

CFD Study of Reactivity Controlled Compression Ignition (RCCI) Combustion in a Heavy-Duty Diesel Engine

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Abstract

In this paper, a numerical study is carried out to investigate the combustion and emission characteristics of reactivity controlled compression ignition (RCCI) combustion mode in a heavy-duty, single-cylinder diesel engine with gasoline and diesel fuels using KIVA-CHEMKIN code with a reduced primary reference fuel (PRF) mechanism. Firstly, a comparison is performed between RCCI and CDC performance and emissions to show the superior characteristics of RCCI combustion. Then, the effect of diesel fuel mass fraction in SOI-1 on combustion and emissions of RCCI engine is studied. It is shown that by increasing the diesel mass fraction in SOI-1, combustion event occurs earlier and PPRR is slightly higher. But this parameter has a trivial influence compared to PRF number and SOI timing.

Keywords

Reactivity controlled compression ignition (RCCI), Start of injection, gross indicated efficiency (GIE), NOx emissions, Ringing intensity (RI)

1 Introduction

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, due to the heterogeneous nature of the diesel combustion process, particulate matter (PM) and oxides of nitrogen (NO_x) emissions have been a challenge for diesel engines (Dec, 2009; Stone, 2012; Mickevičius et al., 2014; Andrejszki et al., 2014).

Although after treatment 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 (due to periodic regeneration; periodically rich operation, and need of a secondary reducing agent); thus removing the CI engine's advantages over the SI engine (Johnson, 2006; 2009; 2011; 2014). Therefore, combustion research for the reduction of NO_x 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 NO_x reduction due to the high activation energy of NO formation reactions. 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 (Turns, 2005; Makarevičienė et al., 2013).

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).

Due to the existing fuel infrastructure, most HCCI and PCCI research have 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

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difficulty controlling combustion phasing at high load condition, many researchers have investigated PCI operation using fuel blends. Bessonette et al. (2007), Inagaki et al. (2006) and Kokjohn et al. (2010) 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. (2010). In this strategy, 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.). For example, a small amount of pilot diesel is injected directly into the combustion chamber and ignites a highly diluted gasoline-air mixture. 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. 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. In addition, flame propagation plays a negligible role during the RCCI combustion process due to the very lean equivalence ratios (Kokjohn, 2012; Reitz, 2013; Eichmeier et al., 2014).

Recently, there have been review articles in the literature on RCCI, which provide a comprehensive and thorough study regarding this newly developed combustion mode (Reitz and Duraisamy, 2015; Paykani et al., 2015a). In addition, a number of studies have been carried out that demonstrate the superiority of the RCCI strategy compared to CDC (Kokjohn et al., 2011; 2013; Hanson et al., 2010; Curran et al., 2013). The most comprehensive one is Kokjohn's work (2012) 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 NO_x 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 (2011) 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. (2013) 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 NO_x 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 are required to best capitalize on the high gross efficiencies.

Kakaee et al. (2014) investigated the combustion and emission characteristics resulting from RCCI combustion mode in a heavy-duty, single-cylinder diesel engine with gasoline and diesel fuels using KIVA-CHEMKIN code. The parametric study revealed that the PRR of the RCCI combustion could be controlled by several physical parameters such as PRF number, and the start of injection (SOI) timing of injected diesel fuel.

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.

2 Numerical model and validation

The KIVA-3V code (Amsden, 1997) is selected as a 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. 1, is a 60-degree sector mesh comprised of approximately 30510 cells at BDC with the average cell size of 3 mm. The various physical and chemistry submodels used in KIVA-3V are listed in Table 1.

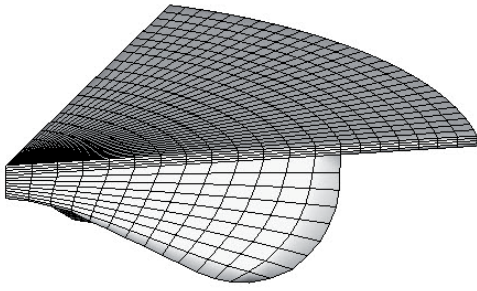


Fig. 1 Computational grid showing piston bowl geometry of the Caterpillar SCOTE engine

Table 1 Models used in KIVA-3V

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

The 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 (Amsden, 1997),

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m u) = \nabla \cdot \left[\rho D \nabla \left(\frac{\rho_m}{\rho} \right) \right] + \dot{\rho}_m^c + \dot{\rho}_m^s \delta_{ml} \quad (1)$$

$$\frac{\partial (\rho I)}{\partial t} + \nabla \cdot (\rho u I) = -P \nabla \cdot u + (1 - A_{kesw}) \sigma : \nabla u - \nabla \cdot J + A_{kesw} \rho \epsilon + \dot{Q}^c + \dot{Q}^s \quad (2)$$

where $\dot{\rho}_m^c$ 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:

$$\dot{\rho}_m^c = \rho \frac{dY_m}{dt} \quad (3)$$

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

where $(\Delta h_f^o)_m$ is the molar heat of formation of species m , W_m is the molecular weight of species m and Y_m is the mass fraction of species m . By referring 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 ($\dot{\omega}_m$) using Eq. (5).

$$\frac{dY_m}{dt} = \frac{\dot{\omega}_m W_m}{\rho} \quad (5)$$

To calculate the molar production rate of chemical species participated in the chemical kinetics mechanism, the gas phase

kinetics library of CHEMKIN-II (Kee et al., 1989) is integrated into KIVA code as shown in Fig. 2. In this procedure, the chemistry routine in the KIVA has been modified to perform chemistry solutions by iterative calling of DVODE (Brown et al., 1989). 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 the 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.

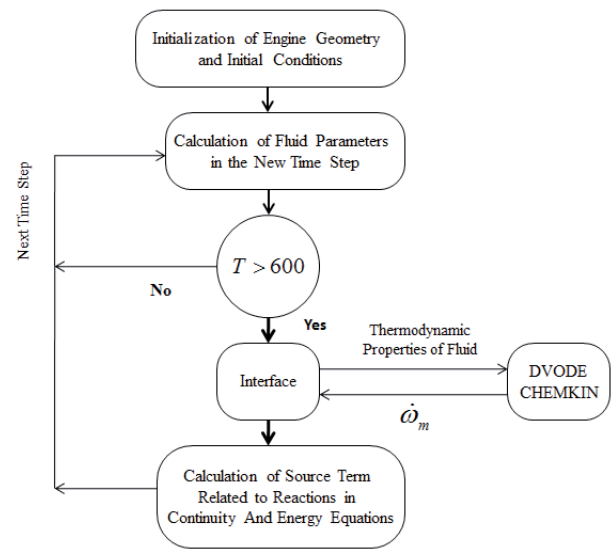


Fig. 2 Flowchart and diagram of coupled KIVA-CHEMKIN-DVODE model

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. (2010) and Nienman et al. (2012). 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 (Ra and Reitz, 2008).

Figure 3 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. 3, there is a slight over-prediction in combustion duration histories. This problem can be regarded to the 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 (Mazi, 2009). However, the experimental and simulation values of GIE, RI and NO_x emissions are in acceptable range.

Table 2 Caterpillar 3401E SCOTE engine geometry (Hanson et al., 2010)

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	335° ATDC
Intake valve closing	-143° ATDC
Exhaust valve opening	130° ATDC
Exhaust valve closing	-335° ATDC

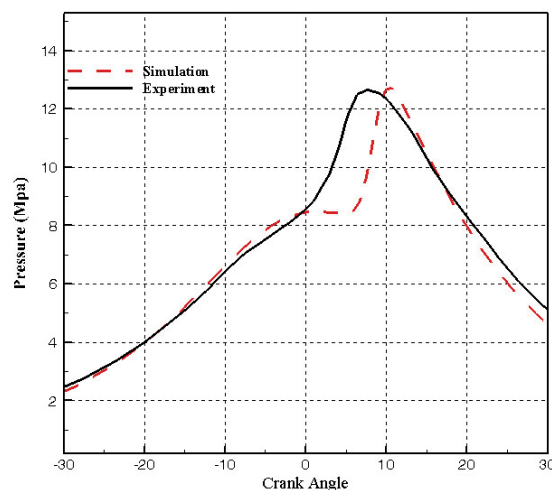
Table 3 Operating conditions for the constant speed RCCI engine (Hanson et al., 2010)

Engine Speed (RPM)	1300
Intake Pressure (bar)	1.74
Intake Temperature (°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 1 st Injection (-)	0.6
EGR (%)	43

3 Results and discussion

3.1 Comparison of RCCI and CDC

In this section, the performance and emissions of RCCI and CDC engines are compared. According to previous results, the GIE of RCCI engine is about 50% and its out NO_x emissions is below the 0.01 gr/KW.hr. For comparison, the diesel engine operation condition is at constant load of 9.9 bar IMEP and the detailed conditions are tabulated in Table 4 (Tess et al., 2011).



	GIE (%)	Ringling Intensity (MW/m ²)	NO _x (g/kW.h)
Experiment	52.2	3.7	0.01
Simulation	49.22	3.83	0.0067

Fig. 3 Comparison of measured and predicted in-cylinder pressure history, GIE, RI and NO_x emissions for RCCI operation

Table 4 Operating conditions for the constant load CDC engine (Tess et al., 2011)

Engine Speed (RPM)	1208
Intake Temperature (°C)	40
Diesel fuel mass fraction (mg)	117
Diesel fuel SOI (deg ATDC)	-10
IVC (deg ATDC)	-143
EVO (deg ATDC)	130
EGR (%)	0

The comparison of in-cylinder pressure histories for RCCI and CDC engines is shown in Fig. 4. Figure 5 illustrates Comparison of predicted GIE, RI and NO_x emissions for RCCI and CDC engines.

As can be seen, it is possible to achieve higher GIEs and lower NO_x emissions in RCCI mode. It can be explained that not only does CDC have regions of the combustion chamber at significantly higher temperatures than the RCCI case, but these regions tend to be located on or near the piston bowl due to the penetration of the fuel jet. These high-temperature regions result in significantly increased piston bowl heat transfer and reduced thermal efficiency. While a majority of the improvements of the GIE can be attributed to reductions in heat transfer losses, the remaining improvement in GIE is due to improved control over the combustion event in RCCI case. On the other hand, high temperature regions in CDC would result in higher NO_x emissions compared to RCCI mode.

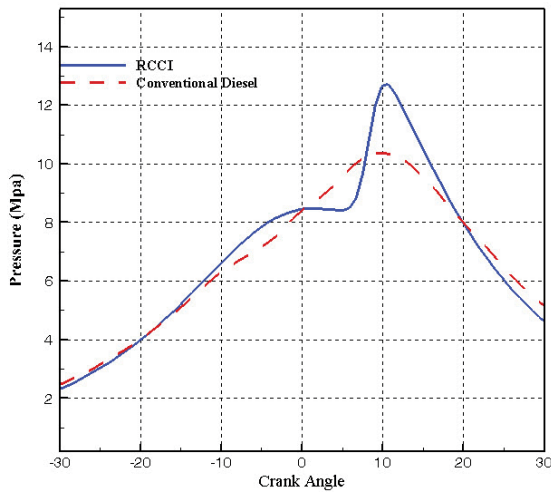


Fig. 4 Comparison of predicted in-cylinder pressure history for RCCI and CDC engines

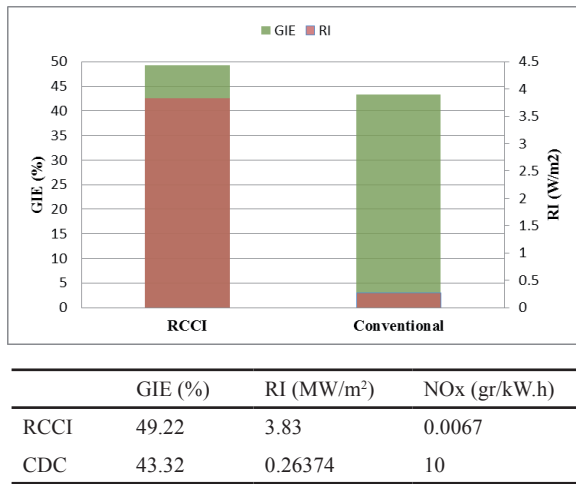


Fig. 5 Comparison of GIE, RI and NOx emissions for RCCI and CDC engines

3.2 Effect of diesel mass fraction

One of the important parameters affecting RCCI engine performance is the mass fraction of injected diesel fuel between two splits. Figure 6 shows the predicted in-cylinder pressure history with the mass fractions of 53%, 60% and 69% in the first split at the case of SOI-1 = -58 and SOI-2 = -37 ATDC. It is evident that as the mass fraction of fuel is higher in the second split, the SOC is earlier and the PPRR is slightly higher. Thus, the second split plays the energy source role for the combustion and it can be used for the combustion event control.

Figure 7 depicts the effect of diesel SOI-1 fraction on the GIE and RI. As expected, by increasing PPRR in the case of SOI-1 fraction=0.53, the RI is increased and exceeds the allowable limit of 5 MW/m² (Paykani et al., 2015b). The variation of in-cylinder temperature history with diesel SOI-1 fraction is plotted in Fig. 8. As can be seen, as the SOC closes to the TDC, temperature increases, and it would eventually results in higher NOx emissions. The NOx emissions trend is shown in Fig. 9.

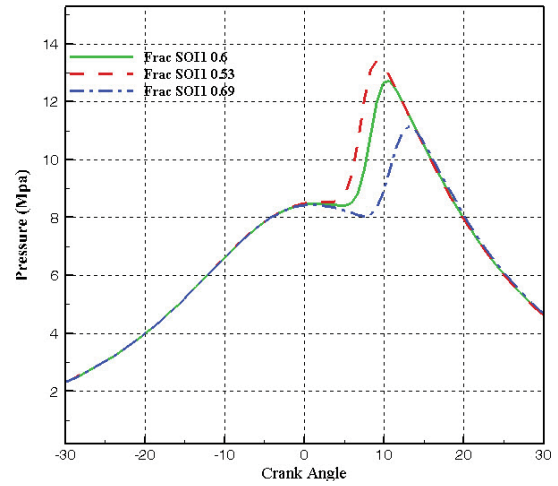


Fig. 6 Comparison of predicted in-cylinder pressure history for various fractions of diesel SOI-1

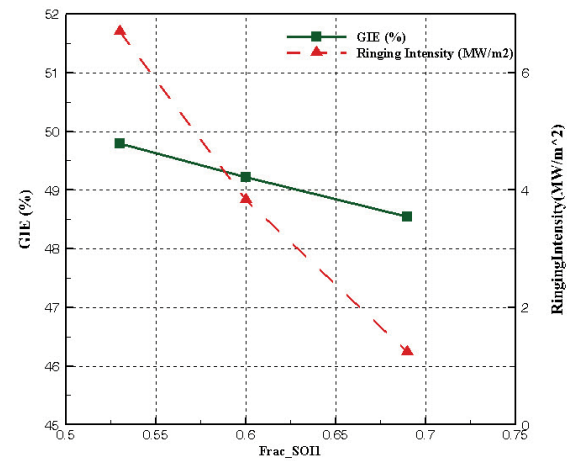


Fig. 7 GIE and RI over SOI-1 diesel mass fraction sweep

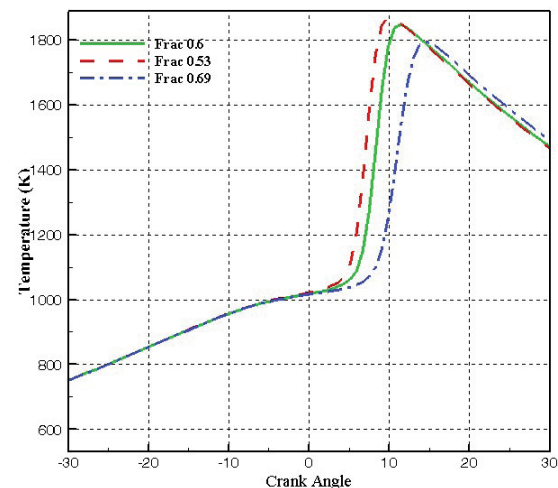


Fig. 8 Predicted in-cylinder temperature history over SOI-1 diesel mass fraction sweep

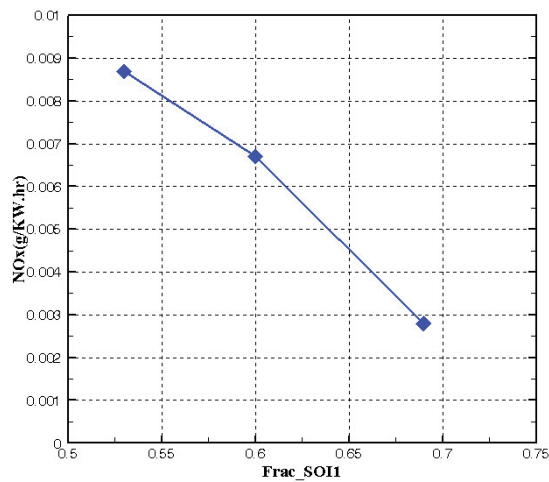


Fig. 9 Variation of NOx emissions over SOI-1 diesel mass fraction sweep

4 Conclusion

This paper numerically studies dual fuel Reactivity Controlled Compression Ignition (RCCI) combustion with gasoline and diesel 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 RCCI combustion mode gives higher GIE and lower NOx emissions compared to CDC. However, its RI is significantly higher, but it is still below the allowable limit.
- As the peak pressure is closer to the TDC, GIE and RI are higher. On the other hand, the effect of combustion duration is adverse regarding RI. Longer durations result in higher GIE and lower RI. This is the important feature of RCCI combustion.
- By increasing the diesel mass fraction in SOI-1, combustion event occurs earlier and PPRR is slightly higher. But this parameter has a trivial influence compared to PRF number and SOI timing.

Abbreviations

ATDC	After Top Dead Center
BTE	Brake Thermal Efficiency
CDC	Conventional Diesel Combustion
CI	Compression Ignition
CR	Compression Ratio
DPF	Diesel Particulate Filter
GIE	Gross Indicated Efficiency
GTE	Gross Thermal Efficiency
HCCI	Homogeneous Charge Compression Ignition
IMEP	Indicated Mean Effective Pressure
LNT	Lean NOx Trap
LTC	Low Temperature Combustion
NOx	Oxides of Nitrogen

PCCI	Premixed Charge Compression Ignition
PCI	Premixed Compression Ignition
PM	Particulate Matter
PPC	Partially Premixed Combustion
PRF	Primary Reference Fuel
PPRR	Peak Pressure Rise Rate
RCCI	Reactivity Controlled Compression Ignition
RI	Ringing Intensity
SCR	Selective Catalytic Reduction
SI	Spark Ignited
SOC	Start of Combustion
SOI	Start of Injection

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