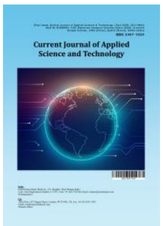

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An Introduction to Automotive Engine Combustion Modeling

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Author's contribution

The sole author designed, analysed, interpreted and prepared the manuscript.

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ABSTRACT

Combustion model is the key basic part of the progress of internal combustion engine technology, and it is a major direction of the future research of internal combustion engine technology. This paper mainly analyzes the advantages and disadvantages of each of the five combustion models, ECFM, ECFM-3Z, SAGE, G-Equation, FGM, CTC and SHELL, and analyzes their respective advantages and disadvantages, as well as the most applicable types of internal combustion engines.

Keywords: Internal combustion engine; combustion modeling; simulation.

1. INTRODUCTION

Internal combustion engine is a kind of heat engine that converts chemical energy into mechanical energy, and its basic principle is to produce high-temperature and high-pressure gases through the mixture of fuel and oxygen combustion, so as to push the piston movement and complete the energy conversion. Therefore, the combustion process of internal combustion

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engine is very critical [1]. The combustion process of internal combustion engine is extremely complex both in space and time distribution, the combustion process is a multi-component and multi-phase chemical reaction process, combustion exothermic will make the fluid transport coefficient increase, the chemical reaction process during combustion is very complex, coupled with the description of the turbulent structure is very difficult to consider the reaction process and spatial distribution of turbulent combustion at the same time is extremely difficult [2].

A combustion model is a mathematical model that describes the combustion process, and its main parameters include mixture concentration, pressure, temperature, and velocity. The accuracy of the combustion model has an important impact on the performance and emissions of internal combustion engines [3], among other things.

At present, internal combustion engine combustion models are mainly divided into two categories: empirical models and semi-empirical models. Each combustion model has its own characteristics and scope of application. The common combustion models are ECFM, ECFM-3Z, SAGE, G-Equation, FGM, CTC, SHELL and so on. In general, the development of combustion model is one of the bases for the progress of internal combustion engine technology, and it is also one of the major directions for the future research of internal combustion engine technology, and this paper mainly introduces five common combustion models.

2. ECFM MODEL

The ECFM (Extended Coherent Flamelet Model) model was developed primarily to describe combustion in direct injection ignition engines and was refined and improved by Colin et al [4] based on the proposed sequential flame model (Coherent Flame Model), which is fully coupled to the spray model and allows for the modeling of stratified combustion that including EGR effects and NO generation, and also predicts detonation [5], the ECFM model relies on the description of the unburned and burned thermochemical conditions of the gas.The ECFM, in order to determine the flame surface density, uses the fuel-to-air equivalence ratio of the fresh gas, the composition (including residual gases), and the temperatures in the vicinity of the flame, and the resulting flame surface densities are used to characterize large-scale burned and unburned stratification . Based on the ECFM model, the ECFM-3Z model was further developed, with 3Z denoting three zones, i.e., a fuel-only zone, an air-only zone and including possible exhaust gases, and a mixing zone in which fuel and air coexist, and the ECFM-3Z model can be used to compute both premixed and non-premixed flames.

For turbulent combustion, ECFM calculates the average reaction rate and the fuel switching is done using a two-step reaction mechanism:

$$C_\alpha \mathrm{H}_\beta \mathrm{O}_\zeta + \left(\alpha + \frac{\beta}{4} - \frac{\zeta}{2}\right) O_2 \rightarrow \alpha \mathrm{CO}_2 + \frac{\beta}{2} \mathrm{H}_2\mathrm{O}$$

$$C_\alpha \mathrm{H}_\beta O_\zeta + \left(\frac{\alpha}{2} - \frac{\zeta}{2}\right) O_2 \rightarrow \alpha \mathrm{CO} + \frac{\beta}{2} \mathrm{H}_2$$

where α, β and ζ are the atomic numbers of C, H and O, respectively.

3. SAGE MODEL

The SAGE model is a combustion model based on a detailed chemical reaction dynamics solver [6], which is the most central combustion model in the CONVERGE software.SAGE calculations are performed using chemical reaction mechanisms in CHEMKIN format.The model can simulate turbulent combustion of any fuel as long as the chemical reaction mechanisms are available.The prediction of detonation, self-fire, and emissions is more accurate than the traditional empirical and semi empirical models. If the reaction mechanism is provided with sufficient accuracy, then SAGE will be able to solve for very accurate results.

When using the SAGE combustion model, the quality control equations for the computational unit are:

$$\frac{d[X_m]}{dt} = \dot{\omega}_m$$

The energy control equation is:

$$\frac{dT}{dt} = \frac{V\frac{dP}{dt} - \sum_m (\bar{h}_m \dot{\omega}_m)}{\sum_m ([X_m]\bar{c}_{p,m})}$$

For fixed-volume combustion, the energy control equation is:

$$\frac{dT}{dt} = \frac{\frac{\dot{Q}}{V} - \sum_m(\bar{h}_m\dot{\omega}_m)}{\sum_m([X_m]\bar{c}_{p,m})}$$

In the above three equations, Xm is the molar concentration of component m, denotes the exothermic rate, V denotes the volume, T denotes the temperature, p denotes the pressure, denotes the molar specific enthalpy of component m, and denotes the molar constant pressure specific heat capacity of component m.

4. G-EQUATION MODEL

The G-Equation model, or G-equation model, is a combustion model based on the Level-set method. The model can be used to simulate premixed combustion and can better reflect the flame propagation development in the cylinder. The G-equation describes the chemical reaction between the region inside the flame surface and the region outside the flame surface with the flame surface as the boundary, and the calculation solves the propagation development of turbulent flame through the flame surface without solving the flow field region inside the flame surface [7-8]. However, at large variations in the mixture equivalence ratio, the G-equation prediction of laminar flame propagation differs significantly from the experimental values [9-10]. In CONVERGE, which can be used alone or in conjunction with SAGE, the G-equation when used alone does not need to solve the detailed chemical reaction mechanism and thus is faster than the SAGE model, and the G-equation when used in conjunction with SAGE needs to solve the detailed chemical reaction mechanism but is computationally faster than the SAGE model alone. However, the G-equation requires more parameters to be calibrated when used, which requires a higher level of experience and knowledge from the user.

5. FGM MODEL

The FGM (Flamelet Generated Manifold) model is a simplified generalized combustion model [11] that reduces the reaction mechanism to two scalars. The model captures kinetic phenomena such as ignition, flame extinguishing and flame quenching and provides accurate flame dynamics, fuel effects and emissions for both premixed and diffusion combustion.The FGM model has a high prediction accuracy in both the high and low temperature regions and allows for natural diffusion of premixed combustion to non-premixed combustion models.

The FGM model decomposes the complex chemical reaction process into global variables that can characterize the complex chemical reaction, which greatly reduces the amount of computation while taking into account the detailed chemical reaction mechanism [12]. The FGM can calculate the detailed reaction mechanism and transfer the results in the form of a table to the three-dimensional CFD software for the simulation of combustion process, and this kind of combustion computation can reduce the computation time significantly.

The principle is that before the 3D calculation, the chemical reaction mechanism is first calculated in one dimension and made into a table, and the results of the one-dimensional calculation are interpolated into the 3D calculation, which makes FGM easy to use the chemical kinetic reaction mechanism containing thousands of steps, which is almost impossible to realize in the SAGE combustion model, however, FGM is currently applicable to fewer models, mainly because of the difficulty of simulating the gas exchange process.

6. SUMMARIZE

An internal combustion engine combustion model is a mathematical model used to describe the combustion process of an internal combustion engine, which mainly involves fuel injection, mixing, ignition, combustion, and emissions. The development of combustion models for internal combustion engines has important theoretical and practical significance, which can help engineers better understand and optimize the combustion process of internal combustion engines, thus improving the performance and efficiency of internal combustion engines [13].

In general, the main advantages of combustion modeling for internal combustion engines include the following:

1. Internal combustion engine combustion modeling can predict the nature and characteristics of combustion and emissions. Parameters such as combustion efficiency, types of combustion products and their contents, temperature and pressure can be predicted by the model for a variety of different scenarios, as well as emission

properties such as NOx and particulate content.
2. Internal combustion engine design and control can be optimized. Using combustion models, the effects of various factors on the combustion process and emissions can be investigated, thus helping to optimize the design and operational control of internal combustion engines to improve their efficiency and reduce pollution [14].
3. Combustion modeling can improve the design and analysis capabilities of internal combustion engine engineers by helping them to better understand the thermodynamic, hydrodynamic, and chemical reaction aspects of the internal combustion engine and thus better design and analysis.

Although combustion modeling for internal combustion engines has many advantages, there are also some challenges and limitations:

1. The combustion process of an internal combustion engine is too complex. The combustion process in an internal combustion engine involves a variety of physical and chemical mechanisms, and it is very difficult to construct an accurate mathematical model.
2. The model requires high computational resources and data input. The establishment and operation of the model requires massive data and computational power, which requires a lot of time and computational resources.
3. The accuracy and validity of the model depends on the accuracy and sufficiency of experimental data. Environmental, fuel and other factors in the actual combustion process may also affect the accuracy and reliability of the model.

In conclusion, combustion modeling for internal combustion engines is a very complex and challenging study that still requires further research and development. However, the development of combustion modeling can provide internal combustion engine engineers with new ideas for thinking and analyzing combustion problems and promote the development and innovation of internal combustion engines.

COMPETING INTERESTS

Author has declared that no competing interests exist.

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