

# NUMERICAL INVESTIGATION ON THE EFFECT OF INJECTION TIMING ON COMBUSTION AND EMISSIONS IN A DI DIESEL ENGINE AT LOW TEMPERATURE COMBUSTION CONDITIONS

*H. Khatamnezhad, S. Khalilarya \*, S. Jafarmadar, H. Oryani*

*Department of Mechanical Engineering, University of Urmia, Postal Code 51723-44115, Iran  
[sh.khalilarya@urmia.ac.ir](mailto:sh.khalilarya@urmia.ac.ir)*

*M. Pourfallah*

*Department of Mechanical Engineering, Babol University of Technology, Postal Code 46169-44484, Iran  
[m.pourfallah@gmail.com](mailto:m.pourfallah@gmail.com)*

\*Corresponding Author

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**Abstract** One promising way to achieve low temperature combustion regime is using 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 that when increasing EGR from low levels to levels corresponding to reduced temperature combustion, soot emission after first increasing is decreased beyond 40% EGR and reaches its lowest value at 58% EGR rate. Advanced injection timing before 20.5 °CA BTDC together with applying 58% EGR leads to simultaneous reduction in NO<sub>x</sub> and soot formation compared with the base engines. The predicted values of combustion process, emissions by this CFD model at high EGR levels show a good agreement with the corresponding data in the literature.

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

**چکیده** به کارگیری نرخ‌های بالای بازخورانی گازهای خروجی (EGR) سرد یکی از راه‌کارهای رسیدن به یک احتراق دما پایین است. در این مقاله با استفاده از دینامیک سیالات محاسباتی (CFD)، تاثیر زمان‌بندی‌های پاشش سوخت بر فرآیند احتراق دما پایین و آلایندگی‌های منتشره از یک موتور دیزلی پاشش مستقیم با کاربرد نرخ‌های بالای EGR بررسی شده است. نتایج نشان می‌دهند هنگامی که نرخ‌های EGR تا مقادیر متناظر با یک احتراق دما پایین افزایش می‌یابند، آلایندگی دوده پس از یک افزایش اولیه تا ۴۰ درصد نرخ EGR، به کمترین مقدار در ۵۸ درصد EGR می‌رسد. به جلو کشیدن زمان‌بندی پاشش قبل از ۲۰.۵ درجه میل لنگ همراه با کاربرد ۵۸ درصد EGR سبب کاهش هم‌زمان تشکیل اکسیدهای ازت و دوده در مقایسه با حالت پایه موتور می‌شود. نتایج پیش‌بینی شده احتراق و آلایندگی با مدل دینامیک سیالات محاسباتی استفاده شده در نرخ‌های بالای EGR توافق خوبی را با ادبیات فن نشان می‌دهد.

## 1. INTRODUCTION

Direct-injection diesel engines have proved to be an efficient option in heavy-duty applications like transportation or power generation. However, due

to the natural conditions of high pressure and temperature in the combustion process, diesel engines emit considerable amounts of pollutants, especially nitrogen oxides (NO<sub>x</sub>) and soot [1]. International regulations ratified in recent years have imposed more stringent limits on pollutant emissions in internal combustion engines. To

comply with these regulations with the common rail injection system which is widely used in recently developed engines; several new fuel injection strategies on conventional diesel combustion have been investigated in direct injection diesel engines.

Variable injection timing is a possible way to meet increasingly restrictive emissions' requirements for direct injection diesel engines. Jafarmadar and Zehni [2] investigated the effect of injection timing and split injection parameters on combustion and emissions of a DI diesel engine via Fire CFD code. Results indicated that 25 % of total fuel injected in the second pulse, reduces the total soot and NO<sub>x</sub> emissions at 25°CA delay dwell between the pulses. Sayint et al [3] explored the effects of fuel injection timing on the exhaust emission characteristics of a direct-injection diesel engine fueled with canola oil methyl ester–diesel fuel blends. They indicated similar trends for diesel fuel and canola oil methyl ester–diesel blends on the exhaust emissions for different injection timings. Results show that the advanced injection timings reduce soot emission and NO<sub>x</sub> emission boosted for all test conditions.

In order to further reduce both NO<sub>x</sub> and soot emissions, new diesel combustion concepts should be developed in conjunction with suitable injection strategies.

One concept of new diesel combustion is homogenous charge compression ignition (HCCI) based on the simultaneous ignition of a highly diluted premixed air-fuel mixture throughout the combustion chamber [4-6]. 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 NO<sub>x</sub> emissions with only a slight decrease in fuel efficiency.

Partial Premixed Charge Compression Ignition (PCCI) is a further possibility for low emission combustion [7, 8]. This concept uses partial premixing of the fuel to reduce the non-premixed part of the combustion. In this concept, low NO<sub>x</sub> 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, increasing the amount of fuel injected

beyond a certain level results in knock, 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 [9] and Akihama et al [10] in a direct injection diesel engine at very low load conditions. They indicated a smokeless and NO<sub>x</sub>-less rich combustion when using EGR above a critical point due to a combustion temperature below the minimum soot formation temperature (i.e., about 1600 °K). Bianchi et al [11] carried out a numerical study to explore low temperature combustion in a diesel engine at medium load conditions. They reported that EGR cooling reduces soot formation, but cannot eliminate it because portions of rich mixture are at high temperature. This high temperature is due the increased heat release from combustion and the reduced dilution effect compared to low load engine conditions. Yun and Reitz [12] demonstrated an optimization of combustion in the low-temperature diesel combustion regime and high EGR fraction. A genetic algorithm scheme was applied to optimize combustion in a diesel engine in order to reduce NO<sub>x</sub>, soot, and brake specific fuel consumption (b.s.f.c.), simultaneously. Start of-injection (SOI) timing, intake boost pressure level, cooled exhaust gas recirculation (EGR) rate, and fuel-injection pressure were used for optimization. Alriksson et al [13] investigated possibilities for extending the range of engine loads using low temperature combustion in conjunction with high levels of EGR to reduce soot and NO<sub>x</sub> emissions. Their results indicate that low soot emissions could not be achieved with high levels of EGR at 50% engine load, and in order to achieve lower soot emission, the charge air pressures should be tuned for higher engine load. Beatrice et al [14] reported that the LTC concept is a better candidate to reduce both the soot and NO<sub>x</sub> forming conditions, because it allows easier auto-ignition control and can be applied to conventional diesel engines with minimal design modifications. However, the differences in combustion between this concept and conventional diesel combustion must be investigated to determine their effects on spray combustion characteristics as well as emissions. Wakisaka et al [15] presented a detailed study of

the effects of increased boost pressure, high EGR level and high injection pressure on exhaust emissions of a light duty diesel engine. They indicated that a combination of increased boost pressure, high EGR level, and high injection pressure reduced  $\text{NO}_x$  and soot emissions significantly.

Therefore, according to the related literature, the low temperature combustion concept by using high cold EGR rates is a better candidate to highly reduce of both soot and  $\text{NO}_x$  emissions at low engine load as well as easier auto-ignition and knock occurrence control compared to HCCI and PCCI concept. Also, this 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. The present study has two major objectives. The first is to investigate the effect of various cooled EGR rates on mixture formation by considering spray characteristics as well as combustion process and emission formation in a DI diesel engine at high engine load condition. The cooled EGR rate is changed from low level to level corresponding to low temperature. As mentioned above, high cooled EGR rate can be made  $\text{NO}_x$ -less condition although soot emissions do not show reduction, because more portion of rich mixture at high temperature exists on high load conditions. Therefore, it is important to consider the mixture formation because operation at real LTC condition is impossible.

The second objective is to examine the effects of advanced injection timing in low-temperature combustion conditions in order to reduce soot engine-out emission using better air-fuel mixing before the start combustion.

The results are obtained by simulation of LTC conditions with three dimensional computational fluid dynamics (CFD) procedures based on FIRE code.

## 2. MODEL DESCRIPTION

The commercial computational fluid dynamics

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(CFD) software FIRE was used to perform the numerical simulation of combustion and emission formation in a diesel engine. The engine specification and operating conditions used in this work are shown in Table 1.

TABLE 1. Engine Specifications

Engine type	Caterpillar 3406 DI diesel engine
Engine speed	1600 rpm
Bore×Stroke	137.19×165.1 mm
Displacement	2.44 Liters
Power	39 Kw
Torque	234 N.m
Compression ratio	15.1
Injector type	Common-rail
Injection pressure	90 MPa
No. of nozzle holes	6
Nozzle hole diameter	0.259 mm
Fuel injected/cycle	0.1625 g

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.

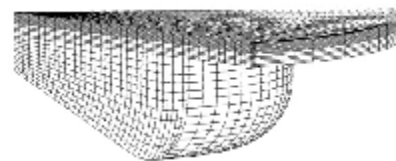


Figure 1. Computational mesh at TDC

In 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 [16]. The turbulent flows within the combustion chamber are

simulated using the RNG k-ε turbulence model which is presented by Han and Reitz [17], modified for variable-density engine flows.

**2.1. Spray and combustion 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 [18]. 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 [19] 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 convected 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. In this generic mechanism, 6 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 have been presented by generalized reactions, described in [20].

Combustion process is modeled by Eddy Breakup model [21]. 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 stoichiometry coefficient, C<sub>R</sub> and C<sub>R</sub>' are model constants; a transport equation for the mass fraction of fuel is solved, where:

$$S_{fu} = -r \frac{e}{k} \min \left[ C_R M_{fu}, C_R \frac{M_{ox}}{s}, C_R' \frac{M_{pr}}{1+s} \right] \quad (1)$$

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.

**2.2. Emission Models** NO<sub>x</sub> 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 [22] describing the thermal nitrous oxide formation. The reaction mechanism can be expressed in terms of the extended Zeldovich mechanism:



The assumption of partial equilibrium provides satisfactory results for the formation of NO<sub>x</sub> at considerably high temperatures.

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 Kennedy and Magnussen [23].

$$\frac{dM_s}{dt} = \frac{dM_{sf}}{dt} - \frac{dM_{so}}{dt} \quad (5)$$

Where:

$$\frac{dM_{sf}}{dt} = k_f \cdot M_{fv} \quad (6)$$

$$k_f = A_f P^{0.5} \exp\left(-\frac{E_f}{RT}\right)$$

$$\frac{dM_{so}}{dt} = a.A\left(\frac{e}{k}\right)M_s, \quad (7)$$

$$a = \min\left[1, \frac{M_{O_2}}{M_s\Phi_s + M_f\Phi_f}\right]$$

All the 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.

### 3. Numerical Model

The numerical method 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 the 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. This is more economical and stable compared to the other algorithms. The upwind scheme is employed for 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:

$$R^f = \frac{\sum_{cells} p \left| \sum_{nb} a_{nb} f_{nb} + b - a_p j_p \right|}{\sum_{cells} p \left| a_p f_p \right|} \quad (8)$$

Where  $\phi_p$  is a general variable at a cell  $p$ ,  $a_p$  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

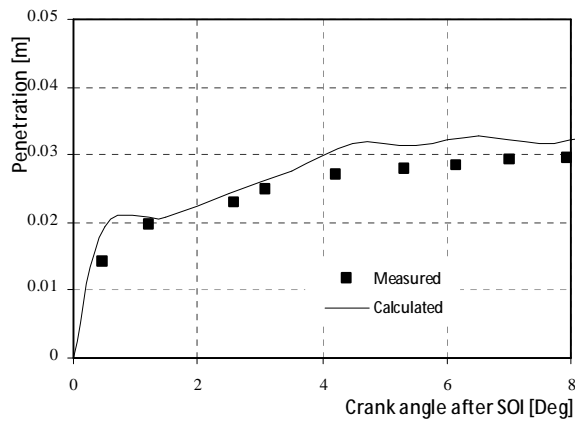
reported in this paper are achieved when the residuals are smaller than  $1.0 \times 10^{-4}$ .

## 4. RESULTS AND DISCUSSION

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

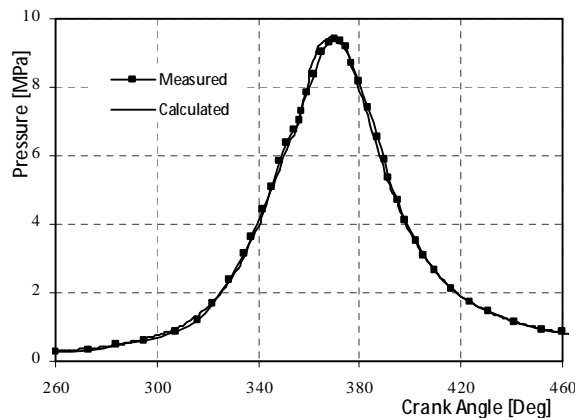
**4.1. Validation of the Model** Before using the three dimensional CFD model to examine the effect of high EGR rate on combustion process and emissions, it is necessary to validate its predictive ability. For this reason we have used experimental data for the single cylinder test engine mentioned above. The model was calibrated at 1600 rpm engine speed. In this condition, start of injection (SOI) was fixed at 351.5 °CA and injection pressure was fixed at 90 MPa. In this work, this condition is so-called a baseline case. The parameters tuned were: liquid spray tip penetration, mean in-cylinder pressure,  $NO_x$  and soot exhaust emissions.

Fig. 2 shows predicted spray penetration for caterpillar diesel engine in comparison with experimental data investigated by Ricart et al [24]. Experimental data for spray penetration exist until about 8°CA after SOI as ignition occurred and the optical measurement system did not contain a narrow pass filter to block out the flame luminosity. There is a good agreement between calculated and measured results and as can be seen, the numerical model tends to over predict the measured spray tip penetration. The accuracy of calculated spray penetration illustrates the ability of this model in prediction of spray characteristics and mixture formation.



**Figure 2.** Comparison of calculated and measured spray tip penetration

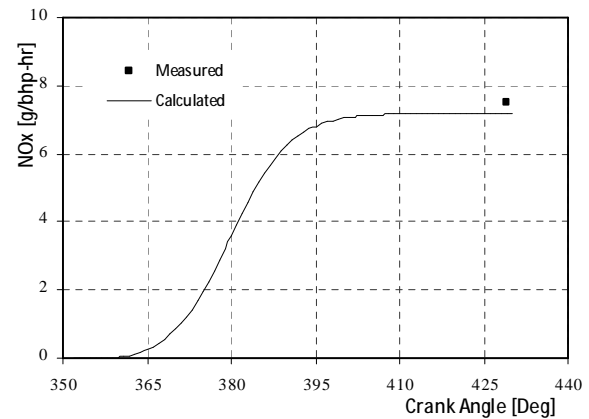
Fig. 3 indicates the comparison of simulated and experimental in-cylinder pressures against the crank angle for the caterpillar diesel engine. The good agreement of predicted in-cylinder pressure with the experimental data [25] can be observed. It is due to time step and computational grid independency of the results.



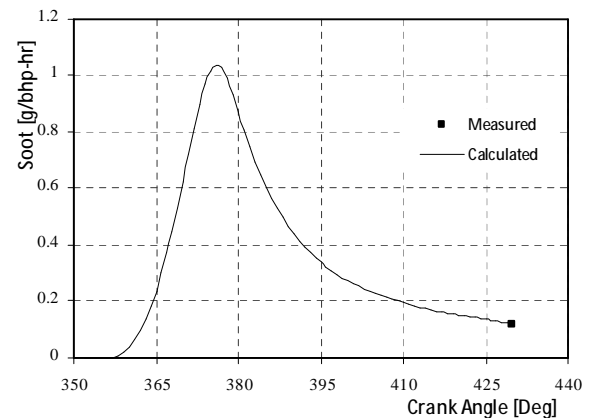
**Figure 3.** Comparison of calculated and measured mean in-cylinder pressure

Figs. 4 and 5 illustrate the total in-cylinder  $\text{NO}_x$  and soot variation with crank angle compared to the experimental values [25] at 430 °CA at baseline condition. It is seen that most of the  $\text{NO}_x$  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 that the calculated total in-cylinder  $\text{NO}_x$  and soot values are in good agreement with experimental values at

430 °CA, which shows the model capability in the assessment of emissions.



**Figure 4.** Comparison of calculated and measured  $\text{NO}_x$  emission



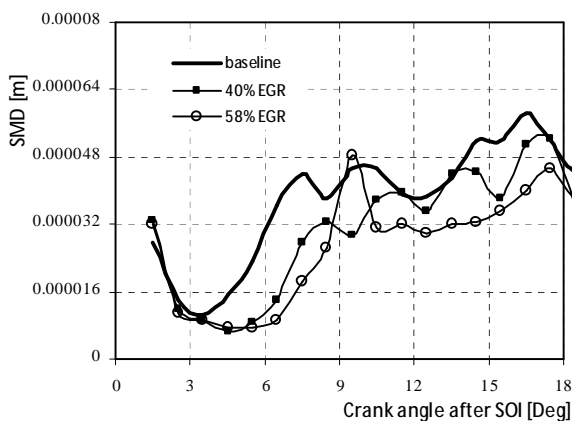
**Figure 5.** Comparison of calculated and measured soot emission

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 EGR rate on air-fuel mixture formation, combustion process and  $\text{NO}_x$  and soot exhaust emissions.

**4.2. Effect of high EGR rates** In this section at the fixed injection timing and injection pressure and for a given amount of fuel in comparison to baseline case, the effect of cooled EGR is investigated on fuel spray characteristics, combustion process and  $\text{NO}_x$  and soot emissions.

EGR temperature in the exit of EGR cooler is considered to be 315 K, which is same as the inlet temperature in baseline case.

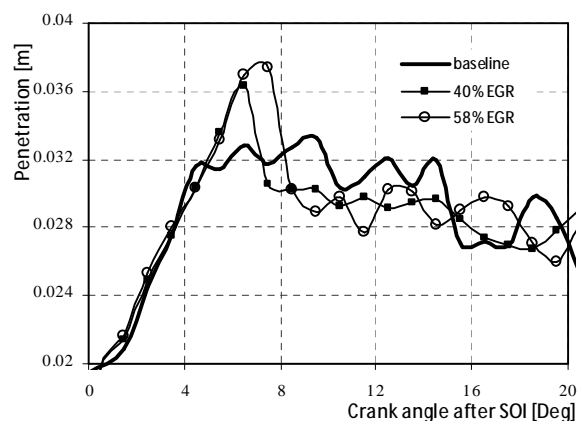
SMD distributions in different EGR rates are shown in Fig. 6, compared to the baseline case. SMD is a quantity characterizing the average droplet size of a spray and is the average volume of all particles in a cell divided by the average surface area of all particles in the cell. Firstly, SMD size is decreased to the lowest value at 354 CA, due to break-up of spray in all cases. The increase of SMD size after the first decreasing appears for all EGR rates in the combustion chamber. When combustion starts after ignition delay, the smaller droplets evaporated and extinguished before the larger droplets. Therefore, larger droplets remained in the fuel jet that led to increase of SMD size. Fig. 6 indicates that the increase of SMD size occurs at later crank angle accompanied by the increase of EGR rate. This reveals that the higher EGR rate causes longer ignition delay.



**Figure 6.** SMD distributions for 40% and 58% EGR rates compared to baseline case

The liquid spray penetration length versus crank angle for different EGR rates are shown in Fig. 7. The liquid spray penetration profile appeared to follow two different phases; an almost linear phase after start of injection and a rapid transition to a steadier penetration length fluctuated around an average value. Increasing the EGR rate to 58% is clearly seen to increase the rate of penetration. This is the result of the reduction of droplets evaporating around the periphery of the penetrating spray in conjunction with the increase of EGR rate and the subsequent decrease of the in-cylinder

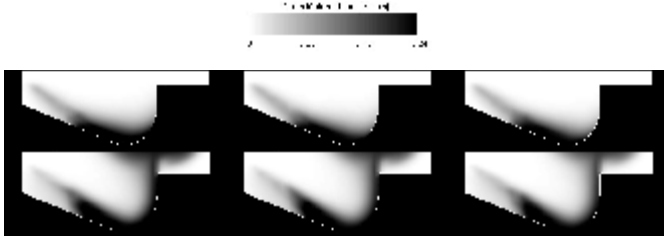
temperature. The increase of first phase penetration leads to a portion of the injected spray droplets impact on the walls of the combustion chamber and form a wall-film. Shortly after the break-up period and ignition delay, the liquid penetration profiles fluctuated around a slowly decreasing average value. These fluctuations could be due to the air entrainment in the liquid jet. The momentum exchange between liquid droplets and inert gas leads to breaking away parcels of droplets around the periphery of the leading edge of the spray tip. During the latter phase, the penetration profile behavior of 40% and 58% EGR rate are almost identical with a slightly higher average at 40% EGR rate. The baseline case has higher average penetration at this moment. This higher penetration leads to the increase of air entrainment in the spray and improving mixture formation. As can be seen in Fig. 6, smaller droplets can be seen at higher EGR rate after the start of combustion. The larger droplets in the baseline case induce the higher momentum and droplet velocity that cause a longer spray tip penetration.



**Figure 7.** Spray tip penetration for 40% and 58% EGR rates compared to baseline case

Fig. 8 shows the contour plots of spray distribution and mixture formation in a cross-section taken diagonally across the bowl and split ting it in half at 360 and 372 °CA, respectively. Mixture fraction is higher in the periphery and tip of the penetrating spray. This is because droplets with smaller SMD are located at these regions that cause higher evaporation rates. As can be seen, spray injected targeted the piston bowl and then progressed along the piston wall. As indicated, mixture fraction

showed a somewhat decreasing trend with the increase of EGR rate. This is because the higher in-cylinder temperature enhances the evaporation rate of the liquid droplet and wall film on piston bowl. This issue influences the deterioration of combustion performance and the formation of incomplete combustion emissions.

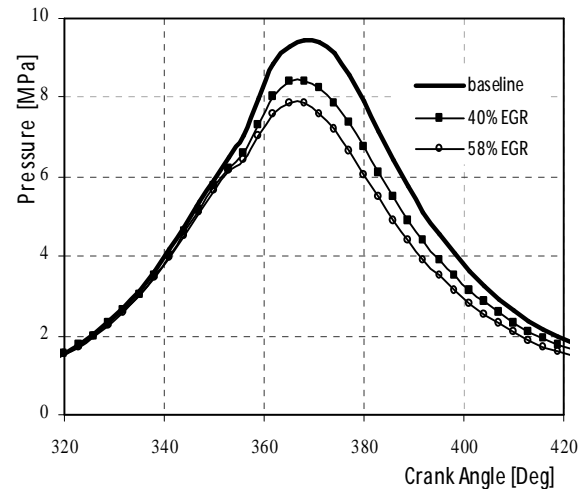


**Figure 8.** Contour plots of spray distribution and mixture fraction in baseline (left column) 40% EGR (middle column) 58% EGR (right column) cases at 360 °CA (first line) 372 °CA (second line)

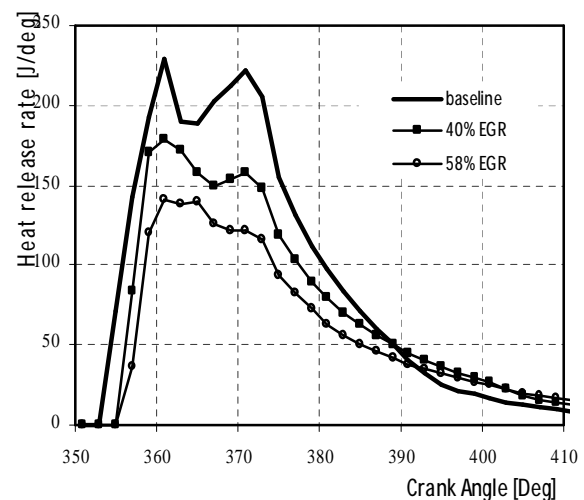
In Figs 9 and 10 the mean in-cylinder pressure and rate of heat release traces for 40% EGR and 58% EGR are compared with the baseline case. It can be seen that the in-cylinder peak pressure is reduced when we use higher rate of EGR. The higher EGR ratio reduces the amount of oxygen. This oxygen deficiency in the cylinder charge reduces the combustion rate leading to retarded combustion and thus lowers peak cylinder pressure values. This is best revealed from the heat release rate curve on various EGR rates (Fig. 10).

Fig. 11 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 as compared to 1504 K for the baseline case. This is due to dilution and thermal effects in conjunction with cooled EGR. The entrance of burnt gases into the cylinder as a substitute for part of the inlet air the reason for reduction of 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<sub>2</sub>) and water vapor (H<sub>2</sub>O), lower end of compression and combustion temperatures are achieved, and heat release rates as well as maximum pressure and temperature are reduced.

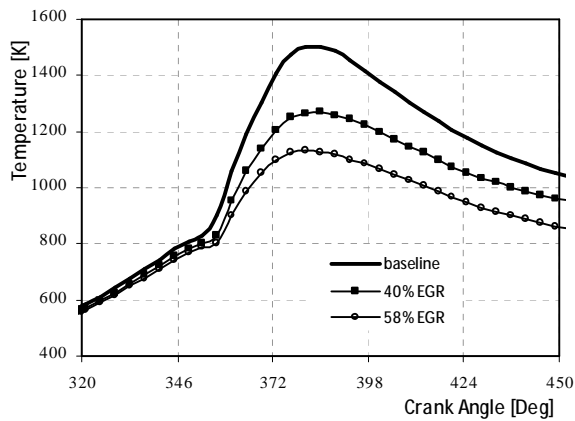


**Figure 9.** Comparison of in-cylinder pressure for different high EGR rate cases and baseline case



**Figure 10.** Comparison of heat release rate for different high EGR rate cases and baseline case





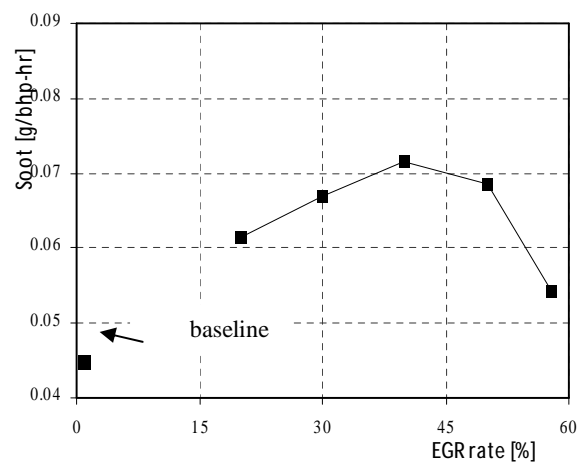
**Figure 11.** Comparing of in-cylinder temperature for different high EGR rate cases and baseline case

The effect of different EGR rates on the overall soot emission at EVO can be seen in Fig. 12. Firstly, high EGR rate accompanied with intake charge dilution and reduction of in-cylinder oxygen concentration decrease air-fuel ratio. Hence, soot formation increases. However, when the EGR rate exceeds a critical point, soot formation decreases sharply. It has also been shown that the soot emission decreases even in the richer condition. Namely, when EGR rate is increased beyond 40 % EGR, soot emission reduced to lower value as compared to 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 that increasing cooling EGR rate to 58%, decreases the soot emission level close to baseline case soot engine-out level. However, it cannot totally eliminate it. In order to explain this reduction from low EGR rate to high one, the effect of temperature on soot formation should be investigated. It has been investigated by Ciajolo et al [26] and explained by Akihama et al [10] at very low load engine conditions.

Oxidization of Polycyclic Aromatic Hydrocarbons (PAH) which are considered soot precursors, take place 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 to 2000 K), which are ideal for both 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 decreases.

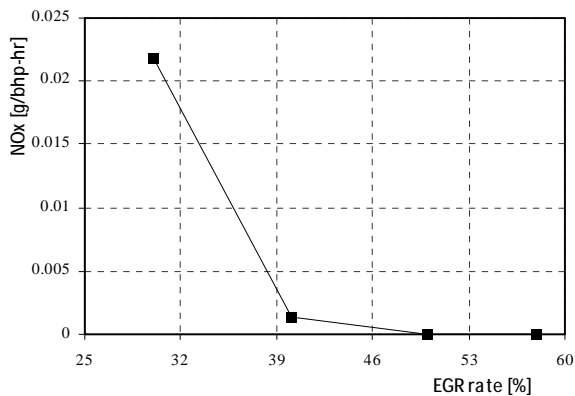
However, when the load is increased to medium and high load conditions, the mass of fuel increases and the air-fuel ratio is reduced. Moreover, the temperature is increased because of the combined effects of lower dilution and greater heat release from combustion. Namely, high EGR rate reduces the soot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



**Figure 12.** Effect of EGR rate on soot emission at EVO for SOI at 351.5 °CA compared to baseline case

Fig. 13 shows  $\text{NO}_x$  emission at different EGR rates. The use of high EGR rate obviously leads to a reduction in the  $\text{NO}_x$  emission rate. When EGR rate is increased above 40%, results show that the amount of  $\text{NO}_x$  moves to nearly zero. As it has been found by many researchers, much of the  $\text{NO}_x$  is formed in the zones up to the peak of the heat release rate. Hence, the heat release rate up to its peak value greatly affects the  $\text{NO}_x$  formation. It is also known that the  $\text{NO}$  formation is very sensitive to the gas temperature during combustion.

In order to further explain  $\text{NO}_x$  and soot emissions reduction, a general comparison is presented to verify the interactions of emissions with temperature and local equivalence ratio distributions for crank angles of interest at baseline case, 40 and 58% EGR conditions.

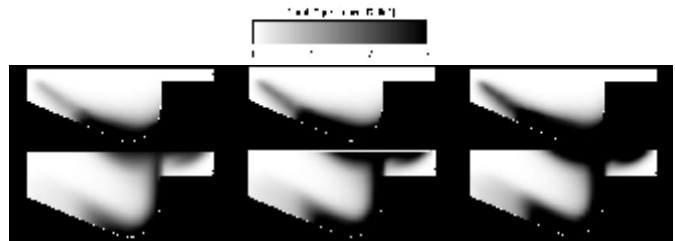


**Figure 13.** Effect of EGR rate on soot emission at EVO for SOI at 351.5 °CA

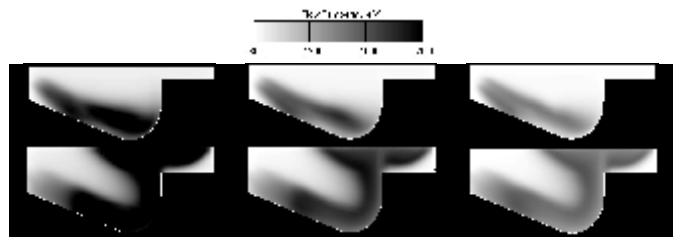
It can be seen from Figs. 14a to d that with both oxygen availability (low local equivalence ratio) and high temperature conditions satisfied,  $\text{NO}_x$  formation increases, but high temperature flame leads to a more  $\text{NO}_x$  formation than the oxygen concentration. As can be seen, the areas with equivalence ratio are close to 1 and the temperatures over 2000 K are the  $\text{NO}_x$  formation areas, which agree well with data in literature [27]. However, high EGR level decreases the local high temperature regions and flame temperature due to reduction in oxygen flow rate to the engine, and increases the specific heat of the charge in conjunction with introducing exhaust gas. Therefore,  $\text{NO}_x$  emissions are gradually reduced, especially for the conditions of combustion temperature below 2000 K (by more than 40% EGR).

As expected, the volume of high equivalence ratio is increased with increased EGR level due to the deeper fuel spray penetration into the chamber and mixing with the more diluted ambient gas. The areas with high equivalence ratio (higher than 3) and the temperature approximately between 1600 and 2000 K in bowl edge and piston surface, have been stated as the soot formation area in literature [27]. Fig. 14c shows the histories for the soot formation region. The combustion condition of the 58% EGR case does not enter the high soot formation region as shown in Fig. 14c despite to the higher equivalence ratio than 40% EGR. Namely, if the temperature is kept below approximately 1600 K, both the  $\text{NO}_x$  and soot formation rates can be reduced regardless of the

equivalence ratio. This concept is referred to as low temperature combustion (LTC) [10]. At 360°CA, there are large fuel rich regions (high equivalence ratio) near wall surface, but the soot levels are low because the turbulence generated by the fuel jet during combustion helps increase mixing which increases soot oxidation rates. When injection ceases at 375°CA, turbulence is no longer generated in the flame by the fuel jet to help increase mixing rates. However, the extent of the fuel rich regions is reduced since adequate time for mixing has been allowed. Thus, the maximum in-cylinder soot is decreased substantially.



**Figure 14a.** Contour plots of equivalence ratio in baseline (left column) 40% EGR (middle column) 58% EGR (right column) cases at 360 °CA (first line) 375 °CA (second line)



**Figure 14b.** Contour plots of temperature in baseline (left column) 40% EGR (middle column) 58% EGR (right column) cases at 360 °CA (first line) 375 °CA (second line)



**Figure 14c.** Contour plots of  $\text{NO}_x$  mass fraction in baseline (left column) 40% EGR (middle column) 58% EGR (right column) cases at 360 °CA (first line) 375 °CA (second line)

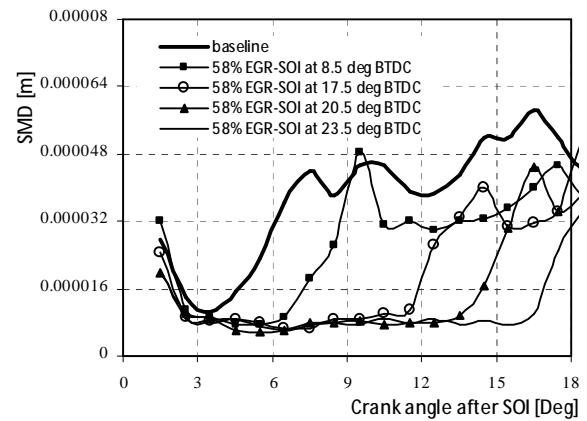


**Figure 14d.** Contour plots of soot mass fraction in baseline (left column) 40% EGR (middle column) 58% EGR (right column) cases at 360 °CA (first line) 375 °CA (second line)

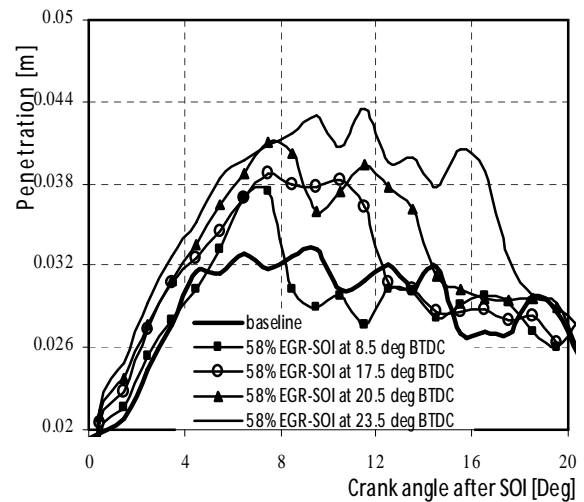
As mentioned above, the high cooled EGR rates remain effective toward NO<sub>x</sub>-less condition while the same result cannot be achieved on soot because large portions of rich mixture exists at intermediate temperatures. In the following section, in order to reduce soot engine-out emissions, advanced injection timings were examined for better air-fuel mixing before the start of combustion and improvement of mixture quality at 58% EGR rate which produces lower soot at low temperature combustion.

**4.3. Effect of injection timing at 58% cooled EGR rate** SMD distributions versus crank angle for different injection timings at 58% EGR rate are shown in Fig. 15. As can be seen, ignition delay increases at advanced injection timings because increasing in SMD size occurs at later crank angle after start of injection. Therefore, longer ignition delay with smaller SMD causes better air-fuel mixing at sufficient time. It is revealed that combustion starts after the end of fuel injection and a premixed mixture is ignited at 23.5 °CA injection timing.

In Fig.16 it is given the comparison of spray tip penetration for advanced injection timings in compared to 8.5 °CA BTDC. The lower in-cylinder temperature and pressure at advanced timing to TDC causes to increase of spray penetration in combustion chamber at advanced interjection timings. This leads to the increase of air entertainment into the fuel spray because of the longer spray path before impinging piston bowl.

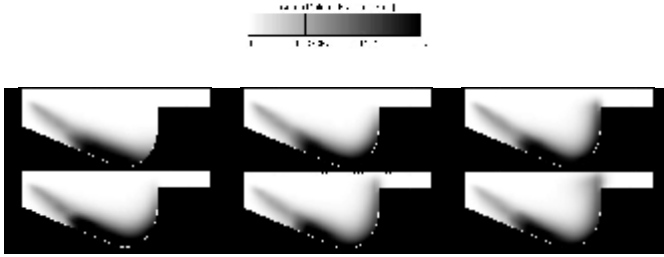


**Figure 15.** SMD distributions comparing between different injection timings at 58% EGR rate and baseline case



**Figure 16.** Spray penetration comparing between different injection timings at 58% EGR rate and baseline case

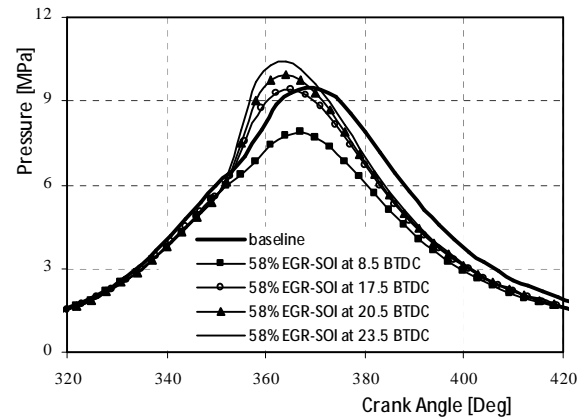
Contour plots of mixture fraction are indicated in Fig.17. Better spray development at advanced injection timings and higher air entrainment in fuel jet increases air-fuel mixture fraction in combustion chamber during injection event. Also, as can be seen, the mixture progressed to the squish area of the piston at advanced injection timing. Consequently, higher oxygen content at this region induces air entrainment and mixture formation.



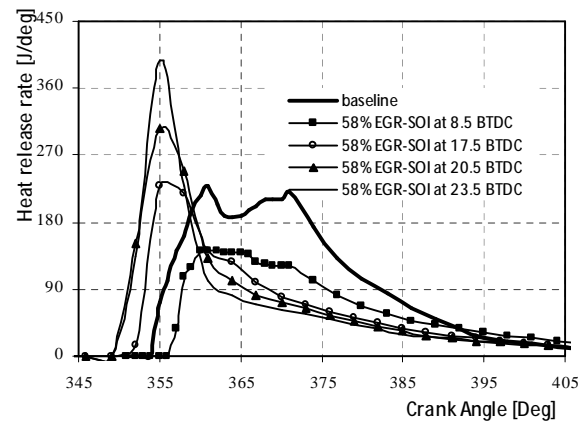
**Figure 17.** Contour plots of spray distribution and mixture fraction, left to right in SOI at 17.5, 20.5 and 23.5 °CA BTDC at 58% EGR for 351 °CA (first line) 354 °CA (second line), respectively

The cylinder pressure and heat release rate for different injection timings at 58% EGR rate, are illustrated in Figs. 18 and 19 as compared to baseline case. Fig. 18 shows that the in-cylinder pressure gets its maximum increase in the case of 23.5 °CA 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 °CA BTDC. The fuel injection is seen to have ended just as main combustion phase began.

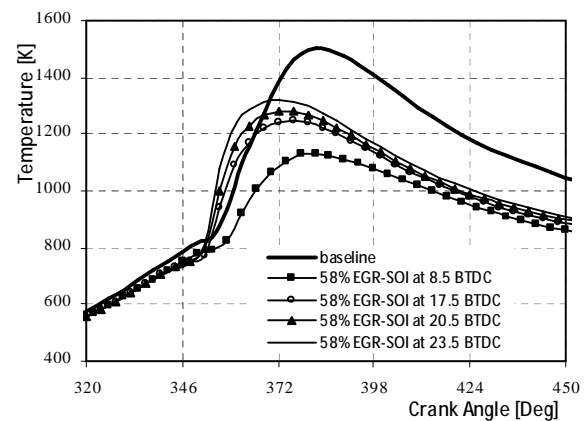
Mean in-cylinder temperature at various injection timings at 58% EGR rate has been shown in Fig. 20 compared with the baseline case. As can be seen, advanced injection timing increases the maximum value of in-cylinder temperature. However, high EGR rate causes this maximum value to become less than the 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 °CA BTDC and 58% of cooled EGR rate, the maximum value of mean in-cylinder temperature is increased up to 1132, 1247, 1283 and 1320K, respectively compared to 1504 K at baseline case.



**Figure 18.** Comparing between in-cylinder pressure for different injection timings at 58% EGR rate and baseline case



**Figure 19.** Comparing between heat release rate for different injection timings at 58% EGR rate and baseline case

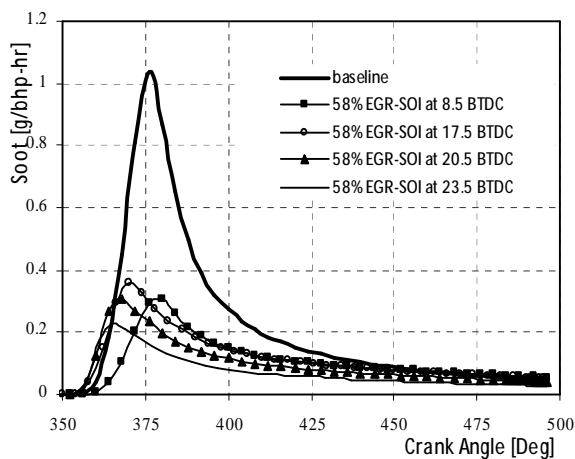


**Figure 20.** Comparing between in-cylinder temperature for different injection timings at 58% EGR rate and baseline case

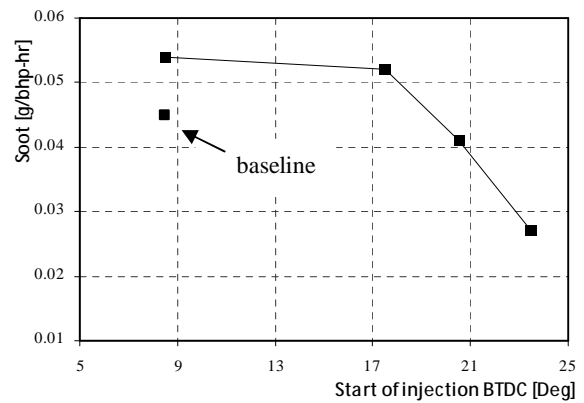
Fig. 21 shows the history of soot production versus crank angle at different injection timings for 58% EGR rate. As can be seen, the peak value of soot

formation is increased at SOI 17.5 °CA BTDC compared to SOI at 8.5 °CA BTDC. This is due to larger wall film formation and insufficient time for mixing at early stages of combustion. But, owing to the increase of soot oxidation rate at homogenous mixture at later crank angle, overall soot is decreased at 17.5 BTDC compared to 8.5 °CA BTDC injection timing. Fig. 22 indicates soot level at EVO for different injection timings at 58% EGR rate and baseline case. As can be seen, soot emission level is for early start of injection timings and specially, in SOI at 23.5 °CA BTDC, consequently the very long ignition delays and adequate time for mixture formation. Therefore, advanced injection timings earlier than 20.5 °CA BTDC at 58% cooled EGR rate obviously reduce the soot emission in compared to baseline case.

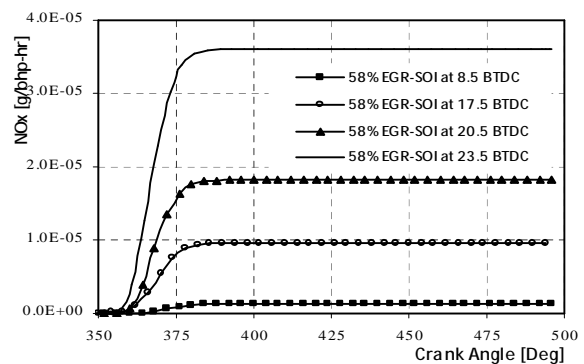
The corresponding NO<sub>x</sub> emission history at different injection timings at 58% EGR rate is displayed in Fig. 23. As the injection timing is advanced, the NO<sub>x</sub> levels increase because the combustion gases spend more time at high temperatures where NO<sub>x</sub> formation rates are high. The NO<sub>x</sub> also decrease 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 NO<sub>x</sub> formation rates. However, relatively low NO<sub>x</sub> is also seen with advance injection timings and high EGR rate compared to baseline case (7.4 g/bhp-hr) and this increase is negligible.



**Figure 21.** Effect of injection timing on soot emission production at 58% EGR rate compared to baseline case



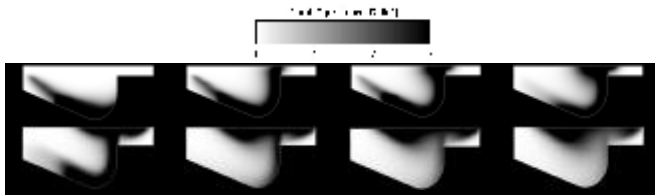
**Figure 22.** Effect of injection timing on soot emission at EVO for 58% EGR rate compared to baseline case



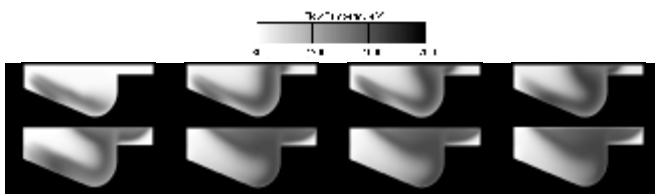
**Figure 23.** Effect of injection timing on NO<sub>x</sub> emission production at 58% EGR

Fig.24a to Fig.24d show equivalence ratio, temperature, NO<sub>x</sub> and soot contours at 360 °CA and 375 °CA with SOI at 8.5, 17.5, 20.5 and 23.5 °CA BTDC for 58% EGR, respectively. The results indicate at advanced injection timing, when the spray targeted the edge of the piston bowl, it flows towards both the piston bowl and squish regions. Therefore, enough time for mixing 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 °CA. Locals with high temperatures (above 2000 K) cannot be seen at different cases that agrees well with no evident NO<sub>x</sub> formation regions. At 375 °CA, 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. Hence, very little soot is formed in the first place. Namely, when

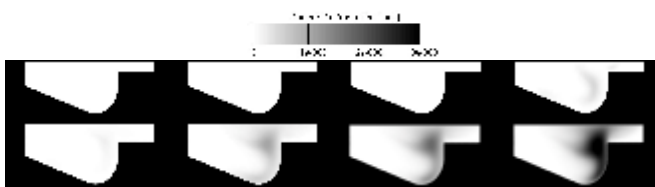
enough mixing occurs before combustion begins, the fuel rich regions (high equivalence ratio) that breed soot formation are reduced in size and so the soot level also decreases. As can be seen from different injection timings, high temperature regions (i.e., above 2000 K) do not exist at 375 °CA owing to high cooled EGR rate. Therefore, NO<sub>x</sub> formation is nearly zero despite the increase of in-cylinder temperature at advanced injection angle.



**Figure 24a.** Contour plots of equivalence ratio, left to right in SOI at 8.5, 17.5, 20.5 and 23.5 °CA BTDC at 58% EGR for 360 °CA (first line) 375 °CA (second line), respectively



**Figure 24b.** Contour plots of temperature, left to right in SOI at 8.5, 17.5, 20.5 and 23.5 °CA BTDC at 58% EGR for 360 °CA (first line) 375 °CA (second line), respectively



**Figure 24c.** Contour plots of NO<sub>x</sub> mass fraction, left to right in SOI at 8.5, 17.5, 20.5 and 23.5 °CA BTDC at 58% EGR for 360 °CA (first line) 375 °CA (second line), respectively



**Figure 24d.** Contour plots of soot mass fraction, left to right in SOI at 8.5, 17.5, 20.5 and 23.5 °CA BTDC at 58% EGR for 360 °CA (first line) 375 °CA (second line), respectively

## 5. CONCLUSION

In the present work, after description of low temperature combustion conditions, the effects of advanced injection timing on spray characteristics, 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, high EGR rates increase ignition delay and spray penetration at this time due to lower in-cylinder temperature. It can be seen that the increase of EGR rate above 40%, to 58% reduces soot formation 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 high load conditions, 58% cooled EGR rate reduces the soot formation but cannot totally eliminate it because some portions of rich mixture are at intermediate temperature. Also, associated with lower peak value of premixed combustion at 58% EGR rate, NO<sub>x</sub> emission is reduced to nearly zero 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 improve the 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 that advanced injection timings before 20.5 °CA BTDC were able to produce combustion with lower soot level compared to baseline case due to better air fuel mixture at longer ignition delay and longer spray penetration. But, the advanced injection timing owing to higher premixed combustion resulted in increase of NO<sub>x</sub> emission which is negligible at 58% EGR level.

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