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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; NO_x; 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.

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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 1bar 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):

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial (\overline{\rho u_i})}{\partial x_i} = \dot{\overline{\rho}}_{spray} \tag{1}$$

Momentum equations (equation 2-3):

$$\overline{\rho}\left(\frac{\partial \overline{u}_j}{\partial t} + \overline{u}_i \frac{\partial \overline{u}_j}{\partial x_i}\right) = -\frac{\partial \overline{p}}{\partial x_j} + \frac{\partial}{\partial x_i}\left(\overline{\tau_{ij}} - \overline{\rho u_i' u_j'}\right) + f_{j,spray} \tag{2}$$

$$\overline{\tau_{ij}} = \left[\mu\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right) - \delta_{ij}\frac{2}{3}\mu\frac{\partial \overline{u_i}}{\partial x_i}\right] + \left[\mu\left(\frac{\partial \overline{u_i'}}{\partial x_j} + \frac{\partial \overline{u_j'}}{\partial x_i}\right) - \delta_{ij}\frac{2}{3}\mu\frac{\partial \overline{u_i'}}{\partial x_i}\right] \tag{3}$$

$$-\rho\overline{u_i'u_j'} = \mu_t\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right) - \frac{1}{3}\rho\delta_{ij}\overline{u_i'u_i'}$$

Energy equations (equation 4-5)

$$\overline{\rho}c_p\left(\frac{\partial \overline{T}}{\partial t} + \overline{u}_i\frac{\partial \overline{T}}{\partial x_i}\right) = -\frac{\partial}{\partial x_i}\left(\overline{\dot{q}_i} + c_p\overline{\rho T'u'_i}\right) + \dot{q}_{spray} + \dot{q}_{comb} \tag{4}$$

$$\overline{\dot{q}}_i = -\lambda\left(\frac{\partial \overline{T}}{\partial x_i} + \frac{\partial \overline{T'}}{\partial x_i}\right) \tag{5}$$

Standard k-ε model (equation 6-7)

$$\rho\frac{\partial k}{\partial t} + \rho\overline{u_i}\frac{\partial k}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{\mu_t}{C_k}\frac{\partial k}{\partial x_i}\right) + \mu_t\frac{\partial \overline{u_j}}{\partial x_i}\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right) - \rho\varepsilon \tag{6}$$

$$\rho\frac{\partial \varepsilon}{\partial t} + \rho\overline{u_i}\frac{\partial \varepsilon}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{\mu_t}{C_\varepsilon}\frac{\partial \varepsilon}{\partial x_i}\right) + C_1\frac{\varepsilon}{k}\mu_t\frac{\partial \overline{u_j}}{\partial x_i}\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right) - \rho C_2\frac{\varepsilon^2}{k} \tag{7}$$

Where terms of C_1 ،C_2 ،Cε ،Ck ،Cμ are equal to 1.92, 1.44, 1.3, 1, 0.09 [16].
Eddy viscosity calculated from eq. 8.

$$\mu_t = C_\mu . \rho\frac{k^2}{\varepsilon} \tag{8}$$

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).

$$N_2 + O \leftrightarrow NO + N \tag{9}$$

$$N + O_2 \leftrightarrow NO + O \tag{10}$$

$$N + OH \leftrightarrow NO + H \tag{11}$$

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):

$$K_1[N_2][O] = K_2[NO][N] \tag{12}$$

$$K_3[N][O_2] = K_4[NO][N] \tag{13}$$

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

$$N_2 + O_2 \longleftrightarrow 2NO \tag{14}$$

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

$$\frac{dm_{soot}}{dt} = \frac{dm_{form}}{dt} - \frac{dm_{oxid}}{dt} \tag{15}$$

$$\frac{dm_{form}}{dt} = A_f m_{fv} p^{0.5} \exp\left(-\frac{E_a}{RT}\right) \tag{16}$$

$$\frac{dm_{oxid}}{dt} = \frac{6M_c}{\rho_s d_s} m_s R_{tot} \tag{17}$$

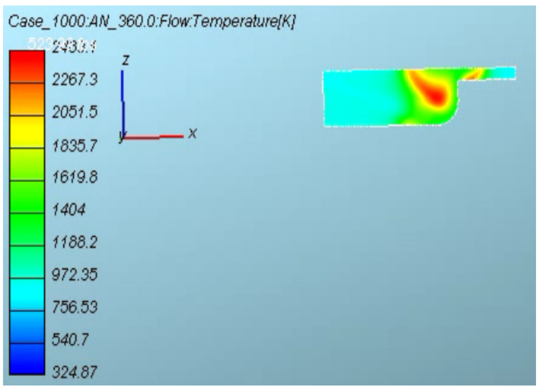
3. Result and discussion

3.1. Validation the numerical results with experimental results

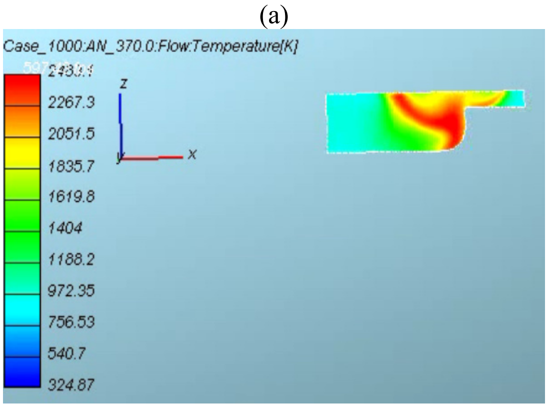
Common method for validation the combustion simulation is the comparison pressure-rank angle curve between the simulation result and experimental result [20]. The result have shown the calculated torque is equal to 89 N.m and the measured torque is equal to 92 N,m. The difference between the experimental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

3.2. Effect of crank angle on temperature.

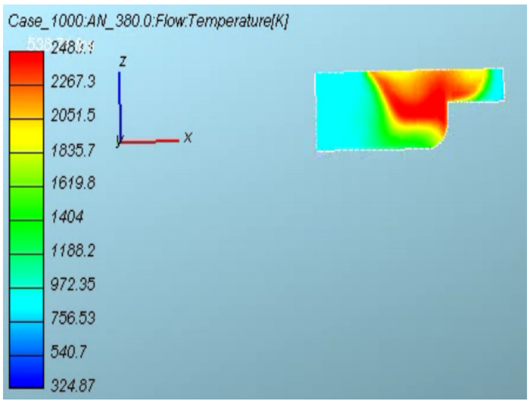
The effect of different crank angle on cylinder inside temperature, for the condition of 900 rpm for engine speed, 200 bar cylinder pressure, and injection timing (15° CA BTDC), shown in figure 1. Due to the non-homogeneous mixture of air and fuel in a diesel engine, the temperature distribution is not 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.



(a)



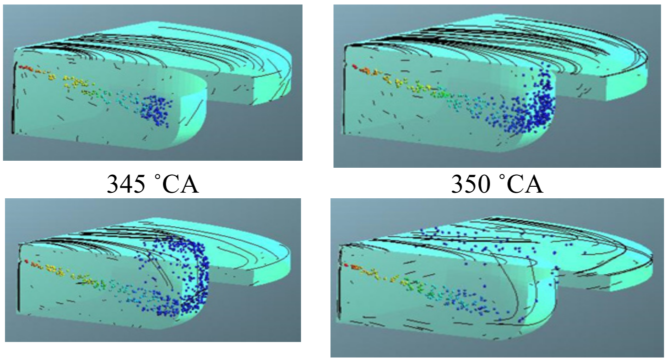
(b)



(c)

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 nuzzle 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 nuzzle fuel spray hits the inside wall of cylinder.



345 ˚CA 350 ˚CA

355 ˚CA 360 ˚CA

Figure 2. Nuzzle fuel spray and the field of flow.

3.3. NO_x 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.

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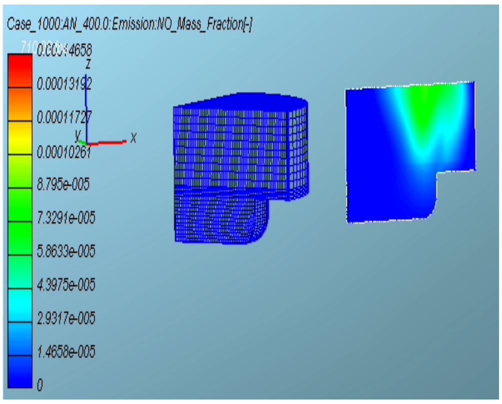
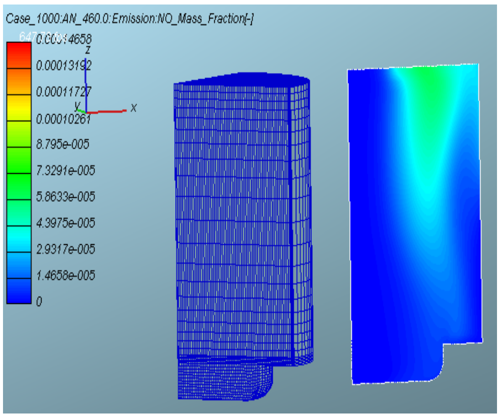


400 ˚CA

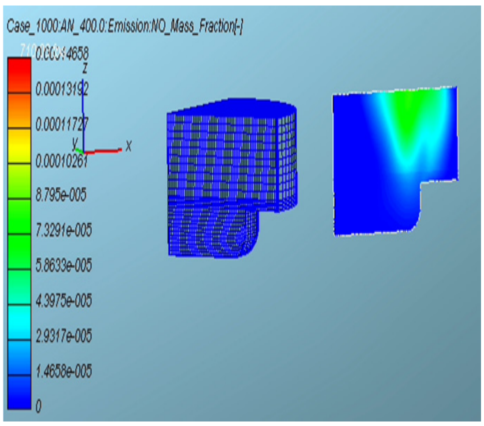


460 ˚CA

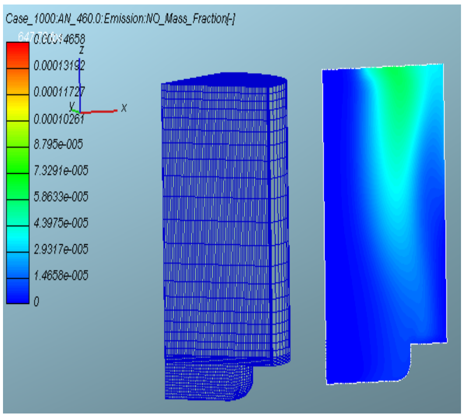
Figure 3. Mass fraction contour nitrogen oxide (NO) in different crake angle.

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.



400 ˚CA



460 ˚CA

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.

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