Investigation of pollutants formation in a diesel engine using numerical simulation

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Abstract
The current study aims to explore the combustion process in a diesel engine and investigate the behavior of pollutant formation at different time events and different locations in the combustion chamber. The time event for maximum rate of production of pollutant soot is also investigated. Further, time events are investigate at which almost all the amounts of pollutants soot and nitric oxide have been produced. The combustion simulation is performed on a 3D sector. Finite volume method is used for numerically solving the partial differential equations that govern the flow along with Transition SST turbulence model. Eddy dissipation model is used for turbulence chemistry interaction. For soot calculation, Moss-Brookes model is used which has less empiricism and theoretically provides superior accuracy.

Keywords: IC Engine, Simulation, Combustion, Soot, Nitric Oxide.

1 INTRODUCTION
Demand for diesel engines is increasing due to its recognized thermal efficiency. So we see them feeding the light and heavy duty vehicles. Contrary to gasoline engines, where gasoline is injected into the air on the way to combustion chamber and therefore there is ample time for mixing of air and fuel uniform before ignition, there is lack of time for making a uniform mixture of air and diesel because diesel is directly sprayed into the compressed hot air in the combustion chamber. This lack of time is not suitable for the burning process. That is why, diesel engines produces more pollution, such as nitric oxide and soot, than the gasoline engines. This pollution is extremely harmful to lives and the environment and so, is a very serious matter. Improving engine design can reduce pollution, but it is a challenging task. It requires the utmost attention and strenuous efforts of researchers and engineers to manufacture efficient and cheaper eco-friendly engines. The task of reducing pollution can only be accomplished by improving the engine design to achieve a complete and perfect combustion which is highly dependent on the uniformity of the air-fuel mixture. Improving engine design involves investigating the design of air inlet and outlet passages, injector nozzle, combustion chamber and fuel blends [1–8].

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Sakata et al. [9] improved the engine design by introducing controlled fuel injection. M. Komno [10] noticed significant reduction in pollutants formation by generating delayed turbulence. The late turbulence increased the air interaction with unburned fuel resulting in increased engine’s efficiency. Lin et al. [11] performed numerical simulations for various combustion chamber designs and investigated one which produce less pollutants. Kim et al. [2] studied the impact of fuel spray direction on the combustion and emission characteristics. Wei et al. [12] examined the impact of nozzle angle on the uniformity of air-fuel mixture and its combustion by numerical simulations. Xu et al. [13] examined the effects of bio-diesel blends on soot formation. EL-Seesy et al. [14] studied the process of formation of nitric oxides and soot from the combustion of diesel/jojoba oil blends. In the current study, we investigate formation of pollutants NO and soot during combustion in a diesel engine under operational conditions.

2 PROBLEM STATEMENT

In this study, we perform a single cylinder combustion simulation to investigate the formation of pollutants soot and nitric oxide (NO) in the combustion chamber. The objective is to analyze the behavior and concentrations of the soot and nitric oxide. Engine specifications are given in Table 1.

Table 1: Engine specifications and operational conditions

| Specification                          | Value                        |
|----------------------------------------|------------------------------|
| Bore × Stroke                          | 150 × 180 mm                 |
| Engine displacement (1 cylinder)        | 3.18086 L                    |
| Compression ratio                      | 13.1                         |
| Nozzle diameter                        | 0.254 mm                     |
| Fuel                                   | Decane C_{10}H_{22}           |
| Fuel injected per orifice              | 29.58 mg/cycle               |
| Injection pressure                     | 120 MPa                      |
| Engine speed                           | 2000 rpm                     |
| Number of nozzle orifices              | 6                            |

2.1 Geometric Model

The three dimensional geometric model of the engine is one-sixth of the engine cylinder which is a three dimensional sector as shown in Figure 1. The top boundary of the model is termed as head. The cylinder head is lying in the plane which contains the point $P(0, 0, 0)$ and its normal is the $y−axis$. The cylinder head is the disk defined by $z^2 + x^2 \leq r^2$, where $r = 75$ mm. If we consider the cylinder head lying in $r\theta$-plane, then cylinder head for the sector is defined by $r = 75$ mm and $-\pi/6 \leq \theta \leq \pi/6$. The head face is extruded along the cylinder axis (negative direction of $y$-axis) for the length of 176.4097 mm followed by the piston bowl space, see Figure 1. Due to consideration of sector, there appear two additional faces, the periodic faces. The period of simulation expands from 570° crank angle (CA) to 833° CA.
2.2 Mathematical Model

Mathematical model contains the following sub models.

2.2.1 Flow Model

Mathematical model, that governs the flow, comprise

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_j} = 0, \quad (2.1)
\]

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = \rho g - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial u_i}{\partial x_j} + \mu \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij}\right) + S_i, \quad (2.2)
\]

\[
\frac{\partial \rho E}{\partial t} + \frac{\partial ((\rho E + p) u_j)}{\partial x_j} = \frac{\partial u_i \tau_{ji}}{\partial x_j} + \frac{\partial}{\partial x_j}\left(k_1 \frac{\partial T}{\partial x_j}\right). \quad (2.3)
\]

In Equation (2.2), it is assumed that \(S_i = 0\). i.e., there is no extra source contributing to govern the flow. In Equation (2.3), \(k_1\) stands for thermal conductivity. These equations are respectively known as continuity, momentum or momentum transport and energy equations.
The general transport equation for any specie \( \phi \) is given by

\[
\frac{\partial}{\partial t} (\rho \phi) + \frac{\partial}{\partial x_j} (\rho u_j \phi) = \frac{\partial}{\partial x_j} \left( \Gamma \frac{\partial \phi}{\partial x_j} \right) + S_\phi.
\] (2.4)

### 2.2.2 Turbulence Model

For turbulence, Transition SST model is used. The model equations are

\[
\frac{\partial \rho k}{\partial t} + \frac{\partial \rho u_i k}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \Gamma_k \frac{\partial k}{\partial x_j} \right) - Y_k + G_k + S_k,
\] (2.5)

\[
\frac{\partial \rho \omega}{\partial t} + \frac{\partial \rho u_i \omega}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \Gamma_\omega \frac{\partial \omega}{\partial x_j} \right) - Y_\omega + G_\omega + S_\omega,
\] (2.6)

\[
\frac{\partial \rho \gamma}{\partial t} + \frac{\partial \rho U_j \gamma}{\partial x_j} = P_\gamma 1 + P_\gamma 2 - E_\gamma 1 - E_\gamma 2 + \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\gamma} \right) \frac{\partial \gamma}{\partial x_j} \right],
\] (2.7)

\[
\frac{\partial \rho \tilde{R} \theta t}{\partial t} + \frac{\partial \rho U_j \tilde{R} \theta t}{\partial x_j} = P_\theta t + \frac{\partial}{\partial x_j} \left[ \sigma_\theta t \left( \mu + \mu_t \right) \frac{\partial \tilde{R} \theta t}{\partial x_j} \right].
\] (2.8)

For details of Transition SST model and model constants, see ANSYS Theory Guide 15.0.

### 2.2.3 Chemical Species Transport

The Transport equation for species produced due to chemical reaction is

\[
\frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho v Y_i) = -\nabla \cdot \mathbf{J}_i + R_i + S_i.
\] (2.9)

### 2.2.4 Spray Breakup Model

For spray breakup, we used Kelvin-Helmholtz and Rayleigh-Taylor (KHRT) model is used which were designed by [15,16]. The model equations are

\[
\Omega_{KH} \sqrt{\frac{a^3 \rho_t}{\sigma}} = 0.34 + 0.38 W e_g^{1.5} \frac{1}{(1 + 1.4 T^{0.6})(1 + Oh)},
\] (2.10)

\[
\Lambda_{KH} \frac{a}{\sigma} = 9.02 (1 + 0.4 T^{0.7}) (1 + 0.45 Oh^{0.5}) \frac{1}{(1 + 0.87 W e_g^{1.67})^{0.6}},
\] (2.11)

\[
\Omega_{RT} = \sqrt{\frac{2 [(\rho_p - \rho_g) (-g \theta)]^2}{3 (\rho_p + \rho_g) \sqrt{3 \sigma}}},
\] (2.12)

\[
K_{RT} = \frac{[(\rho_p - \rho_g) (-g \theta)]^2}{3 \sigma}.
\] (2.13)
2.2.5 Turbulence-Chemistry Interaction

For turbulence-chemistry interaction, Eddy Dissipation model is used which was designed by Magnussen and Hjertager [17]. In this model, the source term $R_{i,r}$ for $i$-th specie from the reaction $r$ is

$$R_{i,r} = \min(R_1, R_2), \quad (2.14)$$

where

$$R_1 = v'_{i,r} M_{w,i} A \rho \frac{\epsilon}{k} \min_R \left( \frac{Y_R}{v'_{R,r} M_{w,R}} \right), \quad (2.15)$$

and

$$R_2 = v'_{i,r} M_{w,i} A B \rho \frac{\epsilon}{k} \sum_P P \frac{Y_P}{\sum_j v''_{j,r} M_{w,j}}. \quad (2.16)$$

In above equations, $N$ denotes number of species, $Y_R$ and $Y_P$ denote respectively the mass fractions of reactant $R$ and product $P$, $A$ is a constant whose value is equal to 4 and $B$ is a constant whose values is equal to 5.

2.2.6 Soot Model

For soot modeling, the Moss-Brookes model is used. The model equations are

$$\frac{\partial \rho Y_{soot}}{\partial t} + \nabla \cdot (\rho \vec{v} Y_{soot}) = \nabla \cdot \left( \frac{\mu_t}{\sigma_{soot}} \nabla Y_{soot} \right) + \frac{d M}{d t}, \quad (2.17)$$

$$\frac{\partial \rho b^{*}_{nuc}}{\partial t} + \nabla \cdot (\rho \vec{v} b^{*}_{nuc}) = \nabla \cdot \left( \frac{\mu_t}{\sigma_{nuc}} \nabla b^{*}_{nuc} \right) + \frac{1}{N_{norm}} \frac{d N}{d t}. \quad (2.18)$$

In above equations $Y_{soot}$ represents the mass fraction of soot, $\sigma_{soot}$ denotes the turbulent Prandtl number for soot, $M$ denotes the mass concentration of soot, $\sigma_{nuc}$ denotes the turbulent Prandtl number for nuclei transport, $b^{*}_{nuc}$ denotes the normalized radical nuclei concentration. For further details of this model, see ANSYS Theory Guide 15.0.

2.2.7 NO Model

The species transport equation for thermal $NO$ is given by

$$\frac{\partial \rho Y_{NO}}{\partial t} + \nabla \cdot (\rho \vec{v} Y_{NO}) = \nabla \cdot (\rho \nabla Y_{NO}) + S_{NO}. \quad (2.19)$$

In above equation, $Y_{NO}$ denotes the gas phase $NO$ mass fraction, $D$ denotes the effective diffusion coefficient. Moreover, the thermal $NO$ formation from the reaction of molecular nitrogen and oxygen is governed by

$$N_2 + O \rightleftharpoons NO + N \quad (2.20)$$

$$N + O_2 \rightleftharpoons NO + O \quad (2.21)$$

$$N + OH \rightleftharpoons NO + H. \quad (2.22)$$
3 SOLUTION PROCEDURE

The underlying combustion simulation is performed using IC Engine tool which is included in ANSYS Workbench 15.0. All the tasks of simulation are completed using this tool. Solution procedure contains the steps described in the following subsections.

3.1 Discretization of Governing Equations

Finite Volume Method is used for numerically solving the governing equations. The model equations are discretized on each finite volume turning them into a system of algebraic equations, which are then solved by multigrid method.

3.2 Meshing

As the piston curve is highly non-linear, so to accommodate the piston boundary for appropriate meshing, the computational domain is divided into very few zones. Mesh on the vertical plane passing through middle of the sector, at three different time events, are given in Figure 2. This figure explores that structured mesh is occupying most of the region of computational domain. In the zone near the piston, there are some cells other than hexahedrons for better adoption of the piston crown. The number of mesh cells at start of simulation (at 570° CA) is 1260257 while at top dead center (TDC) is 201629. This mesh resolution is adequate for the accuracy of the results.

Figure 2: Mesh on the vertical plane passing through middle of the sector at (a) 570° CA, (b) 691° CA and (c) 720° CA (TDC)

Now, we discuss the quality of our mesh. Aspect ratio of the mesh cells lies in the interval [1.0143, 38.572] and the average aspect ratio of the mesh is 3.5036. Skewness of the mesh cells lies in the interval $[1.3057 \times 10^{-10}, 0.6740]$ and the average skewness of mesh is
Orthogonal quality of the mesh cells lies in the interval \([0.4390, 1]\) and the average orthogonal quality of the mesh is 0.98934. The values of the parameters defining mesh quality are in acceptable range.

### 3.3 Initial and Boundary Conditions

In the current study, air is considered as the working fluid. The ideal gas law is used for calculating its density. All cells of the domain are initialized uniformly with; swirl number equal to 1.3, pressure equal to zero Pascal, \(x\) and \(y\) velocities equal to 0 m/s, Turbulent kinetic energy equal to 1 \(m^2/s^2\), turbulent dissipation rate equal to 1 \(m^2/s^3\) and temperature equal to 300 \(K\).

There are five boundaries of the computational domain. The cylinder top face is assigned a temperature of 602 \(K\), wall of the cylinder is assigned a temperatures of 567 \(K\), face of the piston is assigned a temperatures of 645 \(K\). The remaining two vertical faces are periodic faces.

### 4 RESULTS AND DISCUSSION

As the fuel injection starts, and shortly thereafter, the temperature of the compressed air results in burning the fuel. At this stage, the pressure and temperature in the cylinder suddenly increase due to heat of fuel combustion. The pressure in the cylinder achieves the value of 16.745 MPa at 719.75° CA, see Figure 3(a). This high pressure pushes the piston back. After TDC, the pressure gradually comes down due to expansion. In Figure 3(b), maximum temperature is plotted against the crank angle. Initially, the heat is conducted to the cells near boundaries. Then temperature in the cylinder rises due to compression. Injection of fuel is started at 691° CA followed by the start of combustion at 694.05°. The maximum temperature is 894.82 \(K\) at 694.05°. As the fuel starts to burn, the temperature of the burning zone starts rising and achieves a peak of 2993.141 \(K\) at 709.75° CA. After completion of fuel injection and the compression stroke, temperature curve comes down due to expansion. In Figure 3(c), apparent heat release rate (AHRR) is graphed against the crank angle. Its maximum value is 119.064 at 706.5°. In Figure 3(d), particle traces colored by temperature are plotted. This plot shows developed fuel spray as well as high temperature burning zone/particles.

In Figure 4(a), soot mass fraction is plotted against the crank angle. The soot curve starts rising slowly near 695° CA after the ignition of fuel. Slope of the soot curve rises sharply after 704° CA. There is point of inflection at 704° CA where the value of soot mass fraction is 0.001640596 and rate of its production is 0.000278294 per crank angle. After this, rate of soot production decreases which flattens the soot curve. The soot curve looks flatten at 750° CA with soot mass fraction value of 0.005214796. Further, there is minor production of soot. The value of soot mass fraction at the end of simulation is 0.005261718. In Figure 4(b), pollutant NO mass fraction is plotted against the crank angle. The pollutant NO curve starts rising near 700° CA. The major amount of pollutant NO is produced till 720° CA, the top dead center, which is 0.000430189. The value of pollutant NO mass fraction at the end of simulation is 0.000432471.
Figure 3: (a) In-cylinder pressure, (b) temperature, (c) apparent heat release rate and (d) particle traces colored by temperature at 705° CA.

Figure 4: (a) Soot mass fraction and (b) Pollutant NO mass fraction vs Crank Angle degree

Now, we examine the concentrations of soot and pollutant NO on various locations in the cylinder. In Figures 5(a) and 5(b), mass fractions of soot and pollutant NO are given in different horizontal planes in the cylinder at 710° CA. The figures show that concentrations of soot and pollutant NO are higher in the piston bowl, where fuel stream actually strikes.

In Figures 6(a) and 7(a) together, mass fractions of soot can be viewed in the cylinder at the end of simulation. In Figures 6(b) and 7(b) together, mass fractions of pollutant NO
Figure 5: Contours of (a) mass fraction of soot and (b) mass fraction of pollutant NO in various planes which are parallel to cylinder top face and are at a distance from it which is mentioned with each; at 710° CA

can be viewed in the cylinder at the end of simulation. The figures show higher concentrations of pollutants in the piston bowl. These figures further show that the reacting species travel with the piston giving the thrust to the piston by the gradual release of energy.

Figure 6: Contours of (a) mass fraction of soot and (b) mass fraction of pollutant NO in various planes which are parallel to cylinder top face and are at a distance from it which is mentioned with each; at 830° CA
CONCLUSIONS

Conclusions made in this study are as under.

1. The combustion starts after 694° CA which shows an ignition delay of at least 3° CA.

2. Maximum temperate that a cell have is 2993.141 K at 709.75° CA, i.e., near the end of fuel injection.

3. Most of the fuel energy is released before the top dead center.

4. Apparent heat release rate have maximum value of 119.064 at 706.5° CA.

5. Rate of soot production is maximum having value of 0.000278294 per crank angle at 704° CA.

6. Almost all the amount of soot is produced till 750° CA with soot mass fraction value of 0.005214796. Its value at the end of simulation is 0.005261718.

7. Almost all the amount of pollutant NO is produced till 720° CA, the top dead center, which is 0.000430189. Its value is 0.000432471 at the end of simulation.

DECLARATIONS

6.1 Availability of Data and Material

The authors declare that there is no relevant data and material to disclosed in this subsection.
6.2 Competing Interests
The authors declare that they have no competing interests.

6.3 Funding
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6.4 Authors’ Contributions
Mr. Muhammad Zahid is Ph. D. Scholar and Khalid Saifullah Syed is his supervisor.

6.5 Acknowledgements
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