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Multi-Dimensional Modeling of Direct Injection Diesel Engine and Effects of Split Injection

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Abstract- Computations have shown that with high pressure multiple injections two or more injection pulses per power cycle, the Soot - NO_X trade off curves of a diesel engine can be shifted closer to origin than those with the conventional single pulse injections, reducing both the particulate matter and NO_X emissions significantly. In order to understand the mechanism of emissions reduction, multidimensional computations were carried out using CFD for a SCOTE Single cylinder diesel engine with multiple injections. Computations were carried at 9° and 10° with included angle 140° without significant wall impingement using double injections, and the predicted cylinder pressure, heat release rate, particle fate theory, soot and emissions were compared with the measured data. Excellent agreements between predictions and measurements were achieved after improvements in the models were made. The improvements include using a RNG $K-\varepsilon$ turbulence model adopting a new wall heat transfer model and introducing the nozzle discharge coefficient to account for the contraction of fuel jet at the nozzle exit .The present computations confirm that split injection allows significant soot reduction without a NO_X penalty. Based on the computations it is found that multiple injections have retarded injection timings. Regarding soot reduction , it is shown that reduced soot formation is due to the fact that the soot production rich regions at the spray tip are not replenished when the injection is terminated and then restarted .With split injection the subsequently injection fuel burns rapidly and does not contribute significantly to soot production . The present work also demonstrates the usefulness of multidimensional modeling of diesel engine combustion to reveal combustion mechanisms and to provide design insights for low emission engines. The peak pressure obtained for single injection experimental and predicted are 95and 87 bars where start of injection is at 6° btdc, and duration of injection was taken as 20°, NO_X were predicted as 450ppm and that of measured was 529ppm.Predicted PM value is 160ppm where as the measured value is 182.4ppm.In case of double injection the predicted and measured pressures are 93.5 and 88 bars respectively, predicted and measured NO_X were177ppm and 246ppm.As Particulate is concerned the predicted and measured values were 36.2ppm and 42.6ppm respectively.

Index Terms- CFD, Pilot injection, main injection, split injection, start of injection, and duration of injection

I. INTRODUCTION

This Diesel engine is widely used in heavy duty transport applications. Diesel engine is more fuel efficient than spark ignition engine on the other side they have relatively higher emissions and noise levels. Diesel engine manufacturers have to address these problems to meet current and future government regulations which limit particulate and NO_X emissions, while maintaining a quite efficient engine to satisfy the consumers. Particulate matter and NO_X production along with engine noise highly depend on the combustion process Therefore precise control over the fuel injection and spray formation is essential in making improvements to the combustion process .The optimum pressure and optimum nozzle diameter increases the performance and consequently reduces the particulate matter with the better atomization and fuel- air mixing. This in turn unfortunately increases NO_X because of high temperature. To improve the performance and to reduce the NO_X –particulate formation without scarifying the fuel consumption, it is important to understand the relationships between various injection parameters and how they affect the combustion process. Along with the injection pressure and nozzle diameter other injection parameters like such as nozzle hole L/D ratio, rate of injection profile , effect of fuel spray , spray characteristics , that may affect the droplet size, spray penetration exit velocity and spray cone angle. Use of multiple injections can reduce particulate emissions by as much as a factor of three without increasing NO_X emissions. This will be done by better mixing later in the cycle. Optimizing the injection pressure, injection angle and optimizing the nozzle diameter has proven to be an effective way to reduce particulate emissions and consequently improves the engine performance. Multiple injection strategies have been reported for simultaneous reduction of NO_X and PM in a large bore direct injection diesel engine [1, 2, 3].Small bore diesel engines results shown by Nehmer and Reitz [2] that pulsated injection might provide a method to reduce PM and allow for reduction of NO_X from controlled pressure rise. The effectiveness of double, triple and rate shaped injection strategies to simultaneously reduce NO_X and PM was also evaluated. Numerical simulations were carried out to explore the mechanism of soot and NO_X reduction for multiple injections [4]. Multiple injection strategies have a similar effect to the restarted single injection on NO_X reduction. Reduced emissions are due to the fact that the soot producing rich region is **not replenished** when the injection pressure is terminated and restarted. Zang investigated the effect of [5] pilot injection on NO_X, Soot emissions and combustion noise in a small diesel engine, soot emission was seen relevant to the pilot flame and reducing the pilot flame at the main injection starting time can reduce soot emissions. By optimizing pilot injection timings and quantity maintaining and dwell between main and pilot injections simultaneous reduction of NO_X and PM was obtained in a HSDI diesel engine [6].It was also shown that simultaneous reduction of combustion noise and emission is possible by the influence of the pilot burned gas through minimizing the fuel quantity by advancing the pilot injection

timing [7].Combustion concepts like homogeneous charge compression ignition combustion have been shown to be effective for NO_X and PM reduction. The concept of HCCI was applied initially to spark ignition engines because of its volatility property for better homogeneous mixture, where as in diesel engines this concept has been delayed as diesel has low volatility. With the concept of multi pulse injection the problem of homogeneous mixture in diesel engines could be solved and the same has been applied for high speed direct injection diesel engines effectively. Hashizume [8] proposed a low soot solution called multiple stage diesel combustion for higher load operating conditions. Although, soothing luminous flame was observed, this luminous flame disappeared quickly and most of the soot was oxidized rapidly smoke and NO_X were reduced. Su W ,Lin T, Pei Y.A have done work[9]on multi pulse HCCI diesel engine ,they used multiple short injection pulses for early injection and followed by main injection near top dead center and they found that for very early injection a great increase in Hydrocarbon emission was seen. Hasegawa and Yanagihara employed two injections called uniform bulky combustion system .The first injection was used to form a pre- mixture. The second injection was used as an ignition trigger. The ignition of premixed gas could be controlled by the second injection when the early injection maintained a low temperature reaction.

II. METHODOLOGYAND MODEL FORMUALTION

The computer code used in this study was **FLUENT**. The code can solve unsteady, compressible turbulent flows with combustion and fuel spray, and have been used for the computations of various internal combustion engines The code uses a finite volume methodology to solve discredited Nervier-strokes equations. RNGK-ε was used in this study. It could predict more realistic large scale flame structures compared with the K-ε model. The RNG K-ε model is formulated as

$$\frac{\partial \rho k}{\partial t}+\nabla.\left(\rho u k\right)=-\frac{2}{3}\rho k\nabla.u+\tau.\nabla u+\nabla.\left(\alpha_k \mu k\right)-\rho\varepsilon+W^s \quad [1]$$

$$\frac{\partial \rho \varepsilon}{\partial t}+\nabla.\left(\rho u \varepsilon\right)=-\left[\frac{2}{3}C_1-C_3+\frac{2}{3}C_\mu C_\eta \frac{k}{\varepsilon}\nabla.u\right]\rho\varepsilon\nabla.u+\nabla.\left(\alpha_\varepsilon \mu\nabla\varepsilon\right)+\frac{\varepsilon}{k}\left[\left(C_1-C_\eta\right)\tau:\nabla u-C_2\rho\varepsilon+C_s W^s\right] \quad [2]$$

$$C_3=\frac{-1+2C_1-3m\left(n-1\right)+\left(-1\right)^\delta\sqrt{6}C_\mu C_\eta\eta}{3} \quad [3]$$

$\delta=1$ if $\nabla.u<0$

$\delta=0$ if $\nabla.u>0$

And

$$C_\eta=\frac{\eta\left(1-\frac{\eta}{\eta_o}\right)}{1+\beta\eta^3} \qquad \eta=S\frac{k}{\varepsilon}$$

$$S=\left(2S_{ij}S_{ij}\right)^{1/2}$$

$$S_{ij}=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_i}+\frac{\partial u_j}{\partial x_i}\right)$$

In equation (1)-(3) k and ε are turbulent kinetic energy and its dissipation rate .ρ,u,τ and μ are density, velocity, stress tensor and effective viscosity respectively.η is the ratio of the turbulent –to mean –strain time scale . S is the magnitude of the mean strain. m =0.5, and n =1.4.The C3 term accounts for the non-zero velocity dilatation which is closed.

III. GOVERNING EQUATIONS

The governing equations of gas flow consist of mass, momentum and energy conservation equations turbulence equations, gas state relation equations. To take care of physical modeling k-ε turbulence model is employed. The various equations, which are solved**:**

Continuity $\frac{\partial p}{\partial t}+\nabla(\partial u)=0$ [4]

Momentum

$$\frac{\partial \rho u}{\partial t}+\nabla(\rho u)=-\nabla p-\nabla\left[\frac{2}{3}\rho k\right]+\nabla\sigma+\rho g \quad [5]$$

Turbulence Model

K-εquation

$$\frac{\partial(\rho k)}{\partial t}+\nabla(\rho u k)=-\frac{2}{3}\rho k\nabla u+\sigma\nabla u+\nabla.[(\frac{\mu}{pr_k})\nabla k]-\rho\varepsilon \quad [6]$$

ε-Equation

$$\frac{\partial(\partial\varepsilon)}{\partial t}+\nabla.(\rho u\varepsilon)=-(2c_{\varepsilon 1}/3-c_{\varepsilon 3})\rho\varepsilon\nabla.u+\nabla.\left[(\frac{\mu}{pr_\varepsilon})\nabla\varepsilon\right]+\frac{\varepsilon}{k}\left[c\varepsilon_1\sigma:\nabla u-c\varepsilon_2\rho\varepsilon\right] \quad [7]$$

The quantities $c\varepsilon_{1,}c\varepsilon_{2,}c\varepsilon_{3,}pr_{\varepsilon,}pr_k$ are constants whose values are determined from experiments and some theoretical considerations, a feature that establishes certain universality. Standard values of these constants are often used in engine calculations as given below.

$c\varepsilon_1=1.44 c\varepsilon_2=1.92 c\varepsilon_3=-1, pr_k=1.0,$

$pr_\varepsilon=1.3$

IV. MATHEMATICAL MODELS

A Spray model

Spray models used in this study is WAVE break up model suggested by Reitz and could be summarized as follows. [10] Liquid break up is modeled by postulating the new drops are

formed (with drop radius r) from a parent drop or blob (with radius a) with stripping. $r_{new} = B_0 \cdot \Lambda$ (4)Where B_0 =0.61 is a constant, the value of which is fixed. The rate of change of drop radius in apparent parcel due to drop breakup is described by using the rate expression; $\frac{dr}{dt} = \frac{r - r_{new}}{\tau_{bu}}, \tau_{bu} = 3.788 \frac{r}{\Lambda \Omega}$ (5)

The spray –wall interaction model used in the simulations is based on the spray –wall impingement model descried in [8].The model assumes that a droplet, which hits the wall is affected by rebound or reflection based on the Weber number. The Dukowicz model was applied for treating he heat –up and evaporation of the droplet which is described in [11].This model assumes a uniform droplet temperature .I n addition the rate of droplet temperature change is determined by the heat balance which states that that heat convection from the gas to the droplet ether heat up the droplet or supplies heat for vaporization. With higher droplet densities and relative velocities droplet collisions occur. High droplet densities are restricted to the spray kernel. High relative velocities can especially be seen at the tip of the spray, where preceding droplets are decelerated by the gas. Depending on the droplet collision conditions various effects like elastic droplet bouncing, droplet coalescence and droplet atomization are observed.

B. Ignition and Combustion Models

The shell auto ignition model was used for modeling of the auto ignition [10].In this mechanism 6 species for hydrogen 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 [10]. The combustion model used in this study is of the turbulent mixing controlled verity as described by Magnusson and Heritage[11] .This model assumes that in premixed turbulent flames, the reactions (fuel ,oxygen) are contained in the same eddies and are separated from eddies containing hot combustion products . The chemical reactions usually have time scales that are very short compares to the characteristics of the turbulent transport processes .Thus it can be assumed that the rate of combustion is determined by the rate of intermixing on a molecular scale of the eddies containing reactants and those containing hot products in other words by the rate of dissipation of these eddies.

C. NOX and soot Formation Models

The reaction mechanism of NO_X formation is expressed in terms of the extended a Zeldovich mechanism.

$N2+O \leftrightarrow NO+N$ [8]

$N+O2 \leftrightarrow NO+O$ [9]

$N+OH \leftrightarrow NO+H$ [10]

From the fact that in most stoichiometric and fuel –lean flames , the occurring OH concentration very small , the third reaction of the Zeldovich mechanism can be neglected .F or the formation of thermal NO_X , the partial equilibrium approach can be used and the equilibrium of the first two reactions result in one global reaction as follows;

$N2+O2 \leftrightarrow 2N$ [11]

The chemical species appearing in this global reaction are used in the giver single –step fuel conversion equation via:

$\frac{d[NO]}{dt} = 2k_f[N_2IO_2]$ =2kf[N2/O2] [12]

Where only the forward reaction is considered and the reaction rate kf is given as

$Kf = \frac{A}{\sqrt{T}} \exp\left(\frac{-E_a}{RT}\right)$ [13]

The soot formation model currently implemented in fluent is based upon a combination of suitably extended and adapted joint chemical /physical rate expressions for the representation of the processes of particle nucleation, surface growth and oxidation. $\frac{dm_{soot}}{dt} = \frac{dm_{form}}{dt} - \frac{dm_{oxid}}{dt}$ [14]

$\frac{dm_{form}}{dt} = A_f m_{fv} p^{0.5} \exp\left(\frac{-E_a}{RT}\right)$ [15]

$\frac{dm_{soot}}{dt} = \frac{6M_c}{\rho_s d_s} m_s R_{tot}$ [16]

D. Numerical model

The numerical method used in this study is a segregated solution algorithm with a finite volume –based technique. The segregated solution is chosen is 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** algorithm which causes 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 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:

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

Where Φp 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 1.0×10 -4.

V. TURBULENT DISPERSION OF PARTICLES

Dispersion of particles due to turbulent fluctuations in the flow can be modeled using either **Stochastic tracking** (discrete random walk**)** Particle cloud model Turbulent dispersion is

important because it is more realistic, enhances stability by smoothing source terms and eliminating local spikes in coupling to the gas phase.

Table 1: Engine Specifications

Engine	Caterpillar
Bore* stroke	137.19*165.1
Compression ratio	15.1:1
Displacement	2.44 liters
Con rod length	261.62mm
Engine speed	1600 rpm
Nozzle holes	6
Spray angle	140°

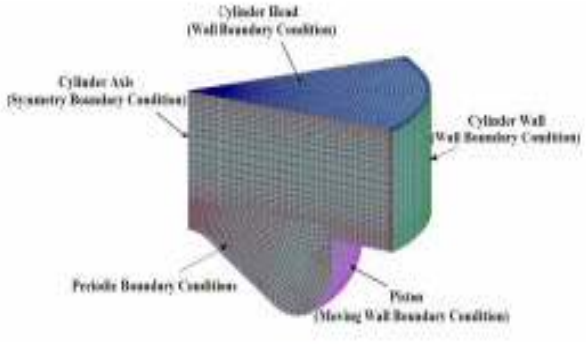

Figure 1: Computational Mesh

VI. RESULTS

Pressure histories for single injection

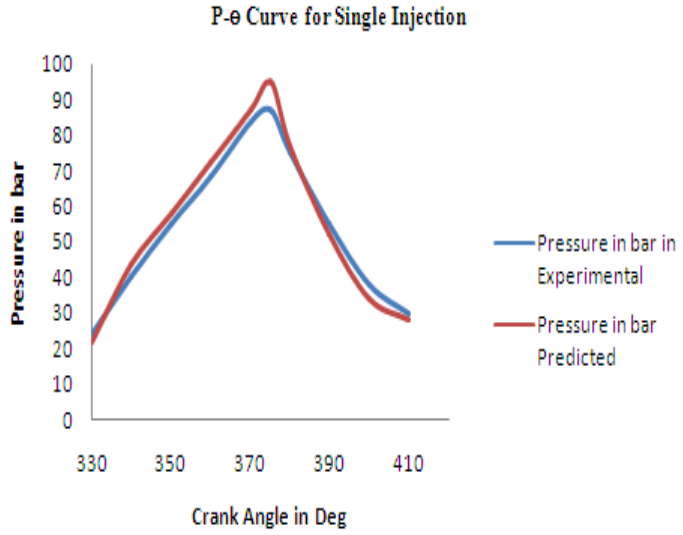

Figure 2

Figure 2 shows the variations of pressure (experimental and predicted) with variation in crank angle for single injection. It is clear from the fig that the predicted results are closely following the experimental results. The major deviation of the predicted pressure from the experimental value is noticed near TDC. From the deviations two important aspects can be observed.

- The predicted peak pressure is higher the experimentally obtained pressure. The peak pressure with RNGK-ε model of diesel computational values and experimental for single injection 95 bar and 87 bar respectively.
- One reason for lower experimental pressure may be due to the greater ignition delay during combustion. The increase in ignition delay causes the combustion to continue even after the piston crosses TDC towards expansion, stroke resulting in lower peak pressure.
- The other reasons for the difference in peak pressure may be due to the residual gases in the clearance volume during exhaust stroke. The higher temperature residual gases are reduces to the fresh charge entry during suction, as it destroys some vacuum by expanding. Blow by and crevice flows also effect the in cylinder pressures. Both these features are not incorporated in this model.
- The occurrence of predicted peak pressure even before TDC indicates that majority of the fuel is consumed in combustion before the piston reaches TDC.This supports the argument that the ignition delay is more in experimental case. Another important observation that can be made is that the RNGK-ε predicts the pressure variations closer to the experimental results.

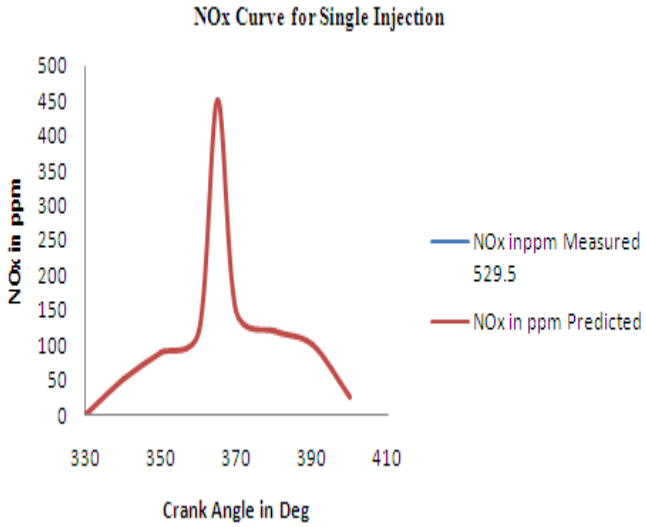

Figure 3

Figure 3 shows the mass fraction of NO variations with crank angle. The fig reveals that the NO formation takes place between 5° bTDC and 25° aTDC. It is a fact that the combustion

generated temperatures during this period will be high. High NO concentration is found in regions with close to stoichiometric mixture fraction and region where the temperature is high. It is understood from the fig the RNG K-ε model prediction agrees well with the measured data.

Figure 4 shows the soot variations with respect to the crank angle. The soot emission predicted with experimental value is 160ppm and 182.7ppm with RNG K-ε model. It is very interesting to note that soot oxidation predominantly takes place in the high temperature regions in which NO_X production is high. The fact that local conditions that favor soot oxidation also favor NO formation is probably major reason for the well known Soot -NO_X trade off typically encountered when optimizing diesel engine. Soot production is given by particle inception rate as a spatial distribution with strong correlation to the mixture fraction field.

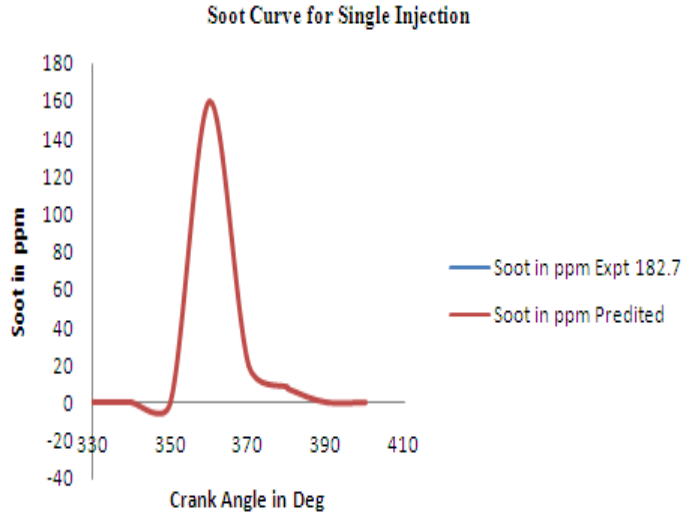

Figure 4

Figure 5 shows the predicted and experimental heat release rate were 550j / ° and that of measured 460j/°. .

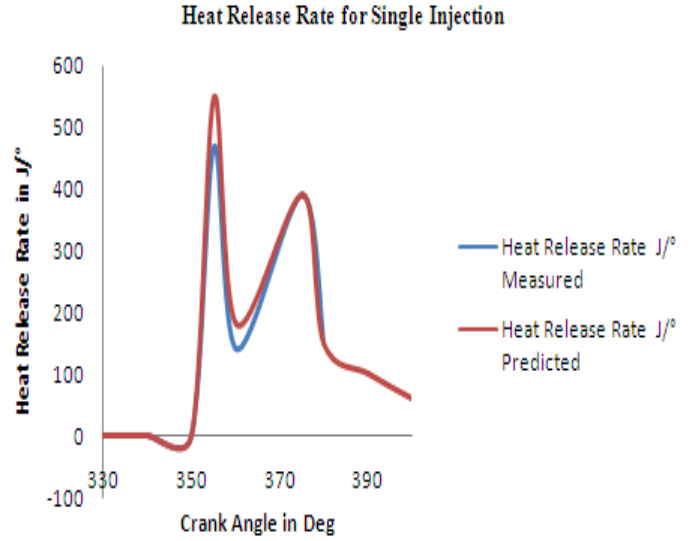

Figure 5

Double Injection

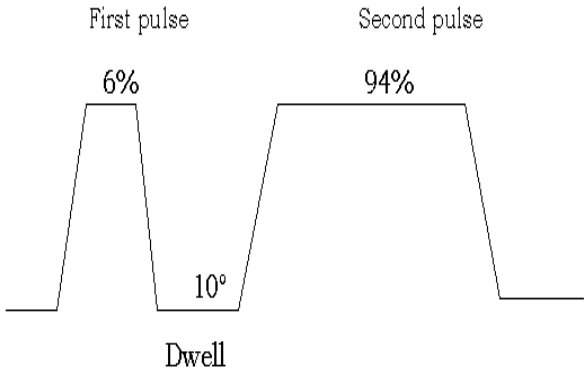

Figure 6: Pressure Histories for Double Injection

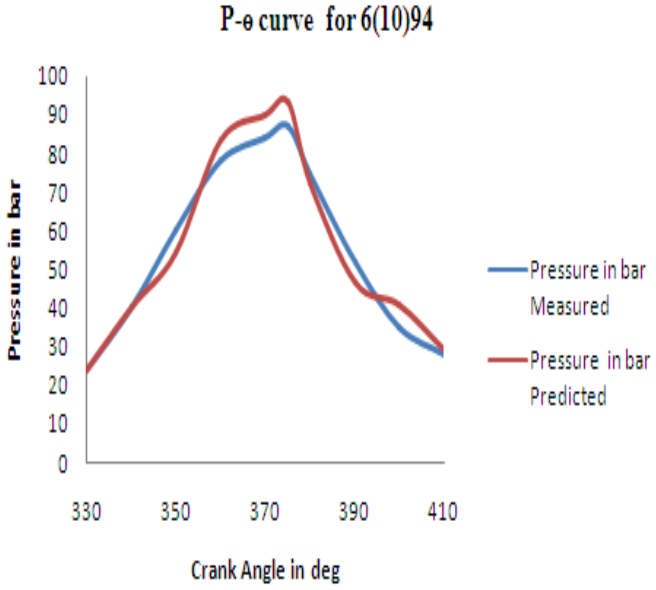

Figure 7

Figure 6 shows the amount of fuel injected in the first pulse as pilot injection and also second pulse as main injection.

Figure 7shows the variations of pressure (experimental and predicted) with variation in crank angle for double injection. It is clear from the fig7.7that the predicted results are closely following the experimental results. The major deviation of the predicted pressure from the experimental value is noticed near TDC. From the deviations two important aspects can be observed.

- The predicted peak pressure is higher the experimentally obtained pressure. The peak pressure with RNGK-ε model of diesel computational values and experimental for double injection 98 bar and 90bar respectively.

- The other reasons for the difference in peak pressure may be due to the residual gases in the clearance volume during exhaust stroke. The higher temperature residual gases are reduces to the fresh charge entry during suction, as it destroys some vacuum by expanding. Blow by and crevice flows also effect the in

cylinder pressures. Both these features are not incorporated in this model.

- The occurrence of predicted peak pressure even before TDC indicates that majority of the fuel is consumed in combustion before the piston reaches TDC. This supports the argument that the ignition delay is more in experimental case. Another important observation that can be made is that the RNGK-ε predicts the pressure variations closer to the experimental results.

- A small injection before the main injection with 0% EGR is not effective in reducing particulate. Thus pilot injection would not be effective in enhancing mixing after the main injection.

- The pilot injection was effective at the 0% EGR condition is that pilot injections are known to reduce the premix burn fraction of burning resulting in lower NO_X production [929461].

Comparison between available experimental and predicted NO_X for double injection

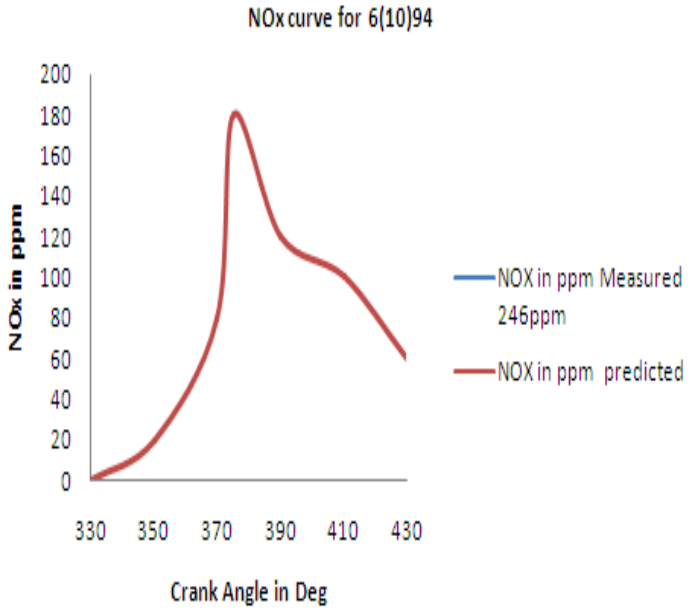

Figure 8

The Nitric oxide (NO) and (NO_2) are usually grouped together as NO_X. How ever NO is the predominant Oxide of Nitrogen produced inside the engine cylinder. The principal source NO is the oxidation of atmospheric Nitrogen. The oxidation of Nitrogen present in the fuel is an additional source of NO. The atmosphere contains both Nitrogen and Oxygen in abundant quantities. But the oxidation of Nitrogen will not take place in atmosphere. It requires high temperatures during to carry out the oxidation reaction. 'Zeldovich Mechanism', which is used in the model, clearly explains the formation of NO.

- Figure 8 shows the mass fraction of NO variations with crank angle. The fig reveals that the maximum NO formation takes place between 5° bTDC and 25° aTDC. It is a fact that the combustion generated temperatures during this period will be high. High NO concentration is found in regions with close to stoichiometric mixture fraction and region where the temperature is high. It is understood from the fig the RNG K-ε model prediction agrees well with the measured data. As pilot injection was initiated ignition delay has been reduced hence the reduction in NO_X and Soot as temperature levels got reduced.
- The measured value from the experiment was 246ppm and where as the computed value from RNG K-ε model is approximately 177.8ppm.

Comparison between Available Experimental and Predicted Soot for Double Injection

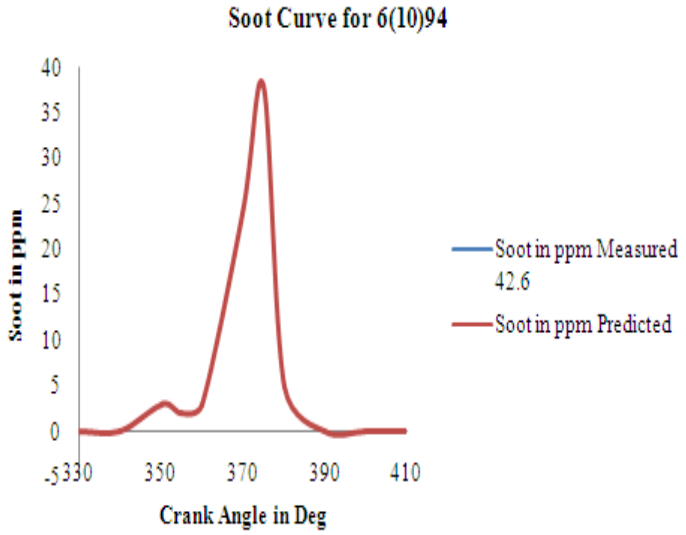

Figure 9

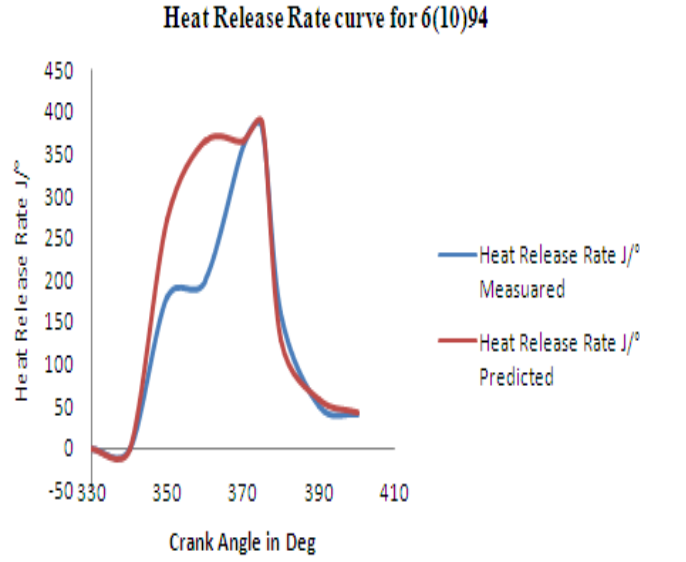

Figure 10

Figure 9 shows the soot variations with respect to the crank angle. The soot emission predicted with experimental value is 36.2ppm and 42.6ppm with RNG K-ε model. It is very interesting to note that soot oxidation predominantly takes place in the high temperature regions in which NO_X production is high. The fact that local conditions that favor soot oxidation also favor NO formation is probably major reason for the well known Soot -NO_X trade off typically encountered when optimizing diesel engine. Soot production is given by particle inception rate as a spatial distribution with strong correlation to the mixture fraction field.

Figure 10 shows the heat release rate in double injection, the measured and predicted values are approximately 400j/° and 490j/° respectively.

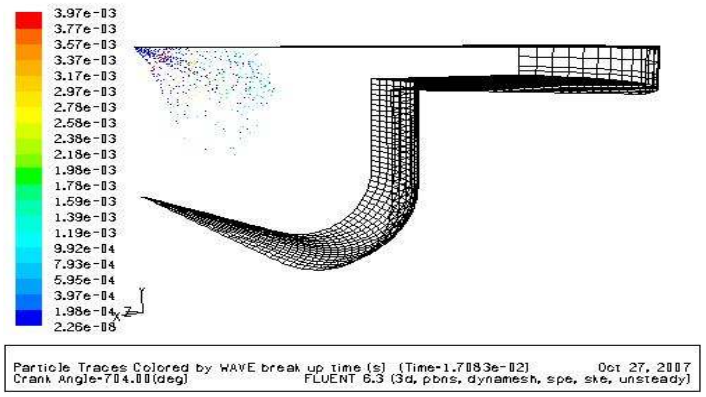

Figure 11

Figure 11 explains particle traces and particle fate theory. This theory enables during simulations how the particles are participated in combustion, how many particles are escaped, how many are trapped, how many are evaporated and how many are aborted. During simulation nearly approximately 1660 to 1734paricles were participated in combustion for every 2000 particles injection. The number of particles participated in combustion could be seen while simulation is under progress.
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VII. Conclusions

A. Single Injection

Based on the above observations the following conclusions are drawn with single injection with start of injections 6° bTDC and duration of injection as 20°.

- It is found that the predicted peak pressure is higher as compared to the available experimental value and are found to be 95bar 87 bar respectively.
- The peak energy (Heat release) predicted during the operating cycle is 537j/° from the fig 6.4,and where as the experimental value is 460j/° .
- It was found that NO emissions obtained from available experimental values are very slightly higher than the predicted value. The NO emission obtained from the available experimental value is 529.5ppm where as the predicted value by RNG K-ε model is approximately 450ppm.
- It was found that the soot emissions are slightly lower for the predicted value by RNG K-ε model when compared to the available experimental value. Soot emission by RNG K-ε is 160ppm approximately and the measured value is 182.7ppm.

B. Double Injection with 10° dwell 6(10)94

Based on the above observations the following conclusions are drawn with double injection with start of injections 6°bTDC and duration of injection as 22° with dwell period of 10°.

- It is found that the predicted peak pressure is higher as compared to the available experimental value and are found to be 93.5bar 88 bar respectively.
- The peak energy (Heat release) predicted during the operating cycle is 489j/° from the fig 6.4, and where as the experimental value is 400j/°.
- It was found that NO emissions obtained from available experimental values are very slightly higher than the predicted value. The NO emission obtained from the available experimental value is 246.05ppm where as the predicted value by RNG K-ε model is approximately 177.8ppm.
- It was found that the soot emissions are slightly lower for the predicted value by RNG K-ε model when compared to the available experimental value. Soot emission by RNG K-ε is 36.2ppm approximately and the measured value is 42.6ppm.

Appendix

bTDC	before top dead center
aTDC	After top dead enter
CA	Crank angle
SOI	Start of injection
DOI	Duration of injection

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