Computational fluid dynamic modelling of NOx formation in diesel engine

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Abstract. The purpose of this study is offering a numerical model to predict the NOx formation of a diesel engine. For this purpose, simulation of combustion and emissions of a diesel engine was performed using CFD FIRE commercial software. The simulation was performed for the condition of 900 rpm for engine speed, 200 bar cylinder pressure, and injection timing (15° CA BTDC). The difference between the experimental and numerical results was reported by about 3.2%. The result of the numerical simulation shown due to the non-homogeneous mixture of air and fuel in a diesel engine, the temperature distribution is not uniform and the temperature in some places reaches 2500 K. In areas with an equilibrium ratio (stoichiometry) and temperatures above 2000 K, nitrogen oxide is the highest. Also, the result shown areas with a temperature range between 1500 and 1900 K are more favorable areas for the formation of soot pollutant.

Keywords. Diesel engine; Computational fluid dynamic; NOx; AVL FIRE; Combustion

1. Introduction
In recent years by increasing the use of fossil fuels, increasing the price, decrease the fossil resources, and the increasing the pollutants optimization of the diesel engine is an important issue. So, decrease fuel consumption, increase efficiency, and decrease the pollutants are the most important issues for the design of the diesel engine. The previous studies have shown combustion process is strongly influenced by the fluid flow inside the cylinder. Therefore, correct understanding of the flow and its characteristics can be useful to provide the condition to optimize the combustion process [1-3]. In order to evaluation the detail of field of speed, pressure, and turbulence intensity it is necessary to solve the some equation such as continues, momentum, energy, and turbulence [4]. These equations are none-linear and they are depend with each other. Also, because of the movement of piston, the boundary conditions inside the cylinder are very complex. Finally, numerical methods use in order to solve these equations [4]. Progress in process speed and accuracy of the computers, has led to introduce the computational fluid dynamic (CFD) as a low cost, fast and reliable methods for simulation the combustion process [5]. Different studies has been conducted in the field of numerical
simulation of the performance and pollutant parameters of the diesel engine [6-10]. Some of these studies reviewed as follow:

Khoshhal et al [7]. Investigated the effect of temperature on NOx formation numerically. In order to numerical simulation, CFD modeling of NOx emission in an experimental furnace equipped with high temperature air combustion system was studied. The result of numerical simulation compared with measured values. The result of comparison between numerical result and experimental result have shown good agreement. The result of the forecast shows that with increasing fuel temperature, some benefits can be gained such as higher fluid velocity, better fuel jet mixing with the combustion air, smaller flame and lower NOx emission. The effect of of injection timing and cone angle on the formation of NOx emissions investigated numerically by Mahran and Paul [11]. Computational fluid dynamics (CFD) method and ANSYS ICE program were used in order to simulating the combustion, injection process, and the formation of NO. The results of the study have shown which computational fluid dynamics (CFD) method can be predict the NO formation. Du et al. [12] investigated the combustion and NOx emission characteristics in a 600 MW wall-fired boiler under high temperature and strong reducing atmosphere. Also, they used the CFD technique in order to simulation the NOx formation and the other combustion phenomenon. The results of simulation have been shown the CFD technique is the good method for simulation the combustion process. Table 1 shows some studies in field of CFD technique for prediction the combustion process.

Table 1. Studies in field of CFD technique for prediction the combustion process.

| Reference | Engine type | Investigated parameters |
|-----------|-------------|-------------------------|
| [13]      | A single-cylinder diesel engine | Cylinder pressure, Thermal of inside the cylinder, Soot emission, NOx emission |
| [14]      | A single-cylinder Dual-Powered Engine | Cylinder pressure, Thermal of inside the cylinder, Soot emission, NOx emission |
| [15]      | Four-Stroke Internal Combustion Engine | Cylinder pressure, Thermal of inside the cylinder, Soot emission, NOx emission, CO emission |

A review of the conducted researches showed that CFD technique can be used as a useful method for prediction the exhaust emission formation in the diesel engine. In the present study, NOx formation in the diesel engine were simulated numerically and the numerical result was verified with the experimental result. All the computational tasks were performed in a personal computer with 16 GB RAM and Intel (R) Core (TM) i7-4750 CPU @ 3.30 GHz.

2. Material and method

2.1. Experimental set-up

In the present study pure diesel fuel used. The specifications measured based on EN 14214 standard for diesel fuel has shown in the table 2.
Table 2. The specifications measured based on EN 14214 standard for diesel fuel.

| Properties                  | Pure diesel | Units |
|-----------------------------|-------------|-------|
| Kinematic viscosity at 40 °C| 3.28        | mm²/s |
| Density                     | 0.85        | g/cm³ |
| Flashpoint                  | 64          | °C    |
| Lower Heating Value         | 36.09       | MJ/Liter |

MF-399 tractor used in order to perform the experimental tests. Specifications of MF-399 tractor engine has shown in table 3. In order to measurement the performance parameters, of diesel engine was coupled to Sigma 5 dynamometer. Emissions were also measured using an emission tester (model MGT5, by MAHA, Germany).

Table 3. Specifications of MF-399 tractor engine.

| Description          | Details                                      |
|----------------------|----------------------------------------------|
| Type                 | six-cylinder, water cooling, four stroke, naturally aspirated |
| Model                | Perkins A63544                               |
| Bore × stroke (mm)   | 98.6 × 127                                   |
| Maximum power in 6000 rpm | 110 hp                                       |
| Maximum torque in 3500 rpm | 376 N.m                                       |

2.2. Numerical analysis

The simulation of combustion process and pollutants have done with CFD FIRE software. Simulation was done for the condition of 900 rpm for engine speed, 200 bar cylinder pressure, and injection timing (15° CA BTDC). Initial pressure and temperature inside the cylinder were 320 °C and 1 bar respectively.

2.2.1. Field flow model. Based on RANS equations and SIMPLE algorithm, standard k-ε model was used for 3D simulation of combustion process. RANS equations as follow:

Continuity equation (equation 1):

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i} \left( \tau_{ij} - \mu \frac{\partial u_i}{\partial x_j} \right) + \rho_{\text{spray}}
\]

Momentum equations (equation 2-3):

\[
\rho \left( \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \tau_{ij} - \mu \frac{\partial u_i}{\partial x_j} \right) + f_{i,\text{spray}}
\]
\[
\overline{\rho} = \left[ \mu \left( \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) - \frac{2}{3} \mu \left( \frac{\partial \overline{u}_i}{\partial x_i} \right) \right] + \left[ \mu \left( \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) - \frac{2}{3} \mu \left( \frac{\partial \overline{u}_i}{\partial x_i} \right) \right] 
\]

\[
- \rho \overline{u}_i' u_j' = \mu \left( \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) - \frac{1}{3} \rho \delta_{ij} u_i' u_j' 
\]

(Energy equations (equation 4-5))

\[
- \rho c_T' \left( \frac{\partial \overline{T}}{\partial x_j} + \overline{u}_i \frac{\partial \overline{T}}{\partial x_i} \right) = - \frac{\partial}{\partial x_i} \left( \overline{q}_i + c_T' \rho \overline{u}_i' u_i' \right) + q_{\text{spec}} + q_{\text{conv}} 
\]

\[
- q_i = - \lambda \left( \frac{\partial \overline{T}}{\partial x_i} + \frac{\partial \overline{T}'}{\partial x_i} \right) 
\]

(Standard k-ε model (equation 6-7))

\[
\rho \frac{\partial k}{\partial t} + \rho u_i \frac{\partial k}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \mu \frac{\partial k}{\partial x_i} \right) + \frac{\partial}{\partial x_i} \left( \mu \frac{\partial \overline{u}_i}{\partial x_i} + \frac{\partial \overline{u}_i}{\partial x_i} + \rho \rho c_T' \rho \overline{u}_i' u_i' \right) - \rho c_T' \frac{\partial \overline{T}'}{\partial x_i} 
\]

Where terms of \( C_1 \cdot C_2 \cdot C_3 \cdot C_4 \cdot C_5 \) are equal to 1.92, 1.44, 1.3, 1, 0.09 [16]. Eddy viscosity calculated from eq. 8.

\[
\mu_s = C_{\mu} \cdot \rho \frac{k^2}{\varepsilon} 
\]

2.2.2. Emission model

2.2.2.1. NOx formation model. For simulation the NOx emission, Zeldovich mechanism used [17].

Governing equations on NOx formation as follow (equation 9-11).

\[
N_2 + O \leftrightarrow NO + N 
\]

\[
N + O_2 \leftrightarrow NO + O 
\]

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

Maximum quantity of NOx formed in equivalence ratio of 0.9. Where burning is in poor or stoichiometric areas, the concentration of OH very low. SO, we can ignore the eq. 11. Equilibrium equations are as follow (eq. 12-13):

\[
K_1 [N_2] [O] = K_2 [NO] [N] 
\]

\[
K_3 [N] [O_2] = K_4 [NO] [N] 
\]

Final NOx formation equation is as follow (equation 14):

\[
N_2 + O_2 \leftrightarrow 2NO 
\]

2.2.2.2. Soot formation model. The rate of Soot formation is as follow (equation 15-17) [18, 19]:

\[
\text{(Equations for model, not fully transcribed due to space constraints.)} 
\]
\[ \frac{dm_{\text{total}}}{dt} = \frac{dm_{\text{form}}}{dt} - \frac{dm_{\text{oxid}}}{dt} \]  \hspace{1cm} (15)

\[ \frac{dm_{\text{form}}}{dt} = A_f m_r p^{0.5} \exp\left(-\frac{E_a}{RT}\right) \]  \hspace{1cm} (16)

\[ \frac{dm_{\text{oxid}}}{dt} = \frac{6M_c}{\rho d_s} m_R \]  \hspace{1cm} (17)

### 3. Result and discussion

#### 3.1. Validation the numerical results with experimental results

Common method for validation the combustion simulation is the comparison pressure-rank angle curve between the simulation result and experimental result [20]. The result have shown the calculated torque is equal to 89 N.m and the measured torque is equal to 92 N.m. The difference between the experimental and numerical results was reported to be 3.2%

#### 3.2. Effect of crank angle on temperature.

The effect of different crank angle on cylinder inside temperature, for the condition of 900 rpm for engine speed, 200 bar cylinder pressure, and injection timing (15° CA BTDC), shown in figure 1. Due to the non-homogeneous mixture of air and fuel in a diesel engine, the temperature distribution is not uniform and the temperature in some places reaches 2500 K. While the temperature in the middle of the piston hole where is far from the flame, the temperature is 1,000 K.

![Temperature distribution](image_url)

(a) Case_1000.AW_360.0.Flow.Temperature(K)

(b) Case_1000.AW_370.0.Flow.Temperature(K)
Figure 1. Contours of temperature inside the cylinder in different crank angles (a) 360 °CA; (b) 370 °CA; (c) 380 °CA.

Figure 2 shown diesel nozzle fuel spray and in-cylinder field flow for different crank angles. Since the injection pressure in the diesel engine is high, the deviation of fuel spray is low. As shown in figure 2, in crank angle of 350 °CA the nozzle fuel spray hits the inside wall of cylinder.

3.3. NOx formation.
NOx formation for different crank angles shown in the figure 3. For the pre-mixed combustion process and the initial stages of none pre-mixed combustion, when the temperatures and pressure of burned gases are very high are, is the best conditions for the formation of nitrogen oxides. In areas with an equilibrium ratio (stoichiometry) and temperatures above 2000 K, nitrogen oxide is the highest. As shown in the figure 3 the accumulation of nitrogen oxide pollutants is highest in the space above the inside of the cylinder.
3.4. Soot formation.
Figure 4 shows soot contours at different angles of the crankshaft. Generally, soot is formed in rich combustion areas, where the volume of oxygen concentration is insufficient to achieve stoichiometric conditions. Areas with a temperature range between 1500 and 1900 K are more favorable areas for the formation of soot pollutant. In a diesel engine, soot is concentrated in two distinct zones, one in the middle of the cylinder and another in the vicinity of the cylinder wall.
Figure 4. Mass fraction contour of soot in different crake angle.

4. Conclusion
In the present study, NOx formation in the MF-399 diesel engine were simulated numerically and the numerical result was verified with the experimental result. Simulation was done for the condition of 900 rpm for engine speed, 200 bar cylinder pressure, and injection timing (15° CA BTDC).

- Due to the non-homogeneous mixture of air and fuel in a diesel engine, the temperature distribution is not uniform and the temperature in some places reaches 2500 K.
- In areas with an equilibrium ratio (stoichiometry) and temperatures above 2000 K, nitrogen oxide is the highest.
- Areas with a temperature range between 1500 and 1900 K are more favourable areas for the formation of soot pollutant.

Acknowledgments
The authors are grateful to the Tarbiat Modares University (http://www.modares.ac.ir) for financial supports given under IG/39705 grant for renewable Energies of Modares research group.

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