



Full Length Article

Large eddy simulation of turbulent combustion by a dynamic second-order moment closure model



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HIGHLIGHTS

- A dynamic second-order moment closure combustion model is developed.
- The model is applicable for all combustion regimes.
- Two experimental flames are predicted by this model.

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ABSTRACT

A dynamic second-order moment closure model is developed for turbulent combustion in the form of large eddy simulation. The filtered reaction rate is directly closed in the form of Arrhenius law, and the whole temperature exponential function is treated as a single variable to avoid the traditional Taylor series expansion. The sub-grid unresolved reaction rate is modeled with a second-order moment closure model. All the coefficients in the sub-grid models are evaluated by the dynamic procedures. To validate and evaluate this model, a priori validation using a DNS database and posteriori validation by LES of the Sandia piloted jet flame (Flame D) and the Sydney bluff-body swirling flame (SM1) are performed. The results demonstrate that the dynamic second-order moment closure model coupled with LES is able to reasonably predict turbulent combustion even with simple chemistry, and has potential to predict more complex combustion with detailed reaction mechanism and acceptable computational cost.

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1. Introduction

In most industrial equipment, such as coal-fired furnaces, combustion gas turbines and internal combustion engines, turbulent combustion has been encountered [1]. Predictive capacity for turbulent combustion is thus of paramount importance to those applications in which experimental measurements are difficult, limited and even not accessible. In the recent years, much more attention has been paid to large eddy simulation (LES) of turbulent combustion, since LES has been demonstrated to be able to provide more accurate information and useful qualitative understanding of turbulent combustion phenomena, compared to the traditional ways on the basis of the Reynolds Averaged Navier-Stokes [2–4].

The most challenging issue in turbulence combustion modeling is proper treatment of the multi-scale coupling process of chemical reaction and molecular diffusion. Many of the current approaches

could be categorized as PDF-like or flamelet-like based on how to deal with the coupling between chemical reactions and molecular diffusion [5]. The steady flamelet model (SFM) put forward by Peters [6,7] is one of the flamelet-like models. It is relatively simple and has been improved in different methods, such as the unsteady flamelet model (UFM) [8], the flamelet/progress variable model (FPV) [9] and so on. The advantage of the flamelet model is that detailed chemistry can be considered with reasonable computational cost. However, it was basically formulated and developed separately for premixed flames and non-premixed flames. The probability density function (PDF) models have been well developed for combustion by Pope [10,11]. Some PDF-like models have also been developed such as the multiple mapping conditioning (MMC) [12] and the one-dimensional turbulence (ODT) model [13]. One advantage of the PDF method lies in the fact that it can be applied to all combustion regimes, even challenging flames, like extinction, ignition flames and bluff-body swirling flames [14]. But the relatively simple mixing models and high computational cost are still the weaknesses in the current application of PDF models.

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However, it has been demonstrated that both non-premixed flames and premixed flames may coexist in either traditionally defined premixed turbulent combustion or non-premixed combustion because of turbulence-chemistry interactions [15]. To predict both premixed and non-premixed flames, Knudsen and Pitsch [16] proposed a multi-regime flamelet model to consider different combustion regimes. This model was further extended to study IC engines by Mittal et al. [17]. In this multi-regime flamelet model, models for both premixed and non-premixed flames are combined to account for turbulent combustion with a regime indicator.

As we mentioned above, the current combustion models, which could be accounted for different combustion regimes, are very difficult for a freshman in CFD to make use of. In this paper, a dynamic second-order moment closure (DSMC) model is developed to account for not only premixed but also non-premixed combustion in the context of large eddy simulation. Also for a beginner in LES of turbulent combustion, there is no difficulty to know well about the model. The chemical reaction rate term is directly closed in the form of Arrhenius law, while the whole temperature exponential function is treated as a variable so that the Taylor series expansion is avoided. The coefficients in the sub-grid model are determined by dynamic procedures. This model is then validated and evaluated by a priori validation using a direct numerical simulation (DNS) database and posteriori validation by LES of the Sandia piloted flame (Flame D) and the Sydney bluff-body swirling flame (SM1), as these flames have been widely selected as benchmark tests to validate various combustion models

2. Governing equations

For low-Mach number and variable-density flow, the filtering continuity, momentum, species and energy equations for LES of turbulent combustion read [18]:

$$\frac{\partial(\bar{\rho})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j)}{\partial x_j} = 0, \quad (1)$$

$$\frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j} = -\frac{\partial\bar{p}}{\partial x_i} + \frac{\partial\bar{\sigma}_{ij}}{\partial x_j} - \frac{\partial}{\partial x_j} [\bar{\rho}(\tilde{u}_i\tilde{u}_j - \tilde{u}_i\tilde{u}_j)], \quad (2)$$

$$\frac{\partial(\bar{\rho}\tilde{Y}_k)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{Y}_k\tilde{u}_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\bar{\rho}\bar{D}_k \frac{\partial\tilde{Y}_k}{\partial x_j} \right) - \frac{\partial}{\partial x_j} [\bar{\rho}(\tilde{Y}_k\tilde{u}_j - \tilde{u}_j\tilde{Y}_k)] + \bar{\omega}_k, \quad (3)$$

$$\frac{\partial(\bar{\rho}\tilde{T})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{T}\tilde{u}_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\bar{\rho}\bar{D}_T \frac{\partial\tilde{T}}{\partial x_j} \right) - \frac{\partial}{\partial x_j} [\bar{\rho}(\tilde{T}\tilde{u}_j - \tilde{u}_j\tilde{T})] + \bar{\omega}_T, \quad (4)$$

where ρ and u are the density and velocity of mixture gas respectively. p is the pressure of the mixture gas. Y_k represents the mass fraction of specie k , and T is the temperature. $\bar{\omega}_k$ and $\bar{\omega}_T$ are the filtered chemical reaction and heat release source terms.

The sub-grid momentum and scalar transport terms in the above equations are modeled by dynamic approach [19,20]. The turbulent stresses are calculated with an eddy viscosity assumption [20]. The residual scalar fluxes are modeled with the gradient-diffusion assumption [1]. The coefficients in the sub-grid models are all calculated by using the dynamic procedures [19]. The closure for chemical reaction source term in Eq. (3) and heat release source term in Eq. (4) will be introduced in the next section in detail.

3. The DSMC combustion model

Considering a chemical system with M reactions, if the filtered reaction rates of all the reactions are evaluated accurately, the reaction rates of the scalars could be calculated. To highlight the effects of the filtering, we consider a rate expression of the form $\bar{\omega}(\rho, Y_F, Y_O, T) = A \exp(-\frac{E}{RT}) \left(\rho \frac{Y_F}{W_F}\right)^m \left(\rho \frac{Y_O}{W_O}\right)^n$. Here m and n are the concentration exponents depending on the chemical kinetics. W denotes molecular weight. Y stands for the mass fraction. A and E denote the pre-exponential factor and the activation energy respectively. R is the universal gas constant. The subscripts F and O represent the fuel and oxidizer respectively. The filtered reaction rate term could be expressed as:

$$\begin{aligned} \bar{\omega} &= A \exp\left(-\frac{E}{RT}\right) \cdot \left(\rho \frac{Y_F}{W_F}\right)^m \cdot \left(\rho \frac{Y_O}{W_O}\right)^n \\ &= B \exp\left(-\frac{E}{RT}\right) \cdot R_1^m \cdot R_2^n \end{aligned} \quad (5)$$

where $R_1 = (\rho Y_F)$, $R_2 = (\rho Y_O)$, $B = AW_F^{-m}W_O^{-n}$. In the previous study, the temperature function is usually treated by the Taylor series expansion, and the filtered source term becomes so complicated that significant error appears [21]. To avoid this problem, the whole temperature function is treated as a variable K in the present study, namely $K = \exp(-\frac{E}{RT})$.

For R_i ($i = 1, 2$), the variance R'_i is assumed to be much smaller compared with R_i , then the expression below can be regarded feasible:

$$R_i^m = (\bar{R}_i + R'_i)^m \approx (\bar{R}_i)^m + m(\bar{R}_i)^{m-1}R'_i. \quad (6)$$

Ignoring the third-order unresolved terms, the reaction rate turns into:

$$\begin{aligned} \bar{\omega} &= B \overline{K R_1^m R_2^n} \approx B \left(\overline{K R_1^m R_2^n} + m n \bar{R}_1^{m-1} \bar{R}_2^{n-1} \overline{K' R_1' R_2'} + m \bar{R}_1^{m-1} \bar{R}_2^n \overline{K' R_1'} \right. \\ &\quad \left. + n \bar{R}_1^m \bar{R}_2^{n-1} \overline{K' R_2'} + m n \bar{R}_1^{m-1} \bar{R}_2^{n-1} \overline{K' R_1' R_2'} \right). \end{aligned} \quad (7)$$

Neglecting the third-order variance correlation term, the mean reaction rate reads:

$$\bar{\omega} = B \left(\overline{K R_1^m R_2^n} + m n \bar{R}_1^{m-1} \bar{R}_2^{n-1} \overline{K' R_1' R_2'} + m \bar{R}_1^{m-1} \bar{R}_2^n \overline{K' R_1'} + n \bar{R}_1^m \bar{R}_2^{n-1} \overline{K' R_2'} \right). \quad (8)$$

As \bar{R}_i can be calculated from the transport Eq. (3), the closure problem of chemical source term is changed into how to model the second-order variance correlation terms $\overline{R_1' R_2'}$, $\overline{K' R_1'}$, $\overline{K' R_2'}$ and the temperature function \bar{K} . The highly non-linearity exponential function \bar{K} is modeled using the fluctuation averaged closure method as:

$$\bar{K} = \frac{1}{2} \left\{ \exp \left[-\frac{E}{R \left(\tilde{T} + \tilde{T}'' \tilde{T}''^{\frac{1}{2}} \right)} \right] + \exp \left[-\frac{E}{R \left(\tilde{T} - \tilde{T}'' \tilde{T}''^{\frac{1}{2}} \right)} \right] \right\}. \quad (9)$$

The variance of temperature \tilde{T}'' is modeled using the sub-grid variance model with the dynamic procedure to determine the coefficient [20]:

$$\bar{\rho} \tilde{T}'' = C_T \bar{\rho} \Delta^2 |\nabla \tilde{T}|^2. \quad (10)$$

The transport equation of $\overline{R_1' R_2'}$ can be derived following the similar method of deriving the transport equation of Reynolds stress as [22]

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