Simulation Study on the Effect of In-cylinder Water Injection Mass on Diesel Engine Combustion and Emissions

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Abstract. Based on Caterpillar 3401 diesel engine, a complete three-dimensional model of the combustion chamber was established in CONVERGE to study the effect of in-cylinder water injection on combustion characteristics and emissions within the water injection mass range from 5mg to 100mg. With the water mass increase, the pressure, power and temperature in the cylinder increase first and decrease later. The changes of CA5 and CA10 of the heat release are not obvious. CA50 of the heat release advances first and delays later. The combustion duration shortens first and increases later. NOx emission is increases as the water injection mass increases from 5mg to 40mg, but it is decrease when the water injection mass increases from 40mg to 100mg. And when the mass of water is 100mg, it has the best suppression effect on NOx. Otherwise, the water injection has the best suppression effect on Soot when the water mass is 60mg.

1. Introduction

Diesel engines have a good power, economy and durability, and are widely used as power output equipment in heavy transportations, engineering operations, etc. especially in scenes that the power requirement is more important. The performance of diesel engines can meet the needs better [1]. However, the problems brought by the rapid development of internal combustion engines have gradually emerged. The increase in oil consumption and the increase in pollutant emissions have to arouse people's attention. While ensuring power, the development of energy-saving and emission-reduction technologies for internal combustion engines is an inevitable choice and requirement, and it is also of very important significance.

In-cylinder Water Injection was applied in aero engines first to solve the knocking problem [2]. Stanglmaier et al. designed a dual-channel in-cylinder injector that can perform coordinated injection of fuel and water in the same nozzle, and verified the synergy. The feasibility of injection to reduce nitrogen oxides, particulate matter, carbon monoxide and unburned hydrocarbons [3]. Jiang et al. achieved water injection in the cylinder through an in-cylinder water injector, and studied the optimal time of water injection in the cylinder with the goal of efficiency optimization [4]. Zhe Kang et al. studied the effect of different water injection temperatures on the performance of in-cylinder water injection diesel engines, and determined that higher water injection temperatures can improve the evaporation rate of water and increase the expansion work [5]. This article mainly focuses on the effect of different water injection
mass on the combustion and emissions of a in-cylinder water-injected diesel engine, and provides a reference for the industrialization of in-cylinder water injection technology in diesel engines.

2. Modeling and validation

2.1. Numerical model

The engine selected in this paper is Caterpillar 3401 diesel engine, and the main parameters are shown in Table 1.

| Engine type         | Caterpillar 3401 |
|---------------------|------------------|
| Stroke*Cylinder bore (mm) | 173.6*165.1 |
| Connecting rod length (mm) | 261.62 |
| Compression ratio | 15.1 |
| Nozzle orifice diameter (mm) | 0.259 |
| Diesel SOI°ATDC | -8.5 |
| Injected duration°CA | 21.5 |
| Included spray angle° | 125 |
| Fuel Injected(mg/cy) | 0.1622 |
| Engine speed (r/min) | 1600 |

The in-cylinder computational fluid dynamics (CFD) model of the engine is established in CONVERGE 2.4. The parameters of the combustion chamber is input in the makefurace tool and a 360° model with water sprary injector,is generated as shown in Figure 1.

![Figure 1. 3D model of combustion chamber with a water injector.](image)

In this paper, the RNG $k - \varepsilon$ model is selected as the turbulent flow model [6], the KH-RT model is selected as the droplet breaking model [7], the O'Rourke model is selected as the turbulence dispersion model, the SAGE detailed reaction model in CONVERGE is selected as the combustion model uses, and the empirical mode is used to simulate the soot formation process. The Hiroyasu model is combined with the Nagle and Strickland-Constable model to simulate the soot oxidation process. Thermal NOx is used to simplify the formation mechanism of NO [8].

In this study, the in-cylinder CFD process is simulated during the period from the intake valve close timing to the exhaust valve open timing. The boundary and initial conditions are shown in Table 2.

| Engine type                      | Caterpillar 3401 |
|----------------------------------|------------------|
| Intake valve closing (CA°ATDC)   | -147 |
| Exhaust valve opening (CA°ATDC)  | 136 |
| Pressure at IVC (bar)            | 1.95 |
| Temperature at IVC (K)           | 330 |
The non-water cycle simulation result and the experimental result of Uludog [9] are compared in Figure 2. It can be seen that the simulation result in this paper are basically consistent with the experimental research, indicating that the established CFD model can be used for subsequent diesel-water combined in-cylinder injection simulation research.

Figure 2. The validation of the established CFD model

2.2. Position of injector of water and spray program
The water injector with 4 spray holes is set at 0.047m away from the center of the cylinder head. the water injection mass is set as 5mg, 10mg, 20mg, 40mg, 60mg, 80mg and 100mg. The spray pressure is 100MPa and the spray temperature of water is 333K. The model adding the water injector is shown in Figure 1.

3. Effect of in-cylinder water mass on combustion characteristics and emissions

3.1. Effect on combustion heat release
It can be seen from Table 3 that as the mass of water injection in the cylinder increases from 5mg to 100mg. The range of CA5 of heat release is within 0.11° CA and the range of CA10 is within 0.01° CA., Both the two results change very little. CA50 is advanced and then delayed with the increase of water mass. When the mass of water is 40mg, CA50 is the earliest, the duration of CA10 to CA90 becomes shorter first and then becomes longer. With the water mass from 5 mg to 40 mg, the change was huge, but the change was little with the water mass from 40 mg to 100 mg. This is because when the mass of water is small, the promotion effect of water on formation and combustion of the mixture is greater than the cooling effect, and when the mass of the water is too much, the cooling effect of the s water plays a leading role.

Table 3. Combustion heat release data under different water mass conditions

| The mass of water | CA5   | CA10  | CA50  | CA10-90 |
|------------------|-------|-------|-------|---------|
|                  | °CA ATDC | °CA ATDC | °CA ATDC | °CA     |
| 5                | 0.214 | 0.806 | 13.821 | 38.410  |
| 10               | 0.220 | 0.824 | 13.619 | 36.379  |
| 20               | 0.220 | 0.819 | 13.115 | 35.536  |
| 40               | 0.220 | 0.814 | 12.507 | 30.861  |
| 60               | 0.220 | 0.804 | 13.109 | 31.025  |
| 100              | 0.220 | 0.819 | 13.418 | 31.393  |
Figure 3 shows that the water mass has little effect on the peak of pre-mixed heat release rate, but has a greater impact on the main combustion period. When the mass of water are 40mg 60mg and 80mg, the peaks of heat release rate are higher than the others obviously, and mixing and combustion process is promoted by the water spray greatly.

![Figure 3. Heat release rates under different water mass conditions](image)

3.2. Effect on in-cylinder pressure and power

![Figure 4. In-cylinder peak pressures and indicated powers under different water mass conditions](image)

As can be seen from the figure 4, the maximum in-cylinder peak pressure is 10.05MPa and the maximum indicated pressure is 43.24 kW when the water mass is 40mg. With the increase of water mass from 5mg to 40mg, the in-cylinder peak pressure and the indicated power gradually increase, but the two indicators decrease accordingly as the water mass increases from 40mg to 100mg. It is because that the water evaporates quickly in a high temperature environment near the top dead center, which can convert heat energy into expansion work. When the water mass is less, the water reacts with the carbon atoms in the diesel, and the hydrogen generated by the reaction can improve the combustion. As the mass of water increases, the water cooling impact become stronger and stronger, which in turn leads to a decrease in in-cylinder peak pressure and indicated power.
3.3. **Effect on temperature in cylinder**

![Figure 5. In-cylinder temperature curves under different water mass conditions](image)

It can be seen from figure 5 that the in-cylinder peak temperature increases firstly and then decreases as the water mass increases from 5 mg to 100 mg. And it reaches the highest value when the water mass is 40 mg. It can also be seen that the in-cylinder temperature gradually decreases as the water mass increases at the same time in the tail stage of the in-cylinder process. This is because when the water is sprayed into the cylinder at the top dead center, it promotes the fuel-air mixing process and the chemical reaction process of the mixture, then the heat release is greater than the heat absorption, which causes the temperature to rise. However, the heat absorption is greater than the heat release in the tail stage of the combustion process.

3.4. **The effect on emissions**

![Figure 6. Soot and NOx under different water mass conditions](image)

The most difficult point in the control of harmful emissions from diesel engines is soot and nitrogen oxides, and these two emissions have a trade-off relationship, so the future development of diesel engines mainly depends on the control of these two emissions [10].

Shown in Figure 6, when the water mass of is less, the cooling effect is not obvious, the effect on NOx is not obvious, and there is even a tendency to increase. When the water mass is 40 mg, the
combustion promotion effect is the best. At this time, the high temperature environment promotes the production of NOx. As the mass of water continues to increase, the cooling effect on the temperature in the cylinder rises. At this time, the NOx emission gradually decreases.

As for the effect of water spray on Soot, from the Figure 6, with the water mass increases, Soot emissions first decrease and then increase. This is because when water is injected into the top dead center, the water gas reaction and the water gas reaction in the high temperature environment occur. The ionized O and OH will promote combustion, make combustion more complete, and reduce soot emissions [11].

4. Conclusion

Through the numerical simulation, the influence of different water injection mass on diesel engine combustion and emissions is studied, and the main findings of the numerical study can be obtained:

1. Less mass of water injection can promote combustion, shorten the combustion duration, increase the instantaneous heat release rate, and increase the temperature in the cylinder. When the mass of water exceeds 40mg, the main combustion duration increases, and the instantaneous heat release rate and cylinder temperature gradually decrease.

2. Less mass of water injection increase the engine indicated power and in-cylinder peak pressure. As the mass of water exceeds 40mg, the two indicators decrease gradually.

3. Water injection promotes fuel-air mixing process and increases in-cylinder peak temperature as the water mass is small. NOx emissions increase with water mass from 5mg to 40 mg and soot emissions decrease with the water mass from 5mg to 60 mg. With the increase of the water mass, the cooling effect of water becomes stronger, the in-cylinder peak temperature decreases obviously. So, NOx emissions decreases but the soot emissions have a increase.

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