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Comparison between a composition PDF transport equation model and an ASOM model for simulating a turbulent jet flame

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Abstract

A composition PDF transport equation (PDF) model and an algebraic second-order moment (ASOM) model of turbulent combustion are used to simulate a methane–air turbulent jet flame, measured by the Sandia National Laboratory. In most regions, both PDF and ASOM predictions are in agreement with the experimental data with not too much difference. The PDF modeling results give the second-order moments with distributions having a similar trend as those given by the ASOM closure model. Although in general the PDF modeling results are somewhat better than the ASOM results, but considering that the computation time of the ASOM model is almost in two orders of magnitude smaller than that of the PDF model, the ASOM model is suggested for simulating large-size engineering facilities.

Keywords: Turbulent combustion; Second-order moment model; Composition PDF transport equation model

1. Introduction

To develop an economical and reasonable turbulent combustion model for simulating practical combustion equipments is obviously important. For simplicity and robusticity in simulating combustors of complex geometry, the eddy break-up (EBU), EBU-Arrhenius model (E-A), and simplified PDF combustion models are widely adopted in commercial codes, such as FLUENT. But in EBU or E-A models, the effect of turbulence is usually dominant, and the effect of chemical kinetics is not properly taken into account. In the simplified PDF model, the assumed PDF is frequently a product of several one-variables PDF's instead of the joint PDF, leading to under-prediction of the reaction rate. At the same time, the PDF transport equation model is more accurate than E-A and simplified PDF models, but computationally is too expensive for simulating practical combustors. The flamelet and CMC combustion models may be a better choice, but they need more studies for their final use. So the engineers are still seeking for an economical and reasonable turbulent combustion model.

Recently, an unconditional second-order moment (SOM) turbulent combustion model was proposed in our laboratory. The computation cost of the SOM model is almost the same as that of the EBU-Arrhenius and simplified PDF models, but the SOM model gives much better results than E-A and simplified PDF models [1]. In the early-developed SOM model, a series expansion approximation is taken for the non-linear exponential term in the reaction rate expression, assuming $E/RT \ll 1$ and $T'/T \ll 1$ and omitting higher order terms [2]. In Ref. [3] this kind of SOM model is used to simulate a methane–air turbulent diffusion flame, including NO formation with a detailed chemical kinetics of 50 species and 300 elementary reactions. The predicted temperature, methane and oxygen concentration are in agreement with the

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Nomenclature

B	pre-exponential factor
C	constant
E	activation energy (J/kmol)
k	turbulent kinetic energy (m/s)
K	reaction-rate coefficient $K = B \cdot \exp(-E/RT)$
$p(\ )$	probability density function (PDF)
R	universal gas constant (J/kmol K)
T	temperature (K)
w	reaction rate (mol/s)
Y	mass fraction

Greek symbols

ε	dissipation rate of turbulent kinetic energy (m^2/s^3)
μ	molecular dynamic viscosity (kg/m s)
ρ	density (kg/m^3)

experimental data, whereas the NO concentration is significantly under-predicted. So, although the early-developed SOM model gives encouraging results in simulating turbulent combustion, but it suffers from serious errors. The reason is that in real combustion processes, especially in NO_x formation, E/RT is much greater than unity and T'/T is not always much less than unity, so the series expansion approximation leads to serious errors. In order to overcome this difficulty, a SOM transport equation model [4] is proposed. In the SOM transport equation model all of the second-order moments, including the correlations of concentration fluctuation with the fluctuation of the reaction-rate coefficient, are closed using a generalized form of transport equations, hence can avoid the series expansion approximation. The SOM transport equation model is already used to simulate a turbulent jet flame [4] and a swirling turbulent combustion with NO formation [1] and the predictions were validated by experimental data. In all those cases, the SOM transport equation modeling results are much better than those obtained using the EBU-Arrhenius model and the simplified PDF model. However, the closure assumptions made in the SOM transport equation model need further theoretical justification. Recently, the validation using large eddy simulation [5] was carried out and it is shown that the closure assumptions are reasonable. Furthermore, for highly shear flows, an algebraic second-order moment (ASOM) model is proposed by dropping the convection and diffusion terms in the transport equations of second-order moments. The correlations in the time-averaged reaction rate expression are closed by algebraic expressions, and they are proportional to the products of the gradients of corresponding time-averaged variables, such as $\overline{Y_1'Y_2'} = C_{YY}\frac{k^3}{\varepsilon^2}\frac{\partial\overline{Y_1}}{\partial x_j}\frac{\partial\overline{Y_2}}{\partial x_j}$. This model is as convenient as the E-A and simplified PDF models, both turbulent and chemical factors are directly considered in the time-averaged reaction rate expression, and it can easily be used with a detailed reaction mechanism.

On the other hand, it is well known that the composition PDF transport equation model is a more accurate and reasonable turbulent combustion model [6] in which the reaction term is an exact one without using any closure models. It can be used in RANS modeling with a detailed chemistry mechanism. The correlation moment of any order can be obtained from the PDF modeling results.

Thus, in this paper, a methane–air turbulent jet flame, i.e. Flame C, measured by the Sandia National Laboratory [7], is simulated using both composition PDF transport equation model and ASOM turbulent combustion model. The predicted time-averaged temperature, species concentration and their root mean square (RMS) values will be compared with the experimental data, and the second-order moments of cross correlations given by the PDF modeling results and the corresponding ASOM modeling results will also be compared.

2. Mathematical models and numerical methods

2.1. The ASOM turbulent combustion model

For an instantaneous reaction rate

$$w_s = B\rho^2 Y_1 Y_2 \exp\left(-\frac{E}{RT}\right) \tag{1}$$

after Reynolds expansion and averaging and neglecting the third-order correlation, the time-averaged reaction rate can be given as

$$\overline{w_s} = \rho^2\left[\left(\overline{Y_1Y_2} + \overline{Y_1'Y_2'}\right)\overline{K} + \overline{Y_1}\overline{K'Y_2'} + \overline{Y_2}\overline{K'Y_1'}\right] \tag{2}$$

where

$$K = B\exp(-E/RT) \tag{3}$$

The concentration fluctuation correlation is closed using a transport equation as

$$\frac{\partial}{\partial t}\left(\rho\overline{Y_1'Y_2'}\right) + \frac{\partial}{\partial x_j}\left(\rho\overline{V_j}\overline{Y_1'Y_2'}\right) = \frac{\partial}{\partial x_j}\left(\frac{\mu_e}{\sigma_{YY}}\frac{\partial\overline{Y_1'Y_2'}}{\partial x_j}\right) + C_1\mu_T\frac{\partial\overline{Y_1}}{\partial x_j}\frac{\partial\overline{Y_2}}{\partial x_j} - C_2\rho\frac{\varepsilon}{k}\overline{Y_1'Y_2'} \tag{4}$$

For highly shear flows, e.g. a jet flame, the correlations of the reaction-rate coefficient fluctuation with the concentration fluctuation $\left(\overline{K'Y_1'}, \overline{K'Y_2'}\right)$ are assumed to be propor-

tional to the products of the gradients of corresponding time-averaged variables, $\frac{\partial \overline{K}}{\partial x_j}\frac{\partial \overline{Y}_1}{\partial x_j}$, $\frac{\partial \overline{K}}{\partial x_j}\frac{\partial \overline{Y}_2}{\partial x_j}$.

It is called an algebraic SOM (ASOM) model, so we have

$$\overline{K'Y'} = C_{K,Y}\frac{k^3}{\varepsilon^2}\frac{\partial \overline{K}}{\partial x_j}\frac{\partial \overline{Y}}{\partial x_j} \tag{5}$$

where $C_{K,Y}$ is a model constant, taken as 0.005. Thus, the ASOM model is a kind of gradient modeling. The time-averaged reaction-rate coefficient is only a function of temperature fluctuation, it is:

$$\overline{K} = \int B\cdot\exp(-E/RT)p(T)\mathrm{d}T \tag{6}$$

where $p(T)$ is the probability density function of temperature, and assuming a bi-delta distribution gives:

$$\bar{k} = \left\{\exp\left[-E/R\left(T+g_T^{1/2}\right)\right]+\exp\left[-E/R\left(T-g_T^{1/2}\right)\right]\right\}\Big/2g_T = \overline{T'^2} \tag{7}$$

2.2. The composition PDF transport equation model

The composition PDF transport equation model solves the mass and the momentum conservation equations using a RANS turbulence model and replaces the energy and species conservation equations by a single-point joint PDF transport equation [6]:

$$\frac{\partial}{\partial t}(\rho P)+\frac{\partial}{\partial x_i}(\rho u_i P)+\frac{\partial}{\partial \psi_k}(\rho S_k P) = -\frac{\partial}{\partial x_i}\left[\rho\langle u_i''|\psi\rangle P\right]+\frac{\partial}{\partial \psi_k}\left[\rho\left\langle\frac{1}{\rho}\frac{\partial J_{i,k}}{\partial x_i}\middle|\psi\right\rangle P\right] \tag{8}$$

where P is the Favre-averaged joint PDF of composition and is solved using a Monte Carlo method. The turbulent scalar flux term is modeled by the gradient diffusion assumption:

$$-\frac{\partial}{\partial x_i}\left[\rho\langle u_i''|\psi\rangle P\right] = \frac{\partial}{\partial x_i}\left(\frac{\mu_t}{\rho Sc_t}\frac{\partial P}{\partial x_i}\right) \tag{9}$$

The mixing term is closed using an IEM model [8].

2.3. Reaction mechanisms and specific heat capacity

A detailed reaction mechanism, i.e. DRM22 [9], with 23 species and 102 elementary reactions is applied in the composition PDF transport equation model, while a global one-step reaction rate [10] is taken in the ASOM model:

$$\omega_{\mathrm{fu}} = 2.119\times10^{11}Y_{\mathrm{ox}}^{1.3}Y_{\mathrm{fu}}^{0.2}\exp(-2.027\times10^{8}/RT) \tag{10}$$

In both models the specific heat capacity is a piecewise polynomial of temperature, for instance, the c_{p} (J/kg K) of methane between 300 K and 1000 K is:

$$c_p = 403.585+9.0573T-0.014425T^2+1.58052\times10^{-5}T^3-6.343\times10^{-9}T^4 \tag{11}$$

2.4. Simulation of a methane–air jet flame

Fig. 1 gives the geometrical configuration and sizes of the simulated piloted methane–air turbulent jet flame, i.e. Flame C, measured in Sandia National Laboratory [7]. The dimensions are for the diameter. The central jet consists of 25% methane and 75% dry air in volume, and its inlet velocity is 29.7 m/s, inlet temperature is 294 K. In the PDF modeling, the annular jet contains hydrogen-air combustion products, composed of 0.11 carbon dioxide, 0.004 carbon monoxide, 0.092 water, 0.056 oxygen and nitrogen in mass fraction with an inlet bulk temperature of 1903 K and inlet velocity of 6.8 m/s. In the ASOM modeling, for the sake of simplicity the annular jet is assumed to be only nitrogen with the same inlet bulk temperature of 1903 K and inlet velocity of 6.8 m/s. The co-flow air velocity is 0.9 m/s, and its temperature is 291 K. The computation domain is taken from 36 mm before the jet exit to 0.72 m after it. Both models use the same two-dimensional grid nodes, as shown in Fig. 2. The total grid number is 2352 and the grid size near the jet inlet is about 0.5 mm.

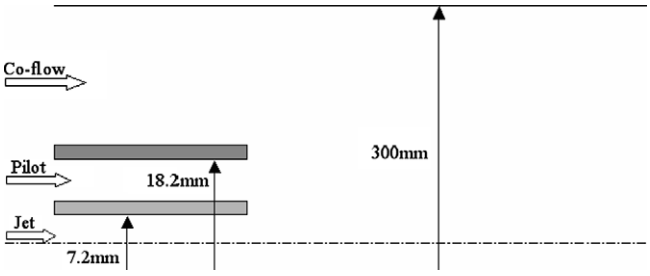

Fig. 1. The geometry of Flame C.

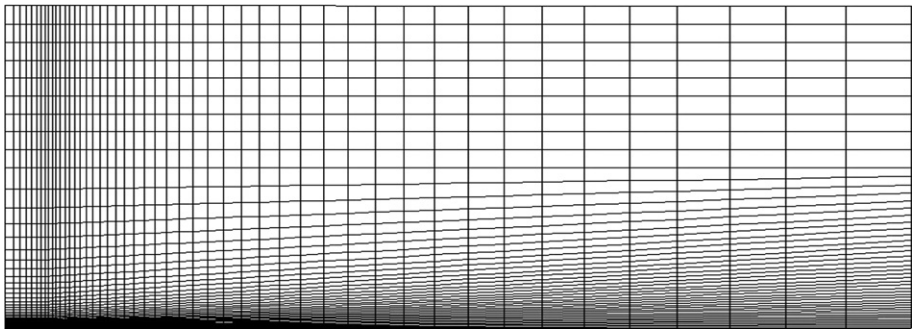

Fig. 2. The grid arrangement.

A second-order upwind scheme is used, and the SIMPLEC algorithm for pressure–velocity corrections is adopted. The composition PDF transport equation model is chosen from FLUENT 6.1 [11] and the ASOM model is incorporated into FLUENT 6.1 by using the UDF (user-defined function) procedure. The Reynolds stress turbulence model (RSM) is used together with the PDF model or the ASOM model. Running a case in a PC with 1.8G CPU and 1024 M memory needs more than 50 h for the composition PDF transport modeling while needs less than 0.5 h for the ASOM modeling.

3. Results and discussion

Fig. 3 shows the predicted time-averaged temperature using two models in comparison with the experimental data. The PDF modeling results are in good agreement with the experimental data; while the ASOM modeling results are also in general agreement with the experimental data, except at cross sections of $x = 7.5d$ and $x = 15d$, where the temperature is over-predicted. So, generally speaking, both models give good results and the PDF model is somewhat better. Figs. 4 and 5 show the time-averaged methane and oxygen concentration respectively. At all cross sections both models give the results near to the experimental data. Again, the PDF modeling results are somewhat better at some cross sections.

Considering that the PDF model uses detailed reaction mechanism and solves Lagrangian equations using the Monte Carlo algorithm, free of numerical diffusion; whereas the ASOM model uses one-step global reaction mechanism and finite-difference method with numerical diffusion, but the average discrepancies between experimental data and PDF model results are about 10%, and are about 17% for the ASOM model, and the ASOM model needs only 1% of the computation time that needed by the PDF model, we can conclude, that the ASOM model is a reasonable and economical one and it is

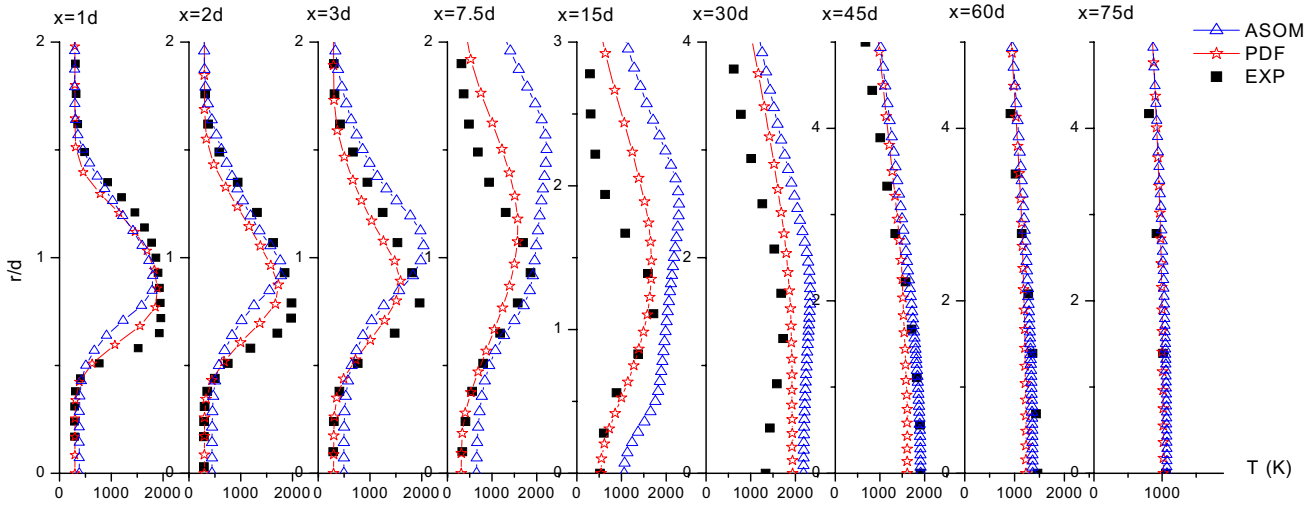

Fig. 3. Time-averaged temperature.

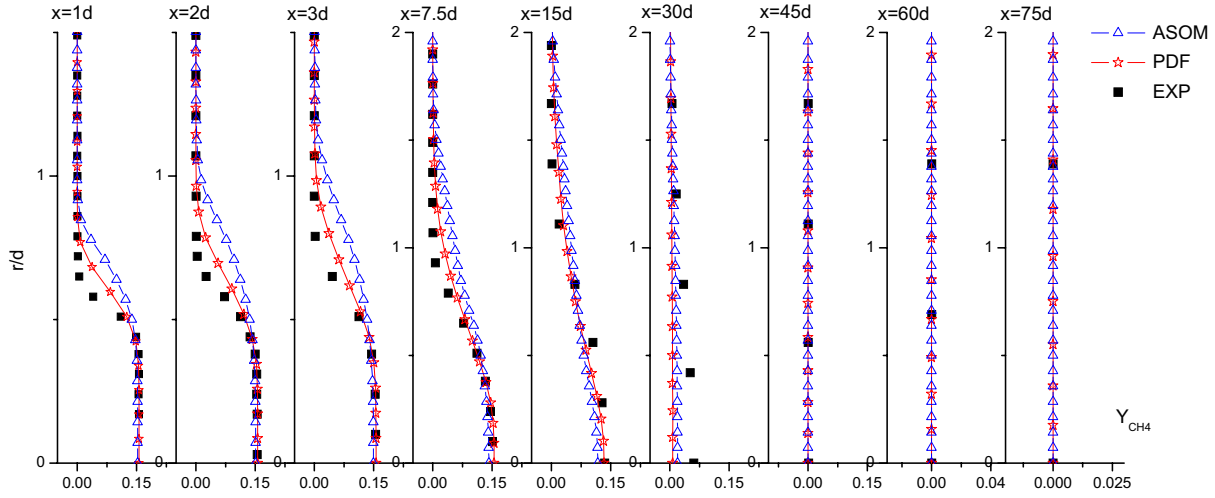

Fig. 4. Time-averaged methane concentration.

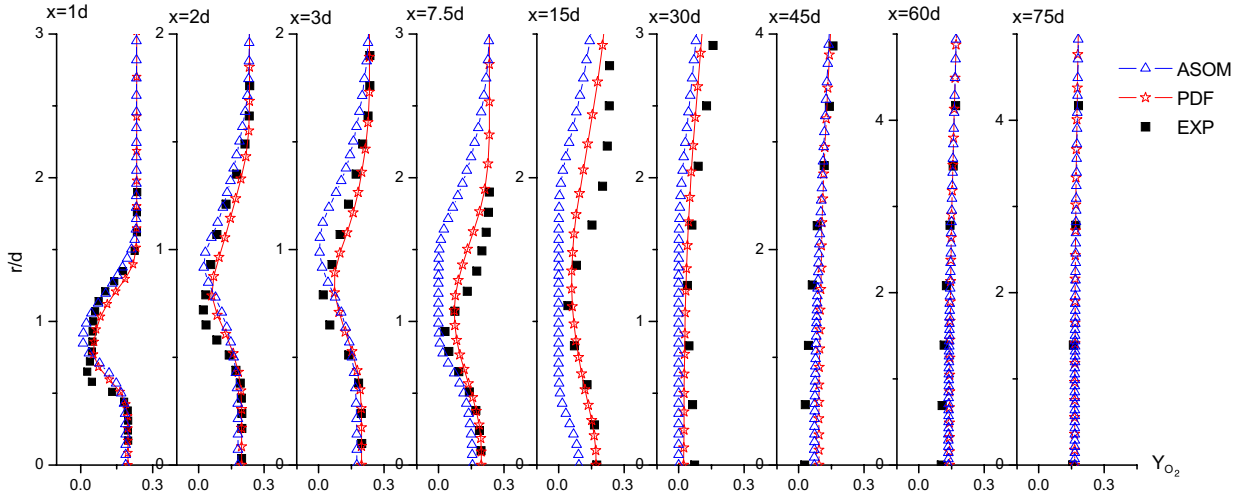

Fig. 5. Time-averaged oxygen concentration.

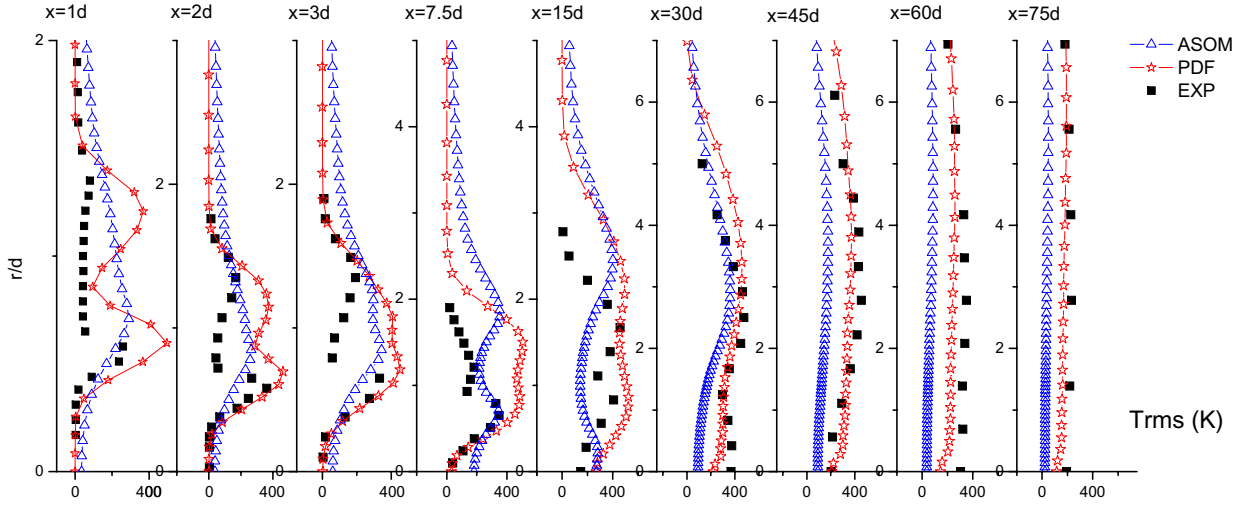

Fig. 6. RMS value of temperature fluctuation.

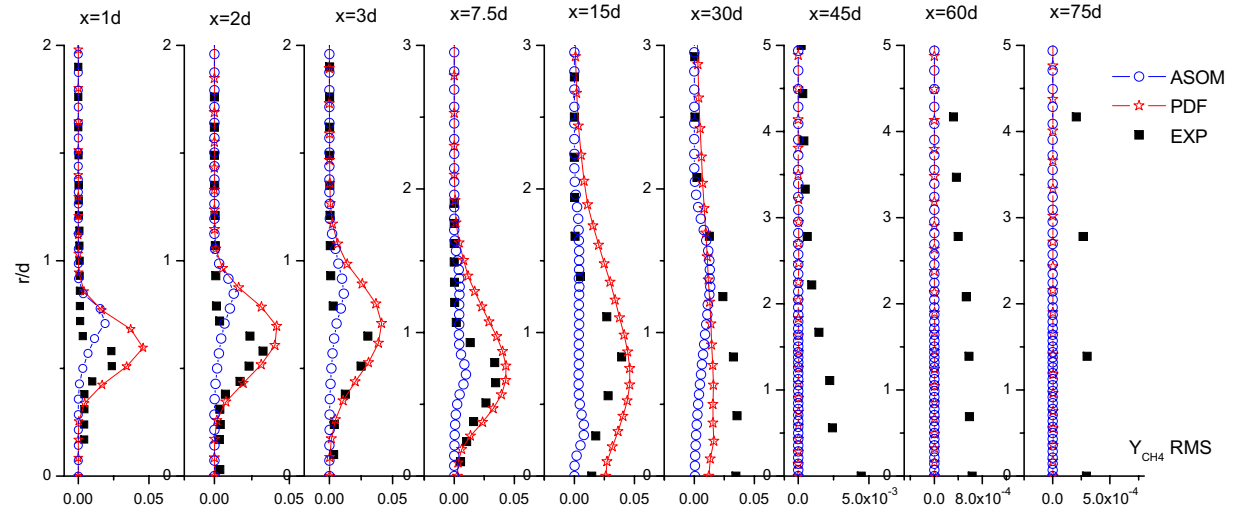

Fig. 7. RMS value of methane concentration fluctuation.

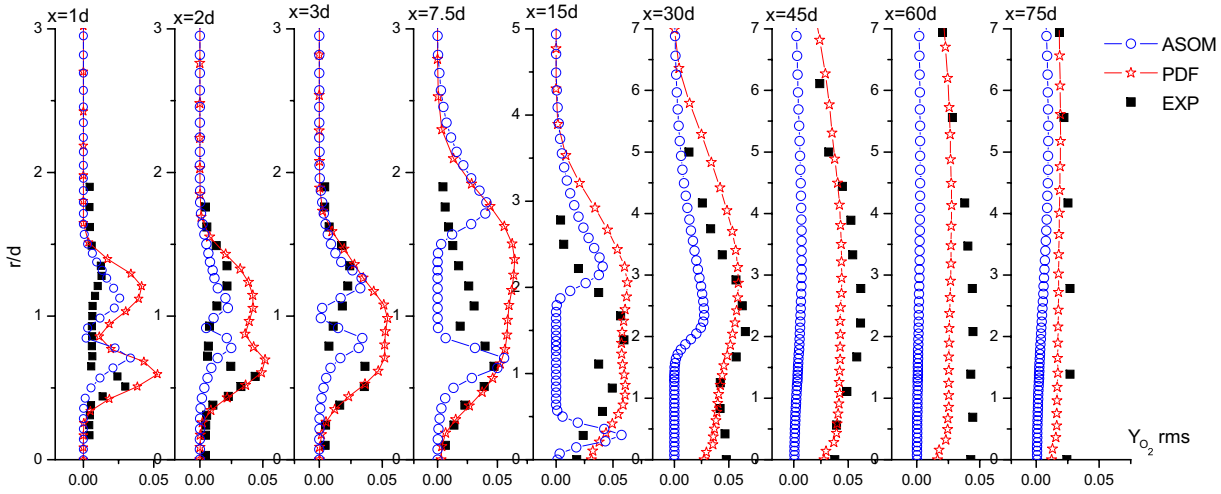

Fig. 8. RMS value of oxygen concentration fluctuation.

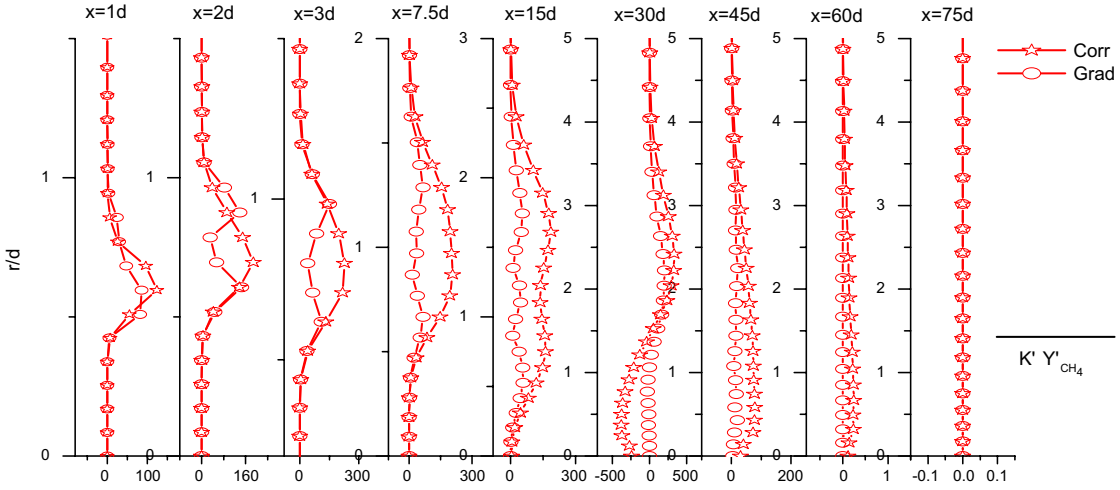

Fig. 9. The correlation $\overline{K'Y'_{CH_4}}$ and the corresponding product of gradients.

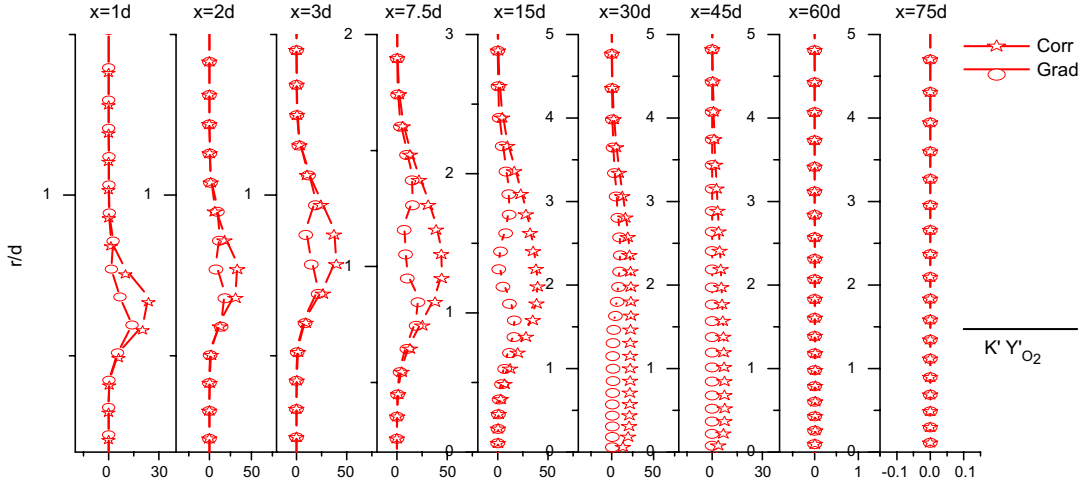

Fig. 10. The correlation $\overline{K'Y'_{O_2}}$ and the corresponding product of gradients.

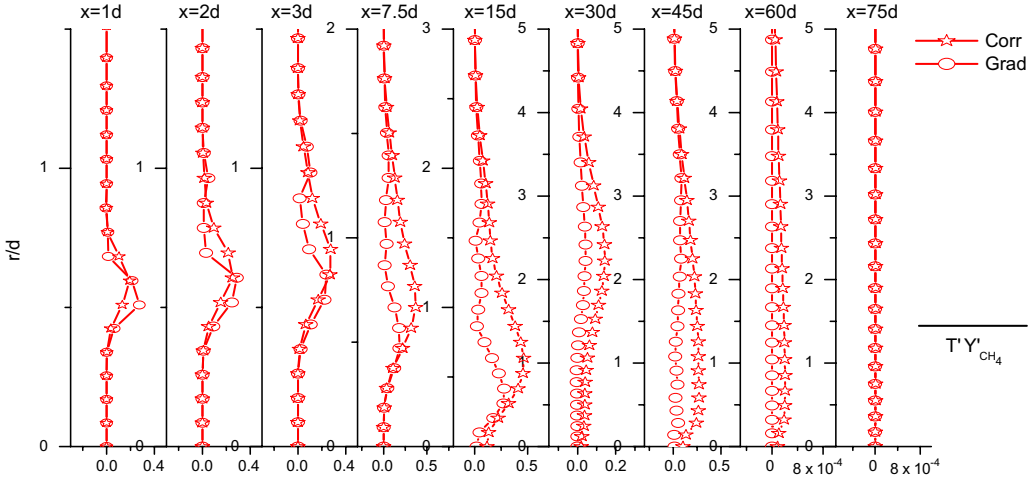

Fig. 11. The correlation $\overline{T'Y'_{CH_4}}$ and the corresponding product of gradients.

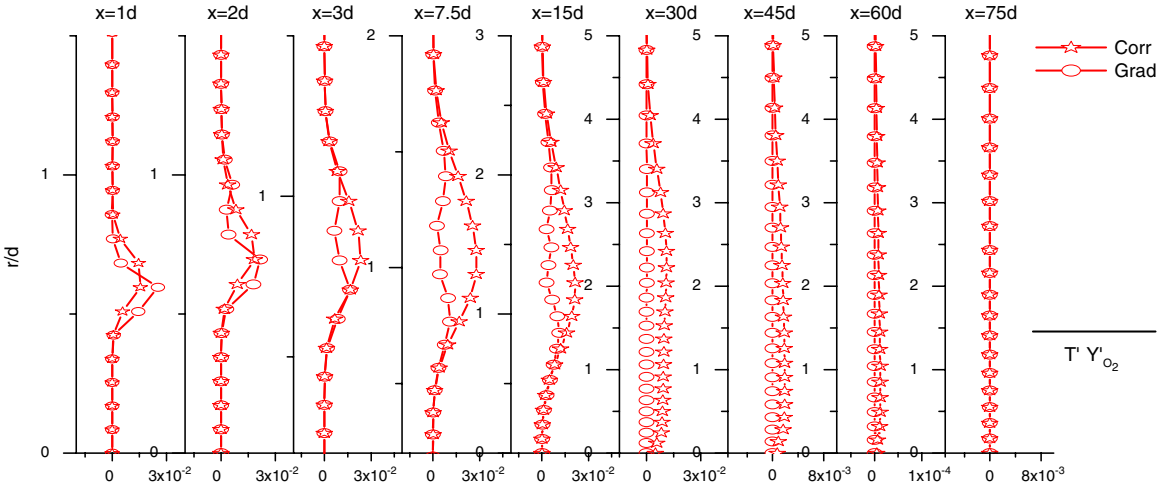

Fig. 12. The correlation $\overline{T'Y'_{O_2}}$ and the corresponding product of gradients.

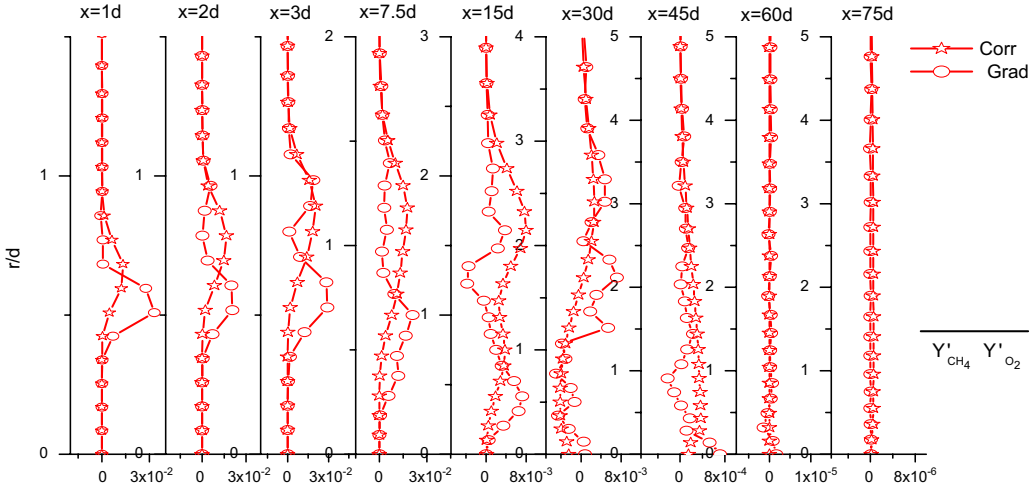

Fig. 13. The correlation $\overline{Y'_{CH_4}Y'_{O2}}$ and the corresponding product of gradients.

suggested to be used in simulating practical large-size engineering facilities.

The root mean square (RMS) values of temperature, methane concentration and oxygen concentration fluctuation are given in Figs. 6–8, respectively. Both models give the results close to the experimental data, but the agreement is not as good as that for the time-averaged values. Again, the PDF modeling results are somewhat better. For example, the PDF model can predict the two-peak RMS value of temperature fluctuation in the region near the jet exit, observed in experiments, whereas the ASOM model cannot.

The correlations (denoted as *corr* in the figure) taken from the PDF modeling results and the products of the gradients (denoted as *grad* in the figure) for corresponding time-averaged variables are shown in Figs. 9–13. It can be seen that in most regions the distributions of correlations of the methane concentration fluctuation with the oxygen concentration fluctuation, the temperature fluctuation with the methane/oxygen concentration fluctuation, and the reaction-rate coefficient fluctuation with the methane/oxygen concentration fluctuation, have a trend similar to that of the product of the gradients of corresponding time-averaged variables. Fig. 14 gives this relationship in a more general way, i.e. the correlation is approximately proportional to the product of gradients (denoted as *PG* in the figure) of corresponding time-averaged variables, which is illustrated as a dash line, the closure assumption in the ASOM model.

Fig. 15 shows the relative values of the correlations, which are the correlations, divided by the product of corresponding time-averaged variables and represent the relative importance of each term in Eq. (2). It can be seen that the correlation terms containing the reaction-rate coefficient fluctuation are larger than unity, whereas the correlation terms containing only concentration fluctuations are smaller than unity. These results can also be obtained from the simulation using the ASOM model.

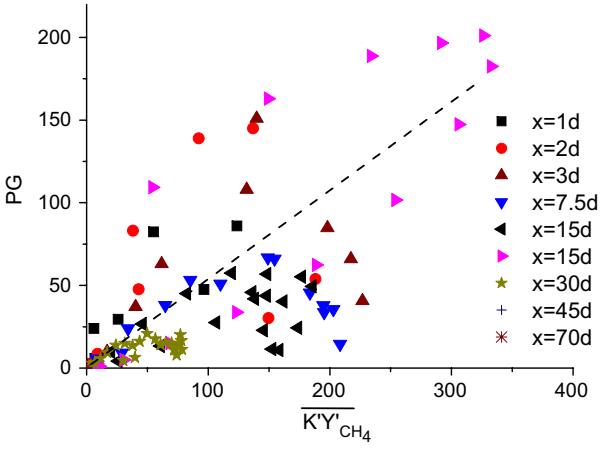

Fig. 14. The relationship between the correlation and the product of gradients.

4. Conclusions

(1) Both PDF and ASOM modeling results for a methane–air turbulent jet flame simulation are in agreement with the experimental data measured by Sandia State Laboratory with not too much difference. Although the ASOM model is not as accurate as the PDF transport model, while the ASOM model can significantly reduce the computational cost, so it is suggested for simulating large-size engineering facilities.

(2) The PDF model gives the second-order moments, similar to those given by the ASOM model.

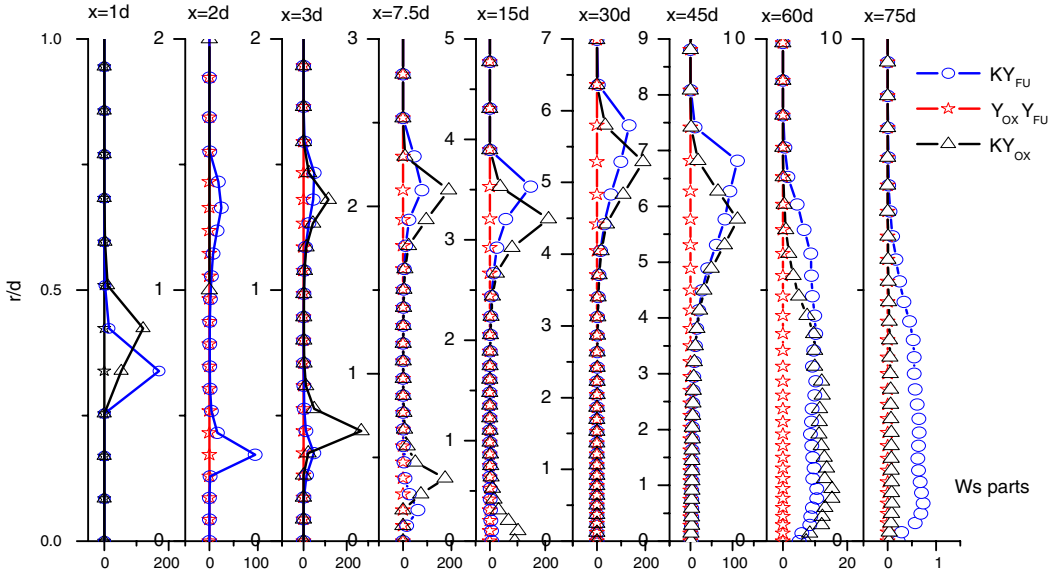

Fig. 15. The relative values of the correlations.

(3) The correlations containing the reaction-rate coefficient fluctuation are more important to the time-averaged reaction rate.

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