On the Effect of Presumed PDF and Intermittency on the Numerical Simulation of a Diffusion Flame

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ABSTRACT

In the present work, the effect of PDF selection and intermittency on the result of the numerical simulation are examined by the simulation of a turbulent methane-air jet diffusion flame. As to the PDFs, beta-function and clipped Gaussian are considered. Results for the pure mixing jet are compared with experimental results. Then, the turbulent flame is calculated for the same conditions and the results obtained for the several models are compared. It is found that the clipped Gaussian distribution coupled with consideration of intermittency recovers the experimental data very well. As to the reacting flow results, the main overall properties of the turbulent jet diffusion flame such as maximum flame temperature are less affected by the choice of the PDF. Flame height and NO emissions, on the contrary, appear to be significantly influenced.

Keywords : PDF, beta-function, clipped Gaussian distribution, intermittency, gaseous fuel, fuel-air mixing, diffusion flame

INTRODUCTION

Probability density functions (PDFs) are widely used for the computation of turbulent flames. Their power lies in the fact that it is possible to consider the effect of concentration variations on reaction rates, heat release and so on. Regarding premixed flames the effect of PDF selection on reaction rate has been theoretically examined by Bray [1]. He found that mean and fluctuation of the reaction rate are quite insensitive to the PDF chosen as long as it does not simply consist of Delta functions (Bray considered uniform, battlement and triangular distributions).

For diffusion flames, it is known [2] that the beta-function cannot reproduce PDFs which show a peak at the fuel (f=1) or oxidizer (f=0) feed and, at the same time, an intermediate maximum as is typically found in fuel jets [3]. Effelsberg and Peters [4] ascribe the intermediate maximum to the contribution from the fully turbulent part of the scalar field.

In this paper, the turbulent jet diffusion flame is chosen as test case because of its importance in industrial furnaces. Although heat transfer and/or heat loss are important phenomena in these actual applications, adiabatic combustion is simulated here, since capturing of PDF selection effects is the main concern of this paper. Heat loss implementations would unnecessarily complicate the discussion here and, therefore, are postponed to be done in future.

THEORETICAL

In this work two PDFs are examined, namely the beta-function, which is used most frequently, and the clipped Gaussian distribution. Both PDFs are defined below. They are used to define the probability for the mixture fraction f which follows the common definition

$$f=\frac{\xi-\xi_O}{\xi_F-\xi_O} \text{ with } \xi=Y_F-\frac{Y_O}{r} \qquad (1)$$

where r denotes the amount of oxygen necessary to burn 1kg of fuel. Together with the standard k-εmodel for the turbulent flow field the two standard equations (e.g. [5]) for the mean $\overline{\overline{f}}$ and variance $\overline{\overline{f''^2}}$ of the mixture fraction are solved. Local mean values $\overline{\overline{\phi}}$, which may be temperature, density and/or chemical species, are obtained by averaging over mixture fraction space, i.e.

$$\overline{\overline{\phi}}=\int_0^1 \phi(f)\,P(f)df \qquad (2)$$

where $\phi(f)$ is obtained from 1D adiabatic flamelet calculations. Determination of the local PDF $P(f)$ from the calculated $\overline{\overline{f}}$ and $\overline{\overline{f''^2}}$ is explained below.

Beta-function

The beta-function PDF P_b is defined as

$$P_b(f;a,b)=\frac{f^{a-1}(1-f)^{b-1}}{\int_0^1 f^{a-1}(1-f)^{b-1}df} \qquad (3)$$

The parameters a and b are calculated from mean and variance of the mixture fraction according to eqs (4) and (5).

$$a=\overline{\overline{f}}\left\{\frac{\overline{\overline{f}}}{\overline{\overline{f''^2}}}\left(1-\overline{\overline{f}}\right)-1\right\} \qquad (4)$$

$$b=a\left(\frac{1}{\overline{\overline{f}}}-1\right) \qquad (5)$$

Clipped Gaussian

The clipped Gaussian PDF P_c is defined as follows.

$$P_c(f;\mu,\sigma)=$$

$$\begin{cases} \int_{-\infty}^{0}\frac{1}{\sigma\sqrt{2\pi}}exp\left[-\frac{1}{2}\left(\frac{f-\mu}{\sigma}\right)^2\right]df & f=0 \\ \frac{1}{\sigma\sqrt{2\pi}}exp\left[-\frac{1}{2}\left(\frac{f-\mu}{\sigma}\right)^2\right] & 0<f<1 \\ \int_{1}^{\infty}\frac{1}{\sigma\sqrt{2\pi}}exp\left[-\frac{1}{2}\left(\frac{f-\mu}{\sigma}\right)^2\right]df & f=1 \end{cases} \qquad (6)$$

For the numerical integration of the integrals in eq.(6) tradeoffs for the lower ($-\infty$) and upper (∞) bounds must be introduced. Here, these bounds are set to the following values

$$f_{L,R}=\mu\pm\sigma\sqrt{-2\ln(\varepsilon\sigma\sqrt{2\pi})} \qquad (7)$$

where typically $\varepsilon\approx10^{-6}$. Mean μ and variance σ of the clipped Gaussian distribution are determined by an iterative numerical procedure such that the conditions

$$\overline{\overline{f}}=\int_0^1 fP_c(f)df \text{ and } \overline{\overline{f''^2}}=\int_0^1\left(f-\overline{\overline{f}}\right)^2P_c(f)df$$

are satisfied.

Intermittency

Intermittency is implemented as summarized by Bilger [6]. The PDF is splitted into a laminar and a turbulent part (eq.(8)), where the laminar part is a Dirac function.

$$P(f) = (1-I)\,\delta(f) + I P_t(f) \tag{8}$$

I denotes the intermittency (i.e. the mean of the intermittency function) which is zero for laminar and one for entirely turbulent regions. When intermittency is considered in the numerical simulation, I is calculated according to

$$\mathrm{I} = \frac{1.25}{1+\left(\overline{\overline{f''^{2}}} \big/ \overline{\overline{f}}^{2}\right)} \tag{9}$$

Note, that I=1 is enforced if eq.(9) should yield larger values or for simulation without intermittency effect. Mean and variance of the turbulent PDF P_t are determined following

$$\overline{\overline{f_t}} = \overline{\overline{f}} \Big/ I \quad \text{and} \quad \overline{\overline{f''^{2}}} = 0.25\,\overline{\overline{f_t}}^{2} \tag{10}$$

These values are then used instead of $\overline{\overline{f}}$ and $\overline{\overline{f''^{2}}}$ to determine the parameters of the PDF P_t. In this paper, P_t is chosen to be P_b or P_c.

TEST CASE

The test problem considered here is the turbulent fuel jet ejected into almost quiescent air. Geometry and flow conditions are adjusted to the experimental setup used by Birch etal. [3] for PDF measurements in non-reacting flow. Natural gas is ejected with a mean velocity of 22.26m/s through a nozzle of 12.65mm inner diameter. Fuel and air temperature is 300K. Air is supplied with a velocity of 0.2m/s.

The numerical simulation is performed for an axi-symmetrical domain of radius 0.5m and length of 1.5m. The nozzle wall thickness is neglected. Fuel is set to 100% methane. The velocity profil at the nozzle exit is set according to the 1/7-power law for fully developed turbulent flow through a pipe. The radial velocity component is set to zero at all boundaries except the outlet where the Neumann condition is applied. For all other variables Neumann conditions are prescribed at radial and outlet boundary.

RESULTS

Numerical simulations have been performed for the non-reacting turbulent fuel jet. The results for mean and variance of mixture fraction are compared with the experimental results of Birch. Then, two simulations are performed for the reacting case using the worst and best matching PDF, namely beta-function without intermittency and clipped Gaussian with intermittency, respectively.

Non-reacting flow

Experimental results for the test case considered here are reported for four radial locations about ten diameters away from the nozzle exit (Birch *etal.* [3]). Values for mean and variance of the mixture fraction are summarized in

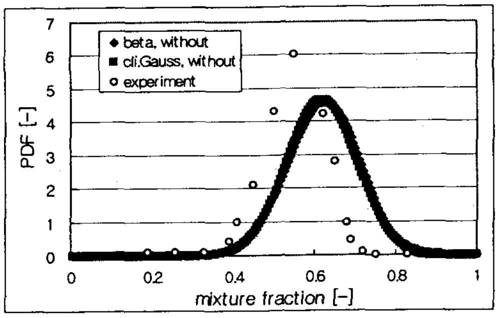
Table 1: Mean and variance of mixture fraction as well as intermittency at z/d=10 for non-reacting flow

	experiment		calculation		
	$\overline{\overline{f}}$	$\overline{\overline{f''^{2}}}$	$\overline{\overline{f}}$	$\overline{\overline{f''^{2}}}$	I
r/d=0.0	0.548	7.06E-3	0.618	7.33E-3	1.0
r/d=1.3	0.181	7.57E-3	0.169	7.64E-3	0.986
r/d=1.49	0.121	6.24E-3	0.122	5.97E-3	0.892
r/d=1.8	0.041	1.68E-3	0.046	1.68E-3	0.7

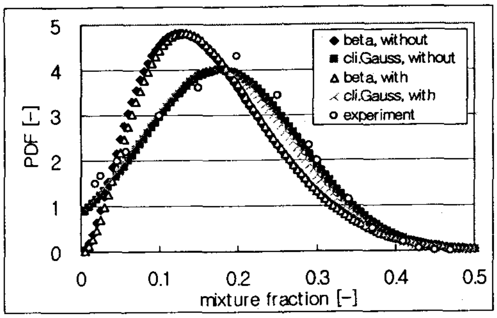
Table 1.

Note that for this calculation the beta-function without intermittency is used for evaluation of local density. The constants of the standard k-εmodel are set to $C_\mu = 0.09$, $C_{\varepsilon 1} = 1.44$ and $C_{\varepsilon 2} = 1.8$ in order to adjust the spreading rate to experimental observations. From Table 1 it is seen that agreement is very good away from the axis of symmetry (r/0.5d=0.0). At the axis disagreement is expected as a known deficiency of the simple turbulence model employed here. Improvement perhaps could be achieved with more sophisticated models, but this has not been tried here, since we are more concerned with the performance of the various PDFs in this work. The last column in Table 1 shows the intermittency as determined from the calculated values for mean and variance of mixture fraction following eq.(9).

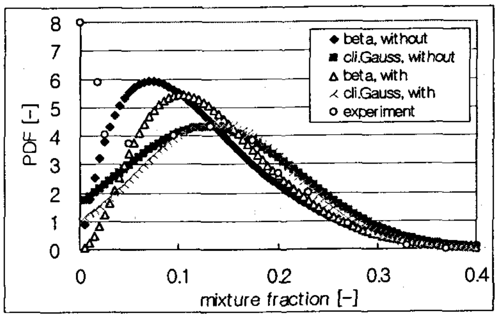
In order to compare the PDFs, the experimentally observed PDF is plotted together with beta-function and clipped Gaussian distribution, with as well as without intermittency, in Figure 1. Since the flow is entirely turbulent (I = 1) at the axis of symmetry, it makes no difference whether intermittency is considered or not. The PDFs are exactly the same. Further it can be observed that the beta-function turns out to be Gaussian here. Beta-function and clipped Gaussian distribution differ considerably away from the axis. At r/0.5d=2.6, the clipped Gaussian with intermittency exactly follows the experiment. It is known [7] that delta functions in the nonturbulent unmixed air (f=0) are smeared into a Gaussian-like peak. Keeping this in mind, the clipped Gaussian at r/0.5d=2.98 also compares quite well, remarkably better than the beta-function. At the outer edge (r/0.5d=3.6) the Gaussian appears to compare poorly at a



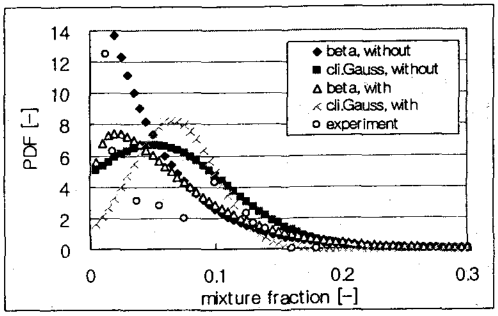
(a) r/0.5d = 0



(b) r/0.5d = 2.6



(c) r/0.5d = 2.98



(d) r/0.5d = 3.6

Fig.1 Assumed PDF shapes for non-reacting jet at z/d = 10 with and without intermittency.

first glance. It must be noted, however, that the intermediate maximum of the clipped Gaussian (with intermittency considered) found at f=0.08 is relatively close to the measured maximum at about f=0.1.

In summary we can conclude that the clipped Gaussian with intermittency recovers the experimental results quite well. In the opposite, the beta-function without intermittency is poor. At the outer edge, it does not behave qualitatively correct. Nevertheless, the beta-function without intermittency is frequently used in numerical simulations. It is implemented in many commercial codes and this is the reason why we decided to perform simulations of the turbulent reacting flow with these two PDFs.

Reacting flow

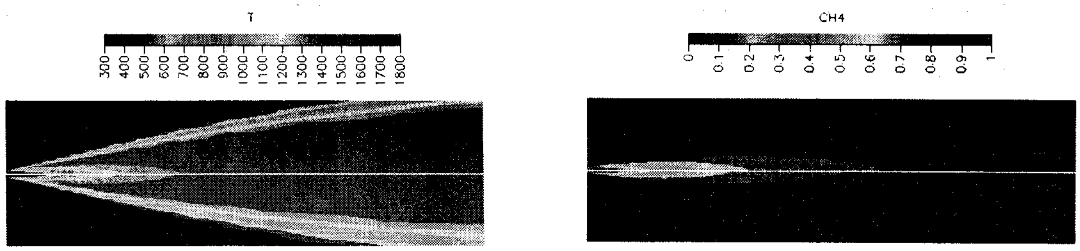
Numerical simulations for the turbulent methane-air jet diffusion flame have been performed for (a) the beta-function without considering intermittency and (b) the clipped Gaussian distribution with intermittency considered. Comparison of the temperature fields (Fig. 2a) reveals no significant differences. For the clipped Gaussian with intermittency the high temperature region appears little bit narrower. The methane concentration fields indicate that the flame height is calculated shorter than obtained with beta-function without intermittency. These results are consistent with former observations [7].

Figure 3 shows a more detailed comparison for temperature and mass fractions of methane, carbondioxide and nitric monoxide 50 diameters away from the nozzle exit. It can be readily seen that the flame is predicted be narrower for the clipped Gaussian PDF. Locally, temperature is predicted more than 300K higher for the beta-function (Fig.3a) which leads to about two times higher NO concentrations (Fig.3d). Such significant effects of the PDF on NO prediction are also found for hydrogen-air flames [8].

CONCLUSIONS

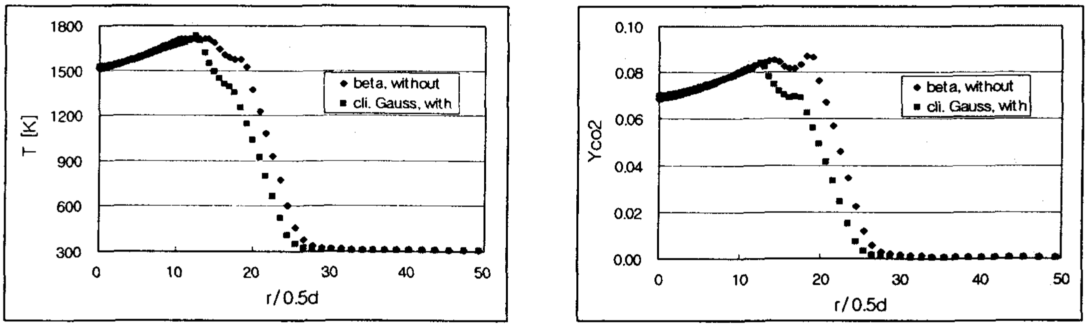
Numerical simulations have been performed for the non-reacting as well as the reacting turbulent jet of methane ejected into slowly coflowing air. The effect of the actual shape of the presumed PDF and the effect of intermittency is investigated. The results can be summarized as follows:

1. The clipped Gaussian distribution accurately models local PDFs. It is important to implement intermittency.
2. Shape of the PDF (and intermittency) mainly affects flame height and NO concen-



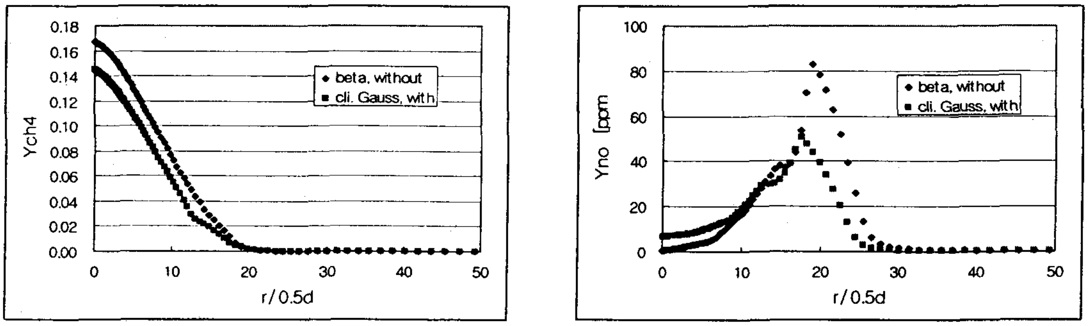
(a) temperature [K] (b) methane mass fractio

Fig.2 Comparison of computated results. Upper half : beta-function without intermittency. Lower half : clipped Gaussian with intermittency.



(a) temperature [K]

(b) mass fraction CO_2 [-]



(c) mass fraction CH_4 [-]

(d) mass fraction NO [ppm]

Fig.3 Computed radial profiles for beta-function and clipped Gaussian, without and with intermittency, respectively, 50 diameters away from nozzle exit.

trations.

REFERENCES

1. Bray, K.N.C. "Turbulent flows with premixed reactants", in *Turbulent Reacting Flows*, ed. by P.A.Libby and F.A.Williams, Springer-Verlag, Berlin, 1980, pp.144-157.
2. Peters, N. *Turbulent combustion*, Cambridge University Press, 2000, pp.197ff.
3. Birch, A.D. *et al.* "The turbulent concentration field of a methane jet", *J.Fluid Mech* 88, 1978, part3, pp.341-449.
4. Effelsberg, E. and Peters, N. "A composite model for the conserved scalar pdf", *Combust.Flame* 50, 1983, pp.351-360.
5. Chomiak, J. *Combustion*, Abacus Press, Gordon and Breach Science Publishers, 1990, p.184.
6. Bilger, R.W. "Turbulent flows with nonpremixed reactants", in *Turbulent Reacting Flows*, ed. by P.A.Libby and F.A.Williams, Springer-Verlag, Berlin, 1980, pp. 79-80.
7. see [6], pp.75ff.
8. Kent, J.H. and Bilger, R.W. "The prediction of turbulent diffusion flame fields and nitric oxide formation", *16th Int.Symp. Combust.*, The Combustion Institute, 1976, pp.1643-1656.