Numerical Simulation of Multiple Injections on the Combustion of Reactivity Distribution in Automotive Engine

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Abstract. To improve the efficiency of the internal combustion engine in a wider range of working conditions, multi-fuel combustion mode has attracted the attention of technicians abroad due to the flexibility to control the activity and concentration stratification of mixture in the cylinder. In this paper, new combustion model was used to analyse the effect of three injections of high-activity fuel in the cylinder on the reactivity stratification. Results showed that the injection strategies of adjusting high-activity fuel, such as early or late injection, the flexible ratio of three injections and injection duration, were able to implement the coupling control of the reactivity and concentration stratification of the mixture.

1. Introduction

Great challenges have been brought into the development of the automotive industry by the increasingly stringent emission regulations, which forced the development of combustion science and technology of internal combustion engines in traditional automobiles.

Homogeneous charge compression ignition (HCCI), which combined with the characteristics of traditional gasoline and diesel engines, can achieve high efficiency of diesel engines and smoke-free emissions of gasoline engines, while the emission of nitrogen oxides is relatively low [1]. However, HCCI combustion mode is dominated by chemical kinetics, the operating conditions are narrow, and combustion is difficult to control. To solve this problem, researchers extended the combustion mode of HCCI to the combustion mode of concentration and active stratified to further expand the range of efficient and clean combustion [2].

In recent years, the working range of high efficiency are expanded by adjusting the inlet temperature, the concentration and composition of the mixture stratification. The high volatility of gasoline is used for stratification in-cylinder, and variable valve is coupled to control the residual gas in the combustion chamber. The low activity of the exhaust gas region and the heating effect of exhaust gas are used to control the ignition and combustion reaction rate of mixture gas. It is very difficult for diesel to achieve high efficiency combustion under all conditions of homogenous charge compression ignition because of its high cetane number and low volatility. Due to the difficulty to volatilize, early injection strategy of diesel will lead into the “wet wall” phenomenon in low pressure environment, while emissions of hydrocarbon and soot will increase because of the fuel dilution [3].
In order to explore the effect of multiple injection on mixture stratification and deepen the understanding of the effect of multiple injection strategy on combustion, new mechanism model of multi-component fuel substitutes for gasoline and diesel was constructed in this paper. The effects of multiple injection strategy on mixture stratification and combustion are analyzed by coupling 3D-CFD fluid code.

2. Construction of combustion simulation model
The chemical kinetics mechanism model of gasoline and diesel surrogates were coupled with KIVA-CFD. The combustion mechanism of gasoline and diesel include n-heptane, toluene, methylcyclohexane, di-isobutene, iso-octane, NOX, and PAH.

The chemical kinetics mechanism at high temperature are from the sub mechanism of TRF and the mechanism of PAH are from Richter [4]. The elementary reactions of methylcyclohexane and di-isobutene in the low and middle temperature stage are from sub-mechanisms [5-6]. This mechanism model concludes 720 reactions and 121 species. The thermodynamic parameters in the model remain unchanged.

In order to improve the computational efficiency of the model, the analysis area is 1/8 of the total combustion chamber volume, with a total of about 20,000 grids. According to the previous experiment and simulation result [7], the boundary conditions for simulation of the three-injection strategy are shown in table 1.

| Table 1. Computational boundary conditions for the three-injection strategy |
|---------------------------------------------------------------|
| **Comparison case** | **SOI1** | **SOI2** | **SOI3** | **SOI4** |
| Total amount of fuel injection(mg/cycle) | 50 | 50 | 50 | 50 |
| Gasoline injection(mg) | 30 | 30 | 30 | 30 |
| Diesel injection(mg) | 20 | 20 | 20 | 20 |
| SOI | -35, -20, -5 °CA ATDC |
| Injection ratio(mg) | 5,5,10 | 5,10,5 | 10,5,5 | 7,7,7 |
| Injection duration (CA) | 3,3,6 | 3,6,3 | 6,3,3 | 4,4,4 |
| EGR ratio | 25(%) |
Comparing the pressure curve and heat release rate of SOI 3, SOI 2 and SOI 1 in Figure1 (a), Results showed that the combustion characteristics do not change linearly according to the growing proportion of the third injection.ignition and combustion started earlier, as showed in the consumption curve of n-heptane and iso-octane in Figure1 (c). Meanwhile, the toluene consumption curve is associated with the ignition sequence of n-heptane, i.e. the toluene consumption of SOI3 started at earliest in Figure2 (d), and the total consumption rate is the fastest in the combustion process.

Figure 2 shows the slice of comparison of the temperature distribution in the cylinder within the three-injection strategy. The concentration distribution of n-heptane (highly active fuel) and iso-octane (low active fuel) are showed in Figures 3 and 4 respectively.

From the analysis on the slices in three groups, SOI4 is the first to ignite and the flame core occurs in the upper part of the combustion chamber pit. The ignition position is neither the pre-mixing zone of iso-octane (low active fuel), nor the root of n-heptane spray (high active fuel), which have high concentration and equivalence, while, the ignition starts at the action zone of mixing and coupling of n-heptane and iso-octane during the third injection.
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The flame propagates along the homogeneous mixing zone of $n$-heptane and iso-octane, which starts from the fire core region to other regions of the cylinder.

After the formation of the ignition core, the combustion sequence of the fuel in cylinder is that the flame diffuses preferentially to the region with higher $n$-heptane concentration and the flame speed is fast due to the higher fuel activity.

After the formation of the ignition core, the combustion sequence of the fuel in cylinder is that the flame diffuses preferentially to the region with higher $n$-heptane concentration and the flame velocity is relatively slow due to the influence of fuel equivalent ratio and activity. The flame diffuses to the whole combustion area in the end. These results proved the conclusion obtained by chemical kinetic analysis that the coupling of cross reactions between fuels can promote the ignition of fuels and accelerate the combustion process of fuels in certain operating conditions.

From the distribution of temperature and fuel concentration in SOI3 and SOI1 in Figure 3, results showed that the stratification of temperature and concentration could be formed with adjusting injection strategy. For instance, temperature stratification gradients in relatively wide range exists in SOI3 fuel combustion, which reflect the effect of active stratification. Due to the higher weight in the third injection of SOI1, the overall temperature of combustion zone is higher, and the temperature gradient formation is not obvious.

![Crank Angle](image)

**Figure 4.** Concentration distribution of iso-octane in three injection strategy

Comparing the temperature and fuel concentration between SOI2 and SOI3, the injection strategies not only affect the formation timing of the fire core, but also affect the flame propagation and fuel consumption. As shown in Figure 4, the fire core of the SOI2 ignition in cylinder is located around the upper part of the pit. The flame propagates along the periphery of the pit in sequence. Meanwhile, the consumption sequence of highly active fuel in SOI2 is progressively upward from the terminal of the fuel spray to the root of the fuel spray. However, the consumption gradually diffused from the mixing zone of low-active fuel and high-active fuel to the high-active region with high equivalence.

In summary, various strategies of injection will cause the differences in activity and concentration stratification, which will lead to the variation of the location of fire core formation, flame propagation mode and combustion temperature distribution. Among three injection strategies, when the weight of first injection is relatively larger, it is easier to form the concentration and active stratification of high active fuel in the cylinder. And the simulation results show that there is considerable effect in three average injection strategy.
4. Conclusion
The effects of injection time and weight on the mixture concentration and stratification are compared in multiple injection strategy, the results are concluded as followed:

1. In multiple injection strategy, the early first injection is beneficial to the formation of mixture concentration and active stratification.

2. The more injection mass at later injection time, the worse effect of concentration and active stratification in cylinder, it will affect the thermal efficiency of combustion. While the concentration and active stratification of SOI2 are better, however, the ignition is latest, which leads to the incomplete combustion and the poor combustion efficiency in cylinder.

3. The coupling control of active stratification and concentration stratification of the mixture can be realized by adjusting the injection strategy of high active fuel, thereby affecting the combustion process.

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