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An evaluation of beta PDF integration using the density-weighted PDF and the un-weighted PDF

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Abstract

In many turbulent combustion models, the mean values of scalars are often calculated by integrating the product of the scalar profile and the probability density function (PDF) over mixture fraction space. For the integration, researchers used the weighted and the un-weighted PDF interchangeably depending on their preference. For both PDFs, a β-function is normally presumed. However, a recent study by Liu et al. [Internat. J. Therm. Sci. 41 (2002) 763–772] showed that the predicted mean values of scalars might be significantly different depending on the employed PDF. This paper determines the reason for the difference and shows that the same result can be predicted by using the proper parameters in conjunction with the un-weighted PDF.

Keywords: Probability density function; Turbulent combustion; Modeling; CFD

1. Introduction

Many advanced turbulent combustion models share the basic assumption that the instantaneous scalar values such as the species concentration, temperature and density are related to a conserved scalar such as the mixture fraction. In these models, their average values may be obtained by integration if such relations and the shape of the probability density function (PDF) of the mixture fraction is previously known. For example, the mean values of any scalars can be calculated by:

$$\bar{\phi} = \int \phi(z) P(z)\,\mathrm{d}z \tag{1}$$

In a similar way, the density weighted Favre mean values are obtained by:

$$\tilde{\phi} = \frac{1}{\bar{\rho}} \int \rho\phi(z) P(z)\,\mathrm{d}z \tag{2}$$

As in the work of Bilger [2], the density-weighted PDF (Favre PDF) can be defined as:

$$\widetilde{P}(z) = \frac{\rho P(z)}{\bar{\rho}} \tag{3}$$

and can be used in the calculation of the mean values. Then, the Reynolds and Favre mean values are obtained by the following ways, respectively:

$$\bar{\phi} = \bar{\rho} \int \frac{\phi(z)}{\rho} \widetilde{P}(z)\,\mathrm{d}z \tag{4}$$

$$\tilde{\phi} = \int \phi(z) \widetilde{P}(z)\,\mathrm{d}z \tag{5}$$

The PDFs, $P(z)$ and $\widetilde{P}(z)$, have been used interchangeably in previous studies depending on the preference of the researchers. Whether the density-weighted PDF is used [4–7] or the un-weighted PDF is used [8–10], the shape of the PDF is normally presumed to be given by the β-function:

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Nomenclature

$P(z)$	un-weighted probability density function of mixture fraction
$\widetilde{P}(z)$	density-weighted probability density function of mixture fraction
$\tilde{z}$	Favre mean mixture fraction
$\widetilde{z''^2}$	Favre mean mixture fraction variance
$\bar{z}$	Reynolds mean mixture fraction
$\overline{z'^2}$	Reynolds mean mixture fraction variance
α	β-PDF parameters
β	β-PDF parameters
Γ	gamma function
ϕ	scalar variable
k	turbulent kinetic energy
ε	dissipation rate of turbulent kinetic energy
ρ	density

Subscript

R	corrected for Reynolds averaging input

$$P(z)=\widetilde{P}(z)=\frac{z^{\alpha-1}(1-z)^{\beta-1}}{\int_0^1 z^{\alpha-1}(1-z)^{\beta-1}\,\mathrm{d}z}=\frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}z^{\alpha-1}(1-z)^{\beta-1} \tag{6}$$

The parameters of the β-PDF are related to the Favre mean mixture fraction and its variance by:

$$\alpha=\tilde{z}\left(\frac{(1-\tilde{z})\tilde{z}}{\widetilde{z''^2}}-1\right) \tag{7}$$

$$\beta=(1-\tilde{z})\left(\frac{(1-\tilde{z})\tilde{z}}{\widetilde{z''^2}}-1\right) \tag{8}$$

The PDF is defined for the region where: $(1-\tilde{z})\tilde{z}/\widetilde{z''^2}-1\geqslant 0$. The Favre mean mixture fraction and its variance are calculated from the computational fluid dynamics code. When it is considered that the PDF is approximated, not the exact form, it seems reasonable that the β-PDF is used for the density weighted PDF as well as the un-weighted PDF as long as the final mean values are reasonably predicted.

However, a recent study by Liu et al. [1] showed that the mean density can be significantly different depending on whether the Favre PDF (density weighted) or the un-weighted PDF is used. The current authors confirm this difference for the mean temperature as well as the mean density through this study. The mean temperature and density field have a significant effect on the flow field. Despite the discrepancy in the results from the two methods, a systematic study has not yet been done to explore the differences between the two methods and their predictions to assess which method is correct. This paper is motivated by this necessity.

From the derivation of the β-PDF parameters, it will be shown that the un-weighted PDF parameters should be based on the Reynolds mean mixture fraction and its variance rather than the Favre means. Since only the Favre mean mixture fraction and its variance are normally available from the combustion fluid dynamics (CFD) simulation, the Reynolds mean mixture fraction and its variance need to be determined from the Favre means and used to define new parameters for the un-weighted PDF. Finally, a comparison of the mean temperature fields using the above two probability density functions as well as the newly defined un-weighted probability density function is performed.

2. Mathematical modeling

2.1. The density weighted PDF and un-weighted PDF

The PDF function may be either presumed or solved from a balance equation [3]. However, for engineering applications, a PDF function is normally presumed to be the β function. Even though alternative forms of presumed PDF for the mixture fraction such as the clipped Gaussian and double delta function have been used in the past, the β-PDF function is a widely chosen because it is well defined on the interval (0, 1) and its shape ranges from a delta function to a Gaussian function [4]. When the β-function is presumed as the PDF, the density-weighted PDF function is defined as shown in (6).

The two non-negative parameters, α and β can be determined from the relations to the mean mixture fraction and its variance by the following equations:

$$\tilde{z}=\int_0^1 z\widetilde{P}(z)\,\mathrm{d}z=\frac{\Gamma(\alpha+1)\Gamma(\beta)}{\Gamma(\alpha+\beta+1)} \tag{9}$$

$$\widetilde{z''^2}=\int_0^1 (z-\tilde{z})^2\widetilde{P}(z)\,\mathrm{d}z=\frac{\Gamma(\alpha+2)\Gamma(\beta)}{\Gamma(\alpha+\beta+2)}-\tilde{z}^2 \tag{10}$$

By inserting the relation, $\Gamma(x+1)=x\Gamma(x)$ into (9) and (10), the two parameters, α and β can be related to the Favre mean mixture fraction and its variance as in (7) and (8). The Favre mean mixture fraction and its variance are calculated by solving two additional balance equations in the flow field using the CFD code,

$$\frac{\partial\bar{\rho}\tilde{z}}{\partial t}+\frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\tilde{z})=\frac{\partial}{\partial x_j}\left[\left(\frac{\mu_t}{\sigma_z}\right)\frac{\partial\tilde{z}}{\partial x_j}\right] \tag{11}$$

$$\frac{\partial\bar{\rho}\widetilde{z''^2}}{\partial t}+\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\widetilde{z''^2}\right)=\frac{\partial}{\partial x_j}\left[\left(\frac{\mu_t}{\sigma_g}\right)\frac{\partial\widetilde{z''^2}}{\partial x_j}\right]+C_{g1}\mu_t\left(\frac{\partial\tilde{z}}{\partial x_j}\right)^2-C_{g2}\bar{\rho}\frac{\varepsilon}{k}\widetilde{z''^2} \tag{12}$$

where model constants are given as $\sigma_z = 0.7$, $\sigma_g = 0.7$, $C_{g1} = 2.0$, $C_{g2} = 2.0$.

Once the two parameters for the PDF is determined from the Favre mean mixture fraction and its variance, the Favre or Reynolds mean values of any scalars can be obtained by Eq. (4) and Eq. (5), respectively.

In a similar way, the un-weighted PDF has been equivalently used in calculating those mean values by researchers. The un-weighted PDF is also assumed as β-function and has the same form as Eq. (6). However, when the un-weighted PDF is used, it is clear that the following relations should be satisfied from the definitions for the Reynolds mean mixture:

$$\bar{z} = \int_0^1 z P(z)\,\mathrm{d}z = \frac{\Gamma(\alpha+1)\Gamma(\beta)}{\Gamma(\alpha+\beta+1)} \tag{13}$$

and for the variance of the Reynolds mean mixture fraction:

$$\overline{z'^2} = \int_0^1 (z-\bar{z})^2 P(z)\,\mathrm{d}z = \frac{\Gamma(\alpha+2)\Gamma(\beta)}{\Gamma(\alpha+\beta+2)} - \bar{z}^2 \tag{14}$$

The parameters for the un-weighted PDF are related to the Reynolds mean mixture fraction and its variance instead of those of Favre averaging in the same form as (7), (8):

$$\alpha_R = \bar{z}\left(\frac{(1-\bar{z})\bar{z}}{\overline{z'^2}} - 1\right) \tag{15}$$

$$\beta_R = (1-\bar{z})\left(\frac{(1-\bar{z})\bar{z}}{\overline{z'^2}} - 1\right) \tag{16}$$

where the subscript, R, indicates Reynolds averaged inputs. This can result in an inconsistency since the Favre mean mixture fraction and its variance are conventionally used to define the parameters even in the un-weighted PDF as in Eq. (7) and Eq. (8). In flow field calculations with large density changes such as in combusting flows, the Favre-averaged governing equations are solved in order to avoid the density correlation terms that appear in the Reynolds averaged equations. Therefore, only the Favre mean mixture fraction and its variance are normally available from the CFD simulation. There is thus motivation to use the Favre averaged values in determining the PDF parameters. However, since the Favre mean mixture fraction and variance are not expected to be the same as the Reynolds mean mixture fraction and variance, this may cause significant errors in the prediction. It is then of interest to compare the Favre mean mixture fraction and its variance with those obtained from Reynolds averaging.

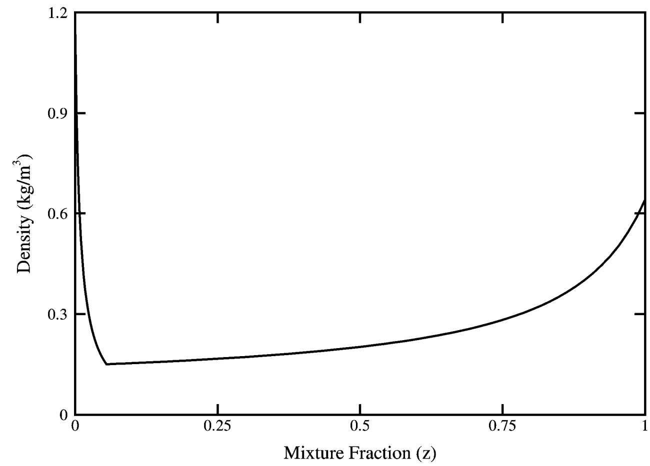


Fig. 1. The density profile used for PDF integration.

2.2. The comparison of the Favre means and Reynolds means

From the Favre mean mixture fraction and its variance, the Reynolds mean mixture fraction can be calculated from (4) in the same way as any other scalars:

$$\bar{z} = \bar{\rho}\int_0^1 \frac{z}{\rho}\widetilde{P}(z)\,\mathrm{d}z \tag{17}$$

The Reynolds mean mixture fraction variance is obtained by:

$$\begin{aligned}\overline{z'^2} &= \bar{\rho}\int_0^1 \frac{(z-\bar{z})^2}{\rho(z)}\widetilde{P}(z)\,\mathrm{d}z \\ &= \bar{\rho}\int_0^1 \frac{z^2}{\rho(z)}\widetilde{P}(z)\,\mathrm{d}z - 2\bar{\rho}\bar{z}\int_0^1 \frac{z}{\rho(z)}\widetilde{P}(z)\,\mathrm{d}z + \bar{z}^2 \\ &= \bar{\rho}\int_0^1 \frac{z^2}{\rho(z)}\widetilde{P}(z)\,\mathrm{d}z - \bar{z}^2\end{aligned} \tag{18}$$

Note that the density weighted PDF is used in the above (17) and (18), requiring only the Favre mean mixture fraction and its variance, which are available from the CFD calculation. Since the Favre mean mixture fraction and variance are available for any location in the domain from the CFD calculation, the Reynolds mean mixture fraction and its variance can be calculated using Eq. (17) and (18), together with a density profile, $\rho(z)$. The density profile used for the current calculation is obtained from the Burke–Schuman flame. However, the profiles from other conditions can be used without loss of generality. In Fig. 1, the employed density profile is presented.

Fig. 2 presents the Reynolds mean mixture fraction as a function of the Favre mean mixture fraction and variance. For convenience, the non-dimensionalized variance is introduced instead of the mixture fraction variance. It is normalized by dividing $\widetilde{z''^2}$ by $\tilde{z}(1-\tilde{z})$ and has a value between

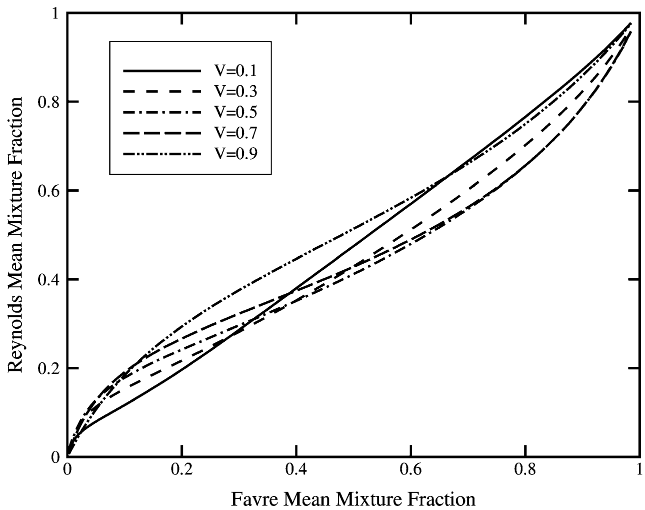


Fig. 2. The comparison of the Reynolds and Favre mean mixture fraction.

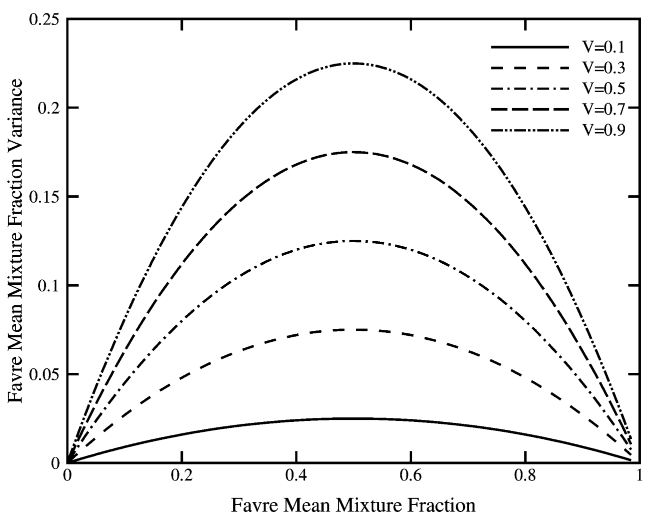


Fig. 3. The Favre mean mixture fraction variance for the Favre mean mixture fraction and the non-dimensionalized variance.

0 and 1:

$$V_n = \frac{\widetilde{z''^2}}{\tilde{z}(1-\tilde{z})} \tag{19}$$

From Fig. 2, it is clear that the Reynolds mean mixture fraction is different from the Favre mean mixture fraction. Depending on the non-dimensionalized variance, the difference may be more than 10% since the Reynolds mixture fraction is skewed by the weighted density profile.

The Reynolds and Favre mean mixture fraction variances are presented in Fig. 3 and Fig. 4, respectively. The Reynolds mean mixture fraction variances are skewed relative to the Favre mean mixture fraction variances.

If the un-weighted PDF is to be used in a consistent manner, the Favre mean mixture fraction and variance obtained from the CFD calculation must be converted to the Reynolds averaged values using Eq. (17) and Eq. (18). The Reynolds average values of scalars such as density and species mass fraction can then be calculated by Eq. (1) using the un-weighted PDF parameters, as defined in Eq. (15) and Eq. (16).

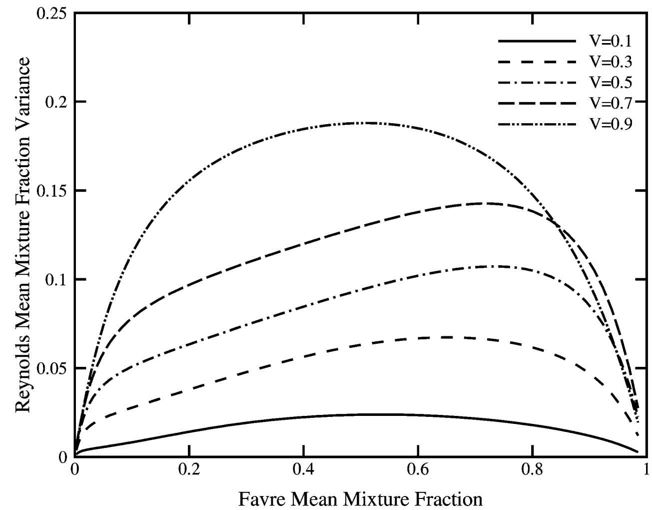


Fig. 4. The Reynolds mean mixture fraction variance for the Favre mean mixture fraction and the non-dimensionalized variance.

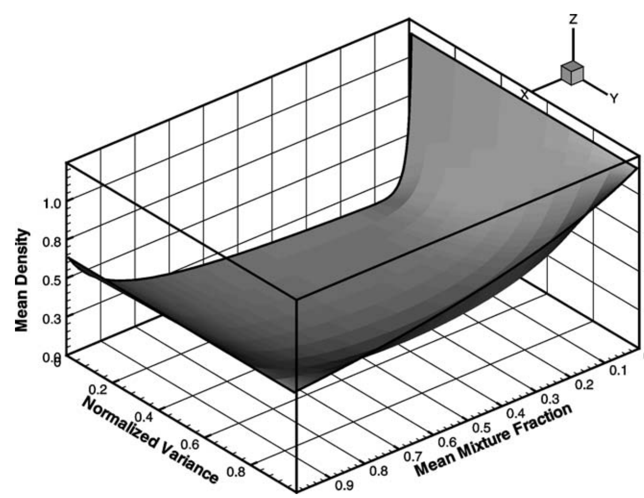


Fig. 5. The Reynolds mean density for the various Favre mean mixture fraction and the non-dimensionalized variance.

The PDFs are ultimately used to calculate expected values of various scalar variables. It is thus of interest to see if the use of different PDFs results in significant differences in the these quantities. The Reynolds mean density is a meaningful variable to examine since it affects both the flow field and the energy equation, and this calculation is repeated frequently during the CFD calculation.

In Fig. 5, the mean density using the density-weighted PDF is presented as a function of the Favre mean mixture fraction and the normalized variance. The Burke–Schuman density profile is used in the calculation. The Favre mean mixture fraction is divided by 100 points from 0 to 1 and the normalized variance is divided by 11 points from 0.01 to 0.99.

In the same way, the Reynolds mean densities are calculated and presented using three different PDFs as follows:

Method I: The un-weighted PDF

The Favre averaged mean and variance of the mixture fraction obtained from the CFD calculation are used to define the un-weighted PDF, $P(z;\tilde{z},\widetilde{z''^2})$, and expected value of ϕ is calculated:

$$\bar{\phi}=\int \phi(z)P\big(z;\tilde{z},\widetilde{z''^2}\big)\,\mathrm{d}z$$

Method II: The un-weighted PDF (corrected)

The Reynolds averaged values for $\bar{z}$ and $\overline{z'^2}$ are first calculated from knowledge of $\tilde{z}$ and $\widetilde{z''^2}$. The Reynolds averaged values are then used to calculate the un-weighted PDF, $P(z;\bar{z},\overline{z'^2})$, and $\bar{\phi}$ is calculated from:

$$\bar{\phi}=\int \phi(z)P\big(z;\bar{z},\overline{z'^2}\big)\,\mathrm{d}z$$

Method III: The density-weighted PDF

$$\bar{\phi}=\bar{\rho}\int \frac{\phi(z)}{\rho}\widetilde{P}\big(z;\tilde{z},\widetilde{z''^2}\big)\,\mathrm{d}z$$

The mean densities are calculated using Methods I, II, and III, respectively and are shown in Fig. 6(a), Fig. 6(b), and Fig. 6(c). The figures show that similar densities are obtained when Method II and Method III are applied. In contrast, Method I, which used Favre-averaged values to define the PDF and then calculated a Reynolds averaged density without correcting the PDF, predicted quite different values for the density. This is further illustrated in Fig. 7 which shows the density as a function of the non-dimensionalized variance for the stoichiometric $\tilde{z}$.

This result shows that the possible reason for the significant difference between the un-weighted PDF and the density weighted PDF is caused by using the inappropriate parameters, that is, the Favre mean mixture fraction and its variance in conjunction with an un-weighted PDF. Therefore, care must be taken to ensure consistency in the calculation of Reynolds values.

3. Numerical simulation

To examine the impact of the PDF integration methods on the predicted flame temperatures, a numerical simulation has been carried out for a turbulent diffusion methane jet flame. Three simulations were performed using the three different integration methods. All other aspects of the simulations are identical.

3.1. Code development

Solutions were obtained using an in-house two-dimensional CFD code. The Favre averaged governing equations

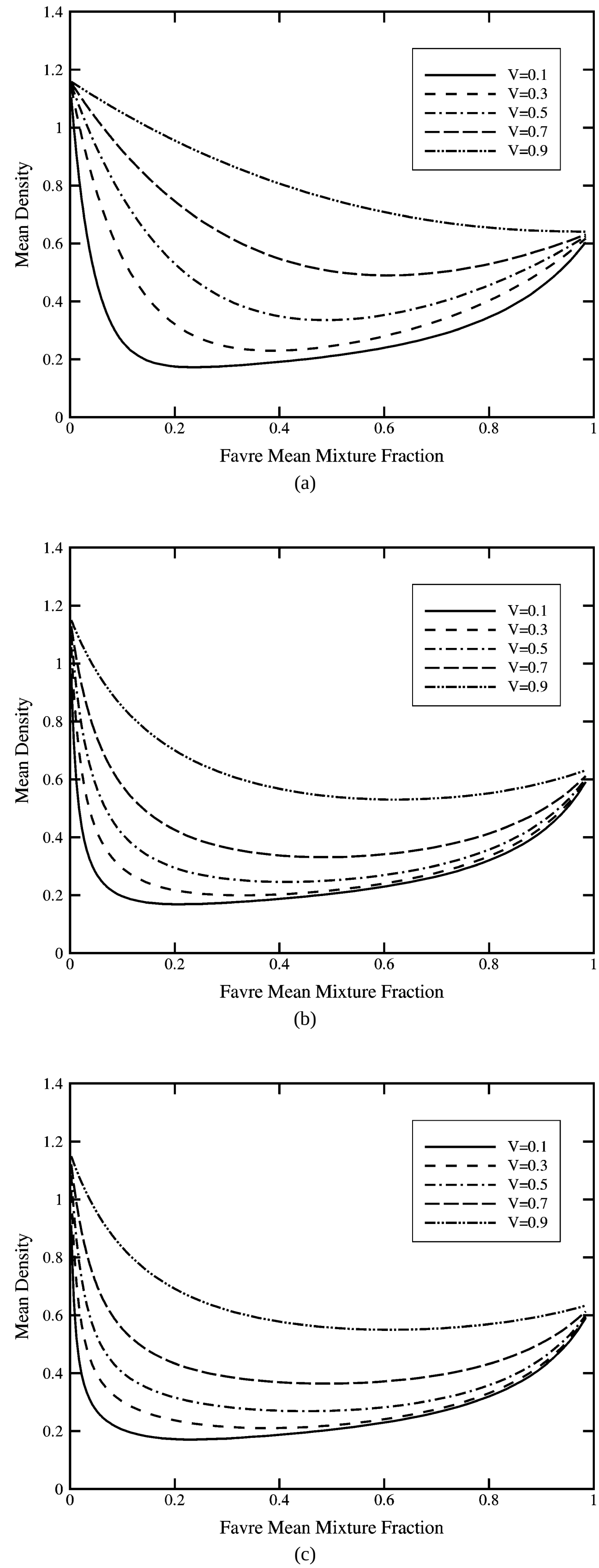


Fig. 6. The mean density for the Favre mean mixture fraction at different normalized variances. (a) The mean density from Method I; (b) The mean density from Method II; (c) The mean density from Method III.

are discretized by the finite volume based approach. The colocated grid scheme is employed and a multigrid solver is used to solve the algebraic equations. The pressure field is corrected using the SIMPLEC algorithm. The k–ε model is implemented for the turbulence. In order to calculate $\tilde{z}$ and $\widetilde{z''^2}$ [11], two additional scalar transport equations are solved simultaneously with the flow field calculation and used in determining the PDF shape. To reduce the computational load, the PDF integration has been performed in advance for the various mean mixture fraction and its variance and stored in a library.

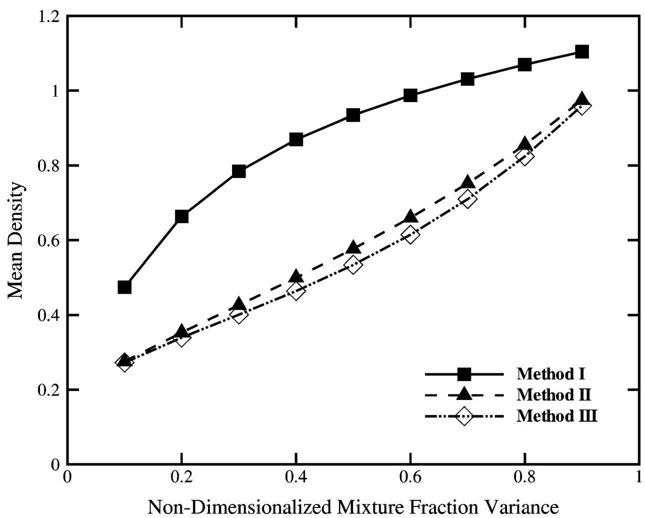


Fig. 7. The mean density for the stoichiometric mean mixture fraction.

3.2. Governing equations

The conservation equations for turbulent kinetic energy, k, and dissipation rate, ε, are given below [11]:

$$\frac{\partial \bar{\rho} k}{\partial t} + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j k) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + P_k - \bar{\rho}\varepsilon \tag{20}$$

$$\frac{\partial \bar{\rho} \varepsilon}{\partial t} + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j \varepsilon) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] + C_{\varepsilon 1}\frac{\varepsilon}{k}P_k - C_{\varepsilon 2}\bar{\rho}\frac{\varepsilon^2}{k} \tag{21}$$

The source term P_k in Eq. (20) and Eq. (21) is given by:

$$P_k = \mu_t\left[\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right]\frac{\partial \tilde{u}_i}{\partial x_j} \tag{22}$$

The model constants are set to the commonly used values of $C_\mu = 0.09$, $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$, $\sigma_k = 1.0$, $C_{\varepsilon 1} = 1.44$, and $C_{\varepsilon 2} = 1.92$. The equations for the mean mixture fraction and its variance are given by Eq. (11) and Eq. (12).

3.3. The test case

The test case considered is a methane jet in a coflow of air. The methane jet velocity is set to 52 $m \cdot s^{-1}$ and the surrounding air flow velocity is set to 2 $m \cdot s^{-1}$. The turbulent

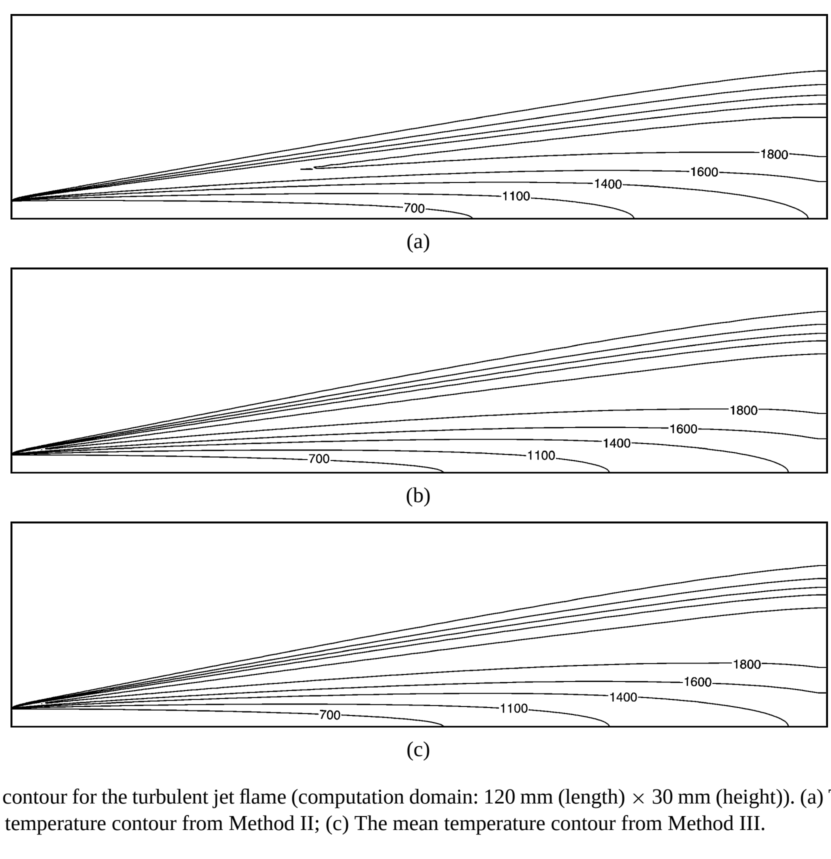
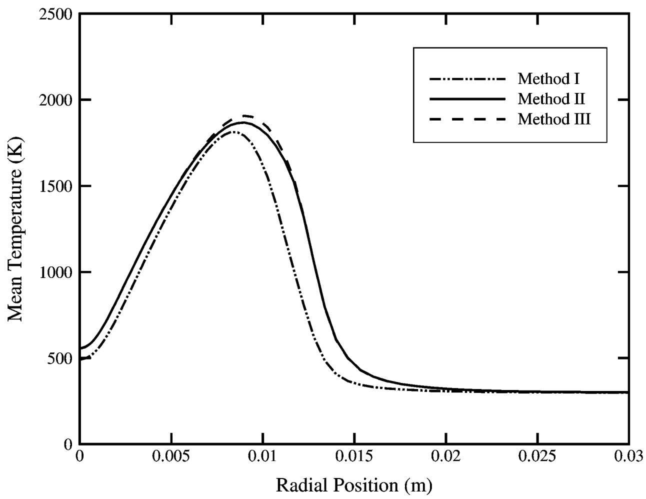
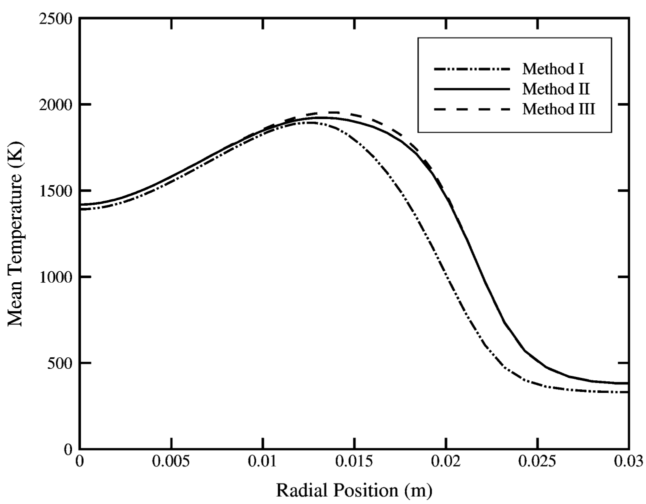


Fig. 8. The mean temperature contour for the turbulent jet flame (computation domain: 120 mm (length) × 30 mm (height)). (a) The mean temperature contour from Method I; (b) The mean temperature contour from Method II; (c) The mean temperature contour from Method III.



(a)



(b)

Fig. 9. The radial profile of mean temperature for the turbulent jet methane flame. (a) The radial temperature profile at $X = 0.055$ m; (b) The radial temperature profile at $X = 0.116$ m.

intensity at the jet inlet is set to 10%. Pure methane is injected from the fuel nozzle with a diameter of 5.2 mm and mixed with the surrounding low speed air. The mean mixture fraction is $\tilde{z} = 1$ at the fuel inlet and $\tilde{z} = 0$ at the air inlet.

4. Results and discussion

Fig. 8(a), Fig. 8(b) and Fig. 8(c) show the predicted temperature contours using the three PDF integration methods. All contours are plotted using the same scale. When the un-weighted PDF is used (Fig. 8(a)), the contours are different from those obtained using the density weighted PDF (Fig. 8(c)). However, when the un-weighted PDF with newly defined parameters is used (Fig. 8(b)), excellent agreement with the results of the density weighted PDF is obtained.

Radial temperature profiles are compared in Fig. 9(a) and Fig. 9(b) at different axial positions. It is clearly seen that the un-weighted PDF with the corrected parameters is in excellent agreement with the density-weighted PDF. In contrast, the use of Favre mean mixture fraction and its variance with an un-weighted PDF results in underprediction of the temperature profile in the outer section of the flame. The slight differences between Methods II and III arise from the numerical integration performed to calculate the expected values.

This trend is consistent with the previous density comparison where the conventional un-weighted PDF shows a higher density for the same mixture fraction. It also agrees with the density comparison of Liu et al. [1].

5. Conclusion

The study has been concerned with examining the impact of the presumed PDF on the expected values of scalars such as density and temperature in combusting flows. The motivation for the work arose from the apparent inconsistency in using the Favre mean mixture fraction and its variance together with an un-weighted PDF in the determination of the expected values of scalars. A systematic comparison between the density-weighted PDF and the un-weighted PDF has been carried out in the study. For mathematical consistency, it is suggested that the parameters for the un-weighted PDF should be related to the Reynolds mean mixture fraction and its variance. For the various combinations of the Favre mean mixture fraction and its variance, the Reynolds mean mixture fraction and its variance are calculated and compared. The differences between the Reynolds and Favre mixture fraction affects the parameters, α and β which are used to determine the un-weighted PDF shape. The mean temperature from the conventional un-weighted PDF and density-weighted PDF are compared with the un-weighted PDF with the corrected parameters. For comparison, a numerical simulation for the methane diffusion jet flame has been carried out. This study leads to the following conclusions:

(1) The predicted mean values using the conventional un-weighted PDF shows significant difference from the result of the density-weighted PDF, which confirms the result of Liu et al. [1].
(2) This difference is caused by using the inappropriate parameters for the un-weighted PDF. The proper parameters for the un-weighted PDF should be related to the Reynolds mean mixture fraction and its variance. Therefore, when the un-weighted PDF is used, newly defined parameters should be used.
(3) Once the proper parameters are used for the un-weighted PDF, it shows excellent agreement with the results of the density-weighted PDF.

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