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Artificial Neural Networks for Chemistry Representation in Numerical Simulation of the Flamelet-Based Models for Turbulent Combustion

Jiarui Zhang¹, Honglan Huang², Zhixun Xia¹, Likun Ma¹, Yifan Duan¹, Yanghe Feng², and Jincal Huang²

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

²College of Systems Engineering, National University of Defense Technology, Changsha 410073, China

Corresponding author: Jiarui Zhang (zhangjiarui@nudt.edu.cn)

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ABSTRACT Turbulent combustion is one of the key processes in many energy conversion systems in modern life. In order to improve combustion efficiency and suppress emission of pollutants, many efforts have been made by scholars to investigate turbulent flames. In the present study, Artificial neural network (ANN) was first employed for the storage and interpolation of the flamelet library in flamelet generated manifolds (FGM) model, in which Eulerian stochastic field (ESF) model was used to directly consider the probability density function of the control variables. This new model had been implemented in OpenFOAM and was validated by simulation of the Sandia Flame D under consideration of the detailed chemical reaction mechanism. By comparing the results of numerical simulations and experimental measurements of the temperature and the mass fraction of main components, the accuracy of the proposed ANN-ESFFGM model was verified. Through the use of ANNs to characterize the chemical reactions, the flame simulation accuracy of the new model is higher than that of the original ESFFGM model, especially in the prediction of the ignition position. With the increase in the number of stochastic fields, the simulation accuracy of the new turbulent combustion model is continuously improved until a certain value of stochastic fields was reached. Moreover, excessively high FGM table resolution has limited improvement in numerical simulation accuracy.

INDEX TERMS Artificial neural network, Eulerian stochastic field methods, Flamelet generated manifold model, OpenFOAM, turbulent combustion.

I. INTRODUCTION

Combustion system is widely used in the field of energy, transportation industries and aerospace, which has brought rapid socio-economic development. It also triggered a series of serious environmental issues, such as resources and pollution problems. The accurate prediction of turbulent flames therefore becomes a critical challenge, and its numerical simulation has been paid more and more attention by researchers from all over the world [1]–[3]. The fundamental mechanism of turbulent flow has not been fully understood yet, and it has a strong nonlinear coupling relationship with the

simultaneous chemical reaction, which makes the prediction of turbulent combustion even more complicated.

Based on how to address the challenge posed by the coupling between chemical reactions and molecular diffusion, the current mainstream combustion models can be divided into Transported probability function (TPDF) models and Flamelet-based models [4]. The TPDF models have the advantages of being free from the limitation of the combustion model and of high calculation accuracy at the cost of consuming a large amount of computing resources [5]. The flamelet models assume that all chemical reactions happen on a thin layer, for which only the changes perpendicular to the flame front is important, the other two dimensions are negligible. These models have successfully decoupled the

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calculations of turbulent flow and chemical reaction process, which makes the simulation of turbulent flame more computationally efficient even when a detailed chemical reaction mechanism is employed [6].

Proposed by van Oijen and de Goey [7], flamelet-generated manifolds (FGM) is one of the most popular flamelet-based models for turbulent combustion in recent years [8]–[11]. In FGM model, scalar properties of combustion system are precalculated by computing a series of 1D laminar flame, in which detailed chemical reaction mechanisms are taken into account, and the results are typically stored in a structured table as a function of the reduced set of reaction coordinates such as mixture fraction, progress variable and enthalpy. Currently, Presumed-PDF (P-PDF) method is widely used for expanding the laminar flamelet look-up table into a turbulent one by considering the interaction between turbulence and chemical reaction [12], [13]. However, evidence shows that there is a noticeable gap between the most widely used PDFs and the actual direct numerical simulation (DNS) data [14]. Then, an investigation on the applicability of the presumed β -PDF approach to modeling of turbulent flames was carried out by a comparison between the DNS data and the corresponding a priori large eddy simulation [15]. The results show that mean and variance are not sufficient as control parameters by means of presumed PDF. To overcome this shortage, a modified laminar flame PDF was proposed by Jin *et al.* [16], and this model was then used by Luo *et al.* [17] to model the reaction rate of premixed turbulent flames.

Recently, our group abandon the P-PDF method and combine the Eulerian stochastic field (ESF) model with FGM model to directly consider the probability density function of the control variables [18]. The new ESFFGM model overcomes the limitations of using the P-PDF model in the original FGM model and reduces the size of the flamelet library since this method does not need to integrate the precomputed table over probability density function. Soon after, a similar work was conducted by Mahmoud *et al.* [19], in which the ESF model was combined with another flamelet-based model termed as Flamelet Progress Variable (FPV) model to investigate turbulent combustion.

However, the storage requirements of FGM lookup table are still extremely large when the table is to be extended to incorporate more physics when required, for example, adding enthalpy h to account for the heat loss/gain [10], adding air dilution level γ to take into account the effect of recirculated burnt gases in a flameless combustion system [20] and adding a second mixing fraction to represent a different stage of combustion in the simulation of pulverised coal combustion (PCC) [21], [22]. In this case, the storage requirement of a look-up table can be as high as several GBs per core and due to the limitation of the computer memory, the resolution of the flamelet library must be reduced, which leads to a decrease in the accuracy of the simulation.

Artificial neural network (ANN), a framework for many different machine learning algorithms to work together and

process complex data inputs, is an attractive alternative to tabulation techniques for the representation of chemical reactions [23]–[26]. The most outstanding advantage of ANN over traditional tabulation method is their negligible memory requirements, since only the architecture and the parameters of the network need to be stored during the simulation. It is reported that this approach reduces the storage size of the chemistry library by three orders of magnitude [27]. At the same time, the smooth function representation of ANN is likely to provide more accurate chemical reaction results over the linear interpolation method used in tabulation techniques.

Therefore, in this study, ANN was first used for the storage and interpolation of the flamelet library in ESFFGM model. Subsequently, the characteristics of the memory requirements and prediction accuracy of this model were analyzed. The rest of the paper is organized as follows: Section II introduces the main models used in this study. Section III gives the simulation setups, the calculated results of Sandia Flame D and gives some discussions. Finally, several conclusions are drawn.

II. METHODOLOGY

A. FGM MODEL

In the FGM model, 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. Therefore, there is no need to solve a large set of scalar transport equations and chemical reactions, and temperature and chemical species mass fractions at each point are identified by referring to the flamelet library. In the present study, the “mixture fraction,” denoted as Z , which describes the mixing state of fuel and oxidizer, and the “progress variable,” denoted as C , which characterizes the progress of the chemical reaction, are elected as control variables in the flamelet look-up table. The FGM turbulent combustion model under the Reynolds Averaged Navier-Stokes (RANS) method can be expressed as follows:

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

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

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

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

$$S_{ij}^D = S_{ij} - \frac{1}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \quad (5)$$

$$S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (6)$$

In equation(1)-(6), (\cdot) stands for a density-weighted or Favre average quantity and $(\bar{\cdot})$ for time average quantity. ρ is the density; u_i is the velocity component of the flow field in different directions ($i = 1, 2, 3$); p is the pressure; μ is the dynamic viscosity; D is diffusion term and subscript t indicates turbulence; S_{ij} is strain rate tensor and τ_{ij} is Reynolds stress, closed with Standard $k - \epsilon$ model in the current study. 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 progress variable, which denotes the progress of chemical reaction from pure mixing ($Y_C = 0$) to fully burnt ($Y_C = 1$), and its definition in this study is as follows:

$$Y_C = \frac{Y_{CO_2}}{W_{CO_2}} + \frac{Y_{H_2O}}{W_{H_2O}} + \frac{Y_{H_2}}{W_{H_2}} \quad (7)$$

where Y_i and W_i is mole fraction and molecular weight of species i respectively.

Then, a normalized progress variable is introduced as:

$$C = \frac{Y_c - Y_c^u}{Y_c^b - Y_c^u} \quad (8)$$

In this way, the high-dimensional chemical reaction system has been projected to a two dimensional manifold:

$$\phi = \phi(Z, C) \quad (9)$$

where ϕ can be any of the scalar properties, such as temperature, mass fraction of a certain species, of this chemical system. This two dimensional manifold is hereinafter referred to as the FGM table (i.e., flamelet library for FGM model). In the present study, the FGM table was created by solving laminar counterflow diffusion flame at different strain rates in physical space and then transfer the results to control variables (i.e., mixture fraction and progress variable) space.

B. ESF MODEL

Probability density function (PDF) method [28] has been demonstrated as one of the predictive and robust approaches for accommodating the effect of turbulence on the reaction rates in turbulent combustion. In this method, transported PDF equations are to be solved and multiple strategies have been developed. Eulerian Stochastic Field (ESF) method in the transported probability density function class model is employed to consider the influence of turbulent fluctuation on the chemical reaction. In the ESF method, the reactive fields are represented by N_f stochastic fields for each of scalars, and it can be expressed as [29]

$$f_\phi(\psi; \vec{x}, t) \approx \frac{1}{N_f} \sum_{n=1}^{N_f} \prod_{\alpha=1}^{N_f} \delta(\psi_\alpha - \varphi_{\alpha,n}) \quad (10)$$

where $\varphi_{\alpha,n}$ is the value of scalar α under \vec{x} position under t time in n th field. δ is the Dirac delta function. In this model, $\varphi_\alpha = [Z, C]$, each stochastic field evolves according to the stochastic partial differential equations (SPDE) derived

from transport equations of the joint-composition PDF. These SPDE can be expressed as [30]:

$$\begin{aligned} d\varphi_{\alpha,n} = & -\tilde{u}_j \frac{\partial \varphi_{\alpha,n}}{\partial x_j} dt + \frac{1}{\langle \rho \rangle} \frac{\partial}{\partial x_j} \left[\frac{\mu_t}{\sigma_t} \frac{\partial \varphi_{\alpha,n}}{\partial x_j} \right] dt \\ & + \left(\frac{\dot{\omega}_\alpha \varphi_n}{\rho} \right) - \frac{1}{2} \frac{\epsilon}{k} C_\phi (\varphi_{\alpha,n} - \tilde{\varphi}_\alpha) dt \\ & + \left(\frac{2\mu_t}{\rho\sigma_t} \right)^{(1/2)} \frac{\partial \varphi_{\alpha,n}}{\partial x_j} dW_{j,n}, \\ & n = 1, \dots, N_f \text{ and } \alpha = \dots, N_s \end{aligned} \quad (11)$$

The first three terms on the right side of the equation correspond to the 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 is varying in time and denotes a random term caused by turbulence.

By solving the stochastic differential equations of each stochastic field, the evolution law of the mixture fraction and the progress variable 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 ANN, which is used for the storage and interpolation of the flamelet lookup table.

C. ARTIFICIAL NEURAL NETWORKS

Artificial neural network is a machine learning algorithm that attempts to mimic how the human brain processes information. It consists of a large number of neurons, which are connected together and are arranged in layers. Generally, neural networks are structured into three layers: one input layer, one or more hidden layers, and one output layer, as shown in Figure 1, and this network will be described in detail in next section.

III. NUMERICAL SIMULATIONS

A. CHEMISTRY REPRESENTATION

1) SETUP

In order to obtain scalar parameters which are required by the RANS model, a neural network, consisting of five hidden layers of non-linear neurons, was created. As shown in Figure 1, mixture fraction and normalized progress variable were selected as inputs, and a vector of the chemical state, the components of which includes temperature, dynamic viscosity and source term of normalized progress variable, was defined as outputs.

The dataset of the ANN, i.e., the laminar flamelets library, was computed by CHEM1D code [31]. As the resolution in the settings of CHEM1D code increases, which also requires an increase in the number of the nodes of flamelet library, the precision of FGM table will be improved. However, it should be pointed out that the library size increases linearly with the number of table nodes in the control variable space, and the time for ANN training and forward propagation will also increase significantly. In the present study, two different levels of table nodes with resolutions of

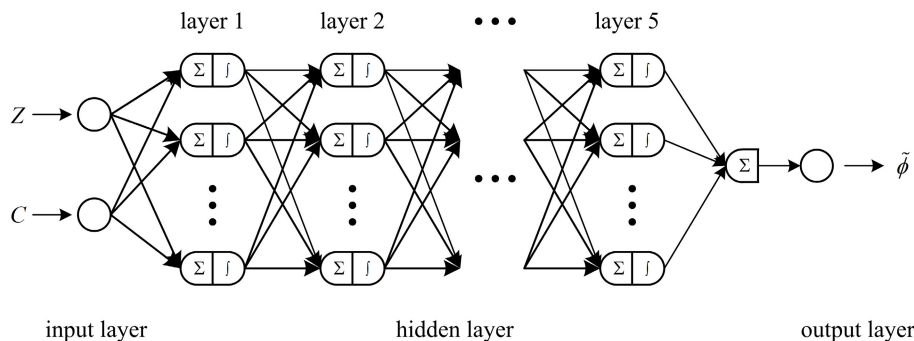


FIGURE 1. Sketch of a multi-layer perceptron that represents the steady flamelet library.

TABLE 1. Memory requirements of different chemistry representation methods. The table size for ANN-ESFFGM refers to the size of the table used for ANN training.

	P-PDF coarse	ESFFGM coarse	ESFFGM fine	ANN-ESFFGM coarse	ANN-ESFFGM fine
Table Size	200×200×200×200	200×200	500×500	200×200	500×500
Memory Requirement	265.6GB	6.9MB	42.2MB	48.9kB	64.6kB

200 × 200 (coarse table) and 500 × 500 (fine table) in the mixture fraction and progress variable spaces, respectively, were applied to check the quality of the ANN-ESFFGM model. Additionally, the number of FGM table nodes in our previous study [18] is the same as the number of the coarse table.

Before training, standardization of all data was performed, which rescales data to have a mean of zero and a standard deviation of unit variance. After a grid search, two different ANNs were selected to be trained with the coarse FGM table and fine FGM table, and the numbers of neurons in each layer in these two ANNs are 30-30-20-20-15 and 30-25-25-30-30, respectively. The network was trained by a multi-layer perceptron regressor with Adam method [32] as the solver for weight optimization. Moreover, 10-fold cross-validation method was used to detect over-fitting, and the scores of 10 tests are all greater than 0.99.

2) MEMORY REQUIREMENT OF CHEMISTRY REPRESENTATION METHODS

Table 1 compares the memory requirements between three structured tables and ANNs. The size of the FGM table for P-PDF method is four orders magnitude than that for ESFFGM method, since both first moment and the second moment of two control variables are needed to generate the flamelet library. Regarding ESFFGM method, library size increases linearly with the number of table nodes in the control variable space, so the cost of memory is affordable when the number of independent variables is less than three. Compared with the previous two FGM table, the memory requirement of ANN is negligible, since only the architecture

and the parameters of the network need to be stored, and as the number of FGM table nodes increases, the memory requirements for the trained ANN does not increase significantly.

B. SIMULATION OF THE SANDIA FLAME D

1) NUMERICAL SETUP

Sandia Flame D in the series of piloted CH_4/air jet flame [33] has been a target of numerous model calculations [18], [19], [27]. The burner investigated was designed by Masri [34] and scalar data was obtained by Raman/Rayleigh/LIF measurements [33], [35]. The Sydney burner consists of a long fuel-pipe that delivers the methane-air mixture with a volume ratio of 1:3 and the Reynolds number is 22400 (average fuel velocity is 49.6m/s and nozzle diameter $d = 7.2$ mm). The experimental database, which includes temperature, velocity and specie mass fraction distributions in both axial and radial directions.

A 2D computational domain (720 × 150mm) with 51957 nodes was used for simulation and a symmetry boundary condition was employed in order to save computational costs. The RANS simulation method used a standard $k - \epsilon$ model and a grid independence study was performed before the numerical investigations.

The simulations were performed with a RANS solver called ANN-ESFFGM, which is based on the open-source finite-volume CFD code OpenFOAM-v2.3.1. Since pressure and velocity are coupled, the solution of both fields were obtained with a two-step approach. The PIMPLE algorithm that originates from merging PISO and SIMPLE was employed in the present study. Second order central differencing scheme was applied for the divergence terms and

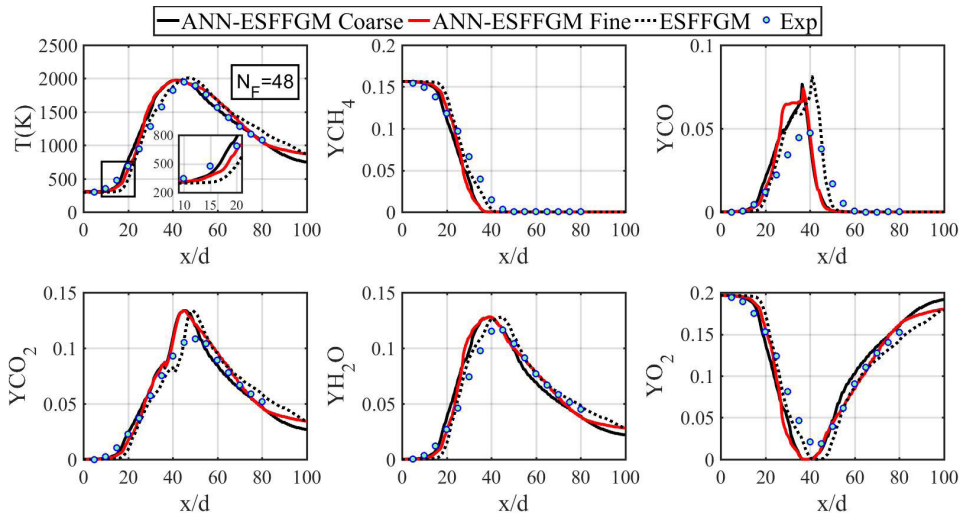


FIGURE 2. Comparison of predicted and measured mean axial temperature and main components mass fraction under the condition of $N_F = 48$.

laplacian terms. The first order Euler integration method was used for the time derivative terms for RANS.

2) RESULTS AND DISCUSSION

In this section, a discussion on the memory requirement of chemistry representation methods was first presented. Then, in order to validate the proposed ANN-ESFFGM model, the simulation results from different table nodes in the flamelet library were compared with the experimental data, including the temperature distribution and species concentrations. To show the advantages of the developed ANN-ESFFGM model, consistent comparisons with our previous numerical results [18] obtained with ESFFGM model were also conducted.

To examine the convergence of the number of stochastic fields N_F , simulations had been carried out for different numbers of N_F (32, 40, 48, 56). Figure 2 shows the comparison of predicted and measured mean axial temperature and main components mass fractions between ANN-ESFFGM model and original ESFFGM model under the condition of $N_F = 48$. The measurement data in the rest of this paper refers to the experimental data in [36]. In general, the proposed ANN-ESFFGM predicts better temperature distribution than the original ESFFGM model and the accuracy of the prediction results of the mass fraction of the main components of the two models is comparable. It is noteworthy that the shortcoming of the original model, which is a delay error of the flame ignition, has been greatly improved. As shown in Figure 2, the ignition position, where the axial temperature began to increase rapidly and CH_4 and O_2 mass fractions began to decline and other products started to appear, was accurately predicted. This advantage of the proposed model can be quantitatively shown in table 2. At the position where $x/d = 20$, the temperature prediction error is shortened

TABLE 2. Comparison of prediction errors of mean axial temperature between different models.

x/d	Measured data (K) [36]	Results in [18]	Coarse ANN	Fine ANN
10	346	14.06%	11.18%	9.63%
20	686	29.77%	12.86%	6.95%
30	1278	9.52%	18.49%	25.62%
40	1825	2.66%	7.78%	7.70%
50	1890	4.80%	2.19%	0.09%
60	1562	7.34%	0.70%	7.74%
70	1277	10.65%	1.27%	5.61%
80	1076	13.48%	0.40%	1.86%
Average error		11.53%	6.86%	8.15%

x/d refers to the flame axial distance divided by the nozzle diameter d. Results in [18] refers to the calculation results of ESFFGM, Coarse ANN and Fine ANN refers to the calculation results of ANN-ESFFGM model trained on a fine and a coarse FGM tables respectively.

to 40%. The reason for this improvement may be that the ANN is able to provide more accurate chemical reaction results over the linear interpolation method used in tabulation techniques, and this advantage is more significant in the flame ignition position where the gradients of scalar properties are relatively large. However, the predicted increase rate of temperature is also a bit faster than the experiment, as reported in our previous study [18], and so are the rates of fuel consumption and the product formation. As can be seen from the average prediction error in Table 2, the usage of ANN to represent chemical reactions significantly improves the accuracy of turbulent combustion simulation under the studied condition. Moreover, it should be noted that the ANN-ESFFGM model with a higher flamelet table resolution (i.e. ANN-ESFFGM fine) does not show a noticeable improvement over the one with a moderate flamelet table resolution (i.e. ANN-ESFFGM coarse).

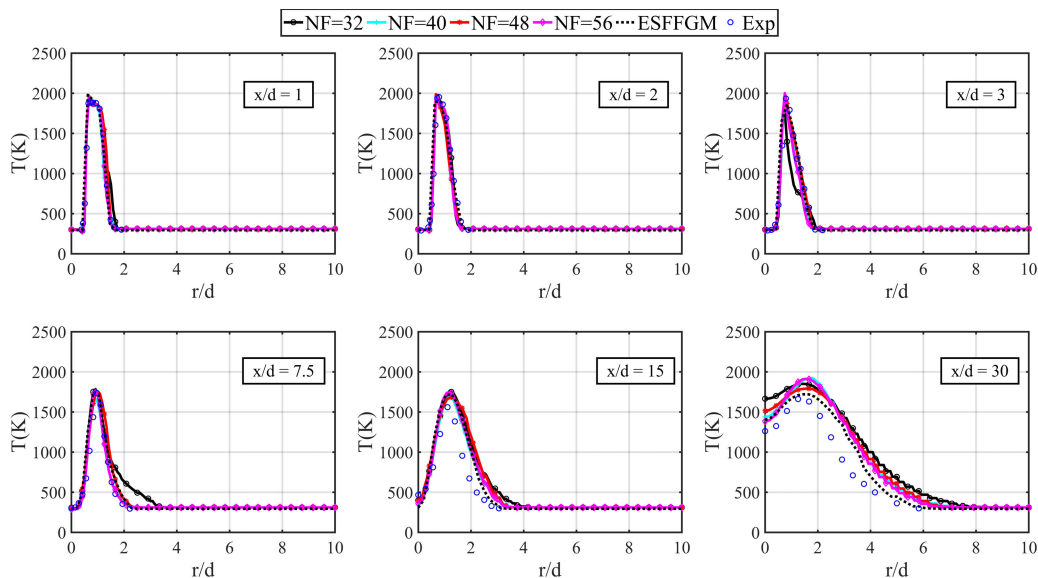


FIGURE 3. Comparison of predicted and measured mean radial temperature at different axial locations.

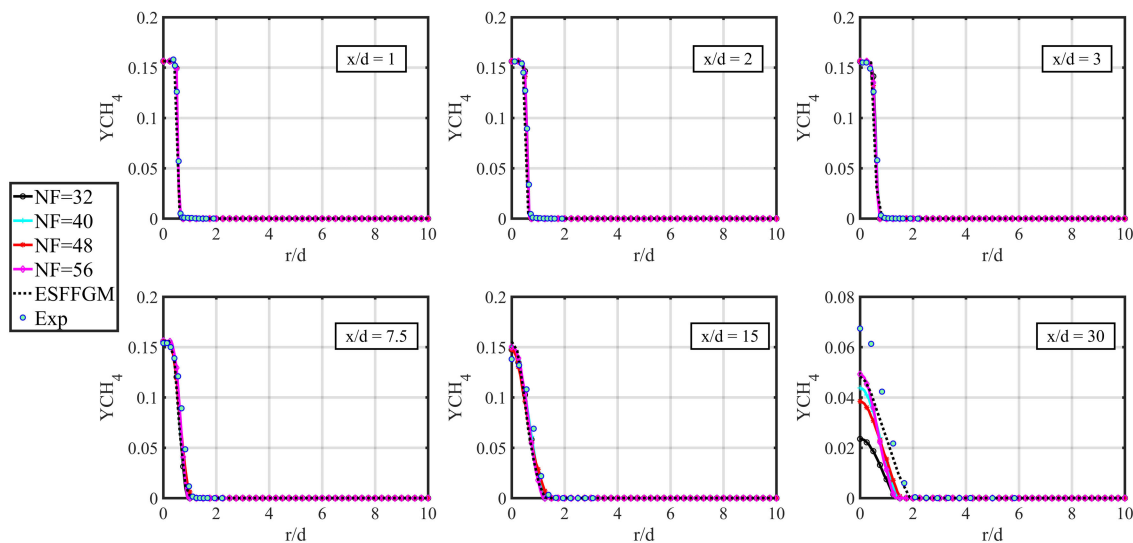


FIGURE 4. Comparison of predicted and measured mean radial CH_4 mass fraction at different axial locations.

Figure 3 shows a comparison of predicted and measured mean radial temperature at the different axial location under the condition of the different number of stochastic fields. The calculated results of the proposed ANN-ESFFGM model with different numbers of stochastic fields and the original ESFFGM with $N_F = 48$ are presented. Overall, these two models show close predictions of the temperature near the fuel inlet (i.e., $x/d < 7.5$), but the ANN-ESFFGM model is better than the original model in prediction of the temperature distribution where flame ignition appears, and both models need to be improved for the temperature prediction of the midstream of the flame. From the results of ANN-ESFFGM

model calculation alone, the temperature distribution can be predicted accurately in 40 fields, which is relatively larger than 24 fields, the number of stochastic fields required by the original model [18]. As shown in Figure 3, with the increase of the number of stochastic fields, the accuracy of the calculated results is constantly improving until the N_F reached to a certain value, 40 in this case, the model results are stable within a certain stage, which indicates that the probability density function of the control variables obtained by the ESF model achieves a statistical convergence.

Figure 4, 6, 5, 6 and 7 show the comparison of predicted and measured mean radial CH_4 , O_2 , CO_2 , and H_2O mass

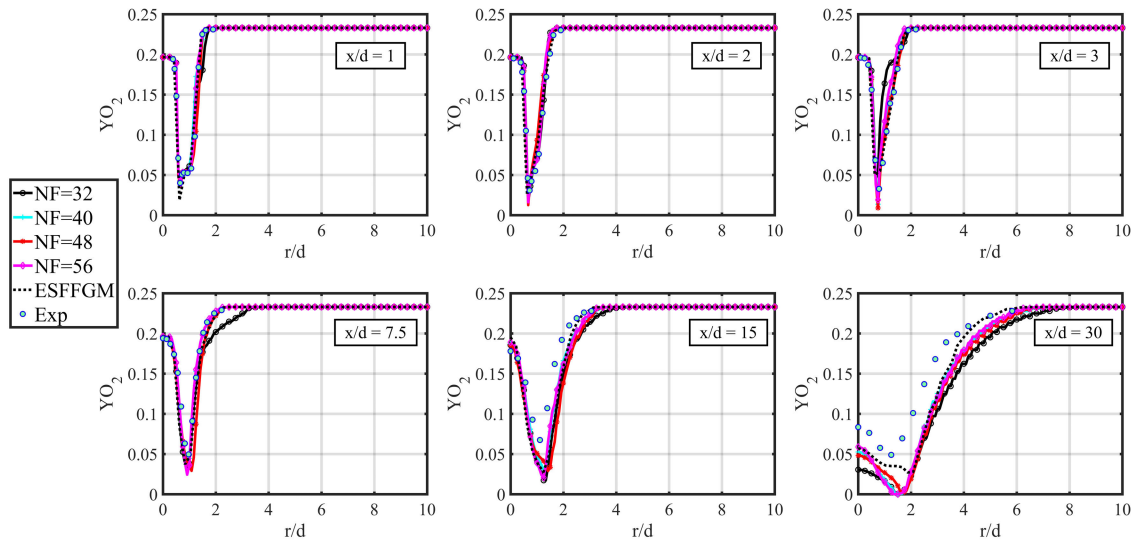


FIGURE 5. Comparison of predicted and measured mean radial O_2 mass fraction at different axial locations.

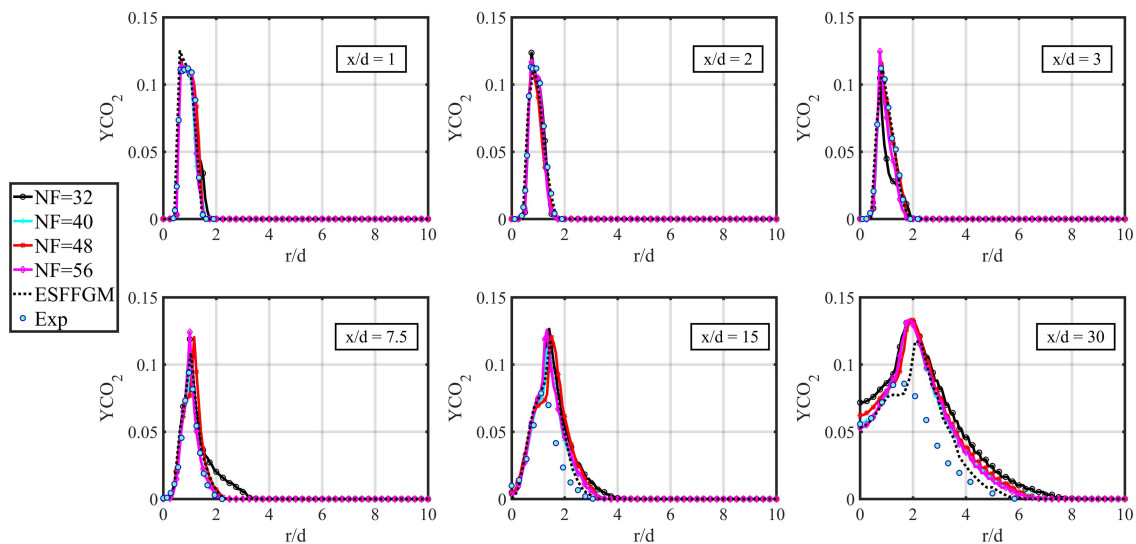


FIGURE 6. Comparison of predicted and measured mean radial CO_2 mass fraction at different axial locations.

fraction at six axial positions respectively. The radial distributions of different axial positions of the ANN-ESFFGM model under different N_F and the original ESFFGM model are presented. As shown in these figures, the more the number of stochastic fields, the more calculated results meet the actual measured values. However, as the distance from the fuel inlet increases, the simulation error continuously increase and the predicted chemical reaction rate is larger than the experiment, and this leads to undervalued mass fraction of reactants and overvalued mass fraction of products. Actually, the prediction of downstream of turbulent flame has always been a challenge, especially for the flamelet-based model, because the flow there is very complicated, and the local chemical

reaction state is difficult to be accurately characterized by a pre-calculated table.

Figure 8 shows the comparison of predicted and measured mean radial OH mass fraction at six axial positions respectively. The radial distributions of different axial positions of the ANN-ESFFGM model under different N_F and the original ESFFGM model are presented. OH is one of the most important intermediate products in the combustion process of hydrocarbon fuels. The detection of OH in a flame can effectively reflect the ignition process of gas fuel. As shown in Figure 8, the accuracy of the predicted OH distributions near the fuel inlet has been greatly improved, so it can be concluded that the ANN strengthens

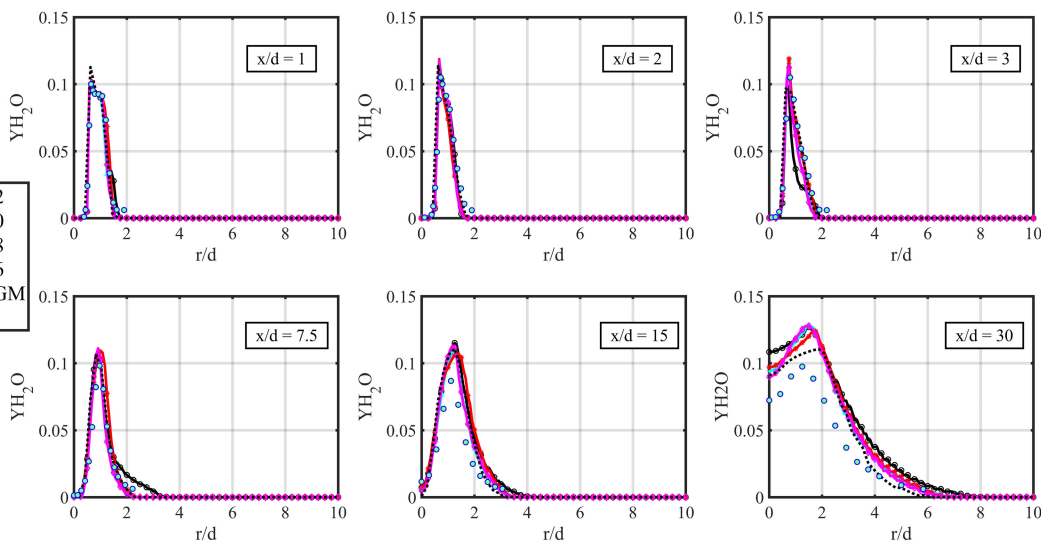


FIGURE 7. Comparison of predicted and measured mean radial H_2O mass fraction at different axial locations.

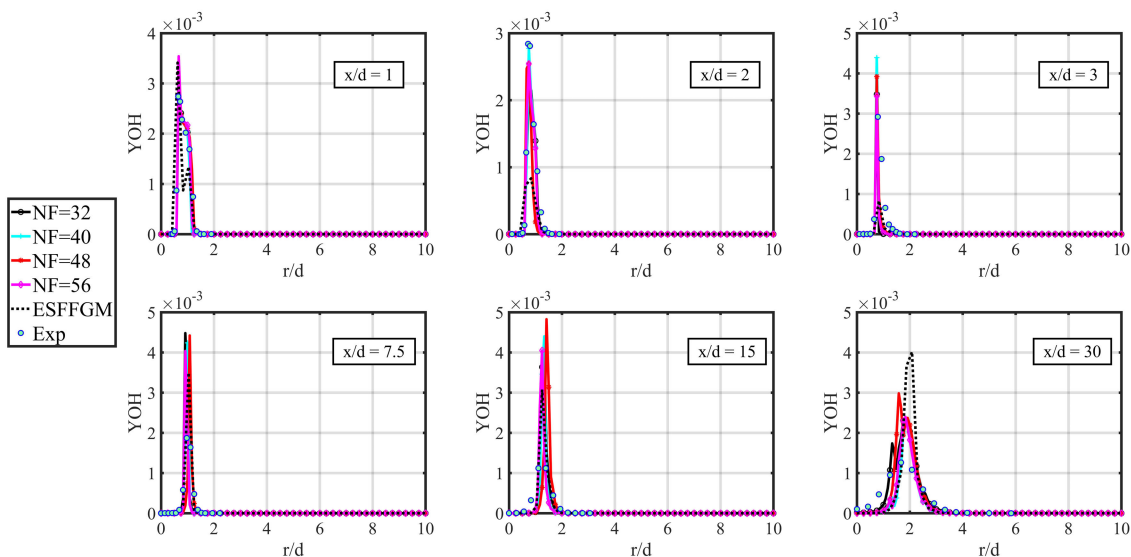


FIGURE 8. Comparison of predicted and measured mean radial OH mass fraction at different axial locations.

the ability to deal with the ignition process of the original model.

IV. CONCLUSION

In the present study, ANN was first employed for the storage and interpolation of the flamelet library in ESFFGM model. In comparison with traditional tabulation method in flamelet-based model, the usage of ANN to store the chemical reactions greatly reduces the memory requirements while ensuring the calculation accuracy. By comparing the results of numerical simulations and experimental measurements of the Sandia Flame D, the accuracy of the proposed ANN-ESFFGM model was verified. Through the numerical investigations on Sandia flame D with different stochastic fields, the following conclusions are obtained:

- 1) By using the ANN to characterize the chemical reactions, the flame simulation accuracy of the new model is higher than that of the original ESFFGM model, especially in the prediction of the ignition position.
- 2) With the increase in the number of stochastic fields, the simulation accuracy of the new turbulent combustion model has been continuously improved until a certain value of N_F is reached.
- 3) Excessively high FGM table resolution has limited improvement in numerical simulation accuracy.

The results presented in this study show that ANN can reliably to characterize the chemical reactions in the flamelet-based models for turbulent combustion simulations. Future work can be carried out from the following two directions. One is to study the applicability of this method in more

complex situations, like spray and coal particles combustion. The second is to employ deep learning method to promote the synergistic melding of physics-based modeling of the governing equations and data-driven modeling of experimental data [37].

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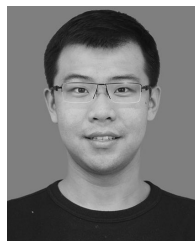
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LIKUN MA received the Doctor of Engineering degree from the Delft University of Defense Technology, in 2016. He was a Lecturer with the National University of Defense Technology. His research interest includes numerical simulation of turbulent spray combustion.



JIARUI ZHANG received the B.S. degree in mechanical engineering from Xi'an Jiaotong University, Xi'an, China, in 2015, and the M.S. degree in aeronautical and astronautical science and technology from the National University of Defense Technology, Changsha, China, in 2017. He is currently pursuing the Ph.D. degree in aeronautical and astronautical science and technology with the National University of Defense Technology.



YIFAN DUAN graduated from the National University of Defense Technology, in 2016. He received the M.S. degree in aeronautical and astronautical science and technology from the National University of Defense Technology, Changsha, China, in 2018. His research interest includes numerical simulation of turbulent combustion.



HONGLAN HUANG was born in Hefei, China, in 1995. She received the B.S. degree in information engineering from Xi'an Jiaotong University, Xi'an, China, in 2017, and the M.S. degree in management science and engineering from National University of Defense Technology, Changsha, China in 2019, where she is currently pursuing the Ph.D. degree in management science and engineering. Her research interests include active learning, reinforcement learning, and one-shot learning.



YANGHE FENG is currently an Associate Research Fellow with the National University of Defense Technology. His research interests include human factors engineering, cognitive computing, deep learning, deep reinforcement learning, and active learning.



ZHIXUN XIA received the Ph.D. degree from the Beijing University of Aeronautics and Astronautics, in 1991. He was a Professor with the National University of Defense Technology. His research interests include aerospace propulsion theory and engineering.



JINCAI HUANG is currently a Professor with the National University of Defense Technology, Changsha, Hunan, China, and also a Researcher of the Science and Technology on Information Systems Engineering Laboratory. His main research interests include artificial general intelligence, deep reinforcement learning, and multiagent systems.

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