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Parametric analysis of Velocity Conditioned Modified Curl's Model (VC-MCM) in the PDF method for Turbulent Non-Premixed Flames

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Abstract

In the probability density function (PDF) method for turbulent combustion, model for molecular diffusion process is required and has large influence on the accuracy of numerical simulations. While most of the existing mixing models can ensure that scalar mean does not change and the scalar dissipation rate is correct, they neglect the possible effect of velocity on the mixing process. However, the Direct Numerical Simulation (DNS) shows that such neglection is only valid if the flow is completely local anisotropic. Therefore, local isotropy requires a velocity-conditioned mixing model. Therefore, in this work, a velocity-conditioned modified Curl's model is introduced and applied for well-known turbulent non-premixed flames, Sandia Flame series D-F. The influence of model parameters such as mixing parameter and the turbulence parameters are investigated based on general Modified Curl's Model and Velocity-Conditioned Modified Curl's Model are compared, together with the experimental data. Moreover, effects of Reynolds number on the model calculations are also investigated. The computational requirements along with the useful results are also discussed in this research work for the both the models.

Keywords: Combustion, Mixing Model, PDF, Sandia Flame, Turbulence

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I. Nomenclature

k	=	turbulent kinetic energy
ϵ	=	turbulent dissipation rate
ς	=	degree of local anisotropy
Re	=	Reynolds number
J_i^{α}	=	Molecular diffusion flux
C_{ϕ}	=	mixing model parameter
$C_{\omega 1}$	=	turbulence model parameter
$\overrightarrow{U_J}$	=	velocity of a particle j
ϕ_a	=	chemical composition of species 'a' at boundary
ξ	=	mixture fraction
$\tilde{A}$	=	Favre-averaged scalar 'A' conditioned over mixture fraction
S_{α}	=	Chemical source term

II. Introduction

The probability density function (PDF) method is widely used in the simulation of turbulent reacting flows and has been quite well known since it came up [1]. By solving the corresponding transported-PDF equation the PDF of velocity and thermo-kinetics scalars and, consequently, their average values and statistical moments of any order can be obtained. The greatest feature in the PDF method is that it overcomes the limitations of conventional models of chemical source term such as Eddy-Breakup (EBU) model and equilibrium-chemistry-assumption model [1]. In another works, chemical source term in the PDF method appears in a closed form, avoiding any modelling.

Despite of this greatest feature that no model is needed for chemical source term, models for the conditional acceleration and for conditional diffusion are necessary. Usually, there is no large difficulty in the modeling of conditional acceleration, which accounts for the effects of the Reynolds stresses fluctuations and the pressure fluctuations. However, modeling of conditional diffusion, describing the molecular diffusion, is a big challenging and has large influence on the accuracy. In order to find a closure for the conditional diffusion, three requirements for this closure must be fulfilled [2,3]: i) the scalar mean remains unchanged; ii) the scalar dissipation rate must be correct; iii) the model must yield the correct local scalar isotropy. Other requirements such as the localness in scalar space are desired properties and not "must" requirements [2,3].

There exist already many mixing models [4-9] for conditional diffusion such as IEM, MCM, EMST, MMC and so on. Although these mixing models fulfill different desired properties, they all satisfy the first two constrains, i) and ii). The constrain iii) is usually largely ignored by most of them [10]. That means, most scalar mixing models assume that molecular diffusion process does not depend on instantaneous velocity, which has already been shown to be inaccurate [11,12]. Theoretically, local isotropy should prevail as Reynolds number increases. For moderate Reynolds number, local anisotropy may be significant [11]. A parameter ς was introduced [11,12], to describe the degree of local anisotropy. For $\varsigma = 0$, flow corresponds to local isotropic, where for $\varsigma = 1$ flow corresponds to complete local anisotropic. Overholt & Pope [12] performed a DNS of a conserved passive scalar with imposed mean gradient in isotropic turbulence, showing clearly that with increasing Reynolds number flow has a lower degree of local anisotropic ($\varsigma \to 0$). It was stated that to preserve local isotropy, scalar mean must be velocity conditioned [11,12].

In this work, a velocity-conditional modified curl's mixing (VCMCM) model has been tested based on algorithm introduced in [11] for well-known turbulent jet diffusion flame, Sandia Flame D. It will be shown that the flame has moderate degrees of local isotropic, requiring the mixing model to be velocity conditioned. The parameters in VCMCM are studied and their influences on the prediction of thermos-kinetic quantities are presented.

III. Probability Density Function (PDF) Method

A joint PDF (JPDF) [1] of velocity, composition and turbulent frequency $f_{\omega \boldsymbol{U\phi}}(\Theta, \boldsymbol{V}, \boldsymbol{\psi}; \boldsymbol{x}, t)$ is employed here. A transported-PDF equation is solved to obtain the PDF, which overcomes the problem that generally the PDF of a flow is a prior unknown. This equation is derived by jointly solving Navier-stokes, continuity This transported-PDF equation for $f_{\omega \boldsymbol{U\phi}}(\Theta, \boldsymbol{V}, \boldsymbol{\psi}; \boldsymbol{x}, t)$ reads:

$$\rho(\underline{\psi})\frac{\partial f}{\partial t} + \rho(\underline{\psi})V_j\frac{\partial f}{\partial x_j} + \left(\rho(\underline{\psi})g_j - \frac{\partial\langle p\rangle}{\partial x_j}\right)\frac{\partial f}{\partial V_j} + \frac{\partial}{\partial \psi_a}\left[\rho(\underline{\psi})S_\alpha(\underline{\psi})f\right]$$
$$= \frac{\partial}{\partial V_j}\left[\left\langle -\frac{\partial \tau_{ij}}{\partial x_i} + \frac{\partial p'}{\partial x_j}\middle|\underline{V},\underline{\psi}\right\rangle\right] + \frac{\partial}{\partial \psi_\alpha}\left[\left\langle\frac{\partial J_i^\alpha}{\partial x_i}\middle|\underline{V},\underline{\psi}\right\rangle\right] \quad (1)$$

where $S_\alpha(\psi)$ denotes the chemical source term, D/Dt denotes to the material derivative and J_α^i being the diffusion flux. While all terms on the left-hand side, including chemical source term, are in closed form, all terms on the right-hand side must be modelled. The conditioned acceleration can be modelled by using the simplified Langevin model (SLM) which reads:

$$\overline{\frac{\partial \tau'_{ij}}{\partial x_j} - \frac{\partial p'}{\partial x_i} | \Theta, V, \psi} = G_{ij}(V - \tilde{U}_j) - \frac{C_o \epsilon}{2f} * \frac{\partial f}{\partial V_i} \tag{2}$$

where G_{ij} is defined as:

$$G_{ij} = \left(\frac{1}{2} + \frac{3}{4} C_o\right) * \frac{\epsilon}{k} \delta_{ij} \tag{3}$$

and usually, the model parameter C_o= 2.1 is chosen as a constant in many studies. However, as shown in [11], C_o is also dependent on the Reynolds number. This will be discussed later. The second term, conditional diffusion, on the right-hand side of Eq. 1 will be discussed in detail in the next section. And the third term, conditional turbulent frequency, is modelled by using the gamma-distribution model.

IV. Velocity Conditioned Mixing Model

As one sees from the original transported PDF equation (Eq. 1), term of conditional diffusion (second term on the right-hand side) is indeed velocity conditioned (Actually the term is turbulent frequency conditioned but no evidence, both from experiments and from numerical studies, shows the importance of turbulent frequency conditioned effect on velocity). Therefore, in the following paragraph, we only focus on velocity conditional effect. However, most of the mixing models do not consider the effect of velocity on the mixing process. In the following, the IEM mixing model [11] is selected to explain the effect of velocity on turbulent mixing more in more detail. The IEM is chosen here because it is a widely used mixing model due to its simplicity and its modification, velocity-conditioned IEM (VCIEM), has already been intensively studied and applied previously in several cases [12-14].

In the original formulation of IEM, the conditional diffusion is modeled as:

$$\overline{\frac{\partial J'_{\alpha,i}}{\partial x_i} | V, \psi} = -\frac{C_\phi}{2} * \omega * (\psi - \tilde{\phi}) \tag{4}$$

where ω is the turbulent frequency and $\tilde{\phi}$ is the scalar mean. C_ϕ is the model parameter that determine the scalar dissipation rate and its standard value is equal to 2.0. We observe clearly that the scalar mixing in IEM is independent of velocity. However, Pope [15] observed that the IEM (Eq. 4) is inconsistent with local isotropy, whereas the alternative

$$\overline{\frac{\partial J'_{\alpha,i}}{\partial x_i} | V, \psi} = -\frac{C_\phi}{2} * \omega * (\psi - \widetilde{\phi | V}) \tag{5}$$

is consistent. In Eq6, $\widetilde{\phi|V}$ is the scalar mean conditioned on $U_i = V_i$. Note that in the absence of mean scalar gradient Eq. 4 and Eq. 5 are equivalent, while in the presence of mean scalar gradient $\widetilde{\phi|V} \neq \tilde{\phi}$. Fox [11] proposed a combination of Eq. 4 and Eq. 5 by introducing the parameter ς describing the degree of local anisotropy:

$$\overline{\frac{\partial J'_{\alpha,\iota}}{\partial x_\iota}|V,\psi} = -\frac{C_\phi}{2} * \omega * (\psi - \varsigma * \tilde{\phi} - [1-\varsigma] * \widetilde{\phi|V}) \tag{6}$$

It can be seen that for local isotropy (ς =0) the mixing process is velocity-conditioned, while for complete local anisotropic (ς =1) the mixing process is independent of velocity. From the DNS analysis in [12], local anisotropy decreases monotone with increasing Taylor-scale Reynolds number $Re\lambda$ and a power-law expression to the ς data yields:

$$\varsigma = 4.15 * Re_\lambda^{-0.65} \tag{7}$$

which is plotted in Fig. 1 (solid line), together with the DNS data in [12] (Points). The Taylor-scalar Reynolds number Re_λ is related to the integral-scale Reynolds number Re_L, in which the characteristic length scale is defined as $L \equiv k^{3/2}/\epsilon$:

$$Re_L = k^{1/2} * \frac{L}{v} = \frac{k^2}{\epsilon * v} \tag{8}$$

and the relationship between Re_λ and Re_L reads [16]:

$$Re_\lambda = \left(\frac{20}{3}.Re_L\right)^{\frac{1}{2}} \tag{9}$$

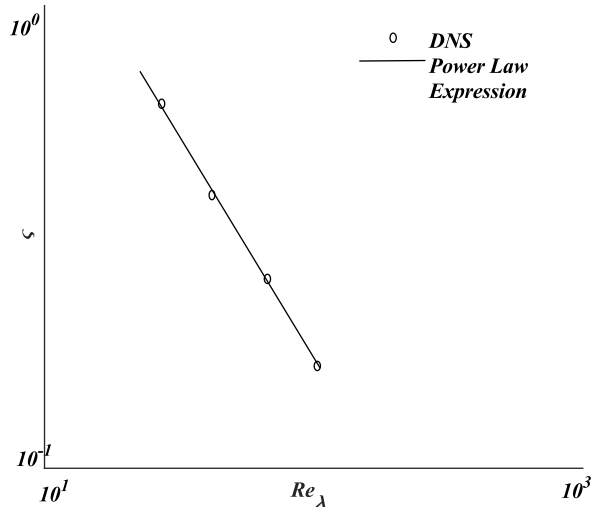

Fig. 1. The quantity "degree of local anisotropy" ς against Taylor-scale Reynolds number $\boldsymbol{Re_\lambda}$. Point: DNS from [12]; Line: power-law expression Eq 8.

In Fig. 2 distribution of ς in the Sandia Flame F is shown. We notice that near the inlet plane of co-flow (z=0, r/D > 10) the flow is mostly local anisotropic ($\varsigma \rightarrow 1$) due to relative low Reynolds number, and the molecular diffusion there does not largely depend on

velocity. However, especially near the centerline (r/D =0), Reynolds number is high and thus more local isotropic ($\varsigma \to 0$). In these regimes, the mixing process is largely velocity-conditioned.

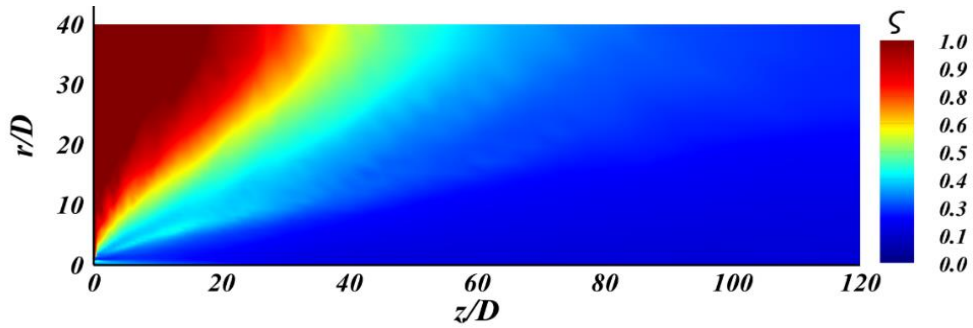

Fig. 2. Example of the distribution of ς in the Sandia Flame D

In this work, we extend the concept of velocity conditioning to the standard MCM model, which was also suggested in [11]. For the velocity-conditioned MCM (VC-MCM) one selects randomly one particle (p_1) and computes its degree of local anisotropy ς . Then another particle (q_2) will be randomly selected from the whole ensemble in the same cell with probability ς , and from the particles with the most similar velocity to p_1 with probability $(1-\varsigma)$. The "most similar velocity" is defined as minimum of the velocity difference between two particles:

$$\min \| \Delta \vec{U}_{ij} \|_2 = \min \left\| \vec{U}_i - \vec{U_j} \right\|_2 \tag{10}$$

The algorithm for VC-MCM is shown in a schematic flowchart in Fig. 3.

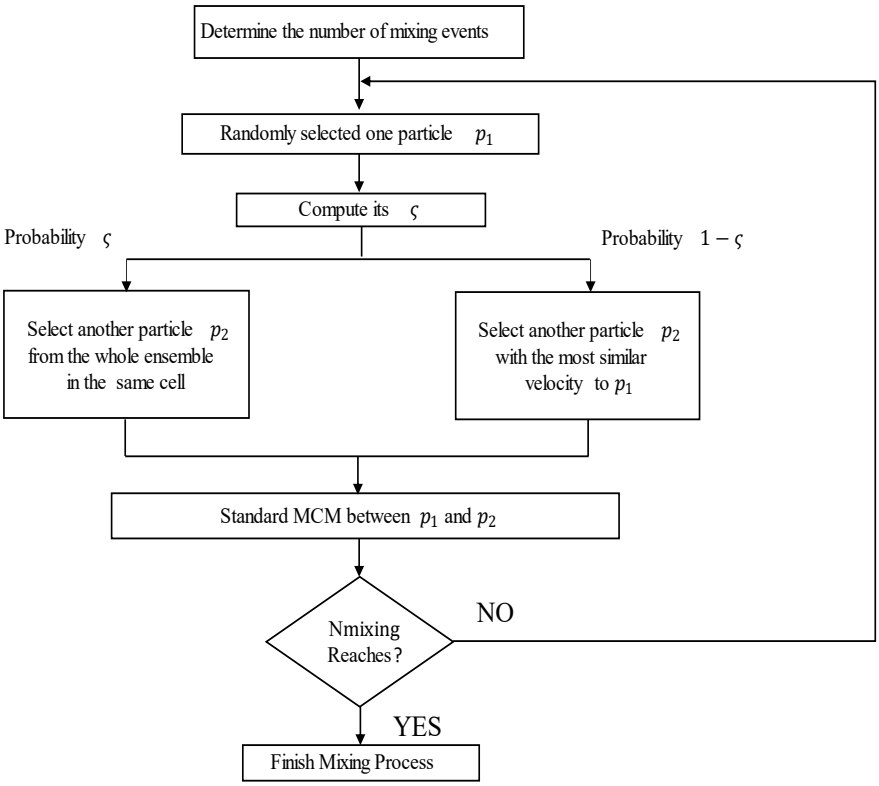

Fig. 3. Schematic flowchart for the numerical implementation of velocity-conditional MCM

V. Methodology and Solution Procedure

Sandia Flame Series D-F consists of a fuel jet with diameter D = 7.2 mm. The fuel is a mixture of 25% methane and 75% air by volume. The mixture is beyond the flammability limits and flame burn like a diffusion flame. The jet is surrounded by the co-axial pilot with an outer diameter D= 18.2 mm with a mixture of C_2H_2, air, CO_2 and N_2 which is operated at a fuel lean condition with equivalence ratio of 0.77 with its regular thermodynamic properties. Experimental studies were conducted by Barlow and Frank [17]. However, as mentioned earlier, in this work only Sandia Flame D will be studied due to the numerous reasons. First, a detailed experimental database in available online [17-19] that makes it possible to judge merits or demerits of the new method. Secondly, it has been the object for numerous modeling attempts for PDF simulations [11,13,20,21]. Last but not the least, this flame exhibits very low levels of local extinction [9,21] hence fulfilling the need to have a valid platform to test different mixing models. Sandia Flame D has a Reynolds number of 22,400 for the jet corresponding to the jet velocity of 49.6m/s. For a better overview of the Reynolds number effect on mixing model's performance, Sandia Flame F is also simulated which corresponds to a Reynolds Number of 44,800 and a jet velocity of 99.2 m/s.

Computational domain or flame is used in an axi-symmetric case as illustrated in Fig. 4 to reduce the computational efforts across the axial direction. Proper boundary conditions across the jet inlet in radial direction are used in order to eliminate jet pipe of the domain, thus saving computational resources. A polar-cylindrical (x, r) coordinate system is applied. The computational domain with 120D (axial)× 40 (radial) is used (with a good agreement with the experimental wind tunnel configuration [17]) and discretized by 51 cells in x direction and 42 cells in r direction (total 2142 cells). The grids are structured and fine near in the regime of symmetric axis (r=0 mm) and inlet (x=0 mm). The simulation starts with 20 particles per cell for Sandia Flame D and 50 particles per cell for Sandia Flame F, and a cluster-and-clone algorithm for particle number control is used. A grid sensitivity study has demonstrated sufficient resolution for the RANS flow and mixing fields.

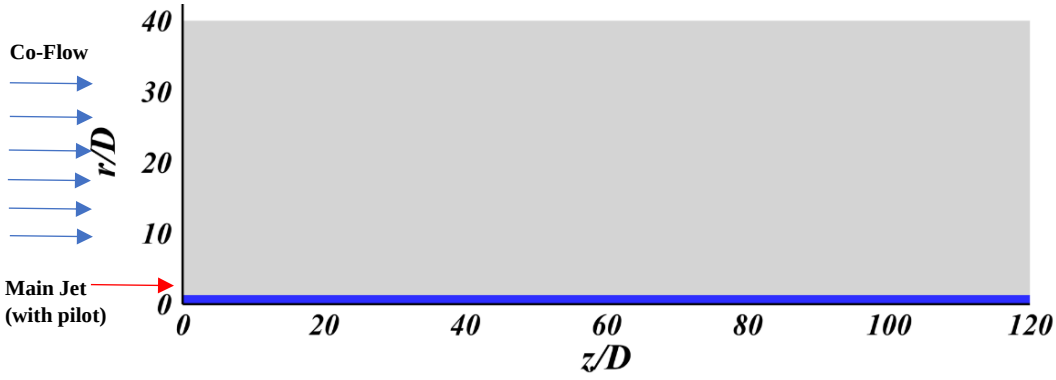

Fig. 4. Computational Model for Sandia Flame Series

Boundary Conditions are provided on the jet exit plane at z/D =0 as they are readily provided [22]. The mean axial velocity, Reynolds stresses $u_1\widetilde{"u_1"}$,$u_2\widetilde{"u_2"}$,$u_1\widetilde{"u_2"}$ are conditioned in a good agreement with [22,23]. Turbulence frequency at the inlet along with its variance are adopted as in [23]. Last, the ratio of dissipation rate and turbulent kinetic energy k is specified as unity.

Table 1.

Thermo-Kinetic States for various Inlet Profiles

Scalar	*Main-jet*	*Co-flow*	*Pilot*
H	*-725.7 KJ/Kg*	*-7.18KJ/Kg*	*-206.7 J/Kg*
p	*1 Bar*	*1 Bar*	*1 Bar*
ϕ_{N_2}	*23.21mol/Kg*	*27.30 mol/Kg*	*26.22 mol/Kg*
ϕ_{O_2}	*6.088 mol/Kg*	*7.35 mol/Kg*	*1.65 mol/Kg*
ϕ_{CO_2}	*0.0 mol/Kg*	*0.0 mol/Kg*	*2.50 mol/Kg*
ϕ_{CH_4}	*9.66 mol/Kg*	*0.0 mol/Kg*	*0.0 mol/Kg*
ϕ_{OH}	*0.0 mol/Kg*	*0.0 mol/Kg*	*0.17 mol/Kg*

Boundary conditions for the thermo-kinetic or the composition state (with a limited number of species) is provided in Table 1. Thermodynamic properties for the main jet were respectively taken as 294 K (Temperature), 1 Bar (Pressure) with a mixture of 25% CH_4 and 75% dry air (species composition). The co-flow consists of pure dry air with a temperature of 292 K and pressure of 1 bar. The pilot composition at the inlet can be a mixture of CH_4/air premixed flame with an equivalence ratio of 0.77. An inlet profile of 1880K and 1 bar is considered in validation with the experimental measurements [23].

In this work, a hybrid RANS/transported-PDF model [24] is applied. The RANS part provides the hydrodynamic quantities (Favre-averaged mean velocity $\tilde{u}_i$) to the PDF part. The PDF part provides the Reynolds stresses $\overline{\rho u_i" u_j"}$ and the temperature $\widetilde{R_g T}$ back to the RANS model.

In the PDF part, the transported-PDF equation is solved by using Monte-Carlo particle method [24,25], where a set of stochastic differential equations (SDEs) are solved for the evolution of notional particles. The position is evolved by its own velocity. The turbulence frequency is modelled by gamma-distribution model, and the velocity is modelled by the simplified Langevin model (Eq. 2). The evolution of the composition due to mixing process is calculated by using the velocity-conditioned MCM, using the algorithm in Fig. 3. Compositions of particles evolved due to chemical reaction are calculated through the Reaction-Diffusion-Manifolds (REDIM) [26] as simplified chemistry. Parameters and their values and corresponding applied models in transported-PDF method are listed in. The parameter in turbulent frequency model and the parameter C_ϕ in velocity-conditioned modified curl's mixing (VCMCM) model were investigated and their influences will be discussed later. Summary for the same is illustrated in Table 2.Note that although in [11] the Re_λ dependence of C_0 in Eq.4 was reported, the C_0 can be considered as a universal constant [1] and good results for reacting turbulent flows can be obtained with C_0 = 2.1 [2,3].

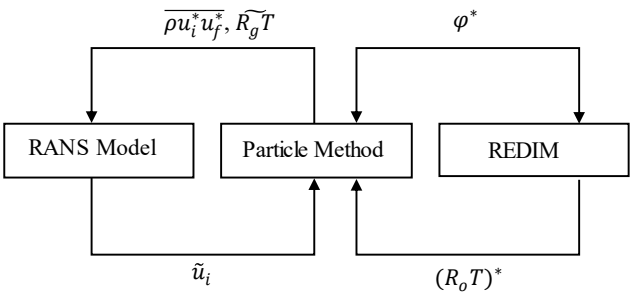

Fig. 5. Overview of coupling between RANS and transported-PDF model (particle method) based on REDIM

In Fig. 5 an overview of coupling between RANS and transported-PDF model (particle method) together with REDIM is represented. It is consistent to the algorithm in the previous works [27,28].

Table 2.

Overview of parametric values and corresponding applied models in transported-PDF method

Turbulence Frequency Model	
C_{Ω}	*0.6893*
$C_{\omega 1}$	*investigated*
C_2	*0.9*
C_3	*1.0*
C_4	*1.25*
Simplified Langevin Model	
C_o	*2.1*
Mixing Model	
$C_{\emptyset}$	*investigated*

VI. Results and Discussions

a) Reynolds number effect of 'Local anisotropy'

In Fig. 6, the Taylor-scale Reynolds number Re_{λ} (using Eq.10) and the degree of local anisotropy ς (using Eqn. 7) for Sandia Flame D (blue solid lines) and Sandia Flame F (red solid lines) along the centerline. The F series has been considered to illustrate the effect of increasing Reynolds number on local anisotropy. It's the same jet configuration but with a Reynolds number of twice that of Flame D i.e., 44800 corresponding to a jet velocity of 99.2 m/s.

It can be clearly observed that due to the higher Reynolds number of main jet in Sandia Flame F, it has also a higher level of Re_{λ} and, thus, lower values of ς. This means that for Sandia Flame F, it has a higher degree of local isotropy/ smaller degree of local anisotropy (smaller ς), corresponding to the hypothesis of local isotropy: in any turbulent flow with a sufficiently large Reynolds number, the turbulence can be well approximated to be local isotropic [16]. Furthermore, both Flames have relatively small values of ς, indicating that the mixing process largely depend on the velocity and velocity-conditioned mixing model is required (compared to e.g., Eq. 6).

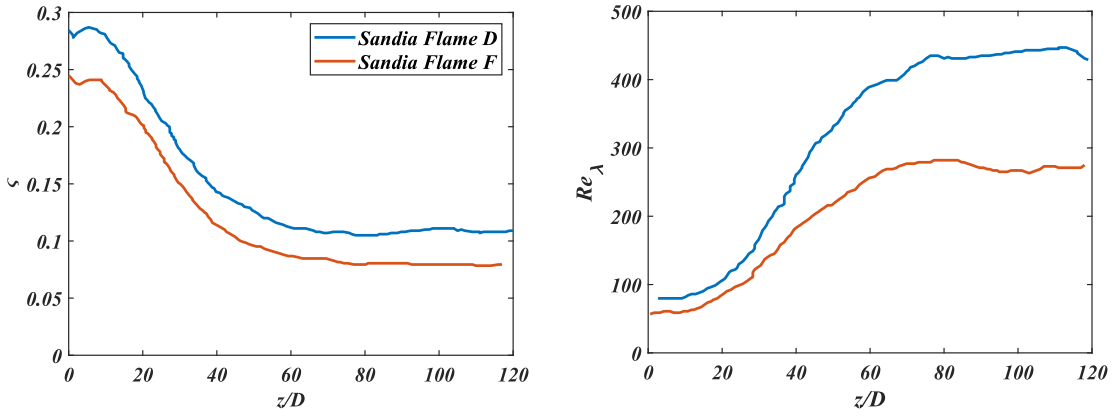

Fig. 6. Comparison of Taylor-scale Reynolds number $\boldsymbol{Re_{\lambda}}$ (left) and degree of local anisotropy ς (right) for Sandia Flame D (blue solid lines) and Sandia Flame F (red solid lines) along the centerline.

Nevertheless, both the flames show the similar behavior in local anisotropy along the centerline despite a major difference in Reynolds Number as observed in Fig. 6.

b) Influence of $C_{\omega 1}$

Although the influence of $C_{\omega 1}$ is well studied in other previous works [21,23], the parameter study shows that using the velocity-conditioned MCM, one needs a larger value of $C_{\omega 1}$ than using the standard MCM.

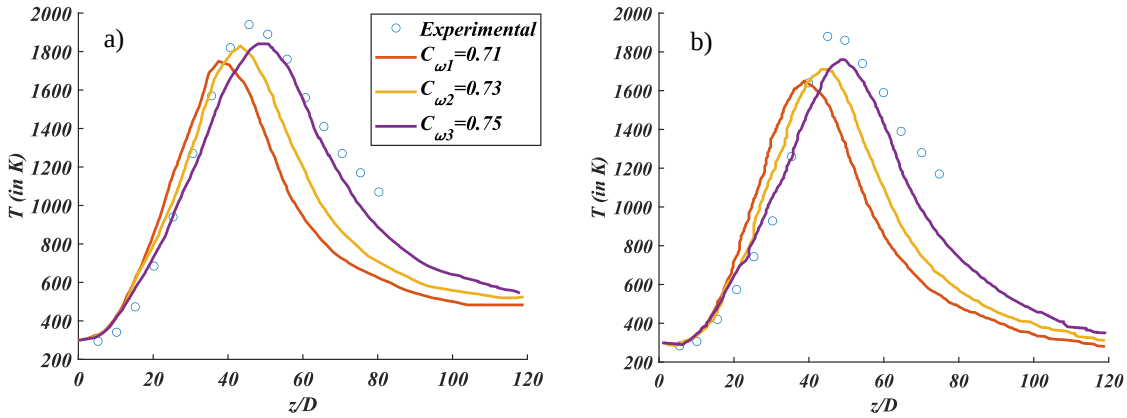

Fig. 7. Dependence of temperatures on $C_{\omega 1}$ in turbulent frequency model along the centerline for Sandia Flame D (a) and Sandia Flame (b). Circles: Experiment data; Lines: simulation results for different $C_{\omega 1}$

In the previous works [21,23], if the standard MCM (not velocity conditioned) is applied, $C_{\omega 1}$ = 0.71 can be used and results are in good agreement with the experimental data. However, for the application of velocity-conditioned MCM using $C_{\omega 1}$ = 0.71 would cause a shorter flame length, which is shown in Fig. 7 for Sandia Flame D and F. As demonstrated, no significant variation is noticed till z/D= 40 but the large variations in the profiles after that state the major influence of turbulence parameter $C_{\omega 1}$ irrespective of the Reynolds Number.

c) Sensitivity Analysis for Mixing Parameter C_{ϕ}

In this section, the influence of model parameter C_{ϕ} in VC-MCM mixing model is investigated. As already studied in other works [3,21], C_{ϕ} controls the scalar dissipation rate, hence affecting the simulation results to a great extent. For the same purpose, the conditional Favre-averaged mean temperatures at four different axial positions are represented in Fig. 8. Results based on $C_{\phi} = 1.3$, 2.0 and 3.0 are plotted together with experimental measurements. Furthermore, the conditional Favre-averaged mean mass fraction of OH is also summarized for a better overview of turbulence-chemistry interactions in Fig. 9. In general, increasing the value of C_{ϕ} yields the higher mean temperatures for Sandia Flame D, which is consistent to the results reported in other works [8,21,25]. Usage of C_{ϕ}=3.0 shows the superior results as shown in Fig. 8 (a)for the Favre-averaged temperature over mixture fraction as it's the most agreeable with the experimental readings. Although, C_{ϕ}= 2.0 also yields remarkable results but it remains a little unpredicted at lower axial positions.

On the other hand, for Favre-averaged mass fraction of OH, a non-linear variation for C_{ϕ}=1.3 across the various axial locations can be observed especially at the oxidizer rich side. Again, C_{ϕ}= 3.0 shows better results as compared to other values. Results based on C_{ϕ}=1.3 show clearly that scalar dissipation rates are much under-estimated, and thus result in over estimation of local extinction effect (much lower values of temperatures and mass fraction of OH).

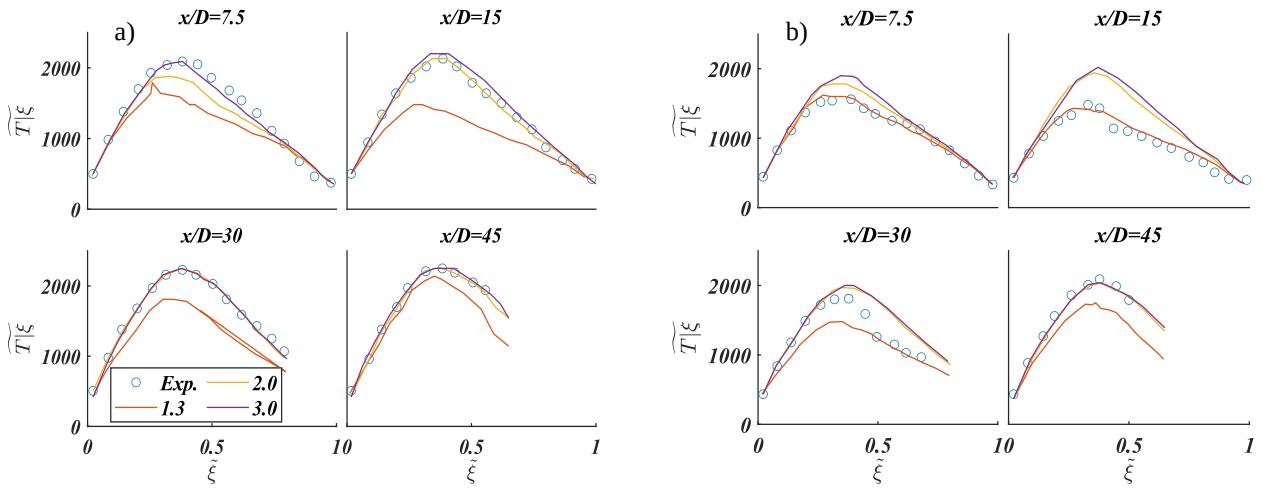

Fig. 8. Conditional Favre-averaged mean temperature $\widetilde{T|\xi}$ over $\tilde{\xi}$ at four different locations for a) Sandia Flame D and b) Sandia Flame F. Circles: experimental measurements; Solid lines: simulation results using different C_ϕ.

The results for Sandia Flame F are quite different. We notice that for locations near the jet exit plan (x/D=7.5 and 15), results of temperatures (Fig. 8 (b)) and mass fractions of OH (Fig. 9 (b)) based on C_ϕ=1.3 agree with experimental measurement much better, while for locations far from jet exit (x/D=30 and 45) value of C_ϕ=3.0 is again more suitable to be used.

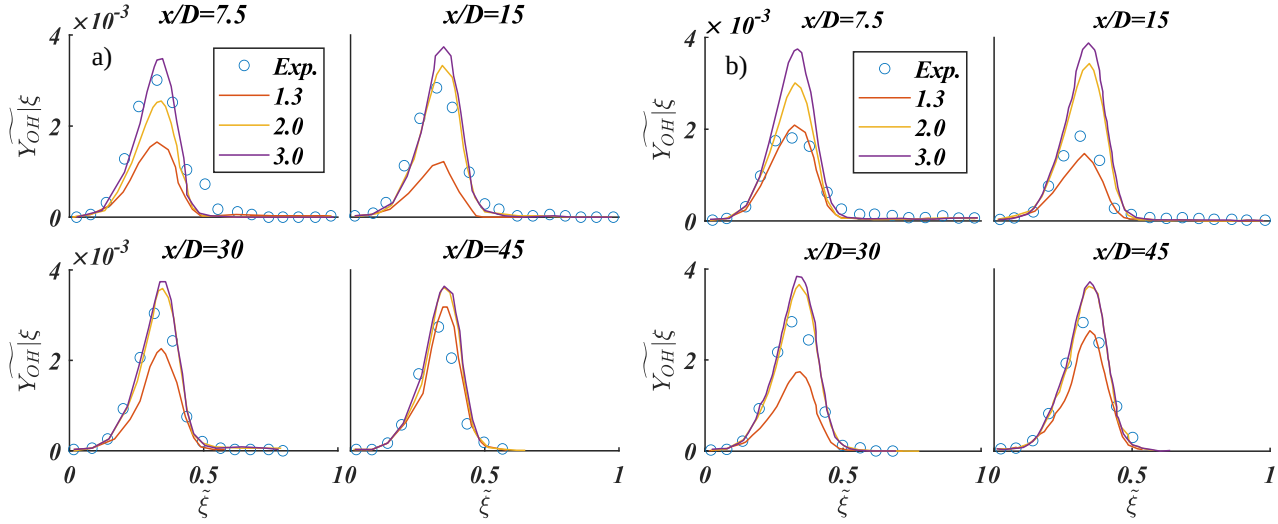

Fig. 9. conditional Favre-averaged mass fractions of OH $\widetilde{Y_{OH}|\xi}$ over $\tilde{\xi}$ at four different locations for a) Sandia Flame D and b) Sandia Flame. Circles: experimental measurements; Solid lines: simulation results using different C_ϕ.

This behavior can be explained by the fact that the mixing model parameter C_ϕ is not a universal constant and dependent on Reynolds number. Compared with the Reynolds number Sandia Flame F, we see that the Reynolds numbers increase with increasing distance to jet exit. Thus, together with the results of conditional quantities shown in Fig. 8 and Fig. 9, it is noticed that C_ϕ increases with increasing Reynolds number. The same observation has also been reported in [10], where values for C_ϕ founded using the DNS data [12] show a definite Reynolds number dependence and the same relationship between C_ϕ and Reynolds number as well.

Conclusion

The velocity conditioned modified curl's mixing model is implemented and applied in the simulation of the well-known turbulent jet diffusion flames (or non-premixed flames), Sandia Flame D and Sandi Flame F. It was shown that the flows have a high degree of isotropy ($\varsigma \to 0$). Hence, the effect of local anisotropy on scalar mixing was significant and a velocity-conditioned mixing model is necessary from physical aspect. The effects of model parameter $C_{\omega 1}$ and C_{ϕ} on flames have been investigated. The results show that a higher value of $C_{\omega 1}$ corresponds a longer flame length and a higher value of C_{ϕ} yields higher mean temperatures. Furthermore, C_{ϕ}=3.0 for Sandia Flame D is found to be the most suitable with respect to the well-matched experimental readings as well. For Sandia Flame F, C_{ϕ}= 1.3 yields good results near the jet exit and C_{ϕ}= 3.0 at far from the jet exit. This phenomenon is attributed to the fact that C_{ϕ} is not a universal constant and increases with increasing Reynolds number. All the simulations for VC-MCM are performed for stochastic 20 particles/cell. It's also concluded that VC-MCM takes a greater number of iterations as compared to general MCM due to sorting and selection through a more vigorous process than general MCM, hence more computationally intensive. The extension of velocity conditioning concept in the simulation of Sandia Flame series D-F is the subject of the current study. Lastly, modelling of Reynolds number dependence on model parameter C_{ϕ} shall be the subject of the further work.

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References

[1] Pope, S. B., "PDF methods for turbulent reactive flows," *Progress in Energy and Combustion Science*, Vol.11, Issue 2, 1985, pp. 119-192.

[2] Pope, S. B., "A Monte Carlo Method for the PDF Equations of Turbulent Reactive Flow," *Combustion Science and Technology*,1981, 25:5-6, pp. 159-174.

[3] Cao, R. R., Wang, H. and Pope, S. B., "The effect of mixing models in PDF calculations of piloted jet flames," *Proceedings of the Combustion Institute*, Vol.31, Issue 1, 2007, pp. 1543-1550.

[4] Dopazo, C. and Edward E. O., "An approach to the autoignition of a turbulent mixture," *Acta Astronautica*, Vol.1, Issues 9–10,1974, pp 1239-1266.

[5] Curl, R. L., "Dispersed phase mixing: I. Theory and effects in simple reactors," *AIChE Journal*, Vol. 9, Issue 2, 1963, pp 175-181.

[6] Janicka, J., Kolbe, W. and Kollmann, W. "Closure of the Transport Equation for the Probability Density Function of Turbulent Scalar Fields", *J. Non-Equilib. Thermodynamics*, Vol. 4, no. 1, 1979, pp. 47-66.

[7] Pope, S. B., "An Improved Turbulent Mixing Model," *Combustion Science and Technology*, 28:3-4, 1982, pp. 131-145.

[8] Nooren, P.A., Wouters, H. A, Peters, T.W.J., Roekaerts, D., Maas, U. and Schmidt, D, "Monte Carlo PDF modelling of a turbulent natural-gas diffusion flame," *Combustion Theory and Modelling*, 1:1, pp. 79-96.

[9] Cleary, M., Klimenko, and Alexander., "A Generalized Multiple Mapping Conditioning Approach for Turbulent Combustion," *Flow, Turbulence and Combustion*. 82., 2009, pp. 477-491.

[10] Fox, R., "Computational Models for Turbulent Reacting Flows," *Cambridge Series in Chemical Engineering*, Cambridge University Press, 2003, Cambridge, England, UK.

[11] Fox, R. O., "On velocity-conditioned scalar mixing in homogeneous turbulence, *"Physics of Fluids* 8, 1996, pp. 2678-2691

[12] Overholt, M. R. and Pope, S. B., “Direct numerical simulation of a passive scalar with imposed mean gradient in isotropic turbulence,” *Physics of Fluids* 8, 1996, pp. 3128-3148.

[13] Stoellinger, M., Efimov, D., and Roekaerts, D., “Monte Carlo simulations of turbulent non-premixed combustion using a velocity conditioned mixing model”. In S. Heinz, & H. Bessaih (Eds.), *Stochastic equations for complex systems: theoretical and computational topics* pp. 143-174. Vol. 20.,2015, Springer, Darmstadt.

[14] Sawford, B. L., “Conditional scalar mixing statistics in homogeneous isotropic turbulence,” *New Journal of Physics,* Vol.6, May 2004, pp. 55-65

[15] Pope, S. B., “Lagrangian PDF Methods for Turbulent Flows,” *Annual Review of Fluid Mechanics,* 1994, pp. 23-63.

[16] Pope, S. B., “Turbulent Flows,” Cambridge University Press, 2000, Cambridge, England, UK.

[17] Barlow R.S. and Frank J.H., “Effects of turbulence on species mass fractions in methane/air jet flames,” *Symposium (International) on Combustion,* Vol.27, Issue 1,1998, pp. 1087-1095.

[18] Schneider, C., Dreizler, A., Janicka, J., and Hassel, E.P. “Flow field measurements of stable and locally extinguishing hydrocarbon-fuelled jet flames”. *Combustion and Flame 135*, pp.185-190.

[19] Raman, Venkat, Pitsch and Heinz, “A consistent LES/Filtered-density function formulation for the simulation of turbulent flames with detailed chemistry,” *Proceedings of the Combustion Institute 31*, 2007, pp. 1711-1719.

[20] de Bruyn Kops, S., Riley, J., and Kosály, G. “Investigation of Modeling for Non-Premixed Turbulent Combustion,” *Flow, Turbulence and Combustion 60*, 1998, pp. 105–122.

[21] Straub C., De S., Kronenburg, A. and Vogiatzaki, K., “The effect of timescale variation in multiple mapping conditioning mixing of PDF calculations for Sandia Flame series D–F,” *Combustion Theory and Modelling*, 20:5, 2016, pp. 894-912.

[22] Barlow, R. S., “Proceedings of the international workshop on measurement and computation of turbulent non-premixed flames,”, United States,1996.

[23] Cao, R.R. and Pope, S. B., “The influence of chemical mechanisms on PDF calculations of non-premixed piloted jet flames”, *Combustion and Flame,* Vol.143, Issue 4, 2005, pp. 450-470.

[24] Jenny, P., Pope, S. B., Muradoglu, M. and Caughey, D. A., “A Hybrid Algorithm for the Joint PDF Equation of Turbulent Reactive Flows”, *Journal of Computational Physics*, Vol.166, Issue 6, 2001, pp. 218-252.

[25] Valiño, L., Ros J., and Dopazo C., "Monte Carlo implementation and analytic solution of an inert-scalar turbulent-mixing test problem using a mapping closure", *Physics of Fluids A: Fluid Dynamics 3,* 1991, pp. 2191-2198.

[26] V. Bykov & Maas U., “The extension of the ILDM concept to reaction–diffusion manifolds,” *Combustion Theory and Modelling*, 11:6, 2006, pp. 839-862,

[27] Yu, C., Minuzzi, F., and Maas, U. “REDIM reduced chemistry for the simulation of counterflow diffusion flames with oscillating strain rates”, *Combustion Theory and Modelling*, 24:4, 2020, pp. 682-704.

[28] Yu, C., Breda, P., Minuzzi, F., Pfitzner M., and Maas, U., “A novel model for incorporation of differential diffusion effects in PDF simulations of non-premixed turbulent flames based on reaction-diffusion manifolds (REDIM)”, *Physics of Fluids 33*, 2021.