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Simulation Studies of Diesel Engine Combustion Characteristics with Oxygen Enriched Air

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Abstract

Based on a six-cylinder direct injection diesel engine, the engine operating condition was simulated by application AVL-FIRE software coupling the n-heptane reduced mechanism containing polycyclic aromatic hydrocarbon (PAH) formation. The simulation and its verification test were both carried out under the maximum torque point. Then, the oxygen enriched combustion was simulated on the model, and the simulated condition was oxygen volume fraction from 21% to 30%. The simulation results show that, the oxygen enrichment (from 21% to 30%) increases the peak cylinder pressure of 3.32%, advances the start of combustion of 1.6 deg and rises the peak of average temperature in cylinder and wall heat flux. Among them, at the condition of 24% O_2, the change of the results is the most significant. Benzene (A1) is one of the precursors of soot generated, the analysis of its impress-cuts of the mass distribution field in cylinder shows that, the increase of oxygen concentration can significantly inhibit the formation of benzene. But the oxygen enrichment makes the combustion more sufficient, cased a rise in the cylinder temperature, an extension in high temperature area, and an increment in the NO_x emission.

Keywords

Diesel Engine, Numerical Simulation, Oxygen Enriched Combustion, Combustion Characteristic

1. Introduction

A lot of researches show that oxygen enriched combustion technology can obviously improve the combustion process of the cylinder, and have a significant effect on the power performance, fuel economy and emission characteristics of diesel engine [1]-[3]. Oxygen enriched intake increased the content of oxygen in the air, cased

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an exacerbation in the combustion, an increment in the flame speed, a rise in the combustion temperature and a decrease in the fuel consumption. In addition, it can also significantly reduce the emissions of soot, but will lead to a substantial increment in NO_x emissions [4]-[6]. The studies by GequnShu [7] and Peter L. Perez [8] show that oxygen enrichment combustion combining with some technologies, such as the controlling of fuel injection timing, water emulsion fuel and EGR technology etc., can make NO_x and soot emissions simultaneously get effective control. At present, there is little research on the oxygen enriched combustion characteristic of diesel engines with the intake oxygen concentration higher than 24%. Although some experimental studies [9] [10] show that, when the intake oxygen concentration is higher than 26%, the effective thermal efficiency of diesel engine will slow decline with the increasing of intake oxygen concentration. However, further exploring the effect of higher intake oxygen concentration on the combustion characteristics of the diesel engine is still significant for improving the combustion process and controlling the pollutant discharge of the diesel engine.

In the present work, the model built by application of AVL-FIRE software and coupling the n-heptane reduced mechanism containing the PAH formation were used for calculating some parameters, such as cylinder pressure curve, rate of heat release and the concentration distribution of emissions, etc. Then, these parameters were used to explore the influence of different inlet oxygen concentration on diesel engine combustion characteristic, so as to accumulate more theory basis in diesel engine.

2. Establishment of Coupling Model

2.1. Selection of Chemical Reaction Mechanism

Because of the cetane number of n-heptane and diesel are the same, the simulation study of diesel engine usually choose n-heptane as a substitute for diesel combustion calculation. Most of the reaction kinetics models are supplied from the Lawrence Livermore national laboratory in n-heptane detailed oxidation combustion mechanism [11] [12]. However, as a result of the mechanism is too complicated for coupling calculation, in this study, the n-heptane-butanol-PAH reduced mechanism which proposed by Hu Wang [13] was selected. The mechanism is verified by the experimental data of the shock tube, the constant volume combustion bomb and the engine , and it can well predict the process of the fuel combustion and the generation of the emissions. As fuel for pure diesel, the new mechanism should get rid of the reduced mechanism of n-butanol in the mechanism part, finally obtained a mechanism including 60 species and 272 elementary reactions to simulate the diesel combustion process and emissions generated.

2.2. Computational Grid and Model

According to the geometric parameters and operating conditions of the diesel engine which was selected by Haozhong Huang [14] for experimental research, the model is established. Diesel engine basic parameters see **Table 1**.

Because of the full size model calculation needs to consume too long and the combustion chamber is in a central symmetry, the 1/7 combustion chamber model is selected according to the number of injector holes. The computational grid is shown in **Figure 1**.

Due to just the combustion characteristics of diesel engine are researched, the calculation will start from the valve closing time of 583 deg to the exhaust valve opening time 845 deg. In the boundary conditions of the model, there are three surface temperatures needing to be set, including the wall of the combustion chamber, the piston head and the inner wall of the cylinder. The temperature of the three surfaces is assumed to be constant, and the temperature value is calculated by reference to empirical formula. In the initial calculation, the temperature and pressure of the cylinder are uniform, the pressure value is set according to the test values, and the temperature value is estimated by the corresponding empirical formula [15]. In addition, according to the engine speed, intake flow and other parameters, the initial kinetic energy intensity is calculated and its direction is defined. In the selection of calculation model, according to the structure characteristics of diesel engine, gas turbulence model selected k-zeta-f, spray model selected Spray Turbulent Diffusion, oil mist evaporation model selected Dukowicz and fuel crushing model selected Wave.

2.3. Combustion Chamber Numerical Model Verification

The accuracy of the model is verified by using the cylinder pressure curve measured by Haozhong Huang [14].

The fuel used in the experiment was pure diesel, and the test conditions were in agreement with the simulation conditions (see **Table 2**).

Table 1. Parameters of the diesel.

Parameters	Unit	Value
Bore × Stroke	mm	105 × 125
Connecting rod length	mm	210
Compression ratio	-	16
Displacement	L	6.5
Maximum torque engine speed	rpm	1400
Number of nozzle holes	-	7
Bore of nozzle hole	mm	0.17
Spray angle	deg	155

Table 2. Conditions of the simulation.

Projects	Value
Fuel	$C_{12}H_{26}$
Fuel delivery per cycle(mg)	47.25
Fuel injection timing(deg)	6.2 deg bTDC
Intake pressure(bar)	1.6
Engine speed(rpm)	1400
Injection rate	HD-Engine Model

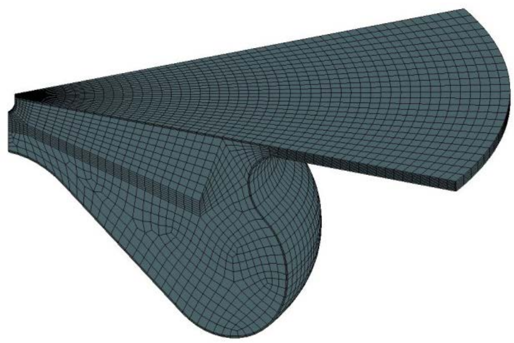


Figure 1. Simulation model of 1/7 combustion chambers.

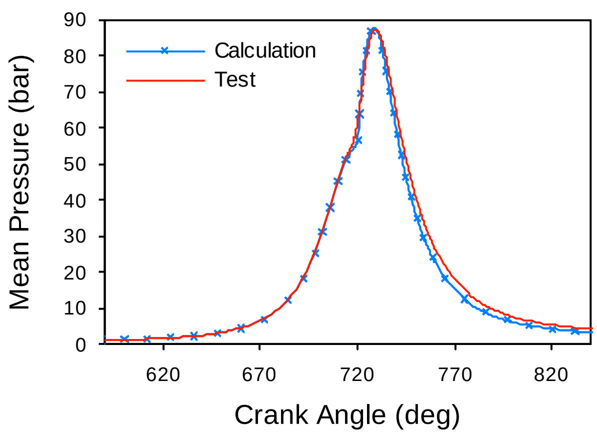


Figure 2. Comparison between the calculation and test in-cylinder pressure.

Figure 2 shows the comparison between the test data and the calculated values of the diesel engine at the intake air (21% O_2), It shows that the pressure in the cylinder is simulated value agrees well with the test results, especially the ignition timing prediction is accurate. It indicates that the boundary conditions are reasonable, calculation model and calculation result is believable. Therefore the model can be used to simulate the combustion process of diesel engine with different intake oxygen concentration.

3. Simulation Results and Discussion

By using the above model, the simulated working condition is kept unchanged, and according to the equal concentration interval, the oxygen mole fraction of the inlet air is respectively selected 21%, 24%, 27% and 30%. Then, some parameters of the diesel engine are simulated under 4 different inlet oxygen concentration conditions, such as cylinder pressure curve, rate of heat release , temperature field and the concentration distribution of emissions, etc., so as to explore the influence of different inlet oxygen concentration on diesel engine combustion characteristic.

3.1. Influence of Oxygen Enriched Combustion on Cylinder Pressure and Rate of Heat Release

Figure 3 is the calculation of cylinder pressure curve. It shows that with the increase of inlet oxygen concentration, there is a slight increment in cylinder peak pressure, a slight advancement in peak pressure point and ignition starting point accordingly. Because of the increase of the oxygen concentration, the fuel and oxygen mix better, the ignition period is shortened and fuel combustion more fully, resulting in the increase of peak cylinder pressure. In addition, in the process of inlet oxygen concentration increasing from 21% to 30%, with the oxygen concentration improving 3% each time, the peak cylinder pressure rise by 1.48%, 1.04% and 0.77% in turn. It can be seen that compared to other inlet oxygen concentration interval, the influence of inlet oxygen concentration on burning process is most significant when the oxygen concentration improve from 21% to 24%. This is because the effect of oxygen concentration decreases with the increase of inlet oxygen concentration, cased a declined in the influence of the oxygen concentration on the combustion process.

Figure 4 shows the rate of instantaneous heat release in the combustion chamber model of 1/7, which indicates that enhanced the oxygen concentration in the intake air makes the cylinder heat release slightly forward. With the promoting of the inlet oxygen concentration, the ignition time is advanced, and then, the heat release of the premixed combustion stage is reduced. As the combustion continued, it shows that the fuel injection continues while mixed diffusion combustion appears, so the heat release of the diffusion combustion stage is increased.

3.2. Influence of Oxygen Enriched Combustion on Mean Temperature Wall Heat Flux

Figure 5 and **Figure 6** respectively show the curve of the average temperature of the combustion chamber and the wall heat flux changes with the Crank Angle under the different inlet oxygen concentration. With the promoting of oxygen concentration, the number of high-energy collisions between molecules combustible mixture molecules and oxygen molecules increases, cased an exacerbation in the combustion and fuel combustion more fully. The average temperature of the cylinder in the ignition stage and the rapid burning stage show an increasing trend, which is favorable for the improvement of the combustion efficiency. At the same time, the temperature of the cylinder increases, cased an increment in the heat flux of the combustor wall. It indicate that the heat loss of the combustor wall is increased, which hinders the improvement of the effective thermal efficiency of the diesel engine.

3.3. Influence of Oxygen Enriched Combustion on Temperature Field and NO Mass Distribution

Figure 7 and **Figure 8** respectively show the combustion chamber temperature field and mole fraction distribution of the NO at the average temperature in cylinder peak point (13 deg a TDC). With the promoting of inlet oxygen concentration, the maximum temperature inside the cylinder is improved and the high temperature region is expanded. Thereinto, the change of oxygen concentration of 24% was the most significant. By comparing the temperature field and NO concentration distribution in cylinder, the changed trend of both is consistent

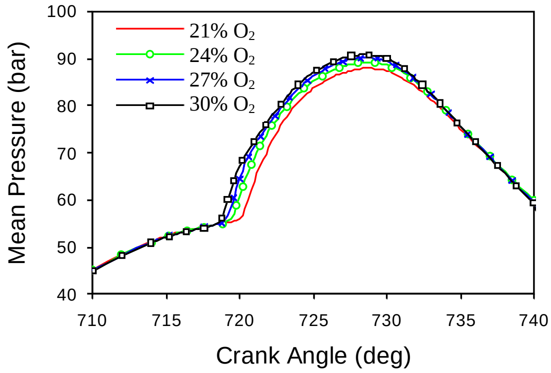


Figure 3. Influence of different O_2 concentration on cylinder pressure.

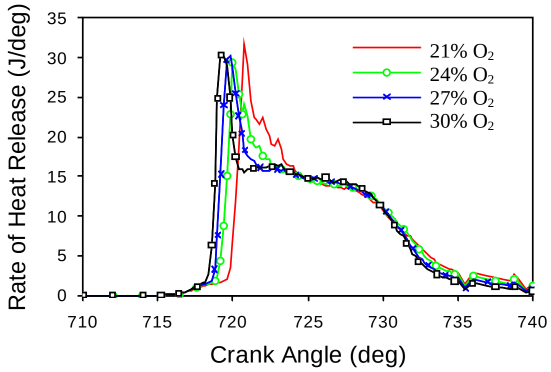


Figure 4. Influence of different O_2 concentration on the rate of heat release.

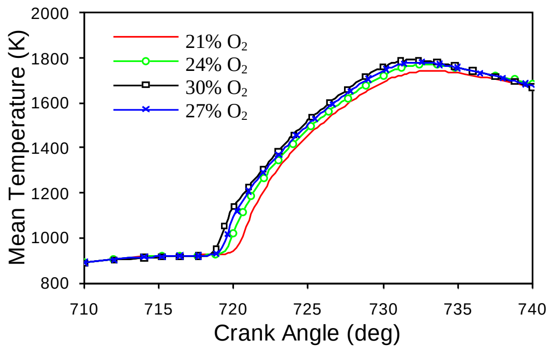


Figure 5. Influence of different O_2 concentration on mean temperature.

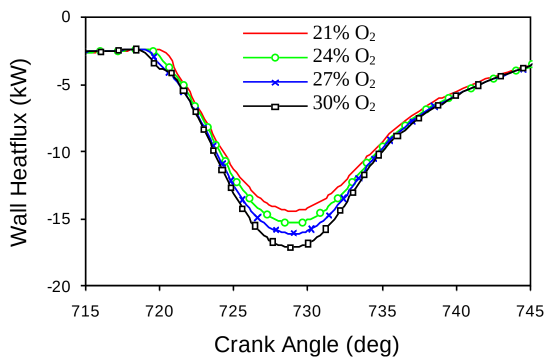
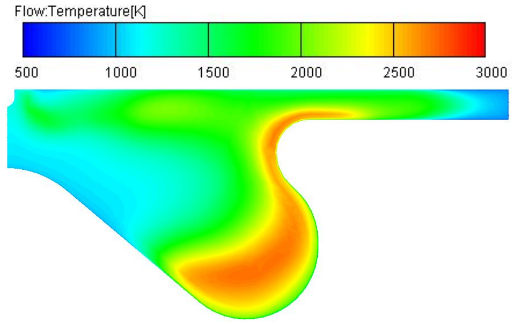
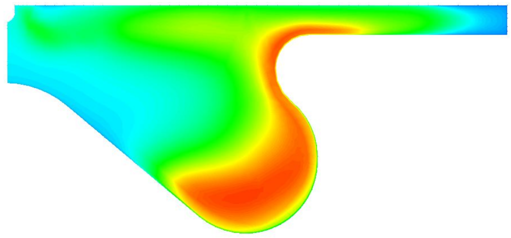


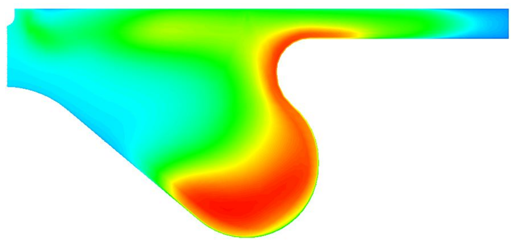
Figure 6. Influence of different O_2 concentration on wall heatflux.



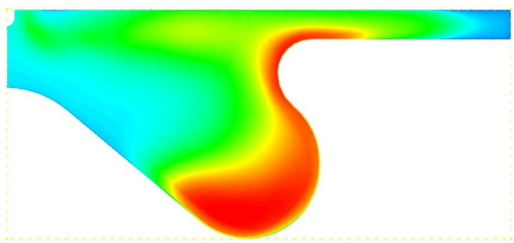
(a)



(b)

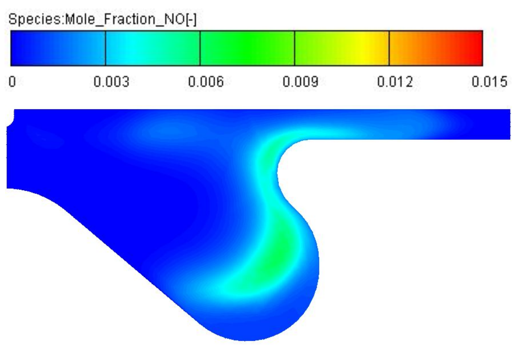


(c)

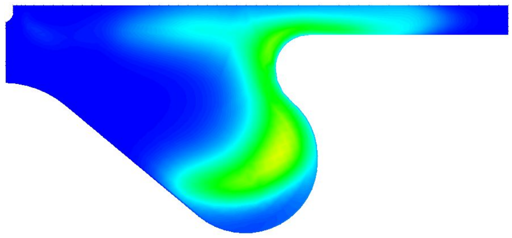


(d)

Figure 7. Temperature field in combustion chamber. (a) 13˚ CA ATDC (V_{O2} = 21%); (b) 13˚ CA ATDC (V_{O2} = 24%); (c) 13˚ CA ATDC (V_{O2} = 27%); (d) 13˚ CA ATDC (V_{O2} = 30%).



(a)



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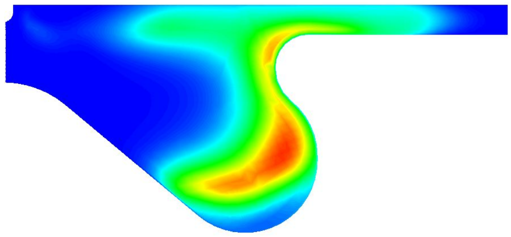

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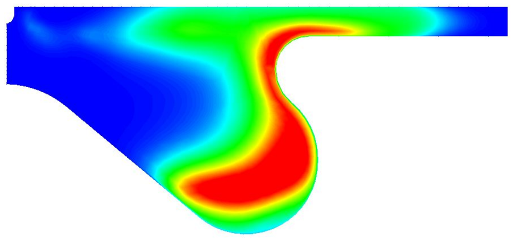

(d)

Figure 8. NO mass distribution in combustion chamber. (a) 13˚ CA ATDC (V_{O2} = 21%); (b) 13˚ CA ATDC (V_{O2} = 24%); (c) 13˚ CA ATDC (V_{O2} = 27%); (d) 13˚ CA ATDC (V_{O2} = 30%).

with the increasing of inlet oxygen concentration. Under oxygen enrichment, the formation rate of NO increases rapidly in the high temperature region.

Figure 9 shows the curve of the average mass fraction of the NO with the crank angle at different inlet oxygen concentrations. From the picture, it can be seen that with the increase of the oxygen concentration, the NO production volume increases sharply, and the curve is getting steeper. This is because the formation conditions of NO are high temperature, rich oxygen and the residence time in high temperature. See **Figure 7**, with the increase of the oxygen concentration, the range of N_2 in high temperature and oxygen enriched conditions becomes larger and the retention time is lengthened, so, the NO emissions increase greatly.

3.4. Influence of Oxygen Enriched Combustion on Soot Emissions

The molecular of the polycyclic aromatic hydrocarbon (PAH) generated by combustion is considered as the precursor of soot, so PAH oxidation reaction mechanism is used to predict soot emissions. However, the changing trend of A1 and soot generation is basically consistent [16], so the changes of soot formation in different oxygen concentrations can be qualitatively studied by observing the changing trend of A1.

As can be seen from **Figure 10**, with the increase of oxygen concentration, the formation of A1 is greatly reduced and the generation time in advance. Among them, when the oxygen concentration increased from 21% to 24%, oxygen enrichment had the most significant effect on the inhibition of A1 formation. This is because the increase of the intake oxygen enriched oxygen makes the fuel burning more fully and the lack of oxygen burning area significantly smaller, caused a decrement in the formation of soot.

4. Conclusions

Under the constant inlet total, with the increase of the inlet oxygen concentration, the peak of the pressure and the average temperature of the cylinder are increased, and the engine power of the diesel engine is enhanced. In

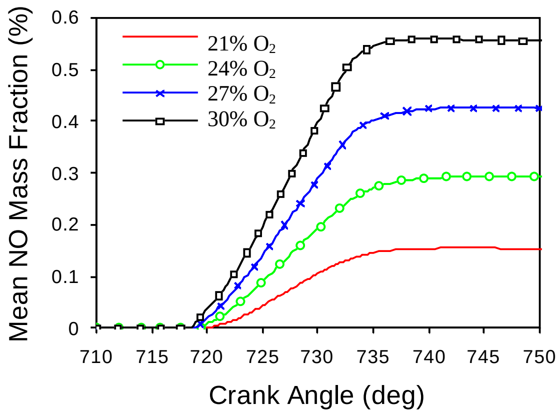

Figure 9. Influence of different O_2 concentration on mean NO mass fraction.

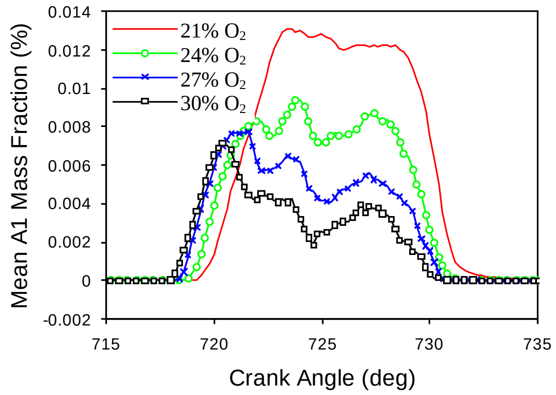

Figure 10. Influence of different O_2 concentration on mean A1 mass fraction.

addition, oxygen enriched combustion can improve the combustion efficiency, and the emissions of soot can decrease greatly. Thus, oxygen enriched combustion is an effective method to improve the diesel engine performance.

However, the performance of the diesel engine is not linear improvement with the increase of the intake oxygen concentration. When the oxygen concentration is over 24%, the effect of oxygen concentration on the combustion of the cylinder is gradually weakened. The cylinder wall heat loss increases greatly, which hinders the improvement of the effective thermal efficiency of the diesel engine. Therefore, the practical application of oxygen enriched combustion in diesel engine also needs to calibrate the best inlet oxygen concentration under different working conditions.

With the improvement of inlet oxygen concentration, the soot emissions are greatly reduced, however, the NO_x emissions increased sharply. Therefore, the future research emphasis should focus on the combination of oxygen enriched combustion and NO_x emissions control technology, in order to achieve the purpose of controlling the emissions of NO_x and soot of diesel engine simultaneously.

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