Numerical Simulation of Pollutants Emitted from Diesel Engine Combustion

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Abstract. Based on the control research of diesel engine combustion emission pollutants, a reasonable numerical simulation study is carried out. At present, hydrocarbon fuel is a common fuel in transportation. Its combustion quality directly affects emissions. Reducing sulfur content and polycyclic aromatic hydrocarbons content in diesel can effectively reduce particulate matter emissions. Because of the poor atomization of diesel fuel, diesel in cylinder cannot be completely burned, resulting in the formation of soot, and diesel additives can increase the degree of combustion completion, and then optimize to achieve the effect of reducing soot. Therefore, the numerical simulation of pollutants is carried out and effective measures are taken to control combustion. The combustion model chosen here is Vortex Cluster Fragmentation Model 20, which is based on turbulent mixing rate.

Keywords: diesel engine; combustion emission; pollutants; environmental pollution; environmental protection.

1. Introduction
With the development of science and technology, the technological level has been continuously improved, emission reduction technology has also been improved, and it has become an increasingly important issue in the use of diesel engines. The extensive application of diesel engine shows that it has many advantages. For example, compared with gasoline engine, diesel engine has better power performance, wider power range and higher compression ratio than gasoline engine [1, 2, 3]. Aiming at the problems of stratified combustion and lean combustion, diesel engine is easier to realize than gasoline engine, which can reflect better economic effect. However, due to the extensive application of diesel engines, the pollution caused by combustion has an impact on human life and the environment. If effective measures are not taken against this situation, it will aggravate the adverse degree of the environment [4, 5, 6].

Diesel engine exhaust contains many harmful substances, such as carbon monoxide (CO), hydrocarbons (HC), nitric oxide (NO), and particulate matter (PM), which can affect human daily life [7]. Diesel engine has high thermal efficiency and excess air coefficient in combustion, so its CO and HC production is less than that of gasoline engine, but its base number is still relatively large. In addition, the particulate matter produced by diesel engine combustion is tens of times more than that of gasoline engine, or even more. Therefore, it is of great significance to select feasible control and optimization methods for the numerical model of pollutants [8].
2. Improvement of pollutant emission from diesel engine combustion

2.1. Pre-processor
The control of diesel engine combustion emission pollutants can be carried out before the engine. Effective pretreatment is needed before the fuel enters the internal combustion engine to ensure that the later emission is controlled. The main technical methods include improving fuel quality, adding diesel additives and using alternative fuels.

2.2. In-machine purification technology
The core of in-plane purification technology is to achieve the optimal combination of intake system, fuel injection system and combustion system, so that fuel and air can be fully mixed, so as to improve the combustion process and reduce the emission of harmful substances. The specific measures are shown in table 1.

Table 1. Main technical measures of internal purification of diesel engine

| Category          | Countermeasure                        | Control object |
|-------------------|---------------------------------------|----------------|
| Fuel system       | Delay injection advance angle          | NOx            |
|                   | Increasing injection pressure          | PM             |
|                   | Optimizing injection rule              | NOPM           |
|                   | Lean burn                              | PM             |
|                   | Turbocharging and turbocharging intercooling | PM         |
| Intake system     | Multi-valve technology                 | PM             |
|                   | Exhaust gas recycling (EGR)            | NOx            |
|                   | New combustion mode                    | NO, PM         |
| Combustion system | Design parameter optimization           | NO, PM         |
|                   | Various combustion chamber shapes      | NO, PM         |
| Electronic control| Electronically controlled high pressure injection, etc. | PM |

2.3. Post-processing technology
The post-processing technology is for the purpose of not affecting other performance of internal combustion engine, and on this basis, the exhaust gas generated by engine is directly treated, and then released to the outside world. According to the effect of in-machine purification technology, whether it can play an effective role is analyzed. Combining with the subsequent situation, effective measures should be taken to deal with it. In general, catalytic conversion technology is mainly used for NO post-treatment, including selective catalytic reduction (SCR), selective non-catalytic reduction (SNCR) and non-selective catalytic reduction (NSCR).
3. Modeling and simulation results of diesel engine combustion

3.1. Calculating object of diesel engine combustion simulation model
The calculation object is a four-cylinder turbocharged and intercooled diesel engine. The main technical parameters are shown in Table 1.

| Table 2. Main performance parameters of diesel engine |
|-----------------------------------------------------|
| **Project** | **Parameter**                    |
| Type        | In-line four-stroke, direct injection and air cooling |
| Combustion chamber | Convex contraction               |
| Cylinder number* Bore diameter(mm)* Stroke (mm) | 4*88*100                      |
| Total displacement (L) | 2.433                           |
| Rated power (kW)/ Rated speed (r/min) | 65/3200                        |
| Maximum torque (N·m)/ Maximum torque and velocity (r/min) | 225/2000                      |
| Idling (r/min) | 800±50                           |
| Fuel system  | Electronically Controlled Monomer Pump |

3.2. Selection of simulation models
There are three main simulation models. The first one is turbulence model, the second one is spray model and the third one is ignition and combustion model.

Turbulence model:
Turbulence is a very complex and irregular three-dimensional unsteady flow. During the working cycle of diesel engine, the gas in cylinder has been undergoing complex and changeable turbulent motion, which has a very important impact on the process of gas compression, mixing, flow and combustion. Therefore, in order to correctly simulate the combustion process in combustion chamber, it is necessary to correctly select the turbulence model.

The turbulence model used here is the standard high Reynolds number k-Ɛ model given by AVL company. k-Ɛ model is an eddy-viscous-dissipation model, which is one of the most mature turbulence closure models. After continuous improvement, it has become a more comprehensive model to simulate three-dimensional flow phenomena in internal combustion engines. It has high computational stability and low requirements for computational resources. In k-Ɛ model, k refers to turbulent fluctuating kinetic energy and Ɛ refers to turbulent dissipation rate. The equation is as follows:

\[
\frac{\partial k}{\partial t} + \rho \frac{\partial \bar{U}_j}{\partial x_j} \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \mu + \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right) - C_1 \varepsilon + C_2 \frac{\varepsilon}{k} \frac{\partial k}{\partial x_j} \frac{\partial k}{\partial x_j}
\]

Spray model:
In the spray process, a two-phase flow phenomenon includes liquid phase and gas phase. Therefore, the conservation equation of gas phase and liquid phase is needed for the simulation calculation. The calculation of liquid phase is based on the Discrete Droplet Method (DDM). The continuous gas phase is described by the standard Euler conservation equation, while the transport process of dispersed phase is calculated by tracking a certain number of representative oil droplet micro-clusters.

The difference equation of the trajectory and velocity of the oil droplet group is as follows:

\[
m_d \frac{d U_{ld}}{dt} = F_{idr} + F_{lg} + F_{ip} + F_{it}
\]

In the formula, \( m_d \) is the mass of the droplet, \( U_{ld} \) is the velocity vector of the oil droplet, and \( F_{idr} \) is the resistance.

Ignition and combustion model:
Combustion models can be used to simulate component changes, ignition, turbulent combustion, and the formation of gaseous hydrocarbon mixtures with air and residual pollutants. The combustion in engine cylinder belongs to turbulent combustion. The turbulent combustion model used in practical simulation can be divided into five categories. Eddy Break Up (EBU), Probability Density Function (PDF) model, Characteristic Time Scale Model, Coherent Flame Model and Turbulent Flame Speed Closure Model 1.

The chemical reactions in premixed flame occur at the interface of vortices formed in the random motion of combustible and unburned gases. The speed of reaction is determined by the speed at which larger gas vortices break up into smaller ones. Because the speed of breakup is proportional to the dissipation rate of turbulent pulsation energy, the reaction rate is related to the basic turbulent parameters $k$ and $\epsilon$.

3.3. Analysis of simulation results

With the increase of injection timing, the ignition delay increases. The longer the ignition delay period is, the longer the diesel and air mix before ignition is, thus resulting in an increase in the number of premixed gases in the combustion chamber. If the injection timing is too large, there will be more mixtures formed during the ignition delay period. These mixtures burn rapidly after ignition, the temperature and pressure in cylinder increase rapidly, the engine works roughly, and the service life of diesel engine decreases. However, if the ignition delay is too short, the formation of mixtures will be adversely affected. Therefore, the length of ignition delay period should be reasonably controlled in order to better group. Weave the combustion process well, thus affecting the optimization of diesel engine emissions, as shown in figure 1.

![Figure 1. Optimized parameters for diesel emissions](image)

In the operation of diesel engine, the fuel evaporation rate at ignition time increases with the increase of injection timing. When the injection timing is 14CABTDC, the fuel evaporation rate at ignition time is close to 50%. A large amount of fuel evaporates and forms premixed mixture with air. When the injection timing is small, the fuel evaporation rate at ignition time is very low, and a large amount of fuel evaporation enters into the diffusion combustion at the same time as combustion. That's ok. It can be explained that the more fuel injection timing increases, the better mixing of fuel and air at the time of ignition is, the more premixed gas volume is, as shown in the following figure.
Figure 2. Comparison of fuel evaporation rate in the lower cylinder of different injection timings at the moment of fire

4. Optimum Direction of Pollutants Emitted from Diesel Engine Combustion

4.1. Optimizing direction of oil supply system

The optimization of diesel engine combustion emission pollutants can start with the fuel supply system. First of all, diesel engines are widely used, so for the use of this equipment, there are strict requirements on power, economy, emissions and noise. In practical use, the intake system, combustion chamber structure and fuel injection system should be rationally equipped. Then, the overall structure and processing technology of the diesel engine are determined to ensure the normal function of the fuel injection system. According to the continuous improvement of direct injection technology, people's requirements for the fuel injection system are also constantly improving. The performance of the fuel injection system and whether it can match reasonably with other systems of the diesel engine largely determine the performance of the diesel engine. Optimum Direction of Pollutants Emitted from Diesel Engine Combustion selects the best composition according to the experimental data. The interaction is shown in the following figure.

Figure 3. Control strategy for low-emission diesel engine combustion process

4.2. Optimization of injection advance angle

In order to optimize this situation, it is necessary to clarify the injection timing, and injection advance angle. For diesel engines, delaying injection is one of the most effective ways to reduce NOX. Through the range analysis of common injection advance angle, it can be verified by reducing NO emission. However, this method also has drawbacks. Excessive delay of injection advance angle will lead to fuel economy deterioration and increase soot emissions. Therefore, compromise control is needed to ensure that both soot and NOx can be reduced to lower emissions. In the use of diesel engine, the fuel injection system of electronic control unit pump is mainly used to control the advance angle accurately by
electronic control system. Through the calibration experiment of different injection advance angle, the best injection advance angle of emission performance can be found, the pulse spectrum of the best injection advance angle can be obtained, and then the best injection advance angle of each working condition obtained from the calibration test can be realized by electronic control system, so as to achieve the effect of reducing emissions.

4.3. Optimization of EGR opening
The EGR valve of the prototype adopts vacuum diaphragm valve, and the opening of the vacuum diaphragm valve is controlled by controlling the vacuum degree produced by an independent vacuum source. The appropriate EGR opening can reduce the emission of NOx under various working conditions. However, EGR may also increase smoke intensity. In addition, under high load conditions, in order to ensure the power of diesel engine, do not open or small open EGR. Under medium and low load, the EGR rate is usually higher. Therefore, it is necessary to optimize the EGR opening of each working condition. Through the calibration test of different EGR valve openings under different working conditions, the optimum EGR openings of diesel engines under different working conditions can be obtained, and the optimum MAP of EGR can be obtained, so that the emission performance, economic performance and power performance of off-road diesel engines can be optimized.

5. Conclusion
From the point of view of in-plane purification, through numerical simulation and emission test comparison, the fuel injection pulse spectrum of a certain type of diesel engine in the unit of practice is set and some parts are matched reasonably to reduce the emission of the diesel engine. Based on the turbocharged and intercooled diesel engine, the numerical calculation model for in-cylinder combustion is established. After verifying the accuracy of the model, the effects of injection timing, nozzle diameter and nozzle extension on mixture formation and combustion process are studied.

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