

Effect of Intake Charge Temperature on Combustion and Emissions Characteristics in a Natural Gas-Diesel Reactivity Controlled Compression Ignition Engine

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Abstract

Partially premixed dual fuel strategy has been suggested as a new strategy for Compression Ignition (CI) engines because it could be effective for simultaneous reduction in NO_x and soot exhaust emission accompanied. This strategy uses premixed low reactivity fuel as main fuel and advanced injection of high reactivity fuel as pilot fuel to reach a Reactivity Controlled Compression Ignition (RCCI) in CI engines. The current paper presents results from a study about NG-Diesel RCCI combustion with variable intake charge temperature in a CI engine. The results from the developed CFD model with a reduced chemical kinetic mechanism verify that the model can simulate the in-cylinder process, accurately. Based on the results, intake temperature impact the engine operation at RCCI combustion, significantly. The high intake temperature could result in advanced combustion phasing and higher ringing intensity (RI) as well as enhanced combustion efficiency. It is due combustion improvement with higher heat release rate (HRR) and peak in-cylinder pressure. On the other hand, the results revealed that RCCI combustion in low intake temperature causes great HC and CO emissions accompanied with low NO_x emission in part load condition.

Keywords

RCCI, Natural gas, Diesel, Combustion, Emissions, CFD Simulation Coupled with Chemical Kinetic, Intake Temperature

1. Introduction

Compression ignition (CI) engines or diesel engines were founded to be an efficient selection in heavy-duty applications like power generation in genset application. However, due to heterogeneous nature and diffusion combustion in diesel engines, a considerable amounts of nitrogen oxides (NO_x) and soot can be seen in this type of engine (Desantes, Benajes, Molina, & Gonzalez, 2004). The current emissions problem as well as limited fuel storage within the world have imposed more tight limits on operation in all types of engines. Hence, different methods have been

suggested, which Low Temperature Combustion (LTC) is a new one in the field of internal combustion engines (Szybist, Edwards, Foster, Confer, & Moore, 2013). In most of LTC strategies, a premixed (or partially premixed) mixture of air and fuel with exhaust gas recirculation (EGR) was used to prevent high pressure rise rate as well as knock phenomena (Khatamnejad, Khalilarya, Jafarmadar, & Nemati, 2011).

Reactivity controlled compression ignition (RCCI) is a modern dual-fuel combustion from LTC strategy for improving thermal efficiency while reducing NO_x and soot compared to

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conventional diesel engines (Reitz & Duraisamy, 2015). In RCCI combustion, a high reactivity fuel, which has good auto-ignition qualities and high cetane number, such as diesel is early injected in a mixture of air and a low reactive fuel with high octane number, for example gasoline or Natural Gas (NG) (Benajes, Molina, García, Belarte, & Vanvolsem, 2014). In fact, the main difference between conventional dual fuel combustion and RCCI is formation of partially premixed mixture of high reactivity fuel in cylinder which can be achieved by early injection of this fuel in compression stroke and enough before top dead center (TDC). High value of HC and CO emissions and in-complete combustion process were reported as the main drawbacks of RCCI combustion at engine part load condition (Dahodwala, Joshi, Koehler, Franke, & Tomazic, 2015).

Fully premixed gasoline and partially premixed diesel fuels have been used by the majority of RCCI combustion studies conducted to date. To study the effect of initial condition on RCCI combustion process, Lim and Reitz (Lim & Reitz, 2014) investigated on a high load operation of RCCI combustion in a heavy duty engine with various intake pressures and EGR rates. The results indicated that high thermal efficiency can be achieved with reasonable peak pressure rise rates in optimum intake charge condition. In another work, the effects of EGR and boost pressure on RCCI combustion were studied by Wu and Reitz (Wu & Reitz, 2014) via a multi-dimensional CFD code. They founded that RCCI combustion is very sensitive to EGR rate, especially at high load. But, combustion and emissions can't change with EGR in higher intake pressure.

More recent efforts for less value of energy consumption and exhaust emission legislations have led to extend of research looking for different alternative fuels in RCCI engines. One of them is NG which is a good alternative low reactivity fuel. Natural gas is a mixture of different gases including methane, ethane, propane, butane, pentane, and other species at different proportions. Methane is the dominate percentage among the mentioned elements. The proportion of mentioned species is related to the area and time of oil discovery, and treatments applied during production or transportation (McTaggart-Cowan, Reynolds, & Bushe, 2006). Based on pervious researches, clean burning take place with NG in compared to liquid alternative fuels like diesel or gasoline. This is related to chemical composition of this fuel and lower carbon to hydrogen atoms ratio in NG.

Moreover, NG fuel has great resources and lower price compared to liquid hydrocarbon fuels, e.g. gasoline and diesel fuel which causes this fuel to be used in internal combustion engines in large scale, recently. In the other side, larger reactivity gradient or reactivity stratification within the cylinder can be achieved by NG compared to other low reactivity fuels (e.g., gasoline) in RCCI combustion (Kakaee & Paykani, 2013).

Due to mentioned advantages of NG, using natural gas in RCCI combustion has been investigated in some researches. A detailed investigation by Nieman et al. (Nieman, Dempsey, & Reitz, 2012) was first attempt to study RCCI combustion using port fuel of natural gas to optimize RCCI engine regarding different parameters such as amount, injection timing and injection pressure of diesel fuel and EGR. Also, he authors compared the results of RCCI combustion with NG and gasoline. They demonstrate that injection parameter can have a significant effect on RCCI combustion features. Also, engine medium load operation was reached without using EGR while maintaining high efficiency and low emission levels. Doosje et al. (Doosje, Willems, & Baert, 2014), explored about NG-Diesel RCCI engine in a full-scale engine between 2 and 9 bar BMEP. They founded that very low NO_x and soot below euro VI emission level can be achieved with the NG substitution higher than 85%. But, high CO and HC emissions were the results of RCCI combustion in this work. In another study, Kakaee et al. (Kakaee, Rahnama, & Paykani, 2015) numerical investigation about the effect NG composition on NG-Diesel RCCI combustion. Their study showed that the higher Wobbe number (WN) of NG increase peak cylinder pressure, temperature and NO_x emissions. But it have good results for reduction of HC and CO emissions at medium engine load condition. Jia et al. (Jia & Denbratt, 2015) had an experimental investigation of diesel injection strategy including injection timing and duration of diesel injection on NG-Diesel RCCI combustion in a heavy duty engine at 9 bar (as medium load) and 1200 rpm. NG-diesel RCCI combustion results in low NO_x and considerably low soot emissions with high HC emission.

Therefore, according to the related literature, RCCI combustion concept is an effective method for reduction of both soot and NO_x emissions, but there is still a lack of detailed study concerning different intake charge condition in a NG-diesel RCCI engine at

low load to reduce high HC and CO emissions content. Therefore, study about the effects of intake charge temperature on combustion and emissions is the main goal and motivation of the current research. Based on a developed and validated three dimensional CFD model coupled with chemical kinetics, the results on combustion features and amount of pollutant emissions such as in-cylinder mean pressure, HRR and values of NO_x, CO, and HC were compared in different cases and discussed in detail.

2. Model Description

A multi-dimensional CFD simulation tool coupled with a reduced chemical kinetic mechanism is used to explore the combustion features and emissions in a six cylinder diesel engine at part load operation. The specifications of mentioned engine depicts on Table 1.

The applied code solves all equations for reacting turbulent flow. Combustion chamber has been modeled in the 45° sector computational mesh which can be seen in Figure 1 at TDC. This is due the mentioned engine uses 8-orifice nozzle, and therefore only a 45° sector has been modeled regarding advantage of symmetry pattern of flow field in combustion chamber. This method significantly reduces computational runtime. The model has 25575 cells at TDC and all computations are carried out on the closed system from IVC at 150 CA bTDC to EVO at 144 CA aTDC. Also, a fully premixed mixture of air and NG is considered for simulation as initial condition at IVC.

Table 1. Engine specification

Characteristics	Values
Type	In-line 6 cylinder, water cooled
Fuel	NG- ULSD
Engine Speed	1500 (rpm)
Compression ratio	16.7
Displacement	12.4 (L)
Intake valve closing	150 (CA bTDC)
Exhaust valve opening	144 (CA aTDC)
Number of nozzle hole	8

In this work, the k-zeta-f model has been used to calculate the effects of turbulent dispersion. Hanjalic et al. suggested this model, recently for flow field of internal combustion engine (Hanjalić, Popovac, & Hadžiabdić, 2004). Diesel injection process is simulated by the standard DDM (Droplet Discrete Model) (Dukowicz, 1980). The break up process of

diesel fuel spray has been simulated by Kelvin-Helmholtz Rayleigh-Taylor (KH-RT) model (Beale & Reitz, 1999). Dukowicz model has been used for evaporation of liquid fuel droplets modeling (Dukowicz, 1980). Also, FIRE standard wall function model was used for wall heat flux calculation.

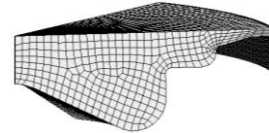


Figure 1. Computational grid at TDC

To detailed simulation of combustion process in current RCCI engine, the FIRE internal chemistry solver has been implemented in this study to include species transport and energy release in combustion simulations, based on CHEMKIN theory (Kee, 1996). Hence, a modified dual-fuel chemical mechanism for n-heptane and methane composed of 50 species and 201 reactions is used for detailed combustion chemistry calculations during engine cycle based on Nieman et. al. (Nieman et al., 2012) simulation. In the present study, methane (CH₄) represents the NG due to mentioned dominate percentage among NG elements and n-heptane (C₇H₁₈) is used as a surrogate for the diesel. NO_x emission formation has been modeled by 4 species and 12 reactions. This is a reduced version of the GRI NO_x mechanism based on extended Zeldovich mechanism (Smith et al., 1999).

3. Experimental Setup and Model Validity

The current experimental test bed on NG-diesel RCCI engine has been previously developed by the same set of authors (Khatamnejad, Khalilarya, Jafarmadar, Mirsalim, & Dahodwala, 2017). The experimental RCCI combustion results achieved at 25% engine load condition. Inline six-cylinder 13L diesel engine equipped with a high pressure common-rail direct injection system and cooled high pressure EGR is used to produce experimental data for the NG substitution investigation and CFD model validation. The engine specifications have been shown in Table 1. The low and high reactivity fuels used in this study are NG and diesel fuel, respectively. The engine was coupled to a 560 kW alternating current dynamometer (HS001779, ABB Innovasys). The NG and diesel fuel flow meter (CMF025M319NRAUEZZZ, Micro Motion) and the air flow meter (14241-7962637, ABB) were

used to measure required flow rates. The NG was induced into the intake using eight NG injectors located downstream of the charge air cooler. Also, a mixer was installed downstream of the NG introduction location to support equal distribution of the NG in the intake manifold. Engine-out and tailpipe gaseous emissions were measured with an emission analyzer (MEXA 7500 DEGR, Horiba). Also, soot emission was determined through the smoke meter (415S, AVL). The engine was instrumented with in-cylinder pressure transducers (6061B, Kistler) to allow cylinder pressure measurements on all six cylinders. Figure 2 represents the 1D diagram of the engine test cell in the current study.

Combustion analysis was conducted from measured cylinder pressure value using the standard first thermodynamic law analysis. Considering the volume trapped in the cylinder when the valves are closed from Intake valve closing (IVC) to Exhaust valve opening (EVO) as a control volume, HRR can be calculated by:

$$HRR = \frac{1}{\gamma - 1} V \frac{dp}{d\theta} + \frac{\gamma}{\gamma - 1} P \frac{dV}{d\theta} \quad (1)$$

where HRR is the heat release rate. This is based on the difference between the chemical heat release rate $\frac{dQ_{chem}}{d\theta}$ and the heat lost to the walls $\frac{dQ_{wall}}{d\theta}$. Also, P is pressure within the

combustion chamber, V is the cylinder volume and γ is the ratio of specific heats of the cylinder content as an ideal gas.

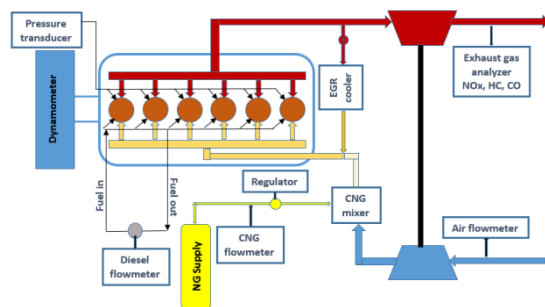


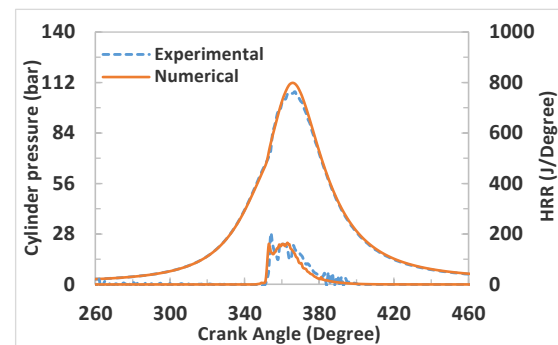
Figure 2. 1D diagram of the engine test cell

Table 2 presents the selected points of RCCI engine operation for simulation results validation at 25% engine load condition. It should be noted that all tests have been carried out in 36% EGR with 80% NG premixed ratio and 1.8 as lambda (excess air).

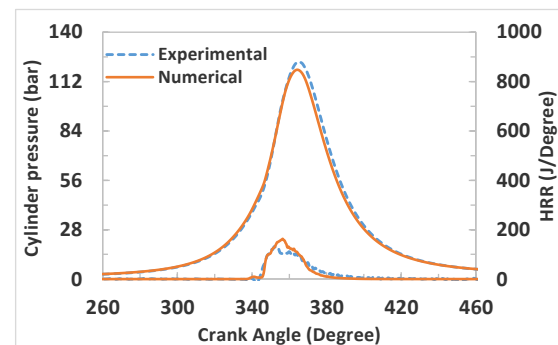
Table 2. Selected engine operating

Case	EGR (%)	SOI (CA bTDC)	IVC temperature (K)
1	36	18	357
2	36	30	384

As can be seen from Figure 3, the predictions of combustion phasing and pressure traces are good. According to the validation cases results, the maximum reported difference between the experimental and simulated peak cylinder pressure is 3.7%. Therefore, it can be concluded that the developed CFD model accurately predicts the engine combustion features with acceptable uncertainty.



Case 1



Case 2

Figure 3. Cylinder pressure, HRR and emissions validation for different cases in Table 2

Regarding to exhaust emissions in different cases, it could be observed from Figure 4 depicts that CO, HC, and NOx emissions variation in two cases are same as with the measurements. It should be noted that the exact matching is not possible due to the fact that one cylinder combustion process simulation is done in CFD simulation; whereas the experimental values are averaged of all 6 cylinders (Mikulski & Bekdemir, 2017). In addition, soot emission is ultra-low in RCCI combustion and is not studied in this study (Kokjohn, Hanson, Splitter, & Reitz, 2011).

Therefore, the developed model is reliable for prediction of combustion and emissions in different conditions including intake charge temperature. Hence, the parametric study of the effect of intake charge temperature on combustion and exhaust emissions formation at part load condition has been done by developed CFD model in current research.

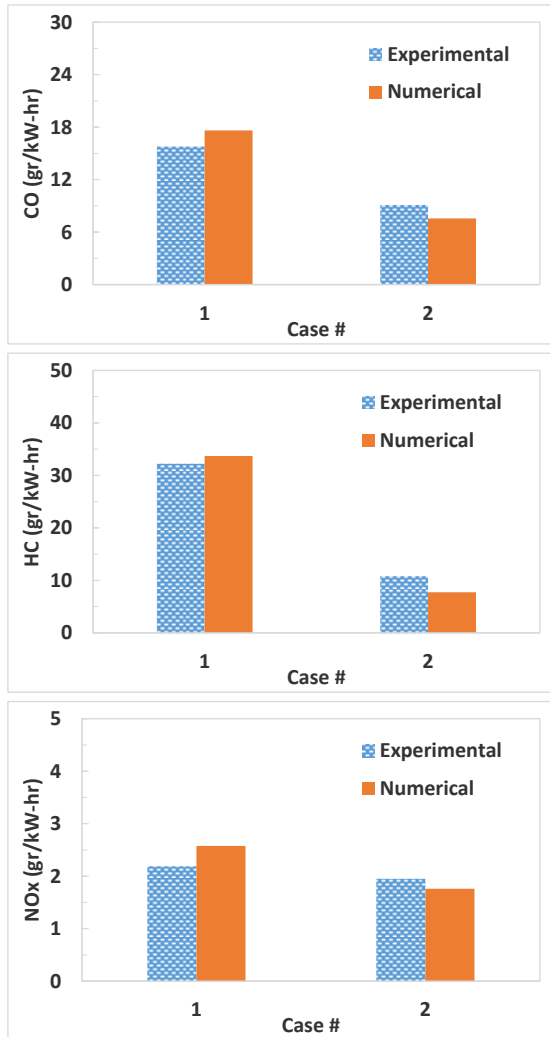


Figure 4. Exhaust emissions validation for different cases in Table 22

4. Results and Discussion

In this section, combustion and emissions of mentioned engine in defined condition is studied at part load. The results related the effect of intake temperature are presented and discussed. It should be noted that other engine parameters including speed, EGR, SOI timing were constant better comparison.

Based on pervios reasech, the combustion process in a RCCI engine is mainly controlled by chemical kinetics due to premixed condition

of NG. Therefore, charge temperature could play a key role in progress of reactions and consequently results in heat relaease of chemical energy (Nobakht, Saray, & Rahimi, 2011). As a result, the effect intake charge temperature on RCCI combustion has been investigated in this section.

The variation of combustion phasing and start of combustion (SOC) in different intake charge temperature has been indicated in Figure 5. The results of combsution phasing and SOC present based on CA50 (i.e., the crank angle position in which the cumulated heat release has reached a value of 50%) and CA10 (i.e., the crank angle position in which the cumulated heat release has reached a value of 10%). It can be seen that the ignition delay is shortened and SOC occurs earlier when the intake temperature increases. This is due to more combustion rate of chemical species in higher charge temperature which is responsible for higher haeat release in less time as well as short ignition delay.

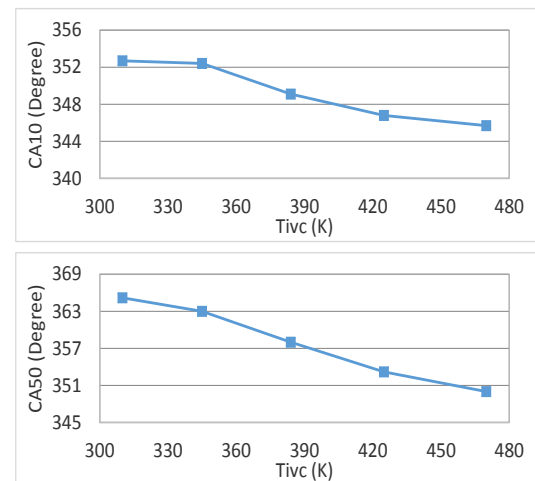


Figure 5. CA10 and CA50 comparison for different cases

In order to further insight into combustion process, the variation of combustion efficiency and RI in different cases have been presented in Figure 5. Combustion efficiency is calculated by the proposed equation as follow (Dempsey, Adhikary, Viswanathan, & Reitz, 2012):

$$\eta_c = \sum (HRR / Q_{in}) \times 100 \quad (3)$$

where HRR is heat release and Q_{in} is the total energy of used fuel. Also, the ringing intensity (RI) was calculated by means of the correlation of Eng (Eng, 2002), finds the intensity of the combustion pressure waves based on amplitude and the speed of sound.

$$RI = \frac{1}{2\gamma} \frac{[0.05(dp/dt)_{\max}]^2}{P_{\max}} \sqrt{\gamma RT_{\max}} \quad (4)$$

where γ is the ratio of specific heats, $(dp/dt)_{\max}$ is the peak pressure rise rate, $P_{\max}$ is the maximum of in-cylinder pressure, R is the ideal gas constant, and $T_{\max}$ is the maximum of in cylinder temperature.

In the other side, the RI is a parameter which has been used in RCCI combustion study to quantify knock level. It was experimentally founded that the maximum RI value is 5 MW/m² for the combustion free of noise and knocking phenomena in heavy duty diesel engine (Nieman et al., 2012). The results clearly indicate an improvement in the combustion efficiency and an increase in the RI values with intake charge preheating higher than 460K. Also, it is indicated that for 480K intake temperature, the RI value is higher than the standard value 5 MW/m².

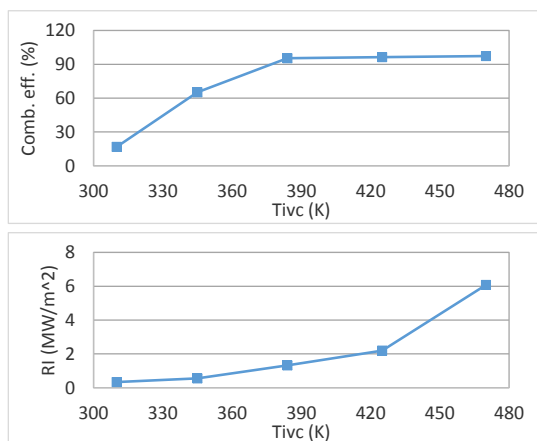


Figure 6. combustion efficiency and RI comparison for different cases

This observed trend can be described by considering HRR and cylinder pressure trends in different cases in Figure 7 and Figure 8, respectively. Based on the results, it can be observed that higher intake temperatures causes advanced combustion phasing with shorter duration as well as higher release rate. This lead to the pressure peak also take place earlier with higher values. As can be seen, misfiring exist in intake temperature at 310K.

The impact of intake charge temperature on emissions is demonstrated in Figure 9. By increasing intake charge temperature HC and CO emissions decrease, significantly. However, NOx emission variation show opposite trend. It is well known that higher in-cylinder

temperature as well as more residence time in high temperature increases NOx emission amount. As can be observed in Figure 10 as contour plots of in-cylinder temperature in different crank angle including CA50 and CA90, increasing intake temperature results in higher combustion temperature which plays a key role in thermal NOx formation. Also, the amount of HC and CO emissions decrease with increasing intake temperature. This is due to combustion improvement and enhanced combustion efficiency in higher intake charge temperature. As can be seen, the increment of HC emission is mainly due to incomplete fuel burning with low temperature within the whole of combustion chamber, especially in near liner and crevices regions which result in unburned HC from wall quenching. Moreover, Figure 10 shows that the engine with lower intake temperature produces more CO. CO emission formation will be increased in rich region with low temperature due to misfiring. Therefore higher cylinder temperature causes lower CO emission formation within the cylinder. It could be concluded that the amount of HC and CO emissions decreases with increasing intake charge temperature.

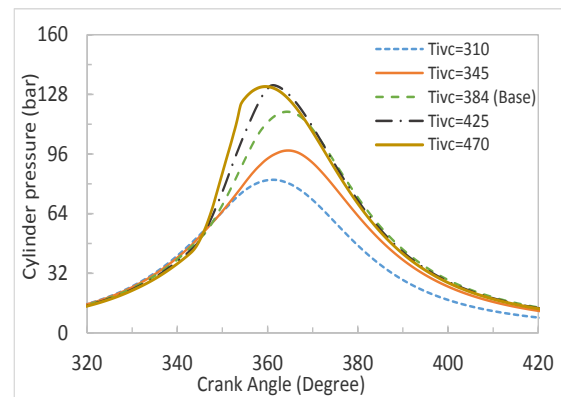


Figure 7. In-cylinder pressure in different intake temperatures

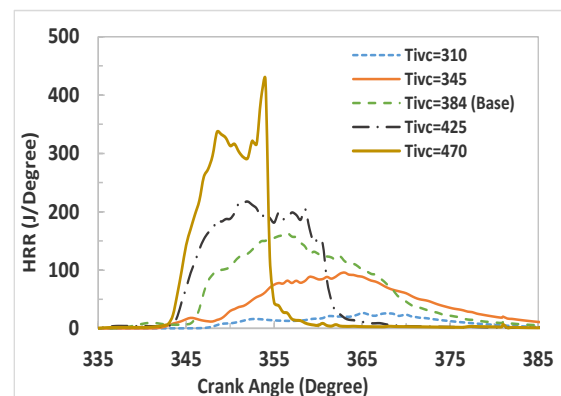


Figure 8. HRR in different intake temperatures

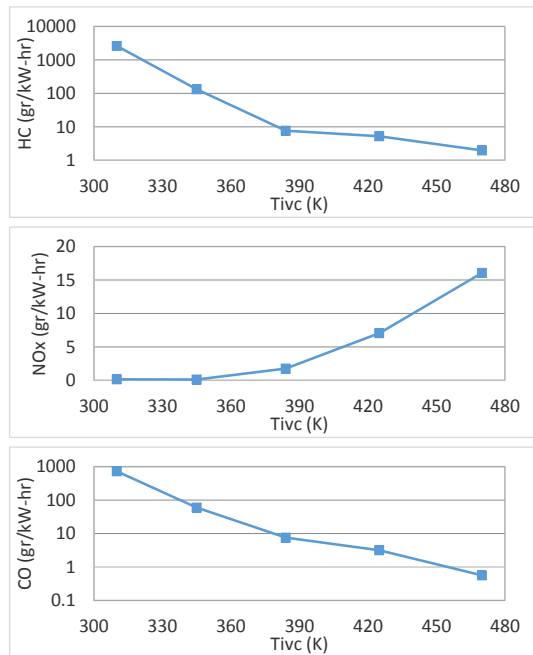


Figure 9. Emissions comparison for different cases

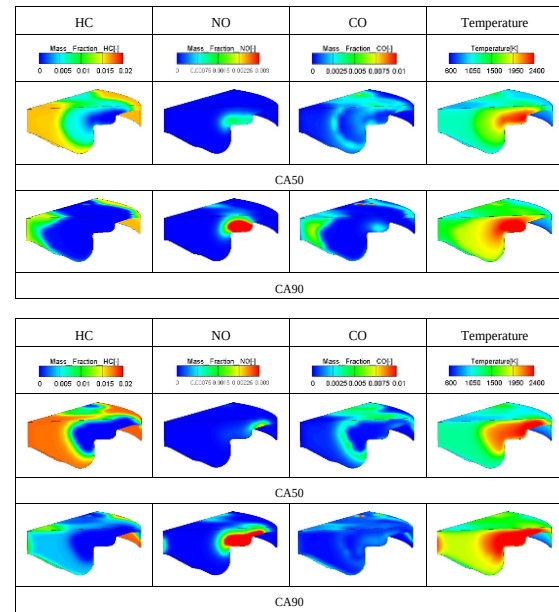
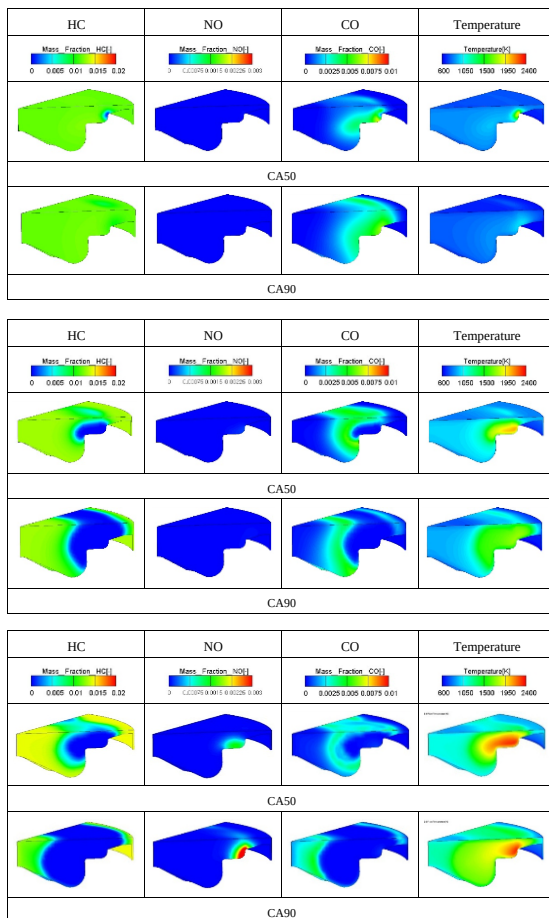


Figure 10. Effects of intake temperature from up to down with 310K to 470K on HC, NO and CO mass fraction and temperature surface planes at CA50 and CA90

To study the results of engine performance variation with different intake charge temperature, ITE (indicated thermal efficiency) has been calculated in different cases as an engine performance parameter. The ITE is calculated by the below correlation where Q_{in} is the total supplied energy by used fuels (Nieman et al., 2012).

$$ITE = \frac{\int_{-180}^{180} PdV}{Q_{in}} \times 100\% \quad (5)$$

Figure 11 shows variation in the ITE and BSFC with respect to the intake charge temperature. As can be seen, when the intake temperature increased from 310 K through to 470 K, ITE and BSFC enhance. The results show that the case with 384 K intake temperature has the highest ITE (41.50%), while the case with 310 K intake temperature has the lowest one (6.70%). There is not enough ignition sources as well as flame kernel formation at 310 K, hence the start of combustion and combustion phasing is retarded with higher losses. In other hand, intake temperature higher than 384 K results in advanced combustion as well as higher negative work at compression stroke. Therefore, early and late combustion phasing decline engine performance including ITE and BSFC and best performance can be achieved with combustion phasing at TDC.

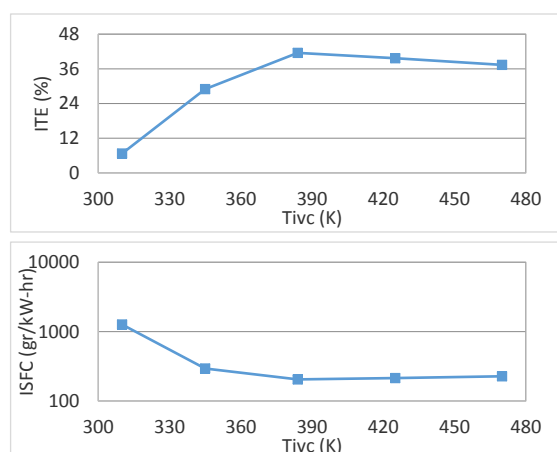


Figure 11. Engine performance comparison for different cases

5. Conclusion

In the present work, a detailed investigation has been conducted to study the effects of intake charge temperature on combustion features and pollutant emissions of a NG-diesel RCCI engine, under 1500 rpm and 25% load operation. To parametric study about the mentioned injection parameters, a detailed three-dimensional CFD model coupled with reduced chemical mechanism was developed. The results of cylinder pressure, HRR and the exhaust emissions including HC, NO_x and CO were validated with obtained experimental results in test bed. Based on the results and discussions, conclusion of the current study can be summarized as follows:

Based on the above results, high intake temperature decreases ignition delay and results in advanced combustion phasing due to more reaction rate of chemical species in higher charge temperature.

Also, associated with lower intake temperature, both RI and combustion efficiency is reduced. This is due to slow rate of heat release accompanied with lower cylinder pressure at low intake charge temperature. But, very high intake temperature results in RI higher than 5 MW/m² and therefore knock phenomena.

It was observed that increasing the intake temperature, HC and CO decrease while NO_x increase. This is due to incomplete combustion within the cylinder.

The best engine performance including ITE and BSFC can be seen with intake charge temperature at 384 K.

In conclusion, to improve the combustion efficiency as well as reduced CO and HC emissions as critical problems of NG-diesel RCCI combustion at part load, increasing

intake temperature up to optimum value is a good method.

5. Acknowledgement

The authors are grateful to FEV for providing the test data used in correlating the baseline simulation models.

Nomenclature

Greek

γ	ratio of specific heats
η_c	combustion efficiency

Abbreviations

γ	ratio of specific heats
η_c	combustion efficiency

Abbreviations

aTDC	after top dead center
bTDC	before top dead center
BMEP	brake mean effective pressure
BSFC	brake specific fuel consumption
CA	crank angle
CA10	crank angle at which 10 percent mass fraction has combusted
CA50	crank angle at which 50 percent mass fraction has combusted
CO	carbon monoxide
CI	compression ignition
CFD	computational fluid dynamics
CN	Cetane number
CNG	compressed natural gas
DI	direct-injection
EGR	exhaust gas recirculation
HD	heavy-duty
HC	unburned hydrocarbon
HCCI	homogenous charge compression ignition
HRR	heat release rate
IC	internal combustion
ITE	indicated thermal efficiency
IVC	intake valve closing
LTC	low temperature combustion
NG	natural gas
NO _x	oxides of nitrogen
RCCI	reactivity controlled compression ignition
RI	ringing intensity
RPM	revolutions per minute
SI	spark ignited
SOC	start of combustion
SOI	start of injection
TDC	top dead center
WN	Wobbe number

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