INTERNATIONAL JOURNAL OF
ENERGY AND ENVIRONMENT

Volume 2, Issue 4, 2011 pp.739-748

Journal homepage: www.IJEE.IEEFoundation.org

Numerical parametric investigation of a gasoline fuelled partially-premixed compression-ignition engine

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Abstract
Parametric studies of a heavy duty direct injection (DI) gasoline fueled compression ignition (CI) engine combustion are presented. Gasoline because of its higher ignition delay has much lower soot emission in comparison with diesel fuel. Using double injection strategy reduces the maximum heat release rate that leads to nitrogen oxides (NO_x) emission reduction. A three dimensional computational fluid dynamics (CFD) code was employed and compared with experimental data. The model results show a good agreement with experimental data. The effect of injection characteristics such as, injection duration, main SOI timing, and nozzle hole size investigated on combustion and emissions.

Keywords: Compression ignition engine; Gasoline fuel; Emission reduction; Combustion; Injection characteristics; Parametric study.

1. Introduction
Conventional compression ignition (CI) engines are known for their high thermal efficiency in comparison with spark ignited (SI) engines. This makes CI engines a potential candidate for the future prime source of power for transportation sector to reduce greenhouse gas emissions and to shrink carbon foot print. However, CI engines produce high levels of NO_x and soot emissions. Conventional methods to reduce NO_x and soot emissions often result in the infamous NO_x-soot trade-off [1].
One of the attractive methods for lowering emissions is low temperature combustion (LTC). Different kinds of low temperature combustion have been explored in the recent years, such as homogeneous charge compression ignition (HCCI), premixed charge compression ignition (PCCI) and high equivalence ratio combustion based on extensive use of high cooled EGR rates.
Homogenous charge compression ignition (HCCI) based on the simultaneous ignition of a highly diluted premixed air-fuel mixture throughout the combustion chamber [2-4]. In this combustion, globally and locally lean mixture produces low soot owing to low local equivalence ratios and low NO_x from low combustion temperatures. However, the control of combustion phasing and hence overall engine control is very difficult in HCCI combustion.
Premixed Charge Compression Ignition (PCCI) is a further possibility for low emission combustion [5, 6]. This concept uses more advanced injection timing than for conventional CI engines. In this strategy, low NO_x and soot emissions achieved by providing a better vaporized air-fuel mixture, which forms

mixture conditions close to a homogenous charge at low temperature combustion condition. Although both the control of combustion phasing and reduction of pollutant emissions can be achieved in the PCCI regime, increase the amount of fuel injected beyond a certain level is resulted in knock that this is limiting the operating range of PCCI combustion.

The use of high cooled EGR rate is other way to gain low temperature combustion condition. The use of EGR is very effective to mitigate NO_x levels by reducing oxygen concentration in the intake system as well as chemical effects of added CO_2 and H_2O [7]. Also, at low engine load condition, lower combustion temperature in the fuel-rich zones (in which normally soot is produced) contributes to greater suppression of soot formation [8]. But higher engine loads leads to higher soot formation because portions of rich mixtures are at high temperatures due to the increase heat release from combustion of higher fuel amount.

Control of fuel injection mode is another method to simultaneously reduction of NO_x and soot emissions that is achievable in advance common rail injection systems. The use of an early small injection (pilot injection) with a large amount injection (main injection) at later crank angle is able to reduce the maximum value of heat release by spreading out the heat release through split injection [9]. In addition, reduction of heat release rate in this strategy is suitable for higher engine load conditions.

Fuels with higher octane number (i.e., gasoline) have higher ignition delay and resistance of auto-ignition. Because of a better air-fuel mixing before the start of ignition, soot emission can be reduced in conjunction with decrease of NO_x formation due to retarded combustion phasing at lower temperature conditions at optimized injection timing. In addition to, fuels with high volatility and diffusivity enhance air-fuel mixing at ignition delay.

Several studies confirmed a possibility of reaching low soot and NO_x emissions using a fuel with high octane number. Kalghatgi et al. [10, 11] investigated effect of fuel auto-ignition quality on engine ignition timings and emissions experimentally for four different fuels with different CN and volatility, including conventional gasoline. Their results indicate that there is significantly higher soot with diesel compared to the gasoline fuel due to lower ignition delay at the same condition. Also for a given IMEP, multiple injection reduces the maximum heat release rate and enables heat release to occur with low cyclic variation compared to a single injection. In addition, the engine could be run at high loads using gasoline fuel with injection timing near TDC due to much larger ignition delay with lower soot and NO_x emissions compared to diesel fuel. More recently, an experimental study of partially premixed combustion with gasoline fuel was performed using a heavy duty comparison ignition engine by Hanson et al. [12]. They use pilot and main injections in their experiment while pilot injection occurs before IVC in their parametric study.

In this work, effect of injection characteristics such as, main SOI timing, injection duration and nozzle hole size have been studied on combustion and emissions in gasoline fuelled engine.

2. Numerical approach

2.1 Model description

In the present model, the compressible, turbulent, three dimensional transient conservation equations are solved for reacting multi-component gas mixtures with the flow dynamics of an evaporating liquid spray by Amsden et al. [13]. The turbulent flows within the combustion chamber are simulated using the RNG k-ε turbulence model which is presented by Han and Reitz [14], modified for variable-density engine flows. The spray module is based on a statistical method referred to as the discrete droplet method (DDM). This operates by solving ordinary differential equations for the trajectory, momentum, heat and mass transfer of single droplets, each being a member of a group of identical non-interacting droplets termed a parcel. Thus one member of the group represents the behavior of the complete parcel. The Kelvin-Helmholtz Rayleigh-Taylor (KH-RT) model was selected to represent spray breakup [15]. In this model Kelvin-Helmholtz (KH) surface waves and Rayleigh-Taylor (RT) disturbances should be in continuous competition of breaking up the droplets. The spray-wall interaction model used in the simulations is based on the spray-wall impingement model that suggested by O'Rourke and Amsden [16]. The Dukowicz model [17] was applied for treating the heat-up and evaporation of the droplets. This model assumes a uniform droplet temperature. In addition, the rate of droplet temperature change is determined by the heat balance, which states that the heat convection from the gas to the droplet either heats up the droplet or supplies heat for vaporization. Combustion process is modeled by Eddy Breakup model [18]. This model assumes that in premixed turbulent flames, the reactants (fuel and oxygen) are contained in the same eddies and are separated from eddies containing hot combustion products. The rate of dissipation of these eddies determines the rate of combustion.

$$\overline{\rho \dot{r}_{fu}} = \frac{C_{fu}}{\tau_R} \bar{\rho} \min\left(\bar{y}_{fu}, \frac{\bar{y}_{ox}}{S}, \frac{C_{\Pr}.\bar{y}_{\Pr}}{1+S} \right) \quad (1)$$

The first two terms of the "minimum value of" operator determine whether fuel or oxygen is present in limiting quantity and the third term is a reaction probability which ensures that the flame is not spread in the absence of hot products. Above equation includes three constant coefficients (C_{fu}, τ_R, C_{pr}) in which Cfu varies from 3 to 25 in diesel engines. An optimum amount was selected according to experimental data. τ_R is the characteristic time for reaction turbulent mixing and is defined as below:

$$\tau_R = \frac{k}{\varepsilon} \quad (2)$$

This specifies the combustible mixture consumption rate.

NO_x formation model is derived by systematic reduction of multi-step chemistry, which is based on the partial equilibrium assumption of the considered elementary reactions using the extended Zeldovich mechanism [19] describing the thermal nitrous oxide formation.

$$N_2 + O \longleftrightarrow NO + N \quad (3)$$

$$N + O_2 \longleftrightarrow NO + O \quad (4)$$

$$N + OH \longleftrightarrow NO + H \quad (5)$$

The overall soot formation rate is modeled as the difference between soot formation and soot oxidation. Soot formation is based on Hiroyasu model [20] and the soot oxidation rate is adopted from Nagle and Strickland-Constable [21].

$$\frac{dm_{soot}}{d_t} = \frac{dm_{form}}{d_t} - \frac{dm_{oxid}}{d_t} \quad (6)$$

$$\frac{dm_{form}}{d_t} = A_f m_{fv} p^{0.5} \exp\left(-\frac{E_a}{RT} \right) \quad (7)$$

$$\frac{dm_{oxid}}{d_t} = \frac{6M_c}{\rho_s d_s} m_s R_{tot} \quad (8)$$

All above equations are taken into account simultaneously to predict spray distribution and combustion progress in the turbulent flow field, wall impingement and gasoline combustion rate using two stage pressure correction algorithms.

2.2 Model validity

The numerical model for Caterpillar 3401 heavy duty gasoline fueled engine with the specifications and operating conditions on the Table 1 is carried out using a three-dimensional CFD code.

Since a 8-hole nozzle is used, only a 45° sector has been modelled. This takes advantage of the symmetry of the chamber geometric setup, which significantly reduces computational runtime. Figure 1 shows the 45° sector computational mesh of combustion chamber in three dimensional at TDC. Number of cells in the mesh is 18,385 cells at TDC. Calculations are carried out on the closed system from IVC to EVO.

Figures 2a and 2b show the comparison between measured [12] and calculated in-cylinder pressure and heat release rate (H.R.R.). The good agreement of predicted in-cylinder pressure and H.R.R. with the experimental data can be observed.

Table 2 shows the comparison of calculated NO_x and soot emissions for the Caterpillar 3401 engine for double injection scheme by the pilot injection (30%) and main injection (70%) with the injection timing of -137˚ATDC and -8˚ATDC, respectively with experimental results [12].

The good agreement between the measured and calculated results for this engine operating condition gives confidence in the model predictions, and suggests that the model can be used for parametric investigations.

Table 1. Engine Specifications

Engine type	Caterpillar 3401 heavy duty
Engine speed	1300 rpm
Bore × stroke	137.20 × 165.1 mm
Connecting rod length	261.6 mm
Compression ratio	16.1:1
Swirl ratio	0.7
Injection strategy	Double
Number of nozzle holes	8
Nozzle hole diameter	0.229 mm
Connecting rod length	261.6 mm
Included spray angle	154 deg
Injection amount (50% load)	5.3 kg/h
Intake valve close timing	-85 ˚ATDC
Exhaust valve open timing	130 ˚ATDC

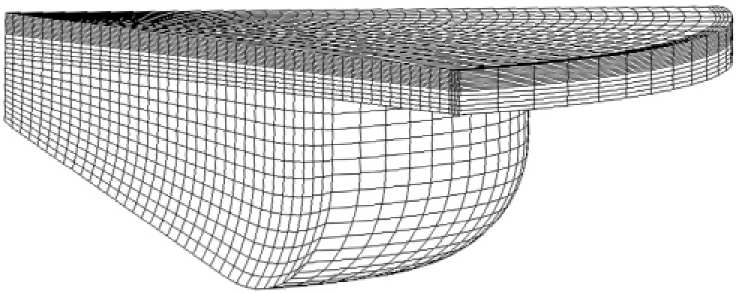
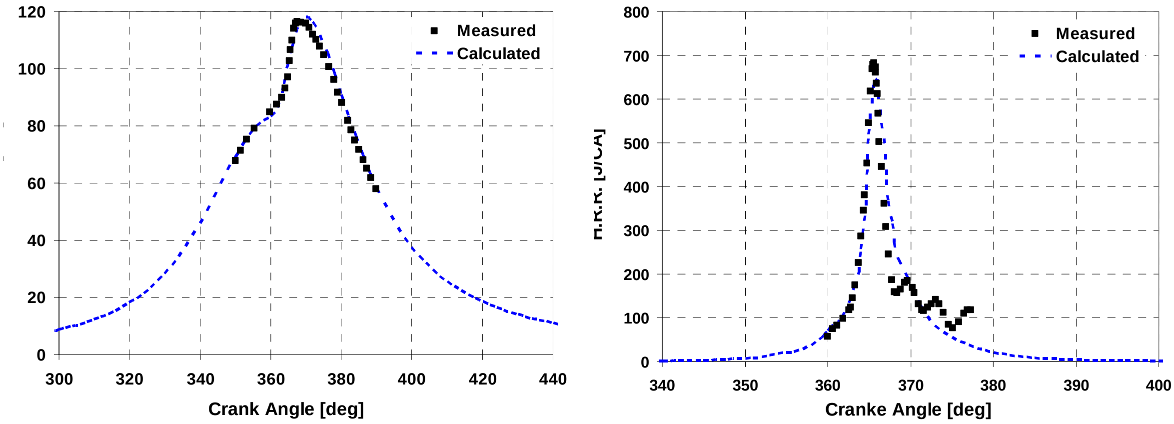


Figure 1. Computational mesh at TDC



(a) (b)

Figure 2. Comparison between calculated and measured in-cylinder pressure, calculated and measured heat release rate, (a) pressure (b) heat release rate

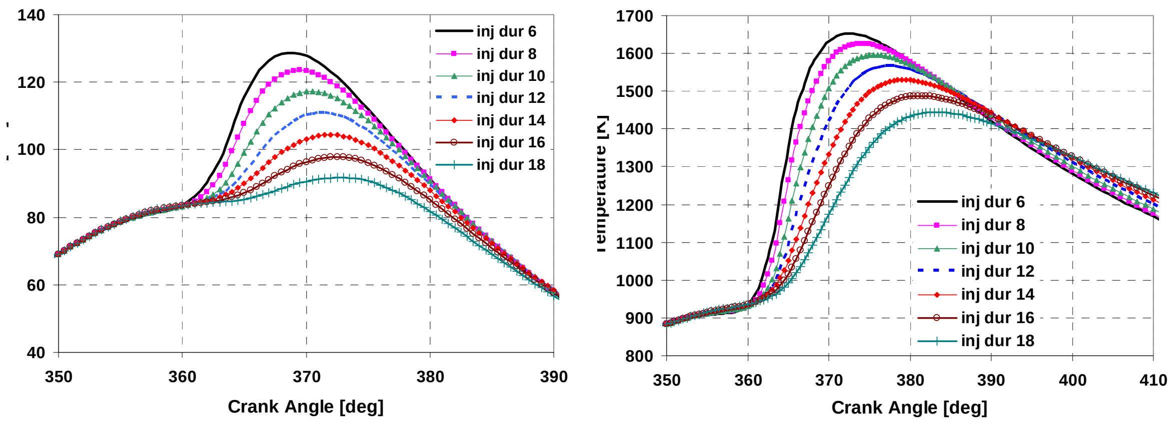
Table 2. Emissions comparison between measured and calculated results

NO_x [g/kWh]	soot [g/kWh]
9.4 (Measured)	0.0391(Measured)
9.37 (Calculated)	0.038 (Calculated)

3. Results and discussion

3.1 Effect of main injection duration

In order to examine the effect of main injection duration on the emissions and combustion characteristics, the injection duration was varied between 6 to 18˚CA. The start of main injection was fixed at -8 deg ATDC. In these simulations, the injection velocity is proportional to the injection duration because the nozzle area size and the amount of total injected fuel were held equal to base case values. Therefore by decreasing the injection duration, the same amount of fuel should inject to the combustion chamber in shorter time and this leads to higher injection velocity. Because of the same start of main injection for all cases decreasing the injection duration leads to an increase of peak cylinder pressures as can be seen in Figure 3a but further decrease in injection duration leads to engine noise an instability. Figure 3b shows the same trend for in-cylinder temperature.



(a) (b)

Figure 3. cylinder pressure and temperature under various injection durations, (a) pressure (b) temperature

Figure 4 shows comparison of IMEP and ISFC under various injection durations. This figure indicates that increase of injection duration causes to a decrease of IMEP and an increase of ISFC. This indicates the dominant effect of injection velocity on engine performance that makes it a key parameter in engine. Atomization of fuel sprays is deteriorated by reduction of injection velocity, resulting in bigger drop sizes. So, homogeneity of air-fuel mixture is reduced and spray impingement is increased, which leads to more fuel stratification. Therefore, the combustion becomes deficient and maximum in-cylinder pressure and temperature decrease. The IMEP is proportional to the in-cylinder pressure and behaves in a same way. ISFC is increased by increase of injection duration.

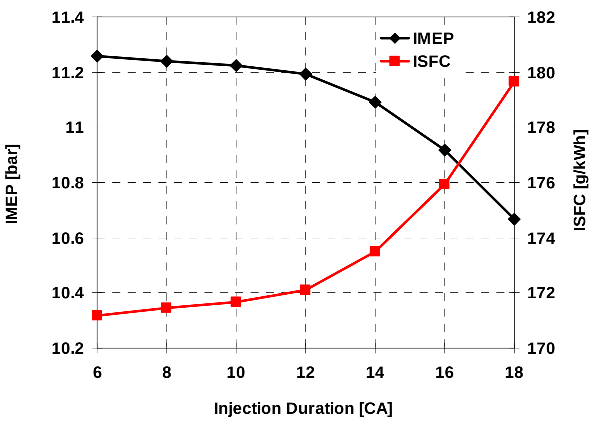


Figure 4. comparison of IMEP and ISFC under various injection durations

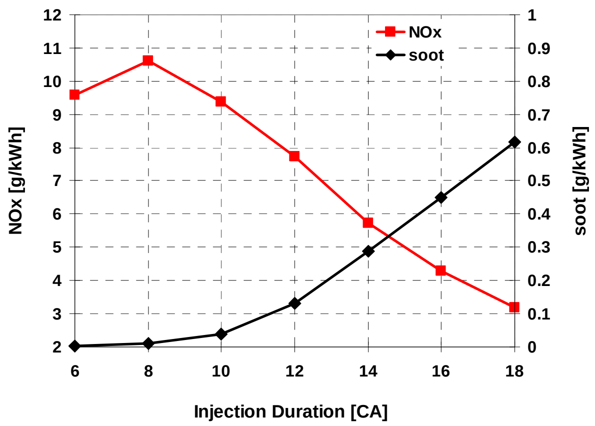


Figure 5. comparison of NO_x and soot under various injection durations

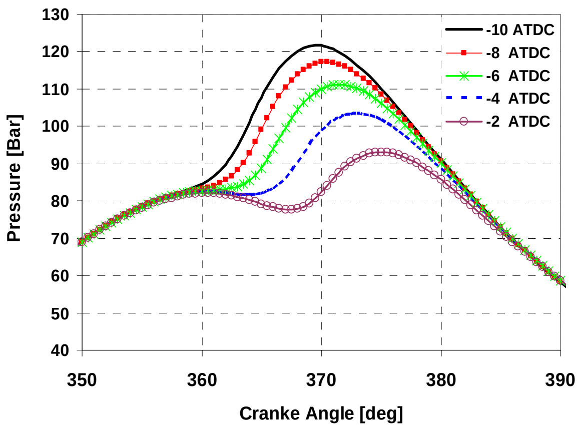
Figure 5 illustrates the NO_x and soot emissions for various injection durations. Reducing the local peak temperatures and the area of high temperature regions by increasing the injection duration, leads to a reduction of NO_x emission formation. Soot emission is very sensitive to homogeneity of air-fuel mixture and it is produced during rich mixtures. Increase of injection duration reduces the injection velocities and this leads to deterioration of the sprays atomization that causes to increase of spray impingement and the fuel wall film formation, which leads to more fuel stratification. Increasing fuel stratification considerably increases soot emissions, as shown in Figure 5.

There is an interesting trend in NO_x and soot diagrams. As can be seen the injection duration is more effective on soot than NO_x formation. On the other hand by reducing the injection duration NO_x approximately remains constant but soot becomes zero. But further decrease in injection duration leads to higher injection velocities that cause to reduce of injector useful life.

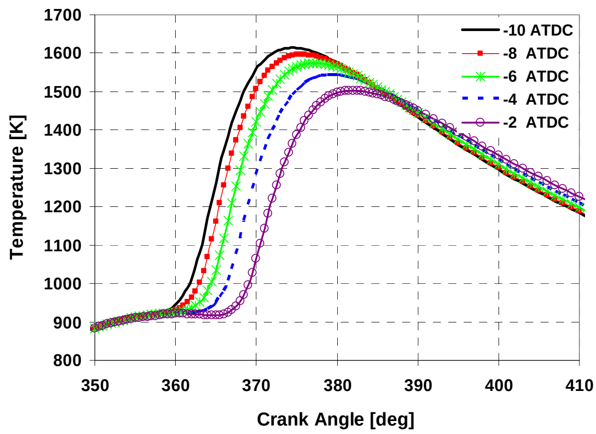
3.2 Effect of main SOI timing

The goal of this section was to investigate the effect of main SOI timing on the emissions and combustion characteristics. Therefore the same conditions such as, engine speed, swirl ratio and initial charge conditions at IVC were used for the simulations. Also for all cases the portion of pilot and main injection were fixed at 30% and 70% respectively.

Predicted in-cylinder pressure and temperature profiles are shown in Figure 6. As can be seen by advancing the main injection timing, the maximum pressure and the maximum of in-cylinder temperature increased. Because of higher ignition delay of gasoline, when the main SOI sweep to the TDC, the combustion becomes poorer due to low gas temperatures, therefore the peak of pressure and temperature is decreased.



(a)



(b)

Figure 6. effect of main SOI timing on cylinder pressure and temperature, (a) pressure (b) temperature

Figure 7 indicates the predicted NO_x and soot for various main SOI timings. As can be seen in this figure by retarding the main SOI timing NO_x emissions decreased. Gasoline ignition delay is increased by retarding the main SOI timing and combustion starts about 14° CA after the SOI .Therefore combustion occurs at low temperature and pressure that leads to deficient combustion and decrease of in-cylinder maximum temperature. NO_x emission formation is very sensitive to in-cylinder temperature and decreased by retarding in main SOI timing. Mixture richness is one of important parameters in soot formation. By retarding the main SOI timing, the time needed for air-fuel mixing reduces that leads to a stratified mixture and an increase of soot emission formation. In Figure 8 a tradeoff IMEP and ISFC is seen, IMEP decreases and ISFC increases by advancing the main SOI timing due to decreasing the peak in-cylinder pressure.

3.3 Effect of nozzle hole size

In this section the effect of nozzle hole size on emissions and combustion is discussed. The nozzle hole diameter was varied between 199 μm to 259 μm and the baseline value is 229 μm as mentioned in Table

2. The injection velocity is inversely proportional with nozzle hole size, because the injection duration and the injection amount were fixed same as baseline case. So increasing the nozzle hole size leads to a reduction of injection velocity.

Figure 9 represents in-cylinder pressure and temperature as a function of crank angle for various nozzle hole diameters. In-cylinder pressure and temperature are decreased by increasing the nozzle hole diameter. Increasing the nozzle hole diameter causes to increase of drop size and decrease of injection velocity. Droplet breakup is very sensitive to injection velocity and droplet size and it is decreased by increasing the initial droplet size and decreasing the injection velocity. By decreasing the droplet breakup the evaporation rate is decreased and leads to un-homogeneity of air-fuel mixture. So combustion occurs incompletely that leads to a decrease of in-cylinder pressure and temperature.

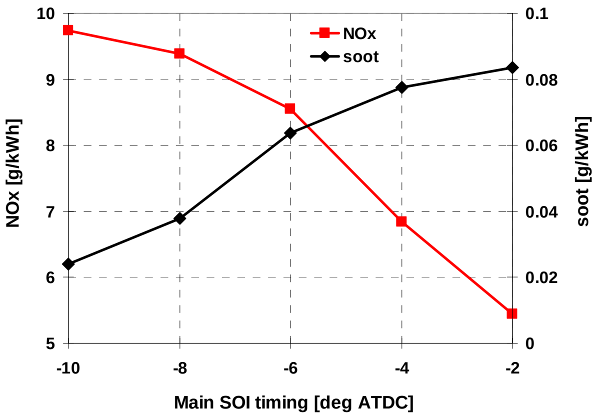


Figure 7. Effect of main SOI timing on NO_x and soot emissions

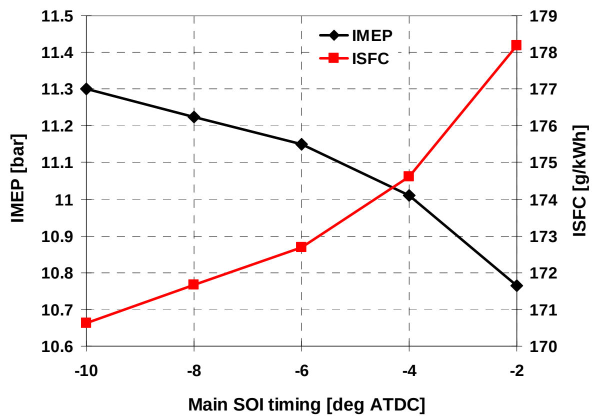
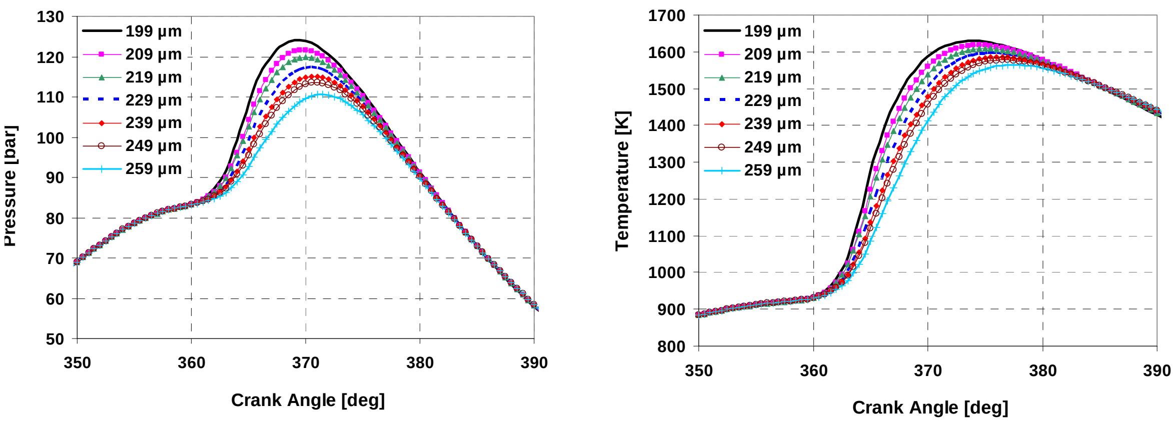


Figure 8. Effect of main SOI timing on IMEP and ISFC



(a) (b)

Figure 9. Predicted cylinder pressure and temperature for various nozzle hole diameters, (a) pressure (b) temperature

Figure 10 depicts the Predicted NO_x and soot emissions for various nozzle hole diameters. Increasing the nozzle hole diameter decreases the in-cylinder temperature that leads to a reduction of NO_x emission formation as can be seen in Figure 10. As mentioned before by increasing the nozzle hole diameter, the droplet size is increased and injection velocity is decreased. This leads to increase of wall impingement of spray droplets and wall film formation that increases the fuel stratification. All of above parameters are effective on soot emission formation and lead to increase of soot by increasing the nozzle hole diameter.

Figure 11 shows the variation of IMEP and ISFC for various nozzle hole diameters. Increasing the nozzle hole diameter deteriorates the gasoline spray evaporation that leads to decrease of in-cylinder maximum pressure and a slight increase of gasoline ignition delay. This leads to decreasing the IMEP and increasing the ISFC. But variation of IMEP by varying the nozzle hole diameter is negligible as can be seen in Figure 11.

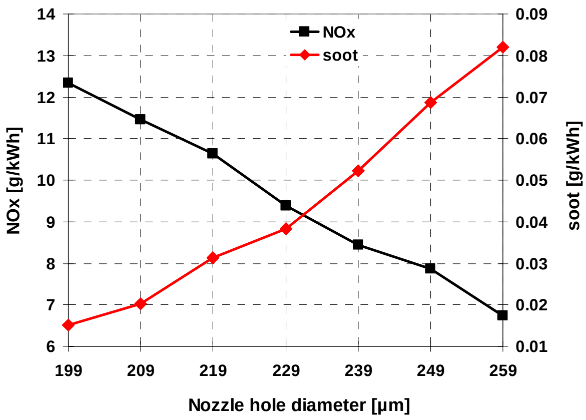


Figure 10. Predicted NO_x and soot emissions for various nozzle hole diameters

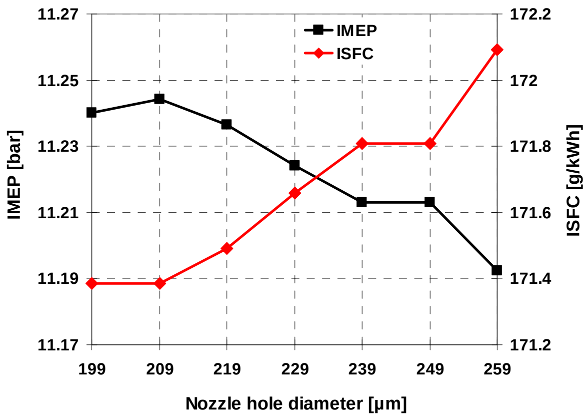


Figure 11. Predicted IMEP and ISFC for various nozzle hole diameters

4. Conclusion

In the present work the effect of injection characteristics have been investigated on combustion and emissions of a gasoline fuelled heavy duty compression ignition engine by using a three-dimensional CFD code.

Results of model for in-cylinder pressure, heat release rate, NO_x and soot exhaust emissions at double injection scheme for the pilot injection (30%) and main injection (70%) with the injection timing of 137 ˚ BTDC and 8 ˚BTDC, respectively is compared with the corresponding experimental data and show good agreement.

- Increasing the injection duration leaded to reducing of in-cylinder pressure and temperature due to decreasing injection velocity and evaporating of gasoline spray. Results depicted that soot emission is very sensitive to injection duration that increasing the injection duration from 6 ˚CA to 18 ˚CA, soot emission increased from 0.0037 g/kWh to 0.6173 g/kWh. There was an interesting trend in NO_x and soot emissions trends that by reducing the injection duration NO_x approximately remains constant but soot becomes zero simultaneous with a slight increase in IMEP.
- By retarding the main SOI timing the in-cylinder pressure, in-cylinder temperature, NO_x emission and IMEP are reduced. The NO_x emission and soot emission were became half and quadruplicate by varying the main SOI timing from 10 ˚BTDC to 2 ˚BTDC respectively. So the main SOI is more effective on soot emission than NO_x emission.
- When nozzle hole diameter is increased, in-cylinder pressure, in-cylinder temperature and NO_x emission formation were decreased and soot emission was increased. It due to increase of droplet size by increasing the nozzle hole diameter that leaded to wall impingement and deficient combustion. The variation of nozzle hole diameter had a negligible effect on IMEP and ISFC.

There is scope for further improvements by using high EGR ratios and optimizing the initial pressure for further reduction of NO_x.

Nomenclature

k	Turbulence kinetic energy [m^2/s^2]
ε	Dissipation rate [m^2/s^2]
T	Temperature
p	Pressure

Greek letters

τ_R	Turbulent mixing time scale
ρ	Density [kg/m^3]

Abbreviations

EGR	Exhaust gas recirculation
ATDC	After top dead center
BTDC	Before top dead center
IVC	Intake valve close
EVO	Exhaust valve open
SOI	Start of injection
CA	Crank angle
IMEP	Indicated Mean Effective Pressure
ISFC	Indicated Specific Fuel Consumption

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