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Simultaneously Reduction of NOx and Soot Emissions in a DI Heavy Duty diesel Engine Operating at High Cooled EGR Rates

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***Abstract*—**One promising way to achieve low temperature combustion regime is the use of a large amount of cooled EGR. In this paper, the effect of injection timing on low temperature combustion process and emissions were investigated via three dimensional computational fluid dynamics (CFD) procedures in a DI diesel engine using high EGR rates. The results show when increasing EGR from low levels to levels corresponding to reduced temperature combustion, soot emission after first increasing, is decreased beyond 40% EGR and get the lowest value at 58% EGR rate. Soot and NOx emissions are simultaneously decreased at advanced injection timing before 20.5 ºCA BTDC in conjunction with 58% cooled EGR rate in compared to baseline case.

***Keywords*—**Diesel Engine, Low Temperature Combustion, High Cooled EGR Rates, Combustion, Emissions

I. Introduction

INTERNATIONAL regulations ratified in recent years have imposed more stringent limits on pollutant emissions and fuel consumption in internal combustion engines. To comply with these regulations and reduce diesel NOx and soot emissions, several new combustion concepts have been developed.

One concept is homogenous charge compression ignition (HCCI) based on the simultaneous ignition of a highly diluted premixed air-fuel mixture throughout the combustion chamber [1], [2], [3]. Close to homogenous conditions are obtained by very early fuel injection. This concept corresponds to combustion in an area with an equivalence ratio leaner than 1 and a temperature lower than 2200 K. HCCI combustion results in minimal soot and NOx emissions with only a slight decrease in fuel efficiency.

Partial Premixed Charge Compression Ignition (PCCI) is a further possibility for low emission combustion [4], [5]. This concept uses partial premixing of the fuel to reduce the non-premixed part of the combustion. In this concept, low NOx and soot emissions achieved by injecting fuel early in the compression stroke in order to form a premixed lean mixture over a long mixing period. Also, increase the amount of fuel injected beyond a certain level is resulted in knock that this is limiting the operating range of PCCI combustion.

Recently, high equivalence ratio combustion, namely low temperature combustion (LTC) concept, based on extensive use of high cooled EGR rates, has been investigated by Sasaki et al. [6] and Akihama et al. [7] in a direct injection diesel engine at very low load condition. They indicated a smoke-less and NOx-less rich combustion when using EGR above a critical point due to a lower combustion temperature below the minimum soot formation temperature (i.e., about 1600 K). Bianchi et al. [8] carried out a numerical study to explore low temperature combustion condition in a diesel engine at medium load condition. They reported that EGR cooling reduces the soot formation but cannot almost eliminate it because portions of rich mixture are at high temperature. This high temperature is due the increase heat release from combustion and the reduced dilution effect in compared to low load engine condition.

The LTC concept is a better candidate to reduce both the soot and NOx forming conditions because it allows easier auto-ignition control and it can be applied to conventional diesel engines with minimal design modifications. However, the differences in chemistry and combustion between this concept and conventional diesel combustion must be investigated to determine their effects on spray combustion characteristics as well as emissions.

This work analyzes the effect of various cooled EGR rates, from low levels to levels corresponding to low temperature combustion, on the combustion and emission formation in a DI diesel engine at medium load condition. As mentioned above, high cooled EGR rate remains effective toward NOx-less condition while the same result cannot be achieved on soot because large portions of rich mixture at high temperature exists at medium load condition. Therefore, the impossibility of operating at real LTC condition increases the importance of mixture formation. Hence, in order to leaning mixture during combustion to reduce soot engine-out emissions the effects of injection timing are investigated in

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low-temperature combustion regimes. The results are obtained by simulating LTC conditions with three dimensional computational fluid dynamics (CFD) procedures based on FIRE code.

II. Model Description

The numerical model for Caterpillar 3406 heavy duty DI diesel engine with the specifications and operating conditions on Table 1 is carried out using FIRE code.

TABLE I
ENGINE SPECIFICATIONS

Engine type	Caterpillar 3406 DI diesel engine
Engine speed	1600 rpm
Bore × stroke	137.19 × 165.1 mm
Displacement	2.44 L
Power	39 kW (52 hp)
Maximum torque at 1600 rpm	234 N.m
Compression ratio	15:1
Injector type	Common-rail, electronic control
injection pressure	90 MPa
Number of nozzle holes	6
Nozzle hole diameter	0.259 mm
Swirl ratio	0.25

Fig.1 shows the 60° sector computational mesh of combustion chamber in three dimensional at TDC. Since a 6-hole nozzle is used, only a 60° sector has been modeled. This takes advantage of the symmetry of the chamber geometric setup, which significantly reduces computational runtime. Number of cells in the mesh is 19,385 cells at TDC. This fine mesh size will be able to provide good spatial resolution for the distribution of most variables within the combustion chamber. Calculations are carried out on the closed system from IVC at -147°CA ATDC to EVO at 136°CA ATDC.

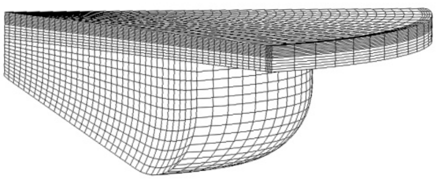

Fig. 1 Computational mesh at TDC

At the applied code, 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. [9]. The turbulent flows within the combustion chamber are simulated using the RNG k-ε turbulence model which is presented by Han and Reitz [10], modified for variable-density engine flows.

A. Spray, combustion and emissions models

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 [11]. In this model Kelvin-Helmholtz (KH) surface waves and Rayleigh-Taylor (RT) disturbances should be in continuous competition of breaking up the droplets.

The Dukowicz model [12] 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.

The Shell auto-ignition model was used for modeling of the auto-ignition [13]. In this generic mechanism, six generic species for hydrocarbon fuel, oxidizer, total radical pool, branching agent, intermediate species and products were involved. In addition the important stages of auto-ignition such as initiation, propagation, branching and termination were presented by generalized reactions, described in reference [13], but this not mean that we used just 6 spices for reaction mechanism.

Combustion process is modeled by Eddy Breakup model [14]. In the eddy break-up model, the rate of consumption of fuel is specified as a function of local flow properties. The mixing-controlled rate of reaction is expressed in terms of the turbulence time scale k-ε, where k is the turbulent kinetic energy and ε is the rate of dissipation of k. With s as the stoicheiometry coefficient, C_R and C_R' are model constants, a transport equation for the mass fraction of fuel is solved, where the:

$$S_{fu} = -\rho \frac{\varepsilon}{k} \min\left[C_R m_{fu}, C_R \frac{m_{ox}}{s}, C_R' \frac{m_{pr}}{1+s} \right] \qquad (1)$$

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.

NOx 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 [15] describing the thermal nitrous oxide formation.

The overall soot formation rate is modeled as the difference between soot formation and soot oxidation. Soot formation is based on Hiroyasu model and the soot oxidation rate is adopted from Nagle and Strickland-Constable [16].

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

III. Numerical Model

The numerical method has been used in this work is a segregated solution algorithm with a finite volume-based technique. The segregated solution is chosen, due to the advantage over the alternative method of strong coupling between the velocities and pressure. This can help to avoid convergence problems and oscillations in pressure and velocity fields. This technique consists of an integration of the governing equations of mass, momentum, species, energy and turbulence on the individual cells within the computational domain to construct algebraic equations for each unknown dependent variable. The pressure and velocity are coupled using the SIMPLE (semi-implicit method for pressure linked equations) algorithm which uses a guess-and-correct procedure for the calculation of pressure on the staggered grid arrangement. It is more economical and stable compared to the other algorithms. The upwind scheme is employed for the discretization of the model equations as it is always bounded and provides stability for the pressure-correction equation. The CFD simulation convergence is judged upon the residuals of all governing equations. This "scaled" residual is defined as:

$$R^{\phi} = \frac{\sum_{cells} p\left|\sum_{nb} a_{nb}\phi_{nb} + b - a_p\varphi_p\right|}{\sum_{cells} p\left|a_p\phi_p\right|} \tag{2}$$

Where p φ is a general variable at a cell p, a_p a is the center coefficient, a_{nb} are the influence coefficients for the neighboring cells, and b is the contribution of the constant part of the source term. The results reported in this paper are achieved when the residuals are smaller than 1.0×10^{-4}.

IV. Results and discussion

In the first part of this section, the possibilities of maintaining low soot and NOx emissions by using high cooled EGR rates to achieve low temperature combustion were investigated. In the subsequent sections, parametric study was conducted to the effects of the injection timing investigated on combustion and emissions at low combustion temperature.

A. Model validity

Before using the three dimensional CFD model to examine the effect of high EGR rate on combustion process and emissions, it is necessary to validate its predictive ability. For this reason we have used experimental data [17] for the single cylinder test engine mentioned above. The model was calibrated at 1600 rpm engine speed and without EGR. In this condition, start of injection (SOI) was fixed at 351.5 and 90 MPa injection pressure. In this work, this condition is so-called a baseline case. The parameters tuned were: in-cylinder pressure, NOx and soot exhaust emissions.

Fig.2 indicates the comparison of simulated and experimental in-cylinder pressures against to crank angle for the caterpillar diesel engine. The good agreement of predicted in-cylinder pressure with the experimental data [17] can be observed. It is due to time step and computational grid independency of obtained results.

Fig.3 and Fig.4 illustrate the total in-cylinder NOx and soot variation with crank angle in compared to experimental values at 430 ºCA at baseline condition. It is seen that most of the NOx is predicted to be produced after the peak heat release (i.e., after peak cylinder pressure) and during this time soot oxidation accounts for the decrease in the in-cylinder soot levels. It can be seen, the calculated total in-cylinder NOx and soot values have good agreement to experimental values at 430 ºCA that represents the model capability in the assessment of emissions.

The good agreement between the measured and computed results for this engine operating condition gives confidence in the model predictions, and suggests that the model may be used to explore new engine concepts about effects of high cooled EGR rate on combustion process and emissions.

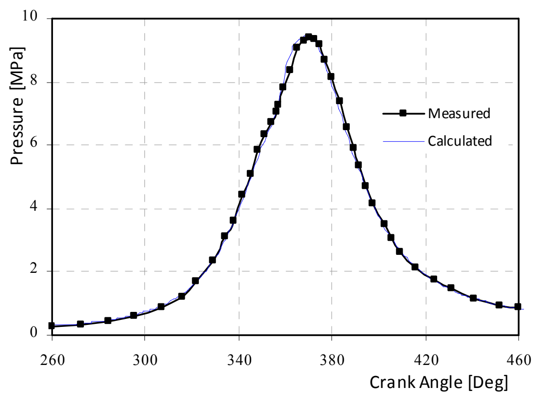

Fig. 2 Comparison of calculated and measured [17] in-cylinder pressure

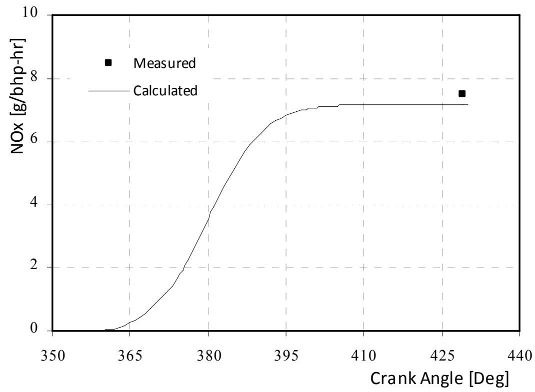

Fig. 3 Comparison of calculated and measured [17] NO_x emission

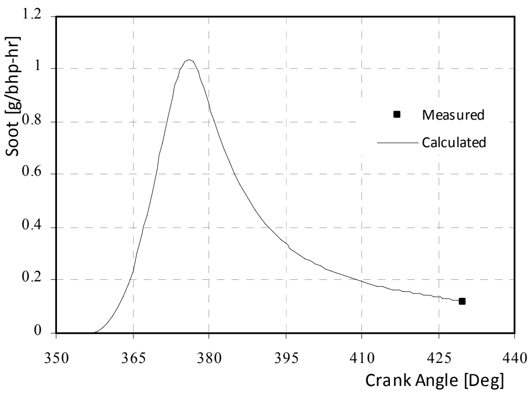

Fig. 4 Comparison of calculated and measured [17] soot emission

B. Effect of high cooled EGR rates

In this section at the fixed injection timing and injection pressure and for a given amount of fuel in compared to baseline case, the effect of cooled EGR is investigated on combustion process and NOx and soot emissions. EGR temperature at the exit of EGR cooler, is simulated 315 K equal to inlet temperature in baseline case.

In Figs.5 and 6 these are given the comparison of mean in-cylinder pressure and rate of heat release traces for 40% EGR and 58% EGR in compared to baseline case. It can be seen that the in-cylinder peak pressure is reduced with increase of EGR. This is because the use of high EGR ratio reduces further the availability of oxygen. This lack of oxygen in the cylinder charge reduces the combustion rate leading to retarded combustion and thus to lower peak cylinder pressure values. This is best revealed from the heat release rate curve on various EGR rates (Fig.6).

Fig. 7 compares the mean in-cylinder temperature for the 40% and 58% EGR rate with baseline case. Operating at 40% and 58% of cooled EGR rate the maximum value of mean in-cylinder temperature is reduced down to 1269 K and 1132 K, respectively in compared to 1504 K at baseline case. This is due to dilution effect and thermal effect in conjunction with cooled EGR [20]. The introduction of burnt gases into the cylinder replaces a part of the inlet air and causes a reduction of the oxygen concentration. This effect slows down the heat release rate if large amounts of EGR are used and leads to reduction in mean in-cylinder temperature. Moreover, during compression and combustion, the inert burnt gases must be heated up together with the rest of the in-cylinder charge. Because the total heat capacity of the charge is higher with burnt gases due to the higher specific heat capacity values of carbon dioxide (CO_2) and water vapor (H_2O), lower end of compression and combustion temperatures are achieved, and heat release rates as well as maximum pressure and temperature are reduced.

The effect of different EGR rates on the overall soot emission at EVO can be seen in Fig.8. Firstly, the soot is increased with increasing EGR rate and decreasing air-fuel ratio accompanied with intake charge dilution with exhaust gas and reduction of in-cylinder oxygen concentration. However, when the EGR rate exceeds a critical point, the soot starts to sharply decrease. Therefore, it was shown that the soot emission decreases even in the richer condition. Namely, when EGR rate is increased beyond 40 % EGR, soot emission reduced to low value at 58% EGR rate. As a result, for a fixed injection timing and injection pressure and for a given amount of fuel, it can be said the increase of cooling EGR to rate of 58%, allows to achieve soot emission level is decreased close to baseline case soot engine-out level but cannot almost eliminate it. In order to explain this reduction from low EGR rate to high one, the effect of temperature on soot formation should be stated which has been investigated in [18] and explained by Akihama et al. [7] at very low load engine condition.

The oxidization of Polycyclic Aromatic Hydrocarbons (PAH), which are considered soot precursors, are improved instead of forming species that transform into soot at high flame temperatures. The maximum soot concentration can be found at intermediate flame temperatures (i.e., 1600 K to 2000 K), which are ideal for both the formation of PAH and tar and their transformation to soot particles. However, in low temperature flames, the rate of oxidation of PAH is very low and the production of PAH is higher than at intermediate temperatures. But, because the temperature is too low to induce the coagulation of PAH into tar and the subsequent transformation of tar into soot, the rate of soot formation is reduced and total in-cylinder soot decreased.

However, when the load is increased to medium load condition, the fuel injected increases and the air-fuel ratio diminishes. Moreover, the temperature is increased because of the combined effects of lower dilution and greater heat release from combustion. Namely, high EGR rate reduces the soot formation but cannot almost eliminate it because portions of rich mixture are at intermediate temperature (above 1600 K).

Fig.9 shows NOx emission comparing between different EGR rates. As Fig.6 reveals that use of high EGR rate leads to an obviously decrease in the NOx emission rate in compared to baseline case (7.4 g/bhp-hr). Also, when EGR level is increased beyond 40 % EGR, NOx emission reduced to nearly

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zero at 58% EGR rate. NOx is formed at high temperatures due to the high activation energy of the $O + N_2 \rightarrow NO + N$ reaction in the Zeldovich mechanism [15].

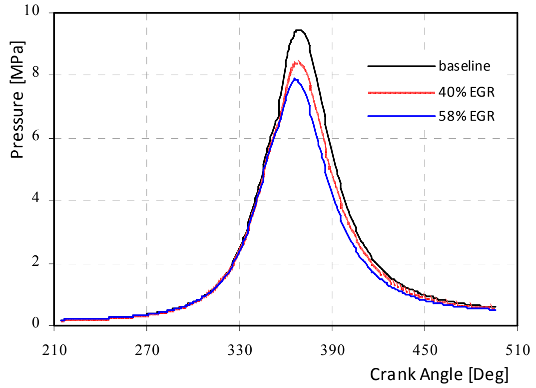

Fig. 5 in-cylinder pressure comparing between different high EGR rate cases and baseline case

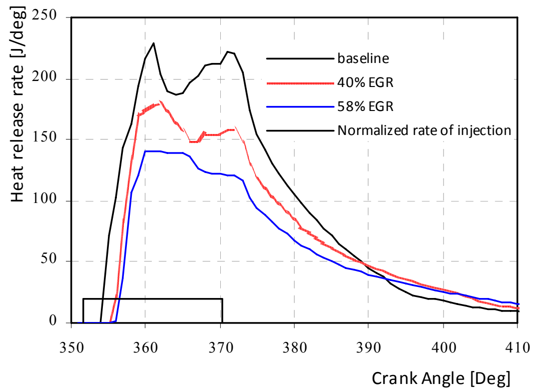

Fig. 6 Heat release rate comparing between different high EGR rate cases and baseline case

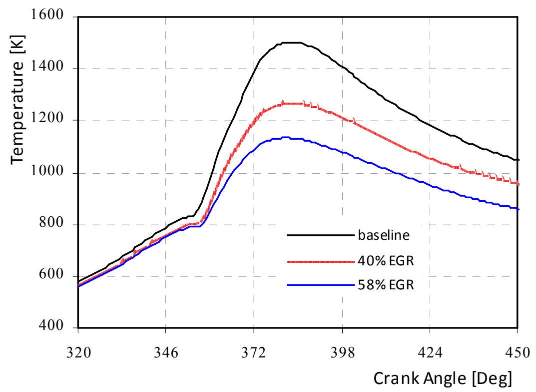

Fig. 7 in-cylinder temperature comparing between different high EGR rate cases and baseline case

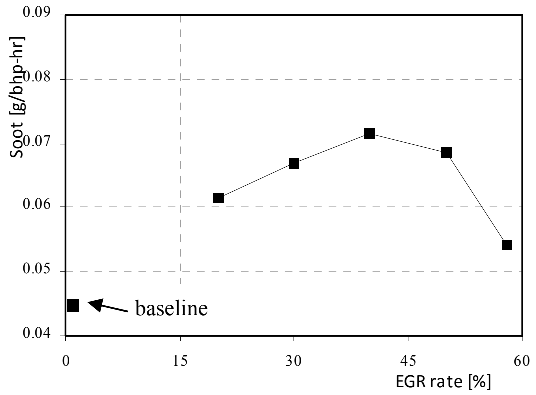

Fig. 8 Effect of EGR rate on soot emission at EVO for SOI at 351.5 ºCA in compared to baseline case

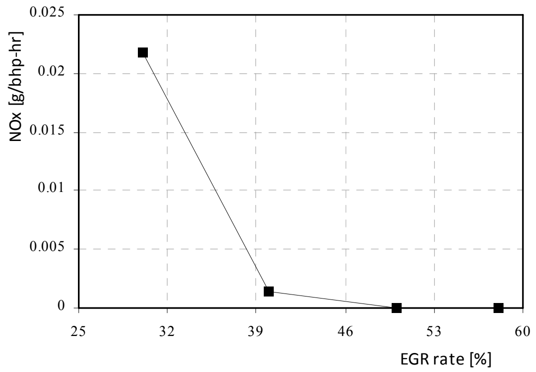

Fig. 9 Effect of EGR rate on NOx emission at EVO for SOI at 351.5 ºCA

As mentioned above, the high cooled EGR rates remain effective toward NOx-less condition while the same result cannot be achieved on soot because large portions of rich mixture at intermediate temperature exists. In the following section, in order to reduce soot engine-out emissions, advanced injection timings were examined for leaning mixture during combustion and improvement of mixture quality at 58% EGR rate which produces lower soot at low temperature combustion.

C. Effect of injection timing at 58% cooled EGR rate

The cylinder pressure and heat release rate for different injection timings at 58% EGR rate, are illustrated in Fig.10 and Fig.11 in compared to baseline case. Fig.10 shows that the in-cylinder pressure gets its maximum increase in the case of 23.5 ºCA BTDC injection timing and shows a slight decrease in both peak pressure value and the rate of pressure rise with the retarding of fuel injection timings toward TDC (top dead center). Similar to the behavior of cylinder pressure versus the fuel injection timings, a slight decrease in heat release rate versus fuel injection timings is observed in conjunction with large increasing tendency in combustion duration. This is due to more ignition delay at advanced injection timing and more fuel injected at this time which leads to more air-fuel mixing and premixed combustion rate. The heat release rate curve shows only a premixed burn phase (there is no evidence of a subsequent diffusion burn) in SOI at 23.5 ºCA BTDC. The fuel injection is seen to have ended just as combustion began.

Mean in-cylinder temperature at various injection timings at 58% EGR rate has been shown in Fig.12 in compared to baseline case. As can be seen, advanced injection timing increases the maximum value of in-cylinder temperature. However, high EGR rate causes to this maximum value becomes less than the baseline case. The higher premixed combustion rates at advanced injection timings lead to increase of mean in-cylinder temperature. As can be seen, SOI at 8.5, 17.5, 20.5 and 23.5 ºCA BTDC and 58% of cooled EGR rate the maximum value of mean in-cylinder temperature is increased up to 1132 K, 1247 K, 1283 K and 1320 K, respectively in compared to 1504 K at baseline case.

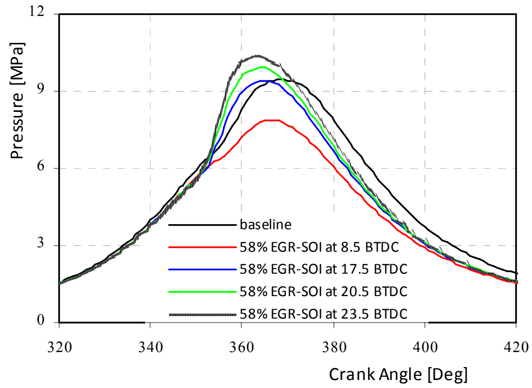

Fig. 10 in-cylinder pressure comparing between different injection timings at 58% EGR rate and baseline case

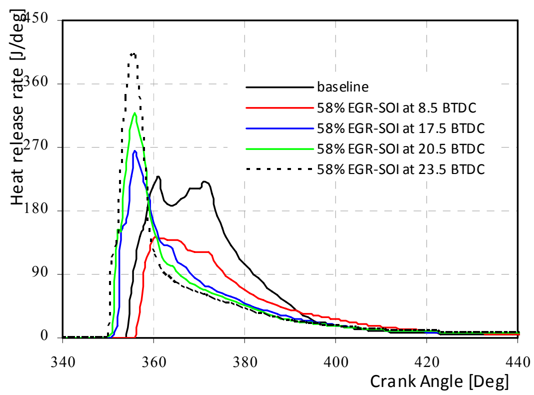

Fig. 11 Heat release rate comparing between different injection timings at 58% EGR rate and baseline case

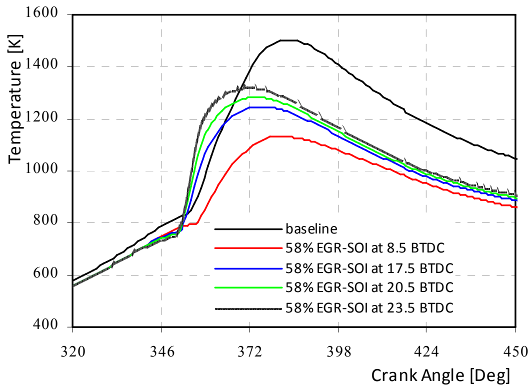

Fig. 12 in-cylinder temperature comparing between different injection timings at 58% EGR rate and baseline case

Fig.13 shows the history of soot production versus crank angle at different injection timings for 58% EGR rate. As can be seen, the peak value of soot formation is increased at SOI 17.5 ºCA BTDC in compared to SOI at 8.5 ºCA BTDC. This is due to larger wall film formation and insufficient time for mixing at early stage of combustion. But owing to increase of soot oxidation rates at homogenous mixture at later crank angle, overall soot is decreased at 17.5 BTDC in compared to 8.5 ºCA BTDC injection timing. Fig.14 shows soot level at EVO for different injection timings at 58% EGR rate and baseline case. As can be seen, soot emission level is seen to be low for early start of injection timings and specially, in SOI at 23.5 ºCA BTDC, consequently the very long ignition delays and adequate time for mixture formation. Therefore, advanced injection timings earlier than 20.5 ºCA BTDC at 58% cooled EGR rate obviously reduce the soot emission in compared to baseline case.

The corresponding NOx emission history at different injection timings at 58% EGR rate is displayed in Fig.14. As the injection timing is advanced, the NOx levels increase because the combustion gases spend more time at high temperatures where NOx formation rates are high. The NOx also decreases with increasing EGR rates. As mentioned above, EGR serves to reduce local temperatures and to reduce oxygen concentrations. This leads to lower reaction rates and lower NOx formation rates. However, relatively low NOx is also seen with advance injection timings and high EGR rate in compared to baseline case (7.4 g/bhp-hr) and this increase is negligible.

In order to further explain for NOx and soot emissions variance, a general comparison is presented to verify the interactions of emissions with temperature and local equivalence ratio distributions for crank angles of interest at different injection timings at 58% cooled EGR rate.

Both oxygen availability (low local equivalence ratio) and high temperature conditions satisfied NOx formation increases, but high temperature flame leads to a more NOx formation than the oxygen concentration. The area with equivalence ratio is close to 1 and the temperature is higher than 2000 K is the NOx formation areas, which agrees well with data in literature [20]. Also, the areas with high equivalence ratio (higher than 3) and the temperature approximately between 1600 K and 2000 K in bowl edge and piston surface, were stated the soot formation area at literatures [20].

Fig.16a and Fig.16b show equivalence ratio, temperature, soot and NOx contours at 360 ºCA for 58% EGR. The results indicate at advanced injection timing, when the spray targeted the piston bowl, it flows towards both the piston lip and squish regions. Therefore, higher air fuel mixture is available at ignition delay which leads to higher peak value of premixed combustion and combustion temperature. However, spray impingement on piston surface and momentum loss due to impingement and wall film formation lead to fuel condensation which increases soot formation at 360 ºCA at advanced injection timing. Locals with high temperature (i.e., above 2000 K) cannot be seen at different cases that agrees well with no evident NOx formation regions.

Fig.17 illustrates corresponding data which mentioned above at 375 ºCA. When the ignition delay is approximately equal to injection duration (SOI at 23.5 BTDC) at 58% EGR, enough time for mixing is available in the squish region with higher available oxygen. So that very little soot is formed in the first place. Namely, when enough mixing occurs before combustion begins, the fuel rich regions (high equivalence ratio) that breed soot formation are reduced in size and so the soot level also decreases. As can be seen from different injection timings, high temperature regions (i.e., above 2000 K) do not exist at 375 ºCA owing to high cooled EGR rate. Therefore, NOx formation is nearly zero despite the increase of in-cylinder temperature at advanced injection angle.

Fig.18 compares the contour plots of NOx, temperature, equivalence ratio and soot at 390°CA. The advanced injection timing produces the most homogeneous charge which leads to low soot emission in conjunction with no evident NOx formation.

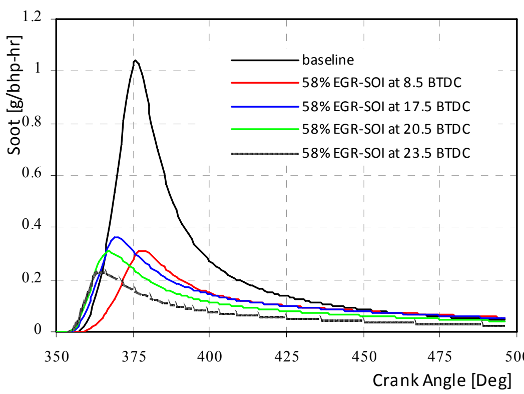

Fig.13 Effect of injection timing on soot emission production at 58% EGR rate in compared to baseline case

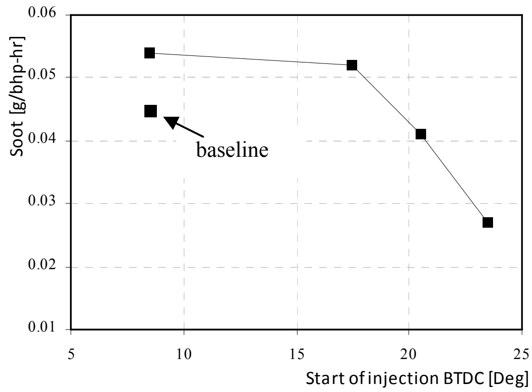

Fig. 14 Effect of injection timing on soot emission at EVO for 58% EGR rate in compared to baseline case

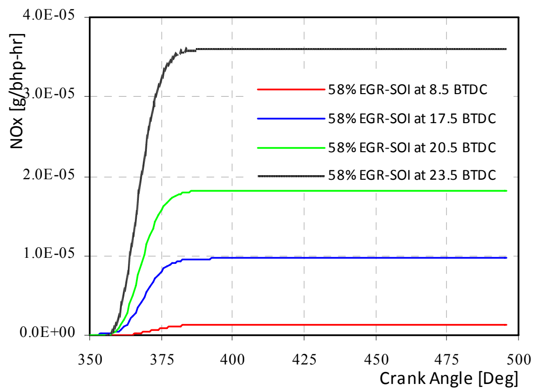

Fig. 15 Effect of injection timing on NOx emission production at 58% EGR

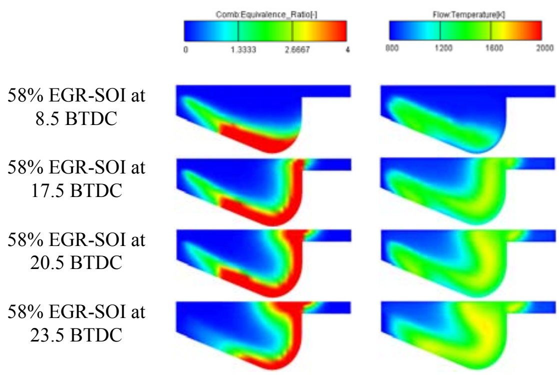

Fig. 16a Contour plots of equivalence ratio (left) and temperature (right) at different SOI at 360 ºCA

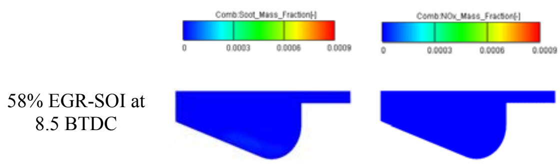

Fig. 16b Contour plots of soot (left) and NOx (right) mass fraction at different SOI at 360 ºCA

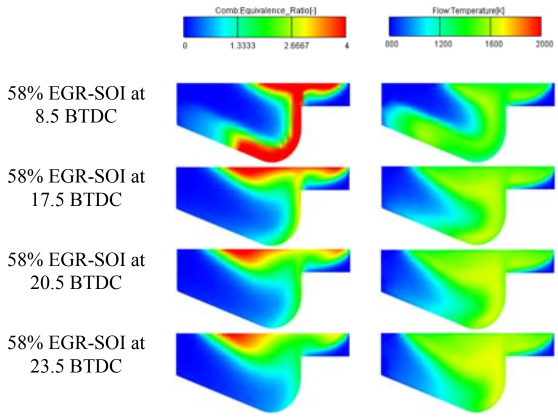

Fig. 17a Contour plots of equivalence ratio (left) and temperature (right) at different SOI at 375 ºCA

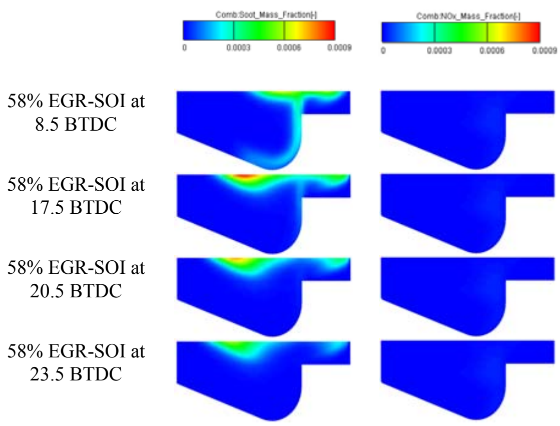

Fig. 17b Contour plots of soot (left) and NOx (right) mass fraction at different SOI at 375 ºCA

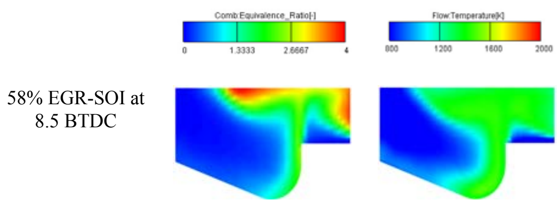

Fig. 18a Contour plots of equivalence ratio (left) and temperature (right) at different SOI at 390 ºCA

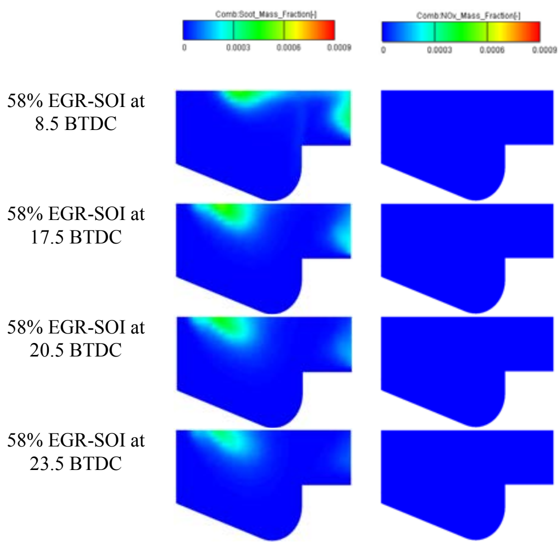

Fig. 18b Contour plots of soot (left) and NOx (right) mass fraction at different SOI at 390 ºCA

V. Conclusion

At the present work, after description of low temperature combustion condition, the effects of injection timing on combustion and emissions have been investigated in low-temperature combustion regimes by using multi-dimensional CFD code in a DI diesel engine and the following results are obtained.

Based on the above results, it can be seen that the increase of EGR rate further than 40%, to 58% rate, reduces soot formation rate despite higher formation to 40% rate because in-cylinder temperature has been kept lower than 1600 K. However, due to the higher fuel injected and higher temperature from greater heat release from combustion at medium load condition, 58% cooled EGR rate reduces the soot formation but cannot almost eliminate it because portions of rich mixture are at intermediate temperature. Also, associated with lower peak value of premixed combustion at 58% EGR rate, NOx emission is reduced to nearly zero value at EVO. The peak value of in-cylinder pressure and temperature is decreased at higher EGR rate. This is because slow heat release rate in conjunction with higher dilution effect and heat capacity effect at higher EGR rate.

In order to improvement of mixture formation at 58% EGR rate to reduce soot emission level, advancing injection timing explored at different advanced SOI timings. The time required for the mixture preparation was made available by injecting the fuel early and having a sufficient ignition delay. The results indicated advanced injection timings before 20.5 ºCA BTDC were able to produce combustion with lower soot level in compared to baseline case due to leaner air fuel mixture at diffusion combustion. But, the advanced injection timing owing to higher premixed combustion resulted in increase of NOx emission which is negligible at 58% EGR level.

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