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Dual-fuel RCCI engine combustion modeling with detailed chemistry considering flame propagation in partially premixed combustion

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HIGHLIGHTS

- A flame propagation model was proposed and validated for RCCI combustion modeling.
- The heat release in the flame front is solved with detailed chemistry with a new formulation.
- This model together with CHEMKIN improves the RCCI modeling accuracy.

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ABSTRACT

In the two limits of a well-mixed charge (e.g. homogenous charge compression ignition (HCCI)) engine, and a well separated charge (e.g. conventional diesel combustion (CDC)) engine, the CHEMKIN coupled computational fluid dynamics (CFD) codes approach has been proved to work well in predicting both chemistry controlled combustion and mixing controlled combustion. In this study, it is shown that for some certain cases in the new combustion mode reactivity controlled compression ignition (RCCI) engine where flame propagation exists, the CHEMKIN approach could fail to predict the combustion characteristics. To extend the capability of the existing CHEMKIN models in combustion, a flame propagation model (FPM) accounting for combustion in partially premixed mixtures was proposed and coupled into the CFD framework KIVA4. In this FPM model, the turbulent flame speed was calculated and the heat release and species conversion rate in the turbulent flame brush was solved with detailed chemical kinetics. A NOx sub-mechanism and a nine-step phenomenological soot model were also coupled into the current integrated model for emission prediction. This model was validated in 3 different dual-fuel experimental engines by comparing the in-cylinder pressure, heat release rate (HRR), NOx emissions and soot emissions. The CHEMKIN and CHEMKIN-FPM were also compared in terms of their capability of predicting the combustion in different combustion regimes. The results show that under certain operating conditions when CHEMKIN failed in the combustion prediction, the current CHEMKIN-FPM shows a superior ability in predicting combustion characteristics.

1. Introduction

The new combustion strategies (e.g. HCCI, RCCI) which could be lumped as low temperature combustion (LTC) have been proved to yield low emission and high thermal efficiency in compression ignition (CI) engines [1]. However, their high engine knocking tendency and high unburnt hydrocarbon emissions are still major obstacles to apply these new combustion modes commercially. Thus, we need in-depth understanding of the combustion process to optimize the fuel combinations and engine management. To get deep insight on the combustion processes in these engines, robust and computationally efficient CFD with specialized combustion models is a crucial tool. However, the broad spectrum of combustion regimes in new combustion mode engines makes the combustion modeling in these engines very challenging [2].

Generally in CI engines under different operating conditions, combustion regimes could be classified into three scenarios: highly stratified combustion (e.g. conventional diesel combustion (CDC)), partially premixed combustion (e.g. PCCI, RCCI) and homogenous premixed combustion (e.g. HCCI) [3]. Considering the ways of complex chemical-turbulence interactions in these three scenarios, we can also classify them in this way: mixing controlled combustion, multimode combustion and kinetically controlled combustion.

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In a mixing controlled combustion (e.g. CDC) engine, the chemistry is much faster than mixing. Hence, typically equilibrium chemistry models are used to simulate the combustion process since the chemical reactions can reach equilibrium rapidly compared to the mixing time. The characteristic time-scale combustion (CTC) model is a classical model in this category [4,5]. To predict CDC combustion, a CTC model should be combined with other models (e.g. SHELL model) since in low temperature range, chemistry is not fast enough to be near equilibrium. In kinetically controlled combustion (HCCI or HCCI-like engine), the chemistry is much slower than mixing (in an ideal HCCI engine, the mixing time-scale is assumed to be zero). Hence, in this homogeneous premixed combustion, chemical kinetics plays the most important role. Models in this category differ from each other because of different chemical mechanisms used, that is, either a global one-step mechanism, generic mechanism for ignition or a detailed/skeletal mechanism to be used. For example, a one-step global Arrhenius formulation is used in the original CFD code KIVA [6] combustion chemistry. It is not accurate since it ignores chemical kinetic details in the combustion. One classical generic mechanism model is the SHELL model [7], which is mainly used for auto-ignition prediction in CI engines. The detailed mechanism model is based on a detailed mechanism chemistry solver such as CHEMKIN [8]. It could be used over the entire phase of HCCI combustion and give accurate species conversion rates and thus energy and temperature prediction, but it suffers from expensive computational cost.

The most complex combustion is partially premixed combustion, in which not only auto-ignition but also flame propagation should be accounted for. Flame propagations are not usually considered in CI engines because unlike the SI engine in which its ignition was triggered by a spark and the combustion was organized by flame propagation, the combustion in a CI engine is initiated by auto-ignition and then controlled by the fuel and oxidizer mixing. However, in the newly-proposed combustion modes such as RCCI, the high reactivity direct-injected fuel could play a role of spark and cause several flame propagations among the low reactivity fuel atmosphere [3]. Under this situation, no flame propagation consideration in the combustion model could cause unacceptable errors under certain operating conditions in RCCI engines.

Even though a lot of numerical investigations have been conducted to study the optimal operating conditions and fuel combinations in these new combustion mode engines [9–12], the flame propagation was ignored in these studies. To consider the flame propagation in the partial premixed combustion, different combustion models have been proposed. Based on the conditional moment closure (CMC) model [13], which solves the combustion and mixing by the conditioned mass fraction, the flame propagation was calculated by adding one reaction progress dimension in the computation in [14]. However, the capability of dealing with flame propagation even exasperates the CPU computational overhead of the CMC model. In addition, Colin et al. [15] proposed an extended coherent flame 3 zones (ECFM3Z) model to simulate the different flame types in the engines. However, it only includes generic chemistry in, thereby not able to calculate detailed chemistry. The level set based flame propagation model G-equation coupled with the SHELL and CTC models, and the G-equation coupled with CHEMKIN was proposed in [3,16], which gives acceptable prediction of RCCI engines under wide operating conditions. However, due to the integration of additive differentiate equations, expensive computation overhead is also encountered in this G-equation model.

Hence, the objective of this study is to develop a unified combustion model coupled with CFD to calculate the diffusion flame, auto-ignition with the consideration of flame propagation in RCCI engines with detailed chemistry. With a new CFD framework KIVA4 which is able to compute unstructured mesh [17] and with a Lagrangian particle based model [18], this study proposed a Lagragian marker particle based flame propagation model to predict the combustion and flame propagation in the RCCI partially premixed combustion. The result shows that this model coupled with CHEMKIN could give better combustion simulation in wide-operating dual fuel engines.

2. Model formulation

2.1. Lagrangian markers

Zero-mass imaginary Lagrangian markers to track flame front position has been used in SI engine ignition model and gasoline direct injection combustion models [18,19]. A certain number of particles which are initially assumed to be distributed uniformly and to describe a sphere will be convected by the in-cylinder gas due to the effect of chemical sources and the flow field. Once one point in the computational domain was ignited (spark ignition in SI or auto-ignition by the high-reactivity fuel in this study), and the physical-chemical conditions allow a self-sustained flame front to develop, the flame front will be tracked and described by the particles. In this study, the computational cell which contains these particles will be separately modeled for a premixed flame. The heat release of other computational cells due to diffusion flame or premixed flame will be modeled by CHEMKIN. The details about the chemistry and combustion modeling in this FPM model and in the CHEMKIN will be described in the following sections.

2.2. CHEMKIN

In the current study, except for the flame front existing cells (containing particles), the chemistry is solved by a chemistry solver – CHEMKIN. The convection and diffusion transport between cells are modeled by the RNG $\kappa-\varepsilon$ turbulence model [20]. The chemical process in a cell is considered as a closed system, in which the sub-grid scale turbulence-chemistry interaction was not considered. The basic principle in CHEMKIN is that the change of each species in one closed computational cell was given by

$$\frac{dY_n}{dt} = v \cdot \dot{\omega}_n \cdot MW_n \tag{1}$$

where v is the specific volume, Y_n is the mass fraction of species n, MW_n is the molecular weight. Within a certain time step, $\dot{\omega}_n$ is the production rate at a given temperature and molar concentration. Hence, if *nsp* is the number of species in the chemical mechanism, a set of ordinary differentiate equations (ODEs) with the number of *nsp* equations will be built and then solved by DVODE [21]. In this way, the energy governing equation can be obtained as

$$\Delta E + v\sum_{n=1}^{nsp} e_n \dot{\omega}_n MW_n = 0 \tag{2}$$

where ΔE is the change of energy in the system due to the chemical reactions, e_n is the internal energy species n. With the newly updated species concentration by CHEMKIN, KIVA4 will solve the energy conservation equation and update the temperature and other thermodynamic data in the system.

Using CHEMKIN to model the combustion in the two limits from chemistry-controlled combustion to mixing-controlled combustion has been proved to work well [22]. However, as pointed in the introduction, flame propagation in premixed or partial premixed combustion cannot be modeled by CHEMKIN due to closed reactor assumption is not valid under these scenarios. For example, the sole CHEMKIN model without flame propagation has been proved to show underestimated in-cylinder pressure in the flame propagation dominant engine simulations [3,16].