IMPLEMENTATION AND VALIDATION OF A NOVEL TABULATED CHEMISTRY TURBULENT COMBUSTION MODLE IN OPENFOAM

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In recent years, Flamelet-Generated Manifolds (FGM) proposed by **Van Oijen** et al. has been widely used in the numerical simulation of various turbulent combustion flames and obtained encouraging results[1-3]. The FGM model builds a look-up table by computing a series of 1D laminar flamelet that takes into account the detailed chemical reaction mechanism. By considering the interaction between turbulence and chemical reaction by the Presumed-PDF (P-PDF) method, laminar flamelet look-up table expanded into a turbulent flamelet look-up table. Due to the limitations of P-PDF assumption itself, for example, the model assumes that the control variables are independent of each other, which is a strong assumption in many cases. And also, with increase of control variables or the reaction mechanism, the size of the look-up table increases exponentially and the memory requirements are huge. With the development and application of FGM model, more and more simulation results prove the limitation of P-PDF method. **Bray** et al. [4] studied the sensitivity of average chemical reaction rates to three P-PDF methods in Sandia Flame D and compared the P-PDF method to DNS data. The results show that there is a remarkable gap between the three most widely used β-PDFs and the actual DNS data, and the assumed shape factors in the P-PDF method greatly affect the chemical reaction rate prediction. In a study of turbulent spray combustion models, **Ge** et al.[5] found that the actual PDFs of the mixture fraction, gas temperature and enthalpy in the model was significantly different from the standard β-PDF. Based on the FGM model, this paper abandon the P-PDF method and combine the ESF model with the FGM model to directly consider the probability density function of the control variables. The new ESF-FGM model has been developed in this study and implemented in OpenFOAM.

In FGM models, there is no need to solve the transported equation for all components and energies, and the chemical reactions in turbulent combustion are thought to occur in low-dimensional manifolds, which means that only a few independent variables are required in the entire component space to characterize Chemical reaction in turbulent combustion. In the model, the "mixture fraction", Z, that characterizes the mixed state of fuel and oxidant and the "progress variable", C, that characterizes the progress of chemical reaction are usually selected as independent variables. Of course, depending on the physical model being simulated, variables such as pressure and enthalpy loss can be added as supplementary independent variables[6]. The FGM turbulent combustion model under the LES method can be expressed as follows:

$$\frac{\partial \bar{\rho}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j}{\partial x_j}=\bar{S}_\rho \tag{1}$$

$$\frac{\partial \bar{\rho}\tilde{u}_j}{\partial t}+\frac{\partial\left(\bar{\rho}\tilde{u}_i\tilde{u}_j\right)}{\partial x_j}=-\frac{\partial \bar{p}}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\bar{2}\mu\tilde{S}_{ij}^{D}-\tau_{ij}\right)+\bar{S}_{u_i} \tag{2}$$

$$\frac{\partial \bar{\rho}\tilde{Z}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j\tilde{Z}}{\partial x_j}=\frac{\partial}{\partial x_j}\left[\bar{\rho}\left(\tilde{D}+D_t\right)\frac{\partial \tilde{Z}}{\partial x_j}\right]+\bar{S}_Z \tag{3}$$

$$\frac{\partial \bar{\rho}\tilde{Y}_C}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j\tilde{Y}_C}{\partial x_j}=\frac{\partial}{\partial x_j}\left[\bar{\rho}\left(\tilde{D}+D_t\right)\frac{\partial \tilde{Y}_C}{\partial x_j}\right]+\bar{\dot{\omega}}_{Y_C} \tag{4}$$

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{5}$$

$$S_{ij}^{D} = S_{ij} - \frac{1}{3}\delta_{ij} S_{KK} \tag{6}$$

Where τ_{ij} is the sub-grid scale (SGS) stress. It is closed with HybridSGS model in the LES. Z is mixture fraction, and defined by **Bilger's** method of element definition with the same diffusion coefficient of all components; Y_C is an un-normalized progress variable, and it's definition in this study is as follows:

$$Y_C = \frac{Y_{CO2}}{W_{CO2}} + \frac{Y_{H2O}}{W_{H2O}} + \frac{Y_{H2}}{W_{H2}} \tag{7}$$

Where Y is molar mass and W is mass fraction, respectively. Export Y_C normalization as progress variable C:

$$C = \frac{Y_C - Y_C^u}{Y_C^b - Y_C^u} \tag{8}$$

Superscripts b and u respectively represent the burned and unburned state. The sum of the equations for Z and C is the independent variable of the look-up table.

Considering the influence of turbulent fluctuation on the chemical reaction, the original FGM model uses the P-PDF method to describe its distribution through the first moment and the second moment of two independent variables. At the same time, the original 2D laminar flamelet look-up table expanded into 4D turbulent flamelet look-up table. In this paper, we abandon this method and choose real-time solutions to components jointing probability density function of two independent variables transported equation and integrate them in the sample space to obtain all the single-point statistics of all the space and time of two independent variables in real time. In this paper, Eulerian Stochastic Field (ESF) model in the transported probability density function class model is used to accomplish this task, and then the ESF model is introduced.

In solving the transported equation of probability density function, when there are many components, the dimension of transported equation is quite high. In this situation, it is difficult to solve the equation with finite volume, finite difference or finite element method. This paper adopts Eulerian Stochastic Field (ESF) model, using a series of stochastic fields N_F to represent joint-composition PDF required by this model. In this N_F stochastic fields, each field contains each component value at each position in the entire flow field. It can be expressed as[7]:

$$f_\varphi(\psi;\vec{x},t) \approx \frac{1}{N_F}\sum_{n=1}^{N_F}\prod_{\alpha=1}^{N_s}\delta\left(\psi_\alpha - \varphi_{\alpha,n}\right) \tag{9}$$

$\varphi_{\alpha,n}$ is the value of scalar α under $\vec{x}$ position under t time in n field. In this model, $\varphi_\alpha = [\mathrm{Z},\mathrm{C}]$, each stochastic field evolvesaccording to the stochastic partial differential equations (SPDE) derived from transport equation of the joint-composition PDF. These SPDE can be expressed as[8]:

$$\begin{aligned} d(\bar{\rho}\varphi_{\alpha,n}) = &-\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\varphi_{\alpha,n}\right)dt + \frac{\partial}{\partial x_j}\left[\left(\frac{\mu}{S_C} + \frac{\mu_t}{S_{Ct}}\right)\frac{\partial\varphi_{\alpha,n}}{\partial x_j}\right]dt + \dot{\omega}_\alpha^n dt - \\ &\frac{\bar{\rho}}{2\tau_{sgs}}\left(\varphi_{\alpha,n} - \tilde{\phi}_\alpha\right)dt + \left(2\bar{\rho}^2\frac{\mu_t}{S_{Ct}}\right)^{1/2}\frac{\partial\varphi_{\alpha,n}}{\partial x_j}dW_{j,n}, \quad for \quad n = 1,\cdots N_F \; and \quad \alpha = 1,\cdots N_s \end{aligned} \tag{10}$$

The first three items on the right side of the equation correspond to convection term, turbulence diffusion term, and source term of the mean flow, respectively. The fourth term indicates micro-mixing due to the attenuation of scalar fluctuations. The last term is the Wiener term, which denotes a random term caused by turbulence, which varies over time but not with spatial location. In a given stochastic field, all scalars use the same $dW_{j,n}$ value, it denotes increments of a vector Wiener process, independent of the spatial location and different for each stochastic field. The turbulent mixing time τ_{sgs} is determined according to the mixing time model proposed by [9]and reads

$$\Omega_{sgs} = \frac{1}{\tau_{sgs}} = C_{\Omega} \frac{\bar{\nu} + \nu_t}{\Delta^2} \tag{11}$$

Where the suitable value for the micro-mixing constant is proposed in the same work as $C_{\Omega} = 2$ and ν denotes the kinematic viscosity.

By solving the stochastic differential equations of each stochastic field, the evolution law of the mixture fraction and the progress variables over time in each stochastic field considering the influence of turbulence is obtained. A statistical average is then used to find the control variables for the flamelet look-up table.

According to the established theoretical model, using OpenFOAM solver that developed in this study, the simulation of flame Sandia Flame (D-F) was carried out under a variety of stochastic fields. This paper first verifies the correctness of the model in the RANS.

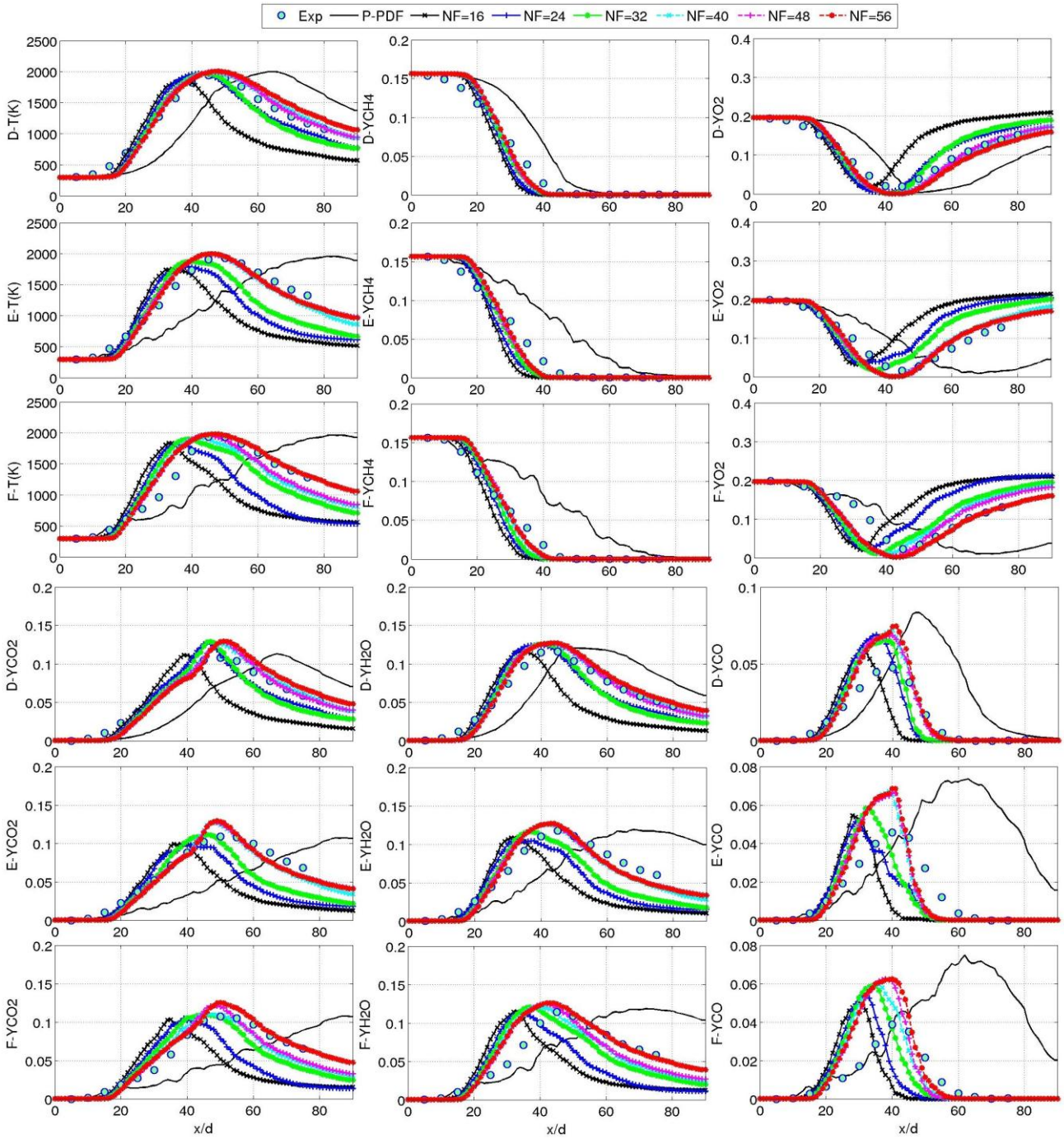

Figure 1: Comparison of predicted and measured mean axial temperature and main components mass fraction in Sandia Flame (D-F) (RANS)

Fig. 1 shows the comparison of predicted and measured mean axial temperature and main components mass fraction between the ESF / FGM model and the original FGM model. Overall, the ESF / FGM model predicts better the

distribution of temperature and main components than the original FGM model using the P-PDF method. For axial components, the ESF / FGM model achieves a more accurate prediction, and as the number of stochastic fields increases, the simulation accuracy is better. With the increase of the number of stochastic fields, the simulation accuracy of the new turbulent combustion model has been continuously improved. However, when the number of stochastic fields is higher than a certain value, the simulation results have little change and tend to be stable. This phenomenon is consistent with the conventional statistical thinking. However, ESF / FGM models were found to simulate the location of the flame ignition later in the experiment, while the position where the axial CH4 and O2 mass fractions began to decline, as well as the positions where other products started to appear, were behind the actual flame positions. It shows that the model simulates the effect of turbulent mixing before flame ignition is weaker than the actual one and the ignition position is further away from the fuel inlet. The rate of temperature rise is also faster than the experiment, and both the rate of fuel consumption and the product formation rate are faster than the experiment. The reason may be that laminar flamelet building does not consider the effect of flow on the flamelet stretching and bending. For the simulation of both CO and CO2 components, the peak position coincides with the experiment, but the simulated value is slightly higher than the experimental value.
So, we use the large eddy simulation to improve the simulation accuracy of the fuel and oxidant mixing process, so as to further improve the accuracy of the simulation results of the new turbulent combustion model.

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