Numerical Study of Reactivity Controlled Compression Ignition (RCCI) Combustion in a Heavy-Duty Diesel Engine Using 3D-CFD Coupled with Chemical Kinetics

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Abstract

In this paper, a numerical study is performed to provide the combustion and emission characteristics resulting from fuel-reactivity controlled compression ignition (RCCI) combustion mode in a heavy-duty, single-cylinder diesel engine with gasoline and diesel fuels. In RCCI strategy in-cylinder fuel blending is used to develop fuel reactivity gradients in the combustion chamber that result in a broad combustion event and reduced pressure rise rates (PRR). RCCI has been demonstrated to yield low NOx and soot with high thermal efficiency in light and heavy-duty engines. KIVA-CHEMKIN code with a reduced primary reference fuel (PRF) mechanism are implemented to study injection timings of high reactivity fuel (i.e., diesel) and low reactivity fuel percentages (i.e., gasoline) at a constant engine speed of 1300 rpm and medium load of 9 bar indicated mean effective pressure (IMEP). Significant reduction in nitrogen oxide (NOx), while 49% gross indicated efficiency (GIE) were achieved successfully through the RCCI combustion mode. The parametric study of the RCCI combustion mode revealed that the peak cylinder pressure rise rate (PPRR) of the RCCI combustion mode could be controlled by several physical parameters – PRF number, and start of injection (SOI) timing of directly injected fuel.

***Keywords**: Reactivity controlled compression ignition (RCCI); start of injection (SOI); primary reference fuel (PRF); gross indicated efficiency (GIE); NOx emissions*

1. Introduction

Growing fossil fuel consumption along with increase in fuel cost and a focus on the reduction of carbon dioxide (CO2) emissions in the transportation sector motivate the need for increased efficiency from the internal combustion engine (ICE). Diesel and gasoline engines are the most common types of ICEs used in the transportation sector. The diesel or compression ignition (CI) engine has superior characteristics compared to petrol or spark-ignited (SI) engines, because of its ability to use high compression ratios (CR) without engine knock, lack of throttling losses, high combustion efficiency, and favorable gas properties for work extraction due to lean operation. However, diesel engines also have benefits and problems in exhaust emissions. They offer reduced emissions of partial combustion products such as carbon monoxide (CO) and hydrocarbons (HC) due to excess air and high in-cylinder temperatures, which combine to oxidize both HC and CO to the complete combustion products, water (H2O) and carbon dioxide. However, due to the heterogeneous nature of the diesel combustion process, particulate matter (PM) and oxides of nitrogen (NOx) emissions have been a challenge for diesel engines [1,2].

Although aftertreatment systems (e.g., DPF, LNT and SCR) are capable of reducing engine emissions to a low level, these efforts generally resulted in poor fuel economy; thus removing the CI engine's advantages over the SI engine [3-6]. Therefore, combustion research for the reduction of NOx and soot emissions while maintaining high thermal efficiency has been led to investigations of advanced combustion strategies based on low temperature combustion (LTC). Lower combustion temperatures

result in NOx reduction due to the high activation energy of NO formation reactions [7]. In addition, utilizing a long ignition delay allows adequate time for mixing prior to the start of combustion; thus, rich regions are reduced and soot formation is inhibited.

There are various LTC strategies, but most are categorized as premixed compression ignition (PCI), including homogeneous charge compression ignition (HCCI), premixed charge compression ignition (PCCI) (also known as partially premixed combustion (PPC)), and reactivity controlled compression ignition (RCCI). Fig. 1 shows the RCCI, PCCI, LTC, HCCI and conventional diesel combustion (CDC) operating regimes plotted on a local equivalence ratio – local temperature space diagram adapted from the work of Neely et al. [8,9].

Due to the existing fuel infrastructure, most HCCI and PCCI research has been conducted using either strictly gasoline or diesel fuel. However, in their neat forms, each fuel has specific advantages and shortcomings for PCCI operation. Since low reactivity fuels like gasoline have difficulty achieving ignition at low-load conditions and high reactivity fuels like diesel have difficultly controlling combustion phasing at high load condition, many researchers have investigated PCI operation using fuel blends. Bessonette et al. [10], Inagaki et al. [10] and Kokjohn et al. [12] showed that different fuel blends will be required at different operating conditions in HCCI and PCCI modes (e.g., a high cetane fuel at light load and a low cetane fuel at high load). Thus, it is desirable to have the capability to operate with fuel blends covering the spectrum from neat gasoline to neat diesel fuel depending on the operating regime.

In recent years, a series of studies on RCCI combustion have been conducted at the engine research center (ERC) of the University of Wisconsin-Madison. RCCI is a dual fuel PPC concept developed by Kokjohn et al. [12]. As shown in Fig. 2, in cylinder fuel blending is arranged using port fuel injection of a low reactivity fuel, (e.g., gasoline, E85, etc.) coupled with optimized multiple direct injections of a high reactivity fuel (e.g., diesel fuel, B20, etc.) [13]. For example, a small amount of pilot diesel is injected directly into the combustion chamber and ignites a highly diluted gasoline-air mixture (see Fig. 2). As the diluted gasoline-air mixture does not ignite without the diesel, the ratio between diesel and gasoline as well as the pilot injection timing can be used to control the combustion process. RCCI relies on the stratification versus homogenization of diesel and therewith the stratification of ignitability. The stratification can be easily controlled by the diesel direct injection [14]. This strategy generates both equivalence ratio and reactivity stratifications in the combustion chamber. Combustion progresses sequentially from the high reactivity regions to low reactivity regions, thereby effectively lowering PRR [15]. In addition, flame propagation plays a negligible role during the RCCI combustion process due to the very lean equivalence ratios [16].

Recently, there have been review articles in the literature on RCCI, which provide a comprehensive and thorough study regarding this newly developed combustion mode [17,18]. In addition, a number of studies have been carried out that demonstrate the superiority of the RCCI strategy compared to CDC [9,19-22]. The most comprehensive one is Kokjohn's work [16] in which RCCI combustion was run on a heavy-duty engine over a wide range of engine loads by varying the gasoline-to-diesel ratio while keeping the diesel injection strategy fixed. The RCCI strategy resulted in lower emissions of NOx and soot, high gross indicated efficiency (GIE), and low PRR (i.e., ringing intensity (RI) compared to HCCI combustion. They also implemented the KIVA-3V CFD code tools to capture the physics of the RCCI combustion process to study the sources of efficiency benefits compared to CDC. The average temperatures are predicted to be very similar; however, the peak combustion temperature for CDC and RCCI is near 2800 and 1700 K, respectively.

Multi-dimensional computational fluid dynamics (CFD) modeling with detailed chemistry can provide the most accurate predictions which would also require great computing power.

Dempsey and Reitz [23] optimized a heavy-duty CI engine to operate with RCCI combustion with gasoline and diesel using the KIVA code incorporating CHEMKIN II and a reduced PRF mechanism, together with a multi-objective genetic algorithm (MOGA) NSGA II, and the COSSO regression model. The main objective of their work was to investigate whether clean and efficient RCCI combustion could be achieved at full load, while maintaining acceptable engine performance at low-loads. According to the above optimizations, it was possible to create engine operating strategies that cover the entire speed-load range of the heavy-duty engine. Splitter et al. [24] tried to achieve 50% BTE or greater in a heavy-duty engine via simulations using GT-Power, and they found that GTEs excess of 59% with corresponding near-zero levels of NOX and PM would be achieved, with use of 18.6 CR with a 50% reduction in both heat transfer and combustion losses. However, the results also demonstrated that improvements to boosting system efficiencies for low exhaust temperatures and overall reductions in

Friction is required to best capitalize on the high gross efficiencies.

Recently, Lim and Reitz [25] optimized the injection strategy for a heavy-duty CI engine for high load RCCI operation using the KIVA3v-Release2 code, featuring a sparse analytical Jacobian chemistry Solver (SpeedCHEM), and the multi-objective genetic algorithm, NSGA II. A series of SOI sweeps was performed with three injections –2 iso-octane injections and 1 n-heptane injection –in order to better understand the roles of those injections in combustion control. They found that when a larger mass is given in the 1st injection, it can effectively reduce the RI.

By this time, there is no research paper published regarding RCCI combustion research in Iran. In this paper, the combustion and emission characteristics in a heavy-duty diesel engine operating on RCCI mode (gasoline/diesel) is investigated using a coupled 3D-CFD/Chemistry model. Model predictions are validated using measured in-cylinder pressure histories. Basing on the in-cylinder reactivity and fuel distributions, the impacts of important parameters, i.e. gasoline mass fraction and diesel SOI timing are understood.

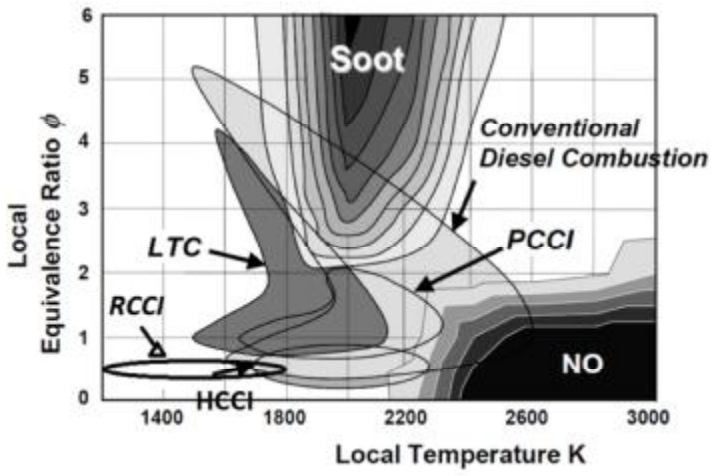


Fig1. RCCI, PCCI, LTC, HCCI and CDC operating regimes plotted on $f-T$ diagram space adapted from the work of Neely et al. and Kokjohn et al. [8,9]

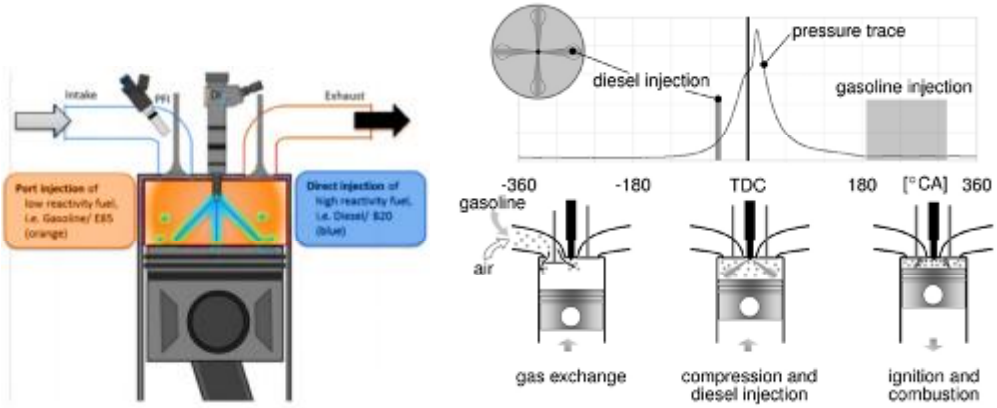


Fig2. RCCI combustion strategy and concept with different fuel characteristics [13,14]

2. Numerical model and validation

The KIVA-3V code [26] is selected as 3D-CFD framework for simulations of reactive fluid flow. KIVA uses finite-volume, temporal-differencing scheme in solution procedures of three dimensional conservation equations and turbulence at the same time. This solution procedure, namely the Arbitrary Lagrangian-Eulerian (ALE) method, decouples calculations of the diffusion and convection terms from chemical source terms. Hence, each computational cell can be treated as a homogeneously mixed reactor at each time-step. The three-dimensional computational grid, seen in Fig. 3, is a 60-degree sector mesh comprised of approximately 30510 cells at BDC with average cell size of 3 mm. The various physical and chemistry submodels used in KIVA-3V are listed in Table 1.

Continuity equation for species m and energy equation in terms of specific internal energy are formulated in KIVA as given in Eqs. (1) and (2), respectively [26],

$$\frac{\partial \rho_m}{\partial t} + \nabla.(\rho_m u) = \nabla.\left[\rho D \nabla\left(\frac{\rho_m}{\rho}\right)\right] + \dot{\rho}^c_m + \dot{\rho}^s \delta_{m_s} \quad (1)$$

$$\frac{\partial (r I)}{\partial t} + \nabla.(r u I) = -P\nabla.u + (1 - A_{ikesw}) s : \nabla u - \nabla.J + A_{ikesw} re + \dot{Q}^c + \dot{Q}^s \quad (2)$$

where $\dot{R}^c_m$ in Eq.(1) and $\dot{Q}^C$ in Eq.(2) are the source terms that need to be calculated by CHEMKIN and DVODE codes. Mathematical descriptions of these terms are as follows:

$$\dot{R}^c_m = r \frac{dY_m}{dt} \quad (3)$$

$$\dot{Q}^c = -\sum_{m=1}^{M} \frac{dY_m}{dt} \frac{(\Delta h_f^{\,o})_m}{W_m} \quad (4)$$

where $(\Delta h_f^{\,o})_m$ is the molar heat of formation of species m, Wm is the molecular weight of species m and Ym is the mass fraction of species m. By refer to above equations, it can be declared that the ultimate goal of a sample combustion model is to determine the chemical species net production rates ($\dot{w}_m$) using Eq. (5).

$$\frac{dY_m}{dt} = \frac{\dot{w}_m W_m}{r} \quad (5)$$

To calculate the molar production rate of chemical species participated in the chemical kinetics mechanism, the gas phase kinetics library of CHEMKIN-II [27] is integrated into KIVA code as shown in Fig. 4. In this procedure, the chemistry routine in the KIVA has been modified to perform chemistry solutions by iterative calling of DVODE [28]. This new unit acts as an interface between KIVA and CHEMKIN and updates the combustion source terms of Eqs. (1) and (2). The binary linking file including species and chemical reactions data in CHEMKIN format is generated by CHEMKIN interpreter prior to each simulation. The KIVA code provides the species concentrations and thermodynamic information of each individual cell at every time step to pass to CHEMKIN solver (when temperature rises above 600 K). The CHEMKIN subroutines construct M-set of stiff ordinary differential equations and DVODE subroutine is then successively called to compute the species net production rates at the end of each time step.

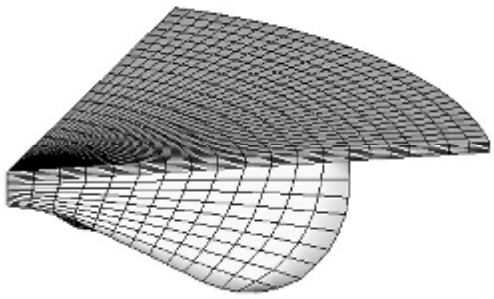


Fig3. Computational grid showing piston bowl geometry of the Caterpillar SCOTE engine

Table 1: Models used in KIVA-3V

Turbulence	RNG $k-e$
Spray break-up	TAB
Spray Collision	O'Rourke
Combustion model	KIVA-CHEMKIN
Fuel chemistry	Reduced PRF mechanism
NOx mechanism	Extended Zeldovich

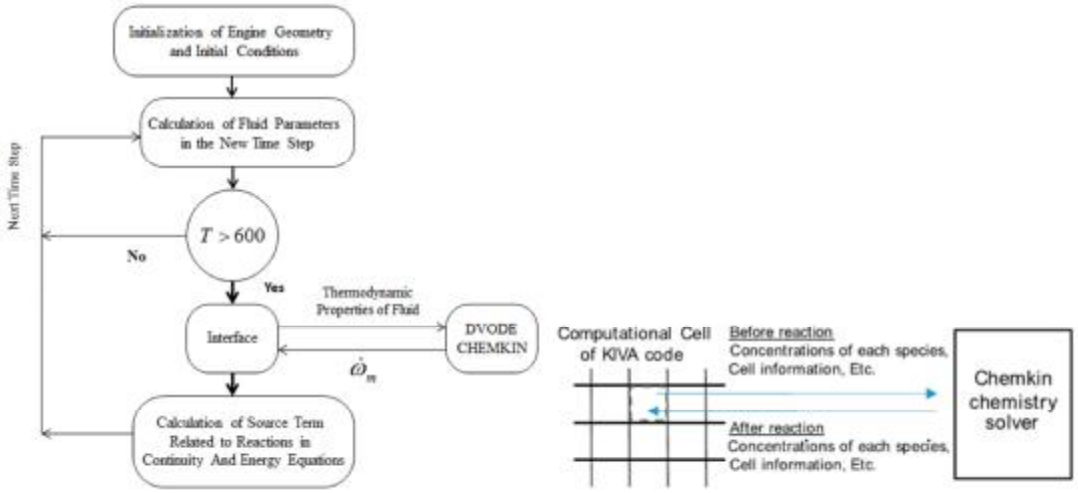


Fig4. Flowchart and diagram of coupled KIVA-CHEMKIN-DVODE model

Table 2. Caterpillar 3401E SCOTE engine geometry [19]

Displacement	2.44 L
Bore × Stroke	13.72×16.51 cm
Connecting rod length	21.16 cm
Compression ratio	16.1:1
Swirl ratio	0.7
Bowl type	Mexican Hat
Number of valves	4
Intake valve opening	3350 ATDC
Intake valve closing	-1430 ATDC
Exhaust valve opening	1300 ATDC
Exhaust valve closing	-3350 ATDC

The model is validated using published experimental data of a heavy-duty Caterpillar 3401E SCOTE engine converted to operate under RCCI mode by Hanson et al. [19] and Nieman et al. [29]. The engine geometry is summarized in Table 2. The engine experiments were conducted at 9 bar IMEP and 1300 rev/min and the operating conditions are given in Table 3.

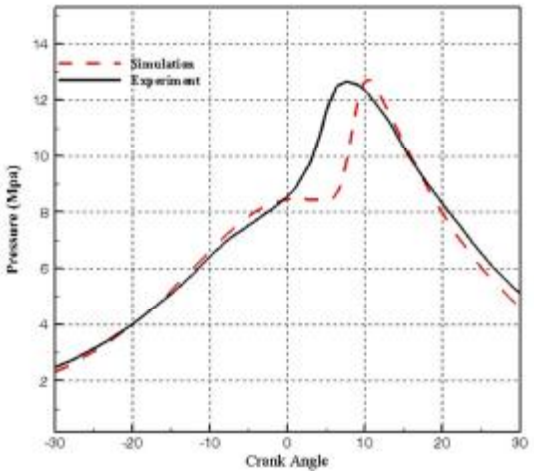
Conventional gasoline and diesel fuels are multi-component fuels and consist of a wide range of hydrocarbon species, and it is thus not practical in engineering applications to kinetically model each species in the real fuel. Therefore, the ignition and combustion characteristics of automotive fuels are typically represented by blends of the primary reference fuels (PRF), namely iso-octane and n-heptane. In this work, the ignition and combustion

characteristics of iso-octane and n-heptane are used to model the kinetics of gasoline and diesel fuel, respectively. A reduced PRF mechanism consisting of 45 species and a 142 reactions, which includes NOx chemistry, was utilized in this study to represent the autoignition and subsequent combustion of gasoline and diesel fuel [30].

Fig. 5 shows predicted cylinder pressure histories compared to experiments. It can be seen that the model predictions of ignition delay, peak pressure location and magnitude are rather in good agreement with experimental data. As it can be seen on Fig. 5, there is a slight under-prediction in combustion duration histories. This problem can be regarded to use of TAB spray breakup model, which models the droplet interaction as a spring-mass system. Such model was observed to over-predict the relative velocity between the liquid droplet and the surrounding gas due to lower drag coefficients. Consequently, the droplet diameter size would be smaller, vaporizes faster and therefore the cylinder pressure are over-predicted [31]. However, the experimental and simulation values of GIE, RI and NOx emissions are in acceptable range.

Table 3. Operating conditions for the constant speed RCCI engine [19]

Engine Speed (RPM)	1300
Intake Pressure (bar)	1.74
Intake Temperature $(^{\circ}C)$	32
Total Fuel (g)	0.094
Premix Fuel Equivalence Ratio (-)	0.35
Percent Gasoline by Mass (%)	89
Diesel SOI 1 (deg ATDC)	-58.0
Diesel SOI 2 (deg ATDC)	-37
Fraction of Diesel in 1st Injection (-)	0.6
EGR (%)	43



	GIE(%)	Ringing Intensity (MW/m2)	NOx(g/KW.hr)
Experiment	52.2	3.7	0.01
Simulation	49.22	3.83	0.0067

Fig5. Comparison of measured and predicted in-cylinder pressure history, GIE, RI and NOx emissions for RCCI operation

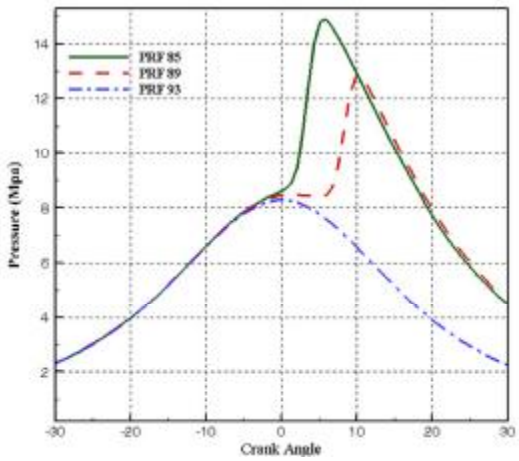
3. Results and Discussion

3.1. Effects of varying the in-cylinder fuel blending ratio (PRF)

Regarding the literature, varying fuel reactivity seems to be a suitable solution to RCCI combustion. Thus, the proportion of premixed fuel (gasoline) was changed to investigate the effect of PRF number on the combustion and emission characteristics of the RCCI combustion mode. The variations of in-cylinder

pressure history, GIE, RI and NOx emissions for various PRF numbers are depicted in Fig. 6. As can be seen, PRF 93 corresponds to the engine misfiring conditions. It can be noticed that, the peak pressure is higher for PRF 85 compared to PRF 89, however its GIE is lower. It may be attributed to the fact that as the PRF is lower, the reactivity and the burning rates are increased as well, leading to increased work done by the system with PRF 89 fuel as shown in Fig. 7. It can also be seen that at start of combustion (SOC) peak pressure is higher for PRF 85, and the work done is higher. But by closing to the EVO timing, it is gradually decreased.

Figs. 8 and 9 illustrate the in-cylinder temperature history and contours for various PRF numbers in RCCI combustion. It is evident that the combustion temperatures of the RCCI combustion mode are significantly lower than those of the CDC mode. Furthermore, the combustion temperatures in the RCCI combustion mode were decreased further as increasing PRF.



	GIE (%)	Ringing Intensity (MW/m^2)	NO_x(g/KW.hr)
PRF 89	49.22	3.83	0.0067
PRF 85	48.9295	11.4163	0.0098

Fig6. Predicted in-cylinder pressure history, GIE, RI and NOx emissions for various PRF numbers

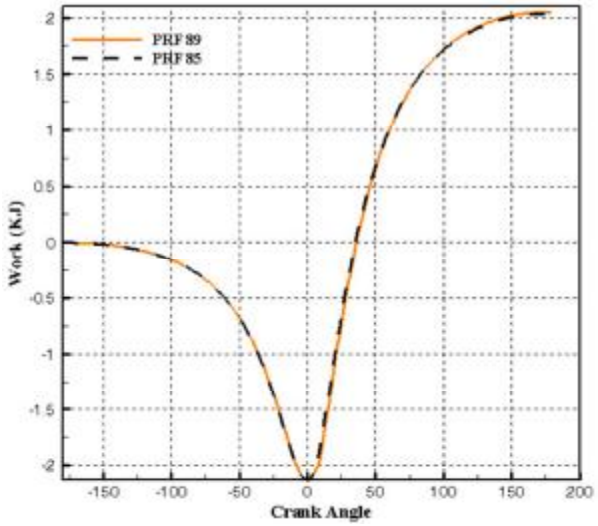


Fig7. Indicated work versus crank angle at two different PRF number

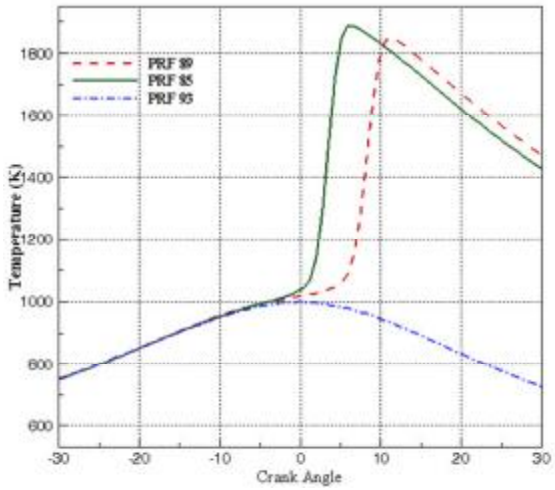
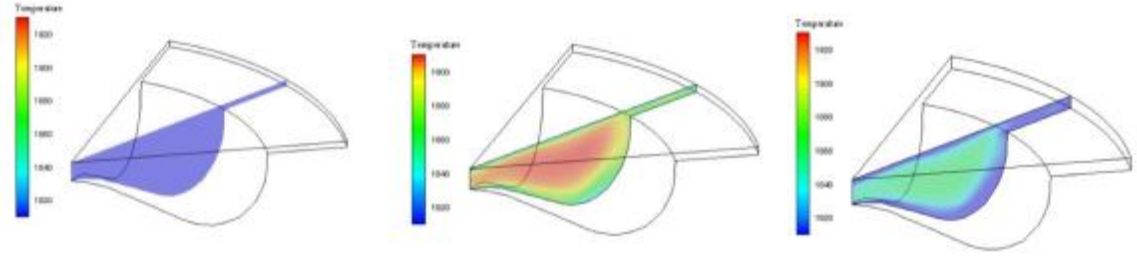


Fig8. Predicted in-cylinder temperature history for various PRF numbers



Crank=0^0 ATDC Crank=5^0 ATDC Crank=10^0 ATDC

Fig9. Contours of predicted in-cylinder temperature for PRF 85 at different crank angles

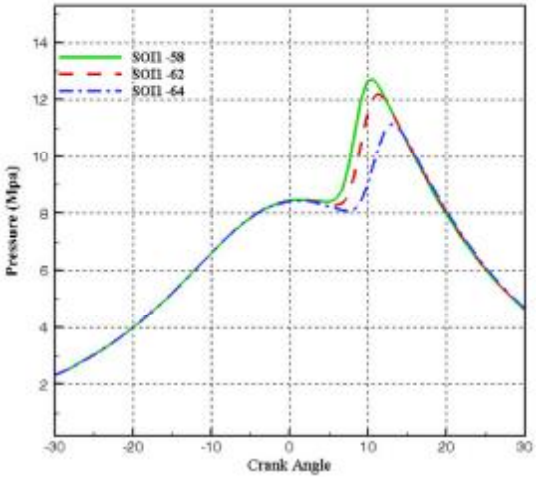


Fig10. Predicted in-cylinder pressure history over SOI-1 timing sweep

3.2. Effect of first main injection (SOI-1) timing

In this section, the investigations are conducted according to the conditions presented in Table 3 with injection timing (SOI-1) sweeps from -58 to -64 ATDC. As the SOI-1 timing was advanced, it was noticed that NOx and PPRR were reduced (see Figs. 10 and 11). This results in reduced in-cylinder temperatures as shown in Fig. 12. It can be seen that, as the SOI-1 is advanced, the increased mixing time between SOI-1 and SOI-2, results in a lower concentration of n-heptane which reduces local fuel reactivity (i.e., the local PRF number is increased) and therefore, leads to increased ignition delay. It could be explained that the advanced SOI-1 timing causes the more-homogeneous fuel-air mixture, due to longer time available for fuel-air mixing. This would eventually lead to lower PPRR and in-cylinder temperatures. In addition, existence of locally fuel-lean regions results in lower local cylinder temperatures that reduce the NOx formation. As shown in Fig. 13, a slightly lower GIE and RI are observed as advancing SOI-1 timing

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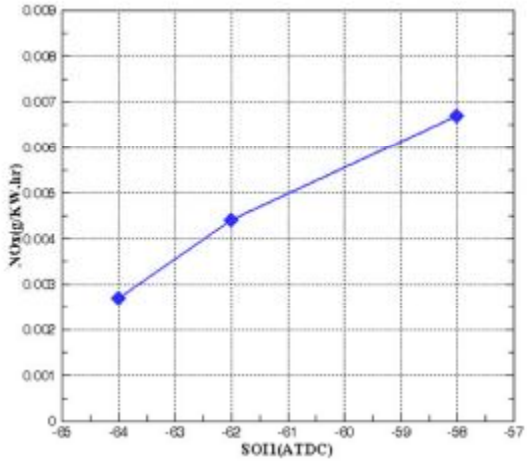

Fig11. Variation of NOx emissions over SOI-1 timing sweep

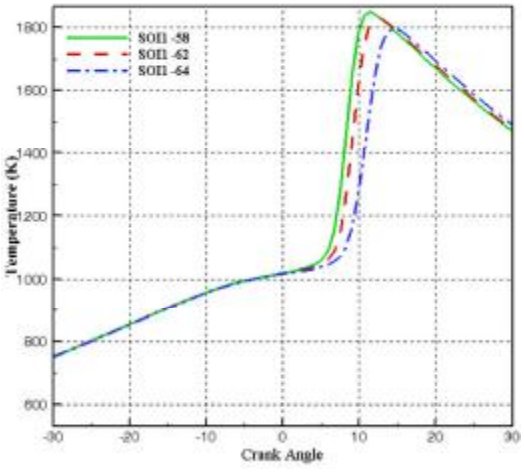

Fig12. Predicted in-cylinder temperature history over SOI-1 timing sweep

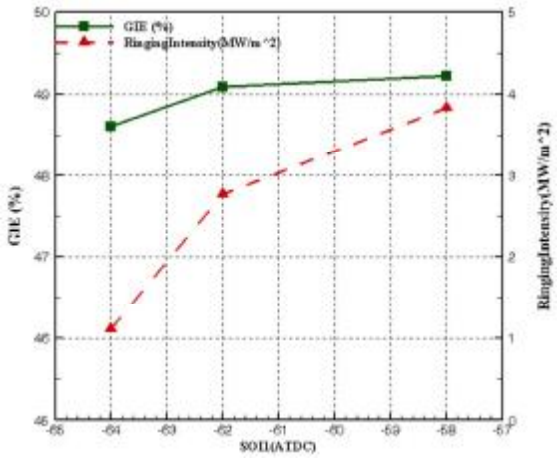

Fig13. GIE and RI over SOI-1 timing sweep

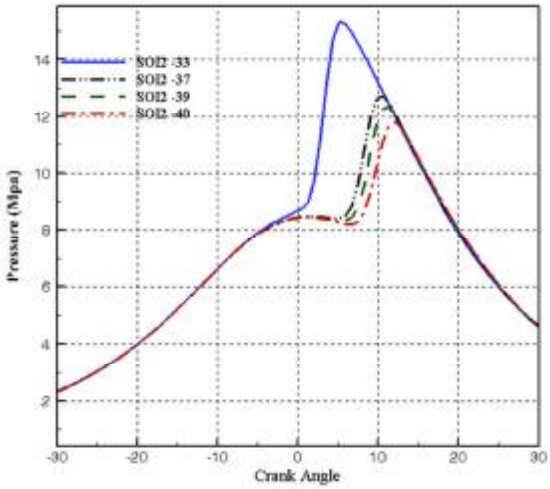

Fig14. Predicted in-cylinder pressure history over SOI-2 timing sweep

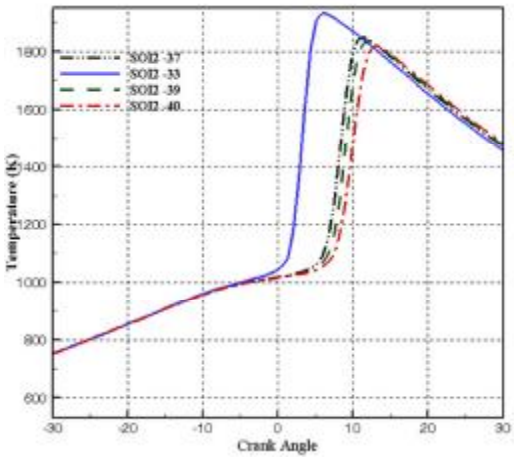

Fig15. Predicted in-cylinder temperature history over SOI-2 timing sweep

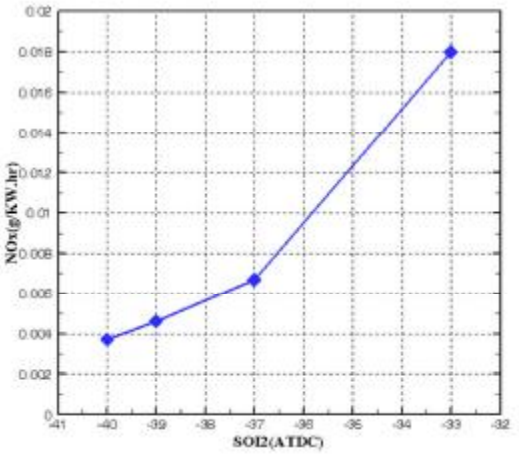

Fig16. Variation of NOx emissions over SOI-2 timing sweep

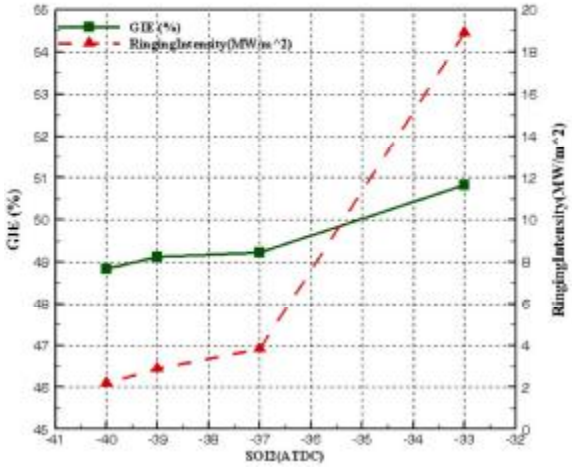

Fig17. GIE and RI over SOI-2 timing sweep

3.3. Effect of second main injection (SOI-2) timing

Similar to the SOI-1 timing sweep, in the case of SOI-2 timings, when the injection timing was retarded, less-homogeneous fuel-air mixture exists within the cylinder, and thus higher concentration of n-heptane enhances local fuel reactivity and the PPRR and in-cylinder temperature as well (see Fig. 14). Due to the advanced combustion phasing and increased PPRR, the cylinder temperature is high as shown in Fig. 15. This increased cylinder temperature is mainly due to the retarded injection timing, since when the time available for mixing is less, fuel-rich regions exist, which causes increased NOx emissions as shown in Fig. 16. Fig. 17 shows the variation of GIE and RI over SOI-2 timing sweep. As can be noticed, the variations of RI with SOI-2 timing is more intense compared to SOI-I. As the SOI-2 is retarded towards -33 ATDC, the RI is greatly increased and exceeds the 10 MW/m2 limit.

Conclusion

In this paper, a heavy-duty compression ignition engine was converted to operate with dual fuel Reactivity Controlled Compression Ignition (RCCI) combustion with gasoline and diesel. This was accomplished using computational tools, namely, the multi-dimensional engine CFD code KIVA incorporating CHEMKIN II and a reduced PRF

mechanism. The conclusions can be drawn as follows:

The numerical study of the RCCI combustion mode revealed that the PPRR of the RCCI combustion mode could be controlled by several physical parameters – PRF number, and diesel SOI timing.

As the in-cylinder fuel blending ratio is varied towards lower global reactivity blends (PRF 89), the ignition delay gets longer and the fuel reactivity stratification is improved. That implies a premixed stage of combustion slightly lowered and combustion duration is shortened.

When using a double injection strategy for the diesel injection, the timing of the first injection (SOI-1) was found to increase mixture stratification as SOI-1 was retarded toward TDC. The increased local equivalence ratio raised combustion temperatures and local fuel reactivity, which then resulted in advanced combustion phasing and increased PRR and NOx emissions.

The timing effect of the second diesel injection (SOI-2) was also found to similar to the SOI-1 timing, with deteriorations in PPRR and RI of the engine in more retarded SOI-2.

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