of n-heptane and natural gas using a genetic algorithm. Proceedings of the Institution of Mechanical Engineers, Part D: Journal of Automobile Engineering, 224(9), 1141–1159. https://doi.org/10.1243/09544070JAUTO1343
34. Amsden, A. A. (1997). KIVA-3V: A block-structured KIVA program for engines with vertical or canted valves (Report No. LA-13313-MS).
35. Kee, R. J., Rupley, F. M., & Miller, J. A. (1989). CHEMKIN-II: A FORTRAN chemical kinetics package for the analyses of gas phase chemical kinetics (Sandia Report No. SAND 89-8009).
36. Agarwal, A., & Assanis, D. (1998). Multi-dimensional modelling of natural gas ignition under compression ignition conditions using detailed chemistry. SAE Technical Paper No. 980136. https://doi.org/10.4271/980136
37. Han, Z., & Reitz, R. D. (1995). Turbulence modeling of internal combustion engines using RNG κ-ε models. Combustion Science and Technology, 106, 267–295. https://doi.org/10.1080/00102209508907782
38. Reitz, R. D. (1987). Modeling atomization processes in high-pressure vaporization spray. Atomization and Spray Technology, 3, 309–337.
39. Hosseini, V., & Checkel, M. D. (2006). Using reformer gas to enhance HCCI combustion of CNG in a CFR engine. SAE Technical Paper No. 2006-01-3247.
40. Handford, D., & Checkel, M. D. (2008). Direct injection assisted HCCI combustion of pre-mixed natural gas. FISITA Student Congress, F2008-SC-007.
41. Handford, D. (2009). Direct injection assisted HCCI combustion of natural gas (Master's thesis). University of Alberta.
42. Mack, J. H., Flowers, D. L., Buchholz, B. A., & Dibble, R. W. (2004). Investigation of HCCI combustion of diethyl ether and ethanol mixtures using carbon 14 tracing and numerical simulations. Proceedings of the Combustion Institute, 30(2), 2693–2700. https://doi.org/10.1016/j.proci.2004.08.136
43. Kokjohn, S., Hanson, R., Splitter, D., & Reitz, R. D. (2011). Fuel reactivity controlled compression ignition (RCCI): A pathway to controlled high-efficiency clean combustion. International Journal of Engine Research, 12(3), 209–226. https://doi.org/10.1177/1468087411401548
44. ANSYS Inc. (n.d.). Introduction to ANSYS ICEM CFD Hexa. http://www.ansys.com/services/training-center/platform/introduction-to-ansys-icem-cfd-hexa
45. Eng, J. A. (2002). Characterization of pressure waves in HCCI combustion. SAE Technical Paper No. 2002-01-2859. https://doi.org/10.4271/2002-01-2859
46. Kokjohn, S., Hanson, R., Splitter, D., Kaddatz, J., & Reitz, R. D. (2011). Fuel reactivity controlled compression ignition (RCCI) combustion in light- and heavy-duty engines. SAE Technical Paper No. 2011-01-0357. https://doi.org/10.4271/2011-01-0357
47. Reitz, R. D., & Duraisamy, G. (2015). Review of high efficiency and clean reactivity controlled compression ignition (RCCI) combustion in internal combustion engines. Progress in Energy and Combustion Science, 46, 12–71. https://doi.org/10.1016/j.pecs.2014.05.003
48. Opat, R., Ra, Y., Krieger, R., Reitz, R. D., Foster, D. E., Durrett, R. P., & Siewert, R. M. (2007). Investigation of mixing and temperature effects on HC/CO emissions for highly dilute low temperature combustion in a light duty diesel engine. SAE Technical Paper No. 2007-01-0193. https://doi.org/10.4271/2007-01-0193
49. Bidarvatan, M., & Shahbakhti, M. (2014). Integrated HCCI engine control based on a performance index. Journal of Engineering for Gas Turbines and Power, 136(10), 101601. https://doi.org/10.1115/1.4027279