Cluster Computing (2019) 22:S15103–S15110
https://doi.org/10.1007/s10586-018-2501-8

Numerical simulation of the Sandia Flame D using the ESF method coupled with FGM model

Yifan Duan[1] · Zhixun Xia[1] · Likun Ma[1] · Zhenbing Luo[1]

Received: 25 February 2018 / Revised: 10 March 2018 / Accepted: 12 March 2018 / Published online: 30 March 2018

Abstract
In this paper, we combine the Eulerian stochastic field (ESF) model with flamelet generated manifolds (FGM) model to achieve a new type of turbulent combustion flamelet model with high accuracy under consideration of the detailed chemical reaction mechanism. It solves the limitations of using the presumed PDF model in the original FGM model and the problems of the FGM model in the promotion of the use of non-applicability and other issues. Using OpenFOAM software and Sandia Flame D experimental data to complete the model to achieve and verify. The results show: the simulation results of the new model are good, which can accurately simulate the axial and radial temperature and the distribution of the mass fraction of the main components, and the accuracy is better than the original FGM model; with the increase of the number of stochastic fields in the ESF model, the accuracy of simulation is continuously improved; when the number of stochastic fields increases to a certain value, the simulation results are stable within a certain range of variation. The above results show that the model is effective for this type of flame simulation and has good prospects for simulating a more complex flame.

Keywords Turbulent combustion · Flamelet generated manifold model · Eulerian stochastic field methods · OpenFOAM

1 Introduction

In the energy, transportation and aerospace research areas, turbulent combustion as one of the most common form of combustion, its numerical simulation has attracted worldwide attention from scholars in the field of combustion. Turbulent combustion is an extremely complex physicochemical process involving turbulent flow, heat transfer, mass transfer and chemical reactions. The fundamental mechanism of turbulent flow is not fully explained and is one of the outstanding problems in classical physics. The flow has a strong non-linear coupling relationship with the simultaneous chemical reaction, which makes the difficulties of numerical simulation of turbulent combustion greatly increased.

✉ Likun Ma
likunma@yeah.net

[1] College of Aerospace Science and Technology, National University of Defense Technology, Changsha 410073, China

The current mainstream combustion models can be divided into Transported PDF method, Flamelet-based model, CMC and other combined models [1]. The transported probability density function class model can be divided into the Eulerian stochastic field model (ESF) and the Monte Carlo transported probability density function model, which has the advantages of being free from the limitation of the combustion mode and of high computational accuracy. But there are also computationally affordable problems that generally requires reducing the computational complexity by simplifying the chemical reaction mechanism. The Flamelet model considers that turbulent combustion consists of a series of laminar flamelets and non-reactive turbulent flow fields that surround these flamelets, has realized the decoupling calculation of turbulent flow and chemical reaction process, which is computationally efficient even when detailed chemical reaction mechanism is employed.

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 the highly consistent with the experimental data of the calculation results [2–4]. 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. [5]. 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. [6] 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. The model was validated by simulation of the Sandia Flame D released by Sandia National Laboratory in the United States.

2 Methodology

2.1 FGM model

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 [7]. The FGM turbulent combustion model under the RANS 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 S_{ij} is strain rate tensor and τ_{ij} is Reynolds stress, closed with Standard $k-\varepsilon$ model. Z is mixture fraction, and is 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: $Y_C=\frac{Y_{CO_2}}{W_{CO_2}}+\frac{Y_{H_2O}}{W_{H_2O}}+\frac{Y_{H_2}}{W_{H_2}}$, where W is molar mass and $Y$is mass fraction, respectively. Export Y_C normalization as progress variable C:

$$C=\frac{Y_C-Y_C^u}{Y_C^b-Y_C^u} \tag{7}$$

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.

2.2 ESF model

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 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 [8]:

$$f_\varphi(\psi;\vec{x},t) \approx \frac{1}{N_F}\sum_{n=1}^{N_F}\prod_{\alpha=1}^{N_s}\delta\left(\psi_\alpha - \varphi_{\alpha,n}\right) \tag{8}$$

$\varphi_{\alpha,n}$ is the value of scalar α under $\vec{x}$ position under t time in n field. In this model, $\varphi_\alpha = [Z, C]$, each stochastic field evolves according to the stochastic partial differential equations (SPDE) derived from transport equation of the joint-composition PDF. These SPDE can be expressed as [9]:

$$\begin{aligned} d\varphi_{\alpha,n} &= -\tilde{u}_j\frac{\partial\varphi_{\alpha,n}}{\partial x_j}dt + \frac{1}{\langle\rho\rangle}\frac{\partial}{\partial x_j}\left[\frac{\mu_t}{\sigma_t}\frac{\partial\varphi_{\alpha,n}}{\partial x_j}\right]dt \\ &+ \left[\frac{\dot{\omega}_\alpha\underline{\varphi}_n}{\rho} - \delta_{\alpha(X_R)}\frac{\dot{Q}_R\left(\underline{\varphi}_n\right)}{\rho}\right]dt - \frac{1}{2}\frac{\varepsilon}{k}C_\varphi\left(\varphi_{\alpha,n} - \tilde{\varphi}_\alpha\right)dt \\ &+ \left(\frac{2}{\rho}\frac{\mu_t}{\sigma_t}\right)^{1/2}\frac{\partial\varphi_{\alpha,n}}{\partial x_j}dW_{j,n}, n = 1,\ldots N_F \; and \quad \alpha = 1,\ldots N_s \end{aligned} \tag{9}$$

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.

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

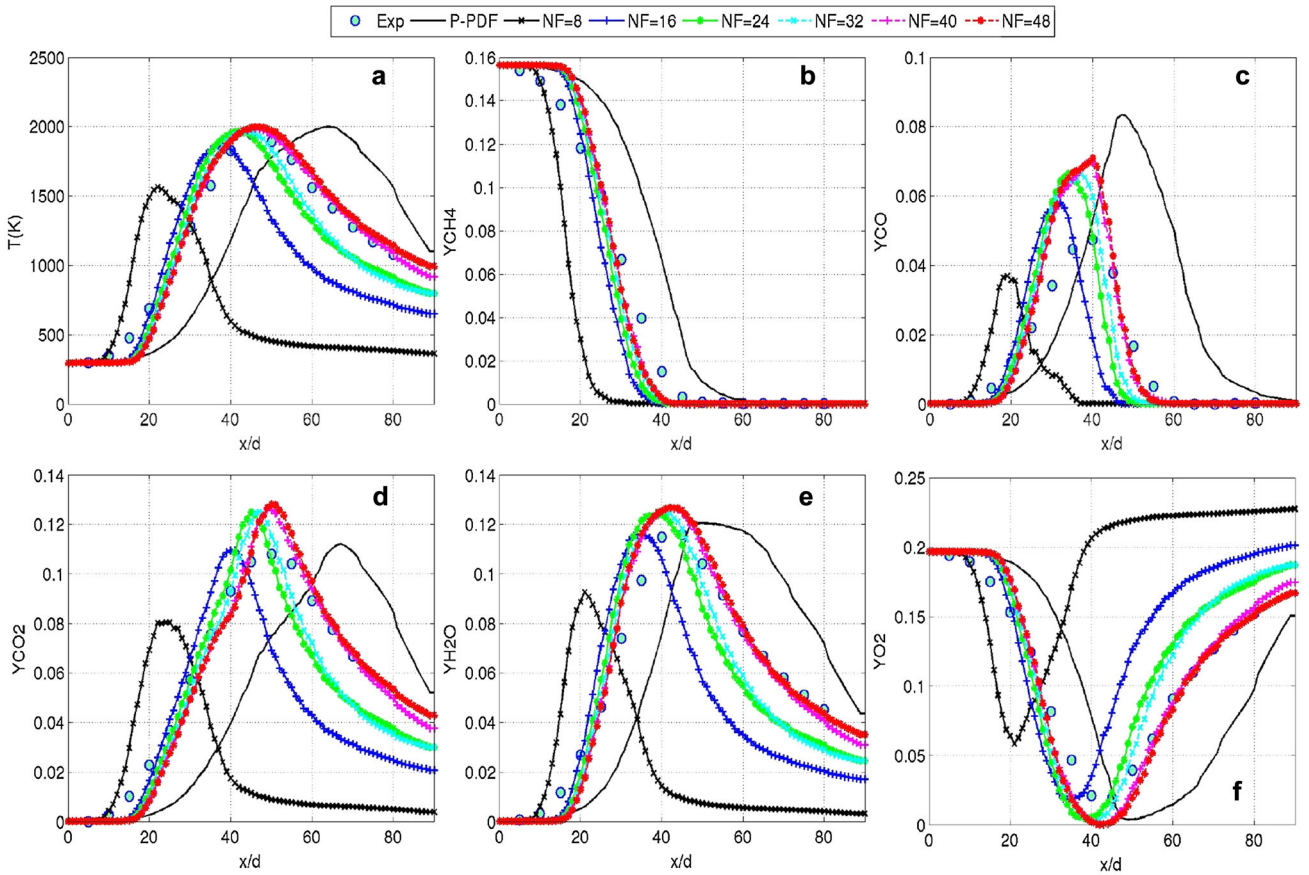


Fig. 1 Comparison of predicted and measured mean axial temperature and main components mass fraction (**a** temperature, **b** YCH_4, **c** YCO, **d** YCO_2, **e** YH_2O, **f** YO_2)

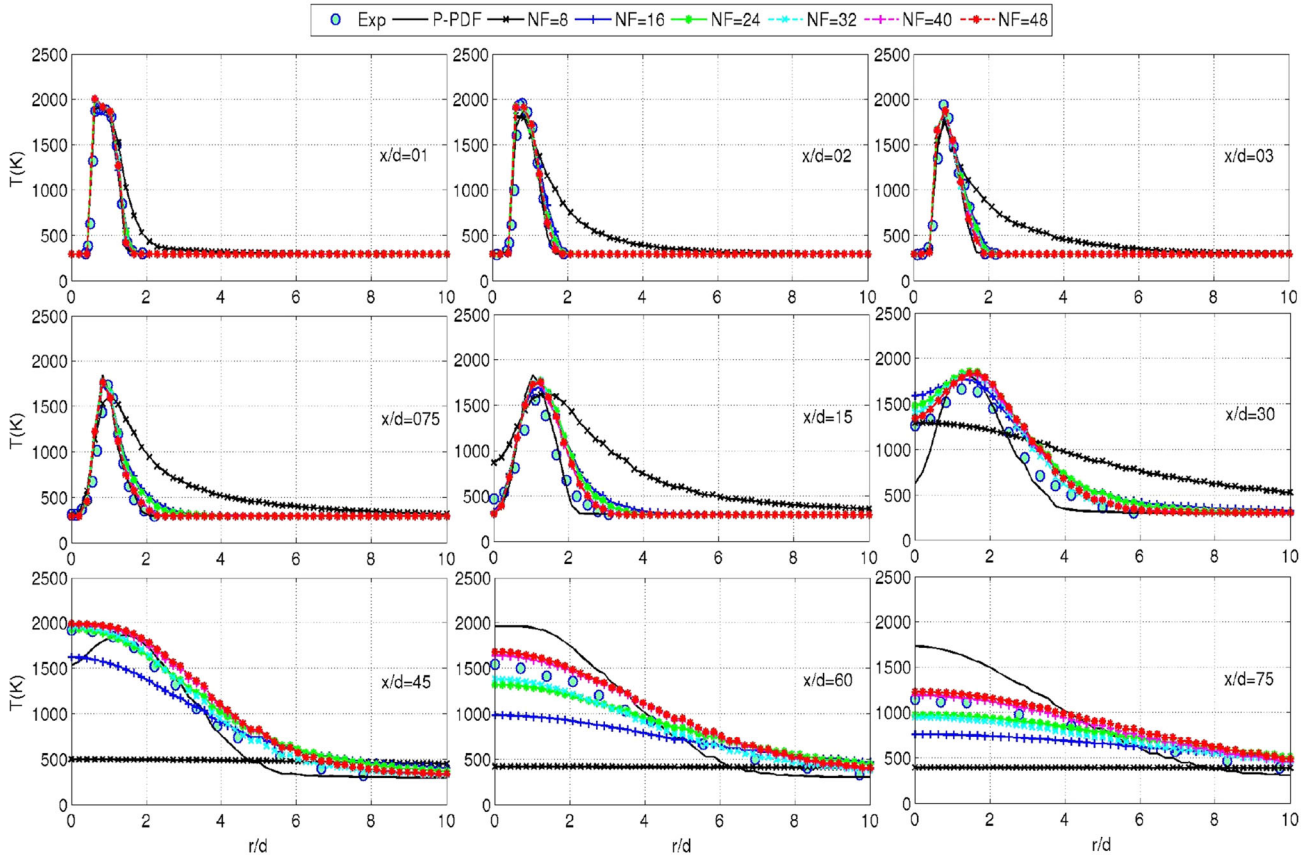


Fig. 2 Comparison of predicted and measured mean radial temperature at different axial location

statistical average is then used to find the control variables for the flamelet look-up table.

2.3 Simulation model

This paper uses Sandia Flame D measured by *Sandia National Laboratory* in the United States. The fuel is a mixed gas of methane and air. The volume ratio is 1:3 and the average velocity of the fuel flow is $u_C = 49.6$ m/s. The pilot fire plays a role of stabilizing the flame. Other flow fields are given in Ref. [10]. The RANS simulation method uses a standard $k - \varepsilon$ model.

3 Result analysis and discussion

According to the established theoretical model, using OpenFOAM solver that developed in this study, the simulation of flame Sandia Flame D was carried out under a variety of stochastic fields. The comparison between the predicted and measured mean axial and radial temperature at different axial location and main components mass fraction, and simulation results of the original FGM model (P-PDF method) are also discussed.

Figure 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 temperature distribution than the original FGM model using the P-PDF method. For axial temperature, the ESF/FGM model achieves a more accurate prediction, and as the number of stochastic fields increases, the simulation accuracy is better. However, ESF/FGM models were found to simulate the location of the flame ignition later in the experiment, while the position where the axial CH_4 and O_2 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 CO_2 components, the peak position coincides with

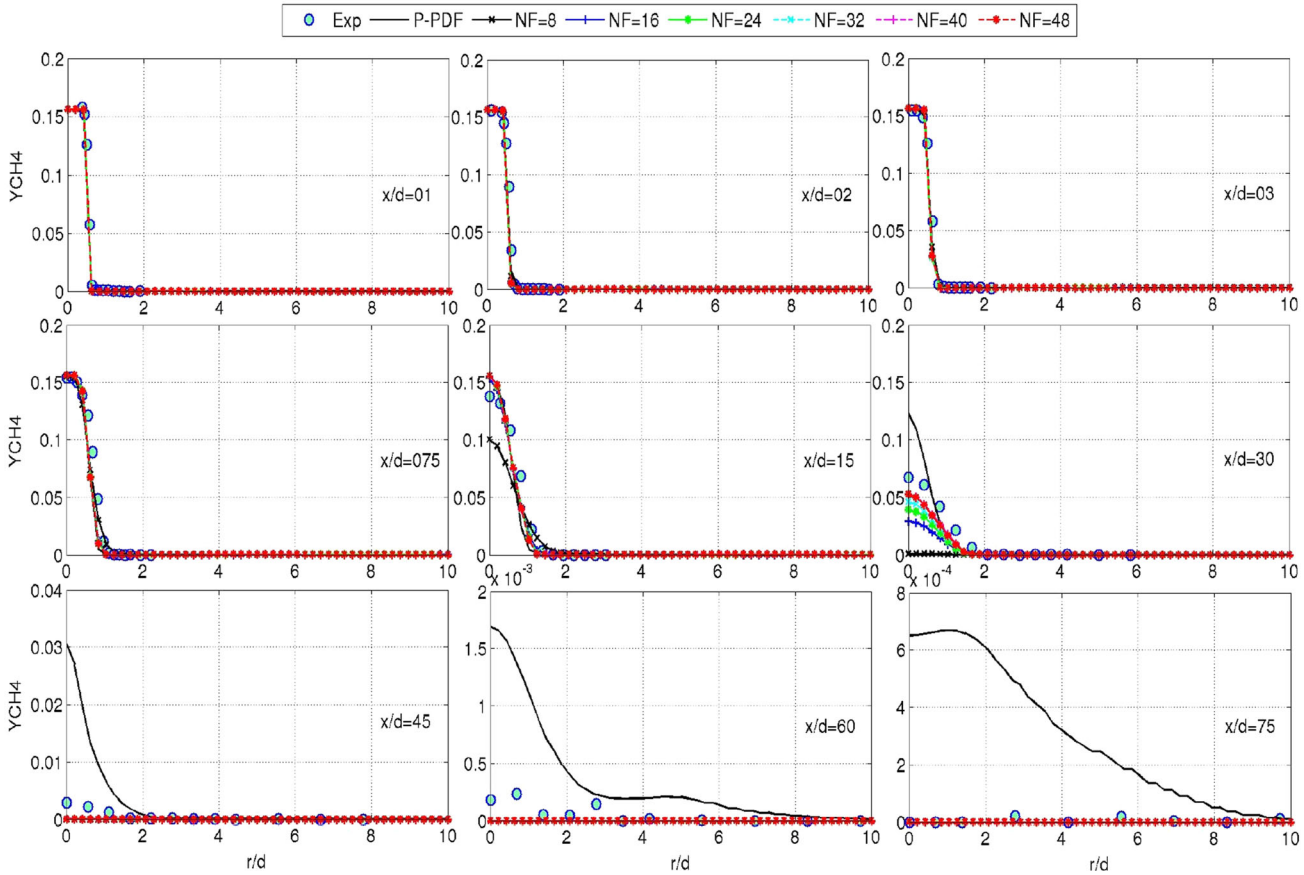


Fig. 3 Comparison of predicted and measured mean radial CH_4 mass fraction at different axial location

the experiment, but the simulated value is slightly higher than the experimental value.

Figure 2 shows the comparison of predicted and measured mean radial temperature at different axial location. The calculated results of the ESF/FGM model and the original FGM model for different numbers of stochastic fields are given. In general, the temperature prediction performance of ESF/FGM model is better than that of the original FGM model using P-PDF method. In the case of *x*/*xd*. *d* less than or equal to 15, the original FGM model is not significantly different from the ESF/FGM model. With the increase of the axial distance, the accuracy of the original FGM model is apparently declining even though its trend is consistent. From the results of ESF/FGM calculation alone, the temperature can be predicted accurately in 24 fields. When the number of stochastic fields is greater than or equal to 24, the calculated values of the radial temperatures in the whole axial position are in good agreement with the experimental results. Simultaneously, with the increase of the number of stochastic fields, the simulated results are in good agreement with the experimental measurements. However, when the number of stochastic fields increases to a certain value, the model results are stable within a certain range, indicating that the probability density function of the control variables obtained by the ESF model achieves a statistical convergence.

Figures 3, 4, and 5 show the comparison of predicted and measured mean radial CH_4, O_2, CO_2 and H_2O mass fraction at nine axial positions respectively. The radial distributions of different axial positions of the ESF/FGM model and the original FGM model under different numbers of stochastic fields are given. In general, the temperature prediction performance of ESF/FGM model is better than that of the original FGM model using P-PDF method. The more the number of stochastic fields, the more the simulated numerical results meet the actual measured values. The original FGM model is better for the simulation of the main components near the fuel inlet. As the distance increases, the error increases continuously and the rate of change is faster than the experiment. However, the ESF/FGM model is more stable with the increase of the number of stochastic fields, and more in line with the

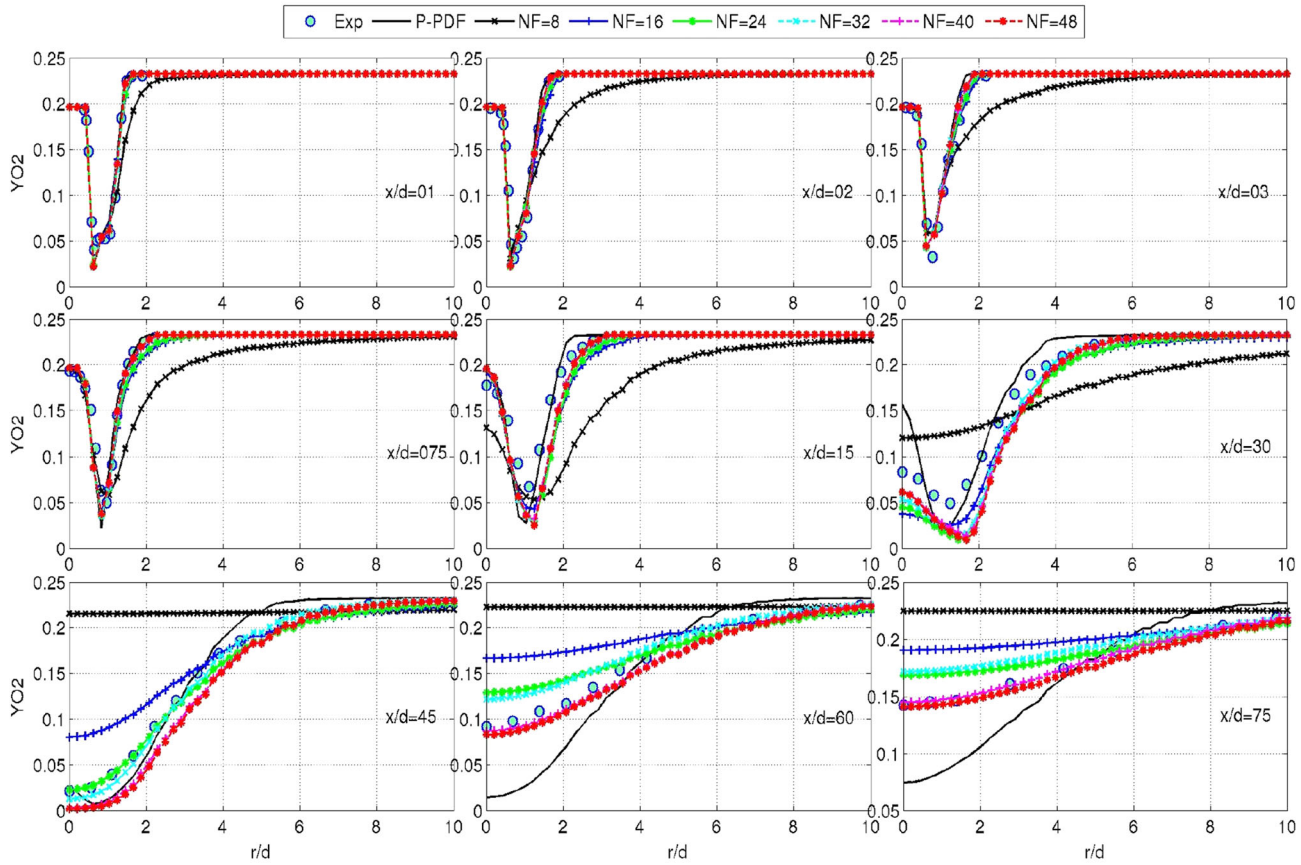


Fig. 4 Comparison of predicted and measured mean radial O_2 mass fraction at different axial location

experimental measurements. From this phenomenon, it can be concluded that the original FGM model using the P-PDF method overestimates the chemical reaction rate and the effect of turbulence on the chemical reaction, While the ESF/FGM model accurately simulates the influence of turbulent pulsation on the control variables, to some extent, to limit the effect of overestimating the side effects of chemical reaction rates.

4 Conclusions

In this paper, by combining the FGM model and ESF model in the transported probability density function class model, a new turbulent combustion model was developed and implemented in OpenFOAM. Through the numerical simulation of the temperature and the mass fraction of each component of Sandia Flame D, the accuracy of the new turbulent combustion flamelet model is verified. By comparing the simulation results of different stochastic fields with the simulation results of the FGM model using the original P-PDF method, the following conclusions are obtained: The flame simulation accuracy of the new model is higher than that of the original FGM model using the P-PDF method. 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. The new turbulent combustion model can to some extent limit the flamelet model overestimation of the chemical reaction rate of side effects. However, the following deficiencies are also found: although imported compared the conventional FGM model, the prediction of the minor species using this new still has room to improve, and that the ignition position and the chemical reaction rate prediction are also not accurate enough. These issues deserve further study. In the next step, large eddy simulation will be used 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.

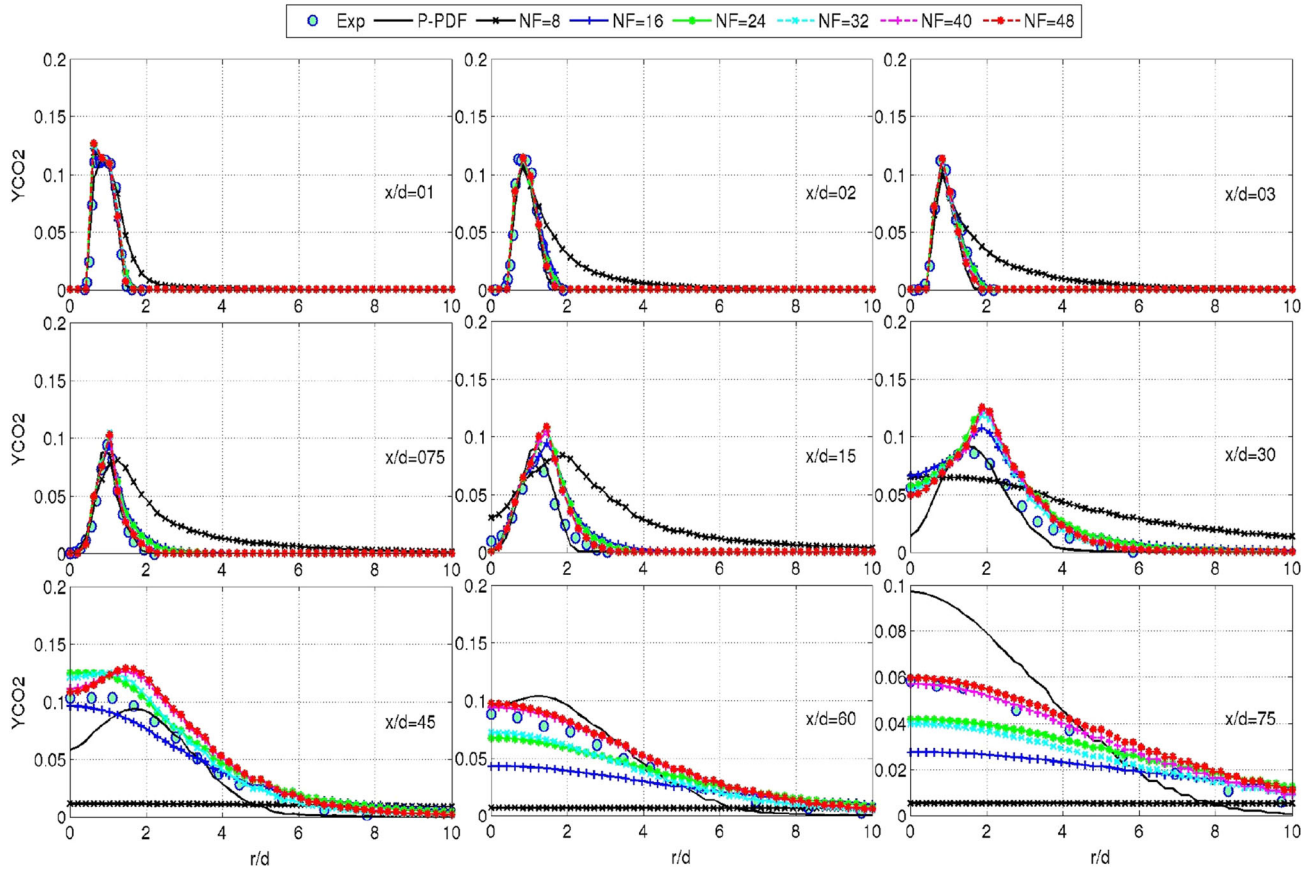
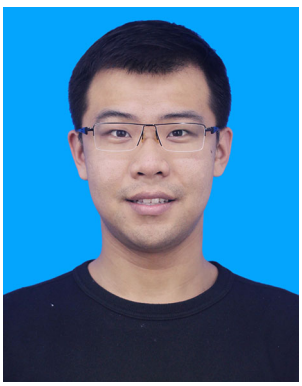


Fig. 5 Comparison of predicted and measured mean radial CO_2 mass fraction at different axial location

Acknowledgements The research was founded within the Project No. 51706241 entitled: "Investigation on the mechanism of droplet/flame interaction and flamelet modeling of turbulent spray combustion" supported by the National Natural Science Foundation of China.

References

1. Pope, S.B.: Small scales, many species and the manifold challenges of turbulent combustion. Proc. Combust. Inst. **34**, 1–31 (2013)
2. Bekdemir, C., Somers, L.M.T., Goey, L.P.H.D.: Modeling diesel engine combustion using pressure dependent flamelet generated manifolds. Proc. Combust. Inst. **33**, 2887–2894 (2011)
3. Donini, A., Bastiaans, R., Oijen, J.A.V., Goey, P.D.: Numerical simulations of a turbulent high-pressure premixed cooled jet flame with the flamelet generated manifolds technique. J. Eng. Gas Turbines Power **137**, 071501 (2015)
4. Ma, L., Roekaerts, D.: Modeling of spray jet flame under MILD condition with non-adiabatic FGM and a new conditional droplet injection model. Combust. Flame **165**, 402–423 (2016)
5. Bray, K.N.C., Champion, M., Libby, P.A., Swaminathan, N.: Finite rate chemistry and presumed PDF models for premixed turbulent combustion. Combust. Flame **146**, 665–673 (2006)
6. Ge, H.W., Gutheil, E.: Simulation of a turbulent spray flame using coupled PDF gas phase and spray flamelet modeling. Combust. Flame **153**, 173–185 (2008)
7. Ma, L., Roekaerts, D.: Numerical study of the multi-flame structure in spray combustion. Proc. Combust. Inst. **36**(2), 2603–2613 (2016)
8. Nmira, F., Burot, D., Consalvi, J.L.: Stochastic Eulerian field method for radiative heat transfer in a propane oxygen-enhanced turbulent diffusion flame. Combust. Theor. Model. **21**, 62–78 (2016)
9. Consalvi, J.L., Nmira, F., Burot, D.: Simulations of sooting turbulent jet flames using a hybrid flamelet/stochastic Eulerian field method. Combust. Theor. Model. **20**, 1–37 (2017)
10. Di Renzo, M., Coclite, A., de Tullio, M.D., De Palma, P., Pascazio, G.: LES of the Sandia Flame D using an FPV combustion model. Energy Procedia **82**, 402–409 (2015)



Yifan Duan Bachelor of Science. Graduated from the National University of Defense Technology in 2016. Continue to study for a master's degree in school. Her research interests include numerical simulation of turbulent combustion.

Zhixun Xia Doctor of Science, Professor. Graduated from the Beijing University of Aeronautics and Astronautics in 1991. Worked in the National University of Defense Technology. Her research interests include aerospace propulsion theory and engineering.

Likun Ma Doctor of Science, Lecturer. Graduated from the Delft University of Defense Technology in 2016.Worked in the National University of Defense Technology. Her research interests include numerical simulation of turbulent spray combustion.

Zhenbing Luo Doctor of Science, Professor. Graduated from the National University of Defense Technology in 2006. Worked in the National University of Defense Technology. Her research interests include active flow control technology.