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Full Length Article

Numerical simulation of premixed combustion using the modified dynamic thickened flame model coupled with multi-step reaction mechanism

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ABSTRACT

Thickened flame (TF) model is one of the effective methods to resolve the flame front in turbulent premixed combustion modeling. The multi-step reaction mechanism is becoming increasingly important for combustion simulations such as pollutant formation, ignition and extinction. The effect of TF model on flame structures when coupling with multi-step reaction mechanism was investigated. The simulation results show that, no matter in laminar or turbulent condition, the global TF model coupling with multi-step reaction mechanism results in an incomplete combustion, which is mainly due to the enhanced species diffusion. Although Durand and Polifke's dynamic thickened flame (DTF) sensor performs well for predicting laminar flame structure when coupling with multi-step reaction mechanism, it underestimates the effective thickening factor. In turbulent premixed flame simulation, the underestimated thickening factor leads to a faster local fuel consumption speed because of the over-predicted sub-grid flame wrinkling factor. A modified DTF sensor suitable for multi-step reaction mechanism is proposed. This sensor using the hyperbolic tangent function of progress variable to calculate thickening factor dynamically. It ensures that both the preheated and reaction zones are thickened effectively. The sub-grid wrinkling factor is hence estimated corresponding to the calculated flame thickness. Results of 1D laminar and 3D turbulent flame show that this method performs well for predicting both burned gas temperature and species concentration in burnt gas, which is important for predicting emissions.

1. Introduction

The investigation of turbulent combustion is of great importance for many industrial applications such as internal combustion engines, aero-engines and gas turbine combustors. Meanwhile, turbulent premixed combustion is more challenging due to the effects of turbulence-flame interaction, which poses more complex problems than it does in non-premixed combustion because of the wrinkled flame front has the feature of propagating normal to itself [1]. Numerical simulation has become an extremely valuable tool for predicting turbulent reacting flows [2]. However, in practical numerical calculation of premixed flames, especially for three-dimensional turbulent cases, the flame thickness (0.1–1 mm) is generally smaller than the computational grid size. Typically, the grid size is about ten-micrometer order. The computational cost in such fine mesh size is far beyond the capacity of general workstation. In purely geometrical approaches, besides using a flame front tracking technique (G equation or level-set) [3–5] or a filter larger than the computational mesh size [6], thickened flame (TF) model is one of the effective methods [7]. Both the geometrical approaches and statistical models have been reviewed by Gicquel et al. [8].

The basic idea of TF model is assuming that there is a flame having the same fuel consumption speed but thicker than the real one. The chemical reaction source term can be calculated using an Arrhenius formulation. Initially, TF model could not be applied in Large Eddy Simulation (LES) because the interactions between thickened flame and turbulence are changed and the lost flame surface must be modeled. Following the lines of Meneveau and Poinsot [9], Colin et al. [7] proposed an efficiency function based on the linear theory to model the sub-grid flame wrinkling in LES. Then a power-law flame wrinkling model was proposed by Charlette et al. [10,11] according to fractal theory. The dynamic methods for determining model parameters have been developed by EM2C [12–14]. More recently, a correction of Charlette et al.'s efficiency functions [10,11] that accounts for the effect of Lewis number was further developed [15]. Some other sub-grid flame model and its verification was conducted in [16–19]. Although TF approach has many advantages [7], the thickened process changes the transport properties of burned and unburned mixture at the same time. To overcome this problem, the dynamic thickened flame (DTF)

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model was proposed by Legier et al. [20]. The DTF model is able to compute the thickening factor dynamically in space and time. Note that the term "dynamic" introduced by Legier et al. [20] is different from the dynamic model in the LES where the parameters of sub-grid combustion model are adjusted dynamically based on the resolved fields [11–14].

In order to achieve a compromise between chemistry details and computational costs, one or two step reaction mechanism coupled with thickened flame model were implemented to simulate turbulent combustion by many researchers [12,20–23]. However, combustion may occur in various regimes simultaneously in a real combustion configuration. It is not easy to describe this complicated phenomenon using simple reaction mechanisms, since they are fitted to reproduce only global flame quantities, such as flame speed and thickness and may not respond accurately to the changes of surrounding physical conditions. Moreover, global mechanisms have some inherent defects in predicting some realistic problems, such as ignition, quenching and pollutant formation. The multi-step reaction mechanism reduced from the detailed mechanism could shows a good performance for many problems. Meanwhile, the computational cost is acceptable for now and decades to come because the multi-step reaction mechanism comprise only ten to twenty components for small-molecular fuels and increase slightly for heavier fuels [24]. Jaravel's work [25] has shown the potential of TF model coupled with multi-step reaction mechanism in predicting emissions. Besides using the global, multi-step or detailed mechanism to describe the chemical reaction directly, tabulated chemistry like FGM [26], FPI [27] and REDIM [28] et al. are very promising methods which have been reviewed by Oijen et al. [29]. In addition, TF model can also be coupled with the tabulated premixed flame chemistry [30–32].

Although thickened flame model can be extended to multi-step reaction mechanism in theory [7], some issues may occur. There are more length and time scales within multi-step reaction mechanism, which have to be resolved on the numerical grid. Therefore, refined numerical grids or larger thickening factor may be required to resolve the intermediate species. Meanwhile, the amounts of intermediate species are increased for the thickening process. The objective of this study is to investigate the effect of TF models on flame structure when coupling with multi-step reaction mechanisms. Both laminar and turbulent combustion were simulated. The rest of the paper is organized as follows. Section 2 presents the combustion and chemistry model and numerical details. In Section 3, the 1D laminar flame structures were compared and a modified DTF sensor was proposed. Then the turbulent flame simulation results obtained by global TF model and the modified DTF sensor were compared in Section 4. Lastly, Section 5 concludes the paper.

2. Numerical model

2.1. The thickened flame model

The basic idea of TF model was originally proposed by Butler and O'Rourke [33]. By solving the three-dimensional balance equations for instantaneous species mass fraction Y_k, Eq. (1), an artificial thickened flame propagation on a coarse grid may be achieved if the thickening factor F is large enough.

$$\frac{\partial \rho Y_k}{\partial t} + \nabla\cdot(\rho \boldsymbol{u} Y_k) = \nabla\cdot(\rho F D_k \nabla Y_k) + \frac{\dot{\omega}_k(Q)}{F} \tag{1}$$

where ρ is the density, $\boldsymbol{u}$ is the velocity vector, $\dot{\omega}_k(Q)$ is the chemical source term of species k. Q denotes any quantity used for calculating the chemical source term. D_k is the mixture-averaged molecular diffusion coefficient of species, $D_k = \frac{1-x_k}{\sum_{j\neq k}^{N}(x_j / D_{kj})}$, where x_k is the mole fraction of species k, D_{kj} is the binary diffusion coefficient of species j and k calculated using Chapman-Enskog expression.

In LES, Eq. (1) is recast as:

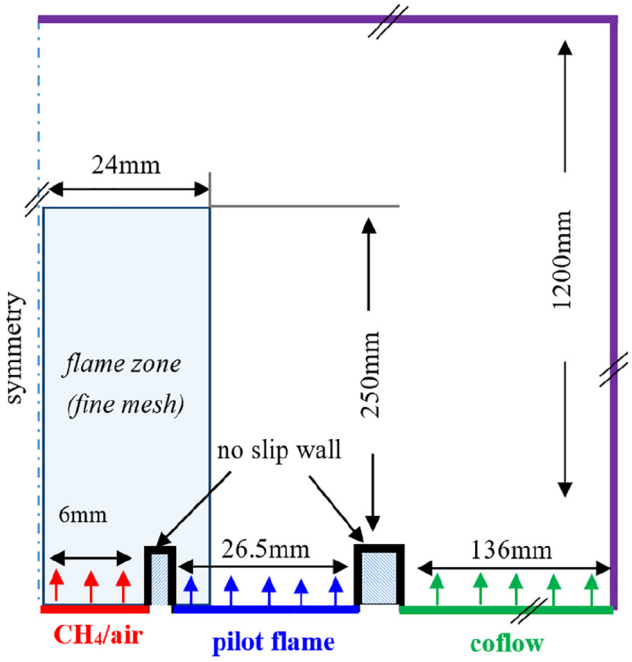

Fig. 1. Half of the numerical domain.

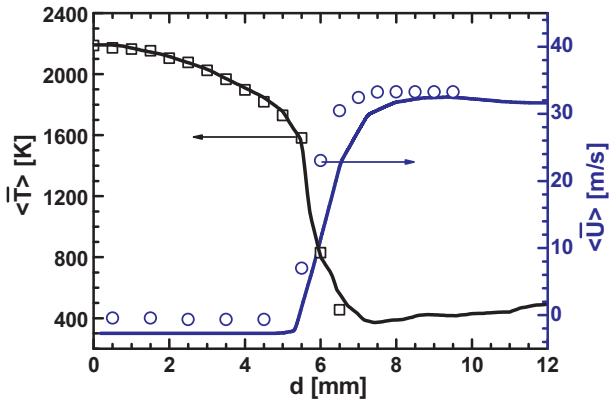

Fig. 2. Mean initial axial velocity and temperature. Symbols: experiment; Lines: simulation results using modified DTF sensor (mentioned in Section 3.2).

$$\frac{\partial \overline{\rho}\widetilde{Y}_k}{\partial t} + \nabla\cdot(\overline{\rho}\overline{u}\widetilde{Y}_k) = \nabla\cdot(\overline{\rho}\Xi_\Delta F D_k \nabla \widetilde{Y}_k) + \frac{\Xi_\Delta \dot{\omega}_k(\widetilde{Q})}{F} \tag{2}$$

where $\overline{Q}$ and $\widetilde{Q}$ denotes filtered and mass-weighted filtered quantities, respectively, ($\overline{\rho}\widetilde{Q} = \overline{\rho}Q$). Ξ_Δ is the sub-grid scale wrinkling factor.

To dynamically determine the thickening factor in space and time, the flame sensor $\Omega = 16[c(1-c)]^2$ suggested by Durand and Polifke [34] is used. The progress variable $c = (Y^u_{ch4} - \widetilde{Y}_{ch4})/Y^u_{ch4} - Y^b_{ch4}$, where Y^u_{ch4} and Y^b_{ch4} is the CH_4 mass fraction in unburnt and burnt mixture respectively, with 1 and 0 representing burned and fresh gas respectively. The dynamic thickening factor is determined as $F = 1 + (F_{max} - 1)\Omega$.

2.2. The power-law flame-wrinkling model

The power-law flame-wrinkling model proposed by Charlette et al. [10,11] is used here to estimate the lost sub-grid scale flame surface due to the thickening process. The original expression has been adjusted by EM2C [12–14] to limit the maximum of the wrinkling factor Ξ_Δ based on fractal theory: