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Combustion modeling in RCCI engines with a hybrid characteristic time combustion and closed reactor model

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HIGHLIGHTS

- A hybrid model based on the classical CTC model and CHEMKIN model was proposed.
- The proposed hybrid model is able to model RCCI combustion with detailed chemistry.
- The hybrid model is robust and efficient for RCCI combustion simulations.

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ABSTRACT

This study proposed a hybrid model consisting of a characteristic time combustion (CTC) model and a closed reactor model for the combustion modelling with detailed chemistry in RCCI engines. In the light of the basic idea of the CTC model of achieving chemical equilibrium in high temperature, this hybrid model uses the CTC model to solve the species conversion and heat release in the diffusion flame. Except for the diffusion flame, the auto-ignition in RCCI combustion is computed by a closed reactor model with the CHEMKIN library by assuming that the computational cells are closed reactors. The border of the transition between the CTC model and closed reactor model is determined by two criteria, a critical temperature and a critical Damköhler number. On the formulation of this hybrid model, emphasis is placed on coupling detailed chemistry into this hybrid model. A CEQ solver for species equilibrium calculations at certain temperature, pressure was embedded with CTC for detailed chemistry calculation. Then this combustion model was integrated with the CFD framework KIVA4 and the chemical library CHEMKIN-II and validated in a RCCI engine. The predicted in-cylinder pressure and heat release rate (HRR) show a good consistency with the data from the experiment and better accuracy than that computed from the sole closed reactor model. More importantly, it is observed that this model could save computational time compared with closed reactor model due to less stiff ordinary differential equations (ODEs) computation. A sensitivity analysis of the critical temperature and critical Damköhler number was conducted to demonstrate the effect of these two parameters in the current model.

1. Introduction

Internal combustion engines are basically classified into compression ignition (CI) engines and spark ignition (SI) engines, both of which have their pros and cons [1]. CI engines have been widely applied in industry such as in ships and trucks because of its high thermal efficiency. The high thermal efficiency of CI engine is attributed to its instinct features of high compression ratio and combustion organization type. However, because of these features, the high temperature and fuel rich zones lead to higher detrimental emissions such as NOx and particulate matter (PM). In contrast, SI engines which employ a spark plug to ignite the premixed fuel/air mixture and organize combustion by flame propagation show lower thermal efficiency but better emission performance. Therefore, efforts have been devoted for proposing advanced engine combustion modes for reducing emissions while maintaining high efficiency. Generally, most of these advanced combustion modes are in an effort to aggregate the advantages of CI and SI engines and at the same time, avoid their disadvantages.

HCCI is one of the first proposed types of advanced combustion modes in engines, which has drawn tremendous attention of engine researchers due to its ideal combustion and emission performance. The fundamental idea of HCCI is to combine the advantages of SI and DICI

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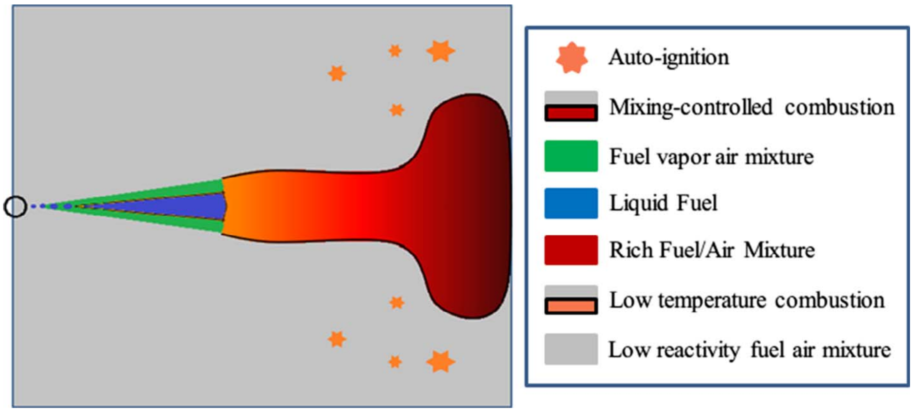

Fig. 1. Schematic figure of RCCI combustion. Different colors mean different combustion zones. The mixing controlled diffusion flame are calculated by the CTC model while auto-ignition are computed by the closed reactor model in the current hybrid model.

engines while to avoid their disadvantages, as SI engine features low soot emission but low thermal efficiency, DICI engine shows high thermal efficiency but high level NOx-soot trade-off relation [2]. In HCCI, the combustion occurs at nearly constant volume and homogeneously. As a result, its low combustion temperature and homogenously lean combustion lead to extremely low emission and a good efficiency. However, because of no direct control strategy of HCCI combustion phasing (the ignition is primarily determined by the fuel/air mixture properties and chemical kinetics), the major challenges in HCCI are the lack of proper combustion phasing control and its undesirably excessive pressure rise rates [2].

To find the best fuels in HCCI engines, Bessonette et al. [3] experimentally investigated the engine performance with different fuel blends for HCCI operations. They concluded that the best fuel should have the auto-ignition ability between diesel and gasoline. Subsequently, motivated by this result, dual-fuel type advanced combustion mode, PCCI, was proposed. Both modelling and experimental investigation suggest that PCCI presents better combustion controllability than HCCI since a strategy of different blending fuel ratios could be used to control the ignition timing in PCCI [4–6]. To extend the combustion controllability more thus engine operating loads, RCCI was proposed by Kokjohn et al. [7]. The distinct fuel intake manner in RCCI (port fuel injection with low reactivity fuel and direct injection with high reactivity fuel) is able to form fuel stratification in the combustion chamber, suppressing the pressure rise rate (PPR) and broaden the operation loads [6–9]. However, as a variant of HCCI and PCCI concept, RCCI, in nature, still has engine knocking tendency especially at high engine loads. In addition, the fuel diversity in RCCI engine makes fuel design and management a necessity. Due to high cost and time-consuming issues in experiment, calibration and fuel design for RCCI engine in combustion modelling would be an effective and efficient way.

Since RCCI combustion involves low-temperature combustion, auto-ignition and partially premixed combustion, rendering substantial complexity for combustion modelling, different researchers proposed RCCI combustion models and integrated them into CFD framework for RCCI engine simulations.

Kong et al. [10] applied a multi-dimensional CFD software KIVA3-V coupled with CHEMKIN library [11] to solve the chemistry kinetics for HCCI modelling. By taking each cell in the computational domain as a closed reactor, ODEs are solved under a constant volume condition. It was proved that this way showed robust prediction in HCCI modelling researches and widely adopted by the following researchers. Because RCCI is a variant of HCCI, this method has been also applied for RCCI engine simulation and has showed good predictability [7,12–15]. In fact, considering that in the KIVA framework, the transport and chemical source terms are solved separately [16], this method has also been used for conventional diesel engine simulations in which the combustion is organized by diffusion flame. However, its computational price is high especially for detailed mechanisms with large size and most of the computational time are consumed by solving the ODEs in CHEMKIN. Moreover, multiple combustion modes including mixing controlled flame and auto-ignition may co-exist in RCCI combustion, an effective method to model the diffusion flame and treat the border between diffusion flame and auto-ignition is important. Thus, efficient and robust methods for integrating the combustion chemistry in RCCI engine simulation are desirable.

This study proposed a CTC model based on the original CTC model for DICI combustion [17] and coupled it with a closed reactor model for RCCI combustion simulation. It is able to solve the detailed chemical kinetics in RCCI combustion and show favorable computational price and accuracy than the commonly used sole closed reactor model with CHEMKIN. This hybrid model was integrated into the KIVA4 codes and validated by comparing with the experimental data from a RCCI engine fueled with gasoline/diesel. It is observed that this model can give reasonable combustion characteristic compared with the measured data. A better accuracy than the sole closed reactor model with CHEMKIN can be found as well. More importantly, an evident computational overhead reduction of the current model can be observed than the closed reactor model with CHEMKIN.

2. Methodology

In conventional simulations of diesel diffusion flame, for the cells lower than a critical temperature T_c, all the chemistry and internal energy change in these cells will be treated by auto-ignition models (SHELL in the classical SHELL-CTC model with generic chemistry; closed reactor model in CHEMKIN with detailed chemistry). In the existing RCCI engine combustion models, all the auto-ignition and diffusion flame are handled by the closed reactor model with the CHEMKIN library without considering the sub-grid turbulence-chemistry interaction. To illustrate the current model in a direct way, a schematic figure is shown as Fig. 1. Compared with the figure of quasi-steady diesel combustion plume as presented from Sandia National Laboratories [18], it is observed that due to the low temperature, the spray vapor transport to the end of the combustion chamber with slight first-stage low temperature combustion. At the end of the spray tip, the mixing between the vapor and the air is still controlling the combustion. This study proposed a hybrid model with computing the auto-ignition cells by closed reactor model with CHEMKIN and calculating the mixing controlled combustion by CTC, as shown in Fig. 1.

Nevertheless, the classical CTC model was formulated with a generic chemical model and is not capable of dealing with detailed chemistry. In the following sections, the formulation of CTC with detailed chemistry is presented; a brief introduction of the closed reactor model treated by CHEMKIN library is then described; the solution algorithm and the couple of these two models are finally introduced.