Modeling of Turbulent Jet Nonpremixed Flames Using a Scalar Combined PDF/Moment Method

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Introduction

The usefulness of probability density function (PDF) approaches has been demonstrated in modeling of a variety of turbulent combustion systems, including premixed and nonpremixed combustion systems. The greatest advantage of this approach against conventional moment approaches is to be able to exactly treat the reaction process as widely documented (Pope, 1985). However, the PDF method also can not avoid a hierarchy of closure problem like conventional moment methods. In one-point PDF methods commonly employed in combustion studies, the PDF transport processes by the molecular mixing, the momentum diffusion and the fluctuating pressure have to be modeled because these processes require high-order information. The modeling of these processes is challenging problems in this approach.

The PDF evolution is solved as an ensemble of notional fine grained particles by the Monte-Carlo method, leading to costly calculations. Therefore, it is very natural that a scalar PDF method is employed together with conventional moment methods in terms of the flow field, without the loss of the above advantage of the PDF method.

There is another problem of the PDF method attributable to the Monte-Carlo method. The numerical error is inversely proportional to a root of the number of Monte-Carlo particles (Pope, 1981). This means an exponential increase of calculations to obtain higher-order accuracy and may decrease the above mentioned advantage. Our previous comparative study between the scalar PDF method and the flamelet model method revealed that relative large errors occur in regions where the transport probability of PDF decreases (Noda, 2002). This problem may be resolved with a help of the moment method which is superior in terms of both the numerical resolution and the calculation cost. The PDF method is modeled to reproduce both the mean and the variance obtained by the conventional moment methods. Thus we can now propose a scalar combined PDF/moment method, in which the scalar PDF transport equation and scalar moment equations are simultaneously analyzed to match the low moments. Therefore, the present scalar combined PDF/moment method does not mean the conventional scalar PDF method which calculates only the flow field by moment

methods. In the present paper, we have verified usefulness of the scalar combined PDF/moment method through a comparison of the scalar PDF, the conventional flamelet model, and the present methods in the configuration of a turbulent jet nonpremixed flame.

Scalar combined PDF/moment method

The present scalar combined PDF/moment method is based on the conserved scalar concept to facilitate the evaluation of accuracy. The flow field is solved by the k-ε 2 equation model. The target flame is a turbulent jet nonpremixed flame (H3 flame) opened on a web site by the international workshop on measurement and computation of turbulent nonpremixed flames.

The present idea is to correct deviations of the mean and the variance of PDF from the corresponding values obtained from the moment equations. This is based on that the modeled transport equation of PDF ensures the conventional moment equations of mean and variance. The deviations take place in regions where the transport probability of PDF decreases, reflecting to the accuracy of the Monte-Carlo method.

A modeled scalar PDF transport equation in terms of the mixture fraction, Z, is as

$$\tilde{u}\frac{\partial \tilde{P}(Z;\boldsymbol{x})}{\partial \mathrm{x}}+\tilde{v}\frac{\partial \tilde{P}(Z;\boldsymbol{x})}{\partial r}=\frac{1}{\bar{\rho} r}\frac{\partial}{\partial r}\left(r\frac{\mu_{eff}}{\sigma_Z}\frac{\partial \tilde{P}(Z;\boldsymbol{x})}{\partial r}\right)+E(Z;\boldsymbol{x}) \quad , \tag{1}$$

where the standard notations are used with the molecular mixing term of E. The Schmidt number σ_Z=0.7. The turbulent diffusion process of the first term on the rhs is modeled by the gradient diffusion concept. The molecular mixing process is modeled by IEM model (Dopazo, 1975). Equations of the mean and the variance of the mixture fraction are as

$$\bar{\rho}\tilde{u}\frac{\partial \tilde{\zeta}}{\partial x}+\bar{\rho}\tilde{v}\frac{\partial \tilde{\zeta}}{\partial r}=\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\mu_{eff}}{\sigma_Z}\frac{\partial \tilde{\zeta}}{\partial r}\right) \tag{2}$$

$$\bar{\rho}\tilde{u}\frac{\partial \tilde{\zeta}''^2}{\partial x}+\bar{\rho}\tilde{v}\frac{\partial \tilde{\zeta}''^2}{\partial r}=\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\mu_{eff}}{\sigma_Z}\frac{\partial \tilde{\zeta}''^2}{\partial r}\right)+C_{g1}\mu_t\left(\frac{\partial \tilde{\zeta}}{\partial r}\right)^2-C_{g2}\bar{\rho}\frac{\varepsilon}{k}\tilde{\zeta}''^2 \quad , \tag{3}$$

where ζ is the random variable of mixture fraction. The constants σ_Z, σ_g, C_{g1} and C_{g2} are ascribed the standard values 0.7, 0.7, 2.8, and 1.92. The modeled scalar PDF equation produces C_{g1}=2.85 and C_{g2}=2.0. Therefore, the mean and the variance of mixture fraction obtained from eq.(1) must be matched the values from the eqs. (2) and (3) within an error coming from the differences of the constants. The present algorithm to match them is simply as follows,

1) the probability density function $\tilde{P}(Z;\boldsymbol{x})$ is corrected to match the mean value obtained by eq.(2), according to the ratio of the Courant number to the Fourier number and 2) the resulting difference of the variance by step 1) is corrected by the molecular mixing process.

Results and discussion

The present scalar combined PDF/moment method is assessed in the configuration of a turbulent jet nonpremixed flame (H3 flame of TNF workshop). Hydrogen/nitrogen mixture of 1:1 by volume is issued from a burner of 8mm i.d. in an ambient air flow with a velocity of 0.2m/s. A number of the Monte-Carlo particles are 400. The flamelet structure is based on the infinite reaction rate chemistry

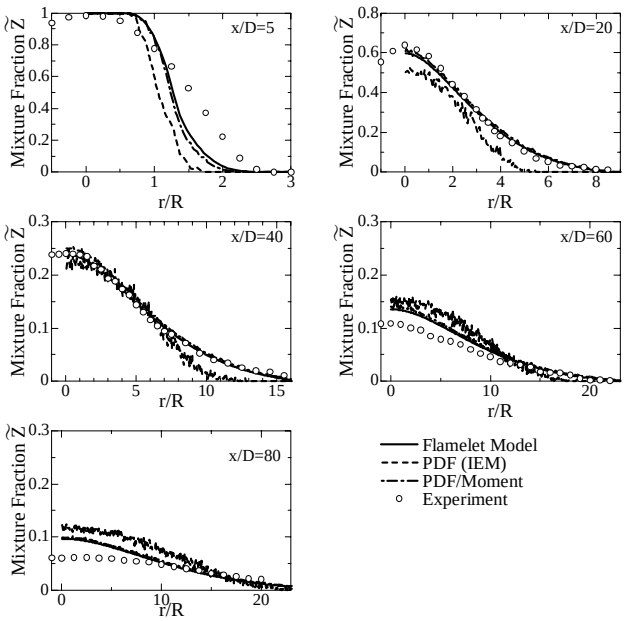

Fig.1 Radial profiles of the measurements and predictions for $\tilde{Z}$.

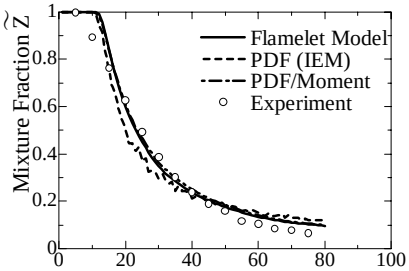

Fig.2 Axial profiles of the measurements and predictions for $\tilde{Z}$.

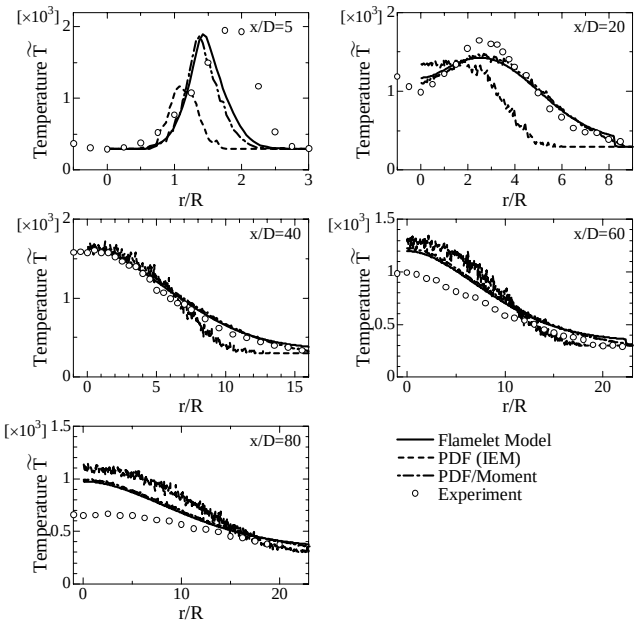

Fig.3 Radial profiles of the measurements and predictions for $\tilde{T}$.

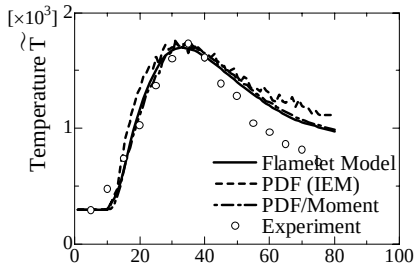

Fig.4 Axial profiles of the measurements and predictions for $\tilde{T}$.

of hydrogen and oxygen.

Figures 1 - 4 show comparisons of the measurements and predictions in terms of the mixture fraction and the temperature. The prediction of the scalar PDF method deviates from the predictions of the flamelet model and the present method. Results obtained by the present method are very close to ones by the flamelet model method.

Figures 5 and 6 show comparisons of PDFs predicted by three methods; the flamelet model, the scalar PDF, and the scalar combined PDF/moment methods. The flamelet model and the present methods show an excellent agreement, but the scalar PDF predictions deviate from the formers. The scalar PDF method must include an error of the transport of PDF's in the downstream region and the boundary region of flame where the transport probability is decreased. The present method has resolved the problem.

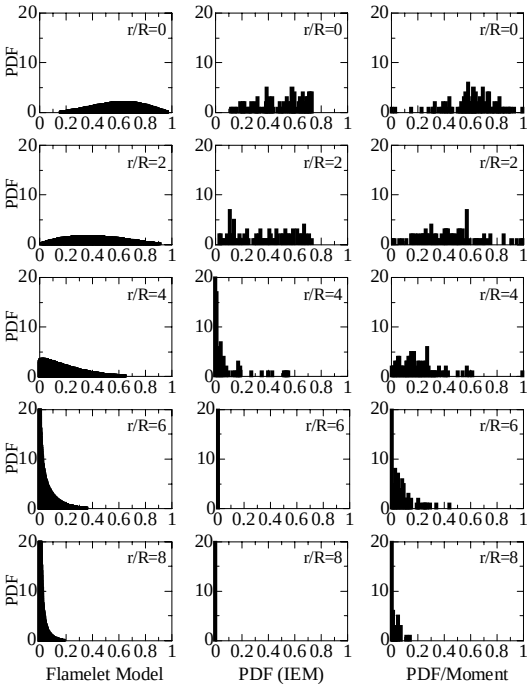

Fig.5 PDFs of mixture fraction at x/D=20

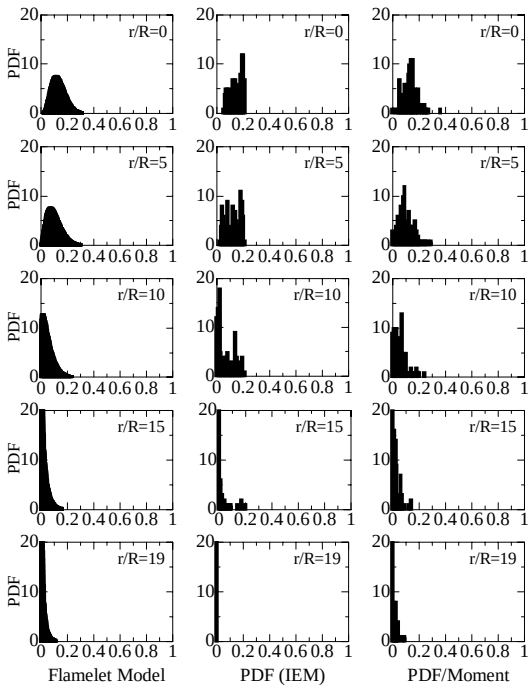

Fig.6 PDFs of mixture fraction at x/D=60

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