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Sensitivity Study of the Model Parameters of a Novel Multiple Mapping Conditioning Mixing Model in the Context of Sandia Flame E

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Abstract

The mixing model is a vital part of Lagrangian Probability Density Function (PDF) methods and is in need of further research. Recently a novel mixing model has been proposed which is based on the concept of Multiple Mapping Conditioning (MMC). It adheres to all the principles of a good mixing model including the localness property. The distinguishing feature of this model is that the mixing is performed in such a way that the mean and the variance of the reference variable and the mixture fraction are nominally the same. This model is physically intuitive due to which the range of its model parameters are small making it convenient to use. However, a thorough sensitivity study of the model parameters is necessary to get an insight into the behavior of the mixing model. An extensive research was conducted in the context of Sandia flame series to determine an ideal set of values for the model parameters. A constant value of 0.71 was used for the model parameter b_o which controls the random walk of particles in reference variable space. In the present work, the effect of varying b_o is studied with Sandia flame E as the test case. It is observed that any value other than 0.71 would cause the variances of the reference variable and the mixture fraction to decay at different rates, in line with the theory. A smaller value will make the reference variable to decay faster and a higher value will force the mixture fraction to decay faster. The determination of values of other model parameters becomes complicated when the reference variable and the mixture fraction do not decay at equal rates. It is concluded that 0.71 is the best value of b_o for inhomogeneous turbulent flows as well. The simulations are in good agreement with the experiments for the ideal set of model parameters.

Introduction

The averaging of the evolution equation of species mass fraction and mixture specific enthalpy results in an unclosed chemical source term. For instance, the Favre averaged mass fraction of species α ($\tilde{Y}_\alpha$) given by

$$\frac{\partial \bar{\rho}\tilde{Y}_\alpha}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{Y}_\alpha}{\partial x_i} + \frac{\partial \overline{J_i^\alpha}}{\partial x_i} = \overline{\omega_\alpha} - \frac{\partial \bar{\rho}\widetilde{u_i''Y_\alpha''}}{\partial x_i}, \tag{1}$$

has an unclosed source term ($\overline{\omega_\alpha}$) representing the production/consumption of species. $\bar{\rho}$, $\tilde{u_i}$ and $\overline{J_i^\alpha}$ represent the averages of density, velocity and molecular flux of species, respectively. The second unclosed term on the right hand side (RHS) represent turbulent transport which is typically modelled using the gradient transport assumption [15]. Since $\overline{\omega_\alpha}$ is a highly nonlinear function of temperature, species concentrations and pressure, and since turbulent fluctuations of these variables are large in flames, closing this term with a model is quite problematic.

The need to model $\overline{\omega_\alpha}$ can be bypassed by using transported Probability Density Function (PDF) methods because $\overline{\omega_\alpha}$ is already closed. The evolution of Eulerian composition PDF (f_{ϕ_k}) is given by [8]

$$\frac{\partial \bar{\rho} f_{\phi_k}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u_i} f_{\phi_k}}{\partial x_i} + \frac{\partial \omega_k f_{\phi_k}}{\partial \psi_k} = -\frac{\partial \bar{\rho} f_{\phi_k} \langle u_i''|\psi\rangle}{\partial x_i} + \frac{\partial}{\partial \psi_k}\left[f_{\phi_k} \left\langle \frac{\partial J_i^k}{\partial x_i}|\psi \right\rangle \right]. \tag{2}$$

ϕ_k is a composition vector and includes all species mass fractions and mixture specific enthalpy. The first unclosed term on the RHS represents turbulent transport in physical space and is modelled using the gradient transport hypothesis. The second unclosed term on RHS determines the turbulent transport in composition space which is calculated using a mixing model in Lagrangian PDF methods [8]. In stochastic Lagrangian PDF methods, notional particles are used to represent samples of the PDF, and the transport in physical space, the transport in composition space and the change in composition due to chemical reactions are calculated in three different fractional sub-steps. The former is modelled by [8]

$$dx_i^* = \tilde{u_i}^* dt + \left(\frac{1}{\bar{\rho}}\frac{\partial \Gamma_{eff}}{\partial x_i}\right)^* dt + \left(\sqrt{\frac{2\Gamma_{eff}}{\bar{\rho}}}\right)^* dW_i', \tag{3}$$

and the next two phenomena affecting the composition vector are represented by

$$\Delta\phi_k^* = \omega_k(\phi^*)dt + d\phi_k^*. \tag{4}$$

In the above, $\tilde{u_i}^*$ is the Favre-averaged particle velocity, Γ_{eff} is the effective diffusivity, $\omega_k(\phi^*)$ is the change in composition due to chemical reactions and $d\phi_k^*$ represents the increment of composition as a result of application of the mixing model. The subscript $*$ indicates particle property, $W_i'(t)$ is an isotropic Wiener process and the Γ_{eff} is defined as

$$\Gamma_{eff} = \mu/\sigma_\phi + \mu_T/\sigma_{T\phi}. \tag{5}$$

In Eq. (5), μ and μ_T are the dynamic molecular and turbulent viscosity, respectively and σ_ϕ and $\sigma_{T\phi}$ are the molecular and turbulent Schmidt number, respectively.

MMC Mixing Model Equations

The main focus of Lagrangian PDF methods is on the mixing model. It has been established that a good mixing model should first satisfy the basic criteria like conservation of mean, decay of variance and boundedness [12]. It should also satisfy a property known as localness, which corresponds to the physical principle for continuum fluids that mixing occurs between fluid regions that have similar compositions. Conventional mixing models like interaction by exchange with the mean (IEM) [4] and modified Curl's [3] do not have the localness property

whereas Euclidean minimum spanning tree (EMST) [12] possesses localness but violates linearity and independence principles and is prone to "stranding" in composition space [12], overdamps conditional fluctuations [7] and has other drawbacks as mentioned in [9]. Multiple Mapping Conditioning (MMC), first proposed in [6], introduces localness property by using a reference variable which is related to the mixture fraction (z) in non-premixed combustion and to progress variable or distance-like variable in premixed combustion using an implicit mapping function. The original RANS-MMC mixing model has been successful in predicting extinction/re-ignition phenomena [16], [11], [17]. A new MMC mixing model has been proposed recently [13] where the reference variable is statistically similar to the mixture fraction. As a result of that similarity the mapping function between the reference variable and mixture fraction PDFs is relatively simple (approaching linearity) so that the new model is both easy to understand and numerically implement. The governing equations of this MMC mixing model are

$$d\xi^* = -\frac{C_\xi}{\tau}(\xi^* - \bar{\xi})dt + b_o\sqrt{\frac{2C_\xi\langle\xi'^2\rangle}{\tau}}dW \tag{6}$$

and

$$d\phi_k^* = -\frac{C_{min}}{\tau}(\phi_k^* - \langle\phi_k^*|\xi^*\rangle)dt, \tag{7}$$

where ξ is the reference variable, $\bar{\xi}$ is the unconditional mean of ξ and $\langle\phi_k^*|\xi^*\rangle$ is the mean of ϕ_k conditioned on ξ, and $\langle\xi'^2\rangle$ is the unconditional variance of ξ. $W(t)$ is a Wiener process and is independent of that in Eq. (3). $\langle\phi_k^*|\xi^*\rangle$ is approximated by

$$\langle\phi_k^*|\xi^*\rangle^n = \frac{(m^{n+1}\phi_k^{n+1} + m^{n-1}\phi_k^{n-1})}{(m^{n+1} + m^{n-1})}, \tag{8}$$

as suggested in [9], where m^{n+1} and m^{n+1} represent the mass of particles in the neighborhood of n-th particle in ξ-space.

The target correlation coefficient (r_t) gives an idea of the strength of correlation between ξ and z and the connection between r_t and other model constants is given by

$$r_t = \sqrt{1 - \frac{C_\xi b_o^2}{C_{min}}}. \tag{9}$$

Here, b_o, C_ξ and C_{min} are the model constants and the recommended values are $b_o = 0.71$, $C_\xi = 2$ and $C_{min} = 8$ corresponding to the correlation between ξ and z of $r_t = 0.935$. The derivation of this model and its application to ideal flow test cases are given in [13]. The details of mixing model implementation in OpenFOAM and its validation using Sandia/Sydney flame experimental data is discussed in [14]. It has been suggested using theory that the model constant b_o, which scales the magnitude of the turbulent diffusion term, should have a value of 0.71 and the same value was used in [14]. However, it is interesting to understand the implications of having a different value for b_o. In this paper, the sensitivity of the model predictions to the value of b_o is analysed.

Experimental Data

The Sandia/Sydney piloted methane-air flame experiments have been conducted to study the effects of increasing jet velocity on flame extinction [1] and will be used in this work to validate the MMC mixing model predictions. The diameter of jet and pilot inlets are $d = 7.2$ mm and $d_p = 18.2$ mm, respectively. The jet composition is 25% methane and 75% air by volume and the pilot mixture consists of C_2H_2, H_2, CO_2, N_2 and air, having the same enthalpy as a methane/air mixture of equivalence ratio 0.77. The jet velocity of flame E is 74.4 m/s which corresponds to $Re = 33600$. Further details can be found in [1]. The mass fraction of CO obtained from laser-induced fluorescence (LIF) is used for validation in this work instead of Raman scattering data as the former is more accurate. The other quantities validated in this work include mixture fraction, temperature and the mass fraction of H_2O, CO_2 and OH.

Numerical Set-up

A hybrid Eulerian/Lagrangian composition PDF algorithm, having a two-way coupling between the finite volume (FV) and particle solvers, is used in the present work [2]. The two-dimensional round-jet flame is simulated in a cylindrical coordinate system with the origin at jet inlet. FV mesh is $50d$ long along axial direction (x-axis) and $12.5d$ wide along radial direction (y-axis). Uniform temperature values given by the experimental data are assigned to the jet, pilot and co-flow inlets. Uniform values are also used for rest of the quantities at pilot and co-flow inlets whereas the profiles given by experiments are used for velocity, turbulent kinetic energy (k) and dissipation (ε) at the jet inlet [10].

The FV mesh has 96 cells along x-axis and 40 cells along y-axis, with refinements near the centerline and inlets. A variable time-step with a maximum Courant number of 0.8 is used which also ensures that $max(\Delta t/\tau) < 1$, where Δt is the time-step and $\tau = k/\varepsilon$ is the turbulent time scale. The standard $k-\varepsilon$ turbulence model with the conventional model constants is used in this work. The number of notional particles representing the PDF per cell is 70 and it has been found to produce converged solution [14]. DRM19 chemical mechanism [5] is used since it is three times computationally cheaper than GRI3.0 mechanism and has been found to produce to satisfactory results. Once the flow has reached statistically stationary state, time-averaging is used to reduce statistical error. The computation of flame E on AMD cluster with 24 processors ($2.1GHz$) takes approximately 36 hours.

Results and Discussion

The validity of using $b_o \neq 0.71$ is investigated in this section. The mean and root mean square (RMS) of ξ and z are compared first since they are significantly affected by b_o. Next, the scatter plot of temperature and mass fraction of CO (Y_{CO}) are analysed to study the effect on conditional statistics. Finally, the graphs of unconditional mean of temperature and Y_{CO} are discussed to highlight the effect of b_o on unconditional statistics. All the simulations discussed in this work have $C_\xi = 2$ and $C_{min} = 8$ as suggested in [14].

By studying the analytical solution of homogeneous turbulent flow, it was concluded that $b_o = 0.71$ ensures that the $\bar{z} = \bar{\xi}$ and $\langle z'^2\rangle \approx \langle\xi'^2\rangle$ [13]. Fig. 1 shows that this is indeed valid for inhomogeneous turbulent reactive flows as there is very good agreement between the mean of ξ and z at all the validated axial locations.

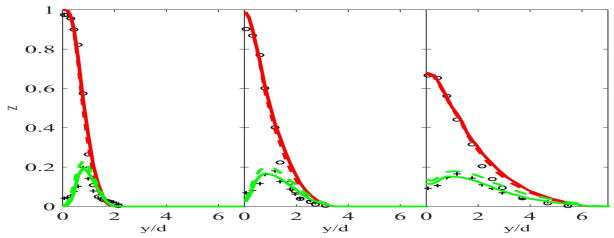

Figure 1: Mean and RMS of ξ and z for a case with $b_o = 0.71$ at $x/d = 7.5$ (left), $x/d = 15$ (centre) and $x/d = 30$ (right). Symbols: experiments; dashed lines: CFD ξ; solid lines: CFD z.

According to the analytical solution of homogeneous turbulent flow, $b_o < 0.71$ causes $\langle z'^2 \rangle$ to decay slower than $\langle \xi'^2 \rangle$ and $b_o > 0.71$ results in faster decay of $\langle z'^2 \rangle$ [13]. Fig. 2 shows that the RMS of z is greater than that of ξ at all three axial locations when $b_o = 0.3$ implying that the decay of mixture fraction variance is slow, which is in line with the theory. When $b_o = 0.9$, the decay of $\langle \xi'^2 \rangle$ is extremely slow which is indicated by higher RMS of ξ as seen in Fig. 3.

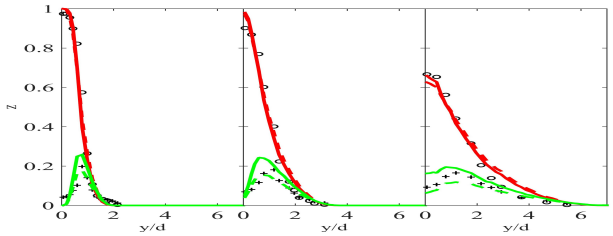

Figure 2: Mean and RMS of ξ and z for a case with $b_o = 0.3$ at $x/d = 7.5$ (left), $x/d = 15$ (centre) and $x/d = 30$ (right). Symbols and lines same as in Fig. 1.

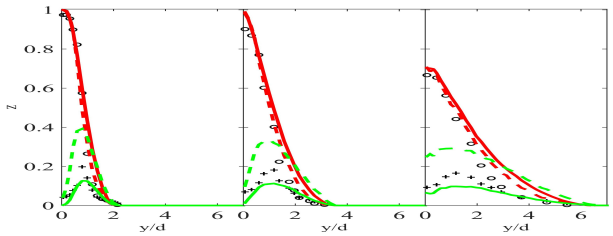

Figure 3: Mean and RMS of ξ and z for a case with $b_o = 0.9$ at $x/d = 7.5$ (left), $x/d = 15$ (centre) and $x/d = 30$ (right). Symbols and lines same as in Fig. 1.

Figures 1-3 show the effect of b_o on the spreading of $\tilde{z}$ and there is a negligible effect of b_o on $\tilde{z}$. However, there is a stark effect of b_o on the RMS of mixture fraction as seen in Fig. 1-3 and the combination of $b_o = 0.71$ and $C_\xi = 2$ reproduce the correct RMS at all the three axial locations.

Equation (9) implies that for a given value of C_ξ and C_{min}, increasing b_o increases r_t and hence the localness of the MMC mixing model. This can be clearly seen in the scatter plot of the temperature and Y_{CO} in Fig. 4 and Fig. 5, respectively. $b_o = 0.3$ decreases the localness of mixing model, due to which the conditional fluctuations are amplified. On the other hand, $b_o = 0.9$ over-damps the conditional fluctuations resulting in higher temperature and Y_{CO} predictions. When compared to experiments, $b_o = 0.3$ slightly over-predicts conditional fluctuations and $b_o = 0.71$ under-predicts the conditional fluctuations. However, $b_o = 0.71$ is preferred since it ensures that $\langle z'^2 \rangle \approx \langle \xi'^2 \rangle$, according to the assumptions of this MMC mixing model.

Figure 6 and Fig. 7 show the effect of b_o on the predictions of the unconditional mean of temperature and Y_{CO}. Increasing b_o increases the localness of mixing model which implies greater mixing resulting in an increase in the unconditional mean of temperature and Y_{CO}.

Conclusions

The sensitivity of the MMC mixing model predictions to the model parameter b_o, which controls the random walk of particles in reference variable space, is investigated in the context

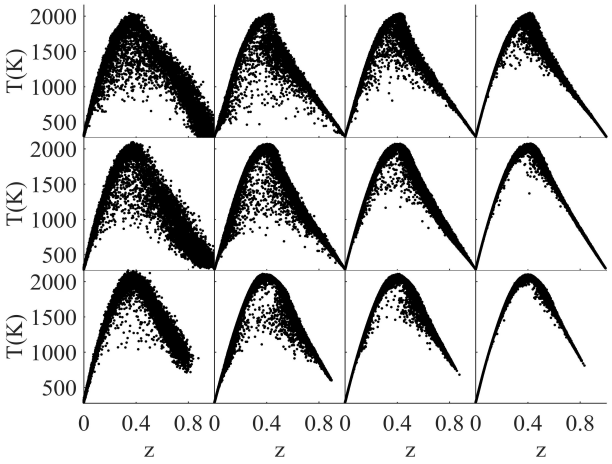

Figure 4: Sensitivity of scatter plot of T to b_o at $x/d = 7.5$ (top), $x/d = 15$ (centre) and $x/d = 30$ (bottom). 1^{st} Column: experiments; 2^{nd} column: $b_o = 0.3$; 3^{rd} column: $b_o = 0.71$; 4^{th} column: $b_o = 0.9$.

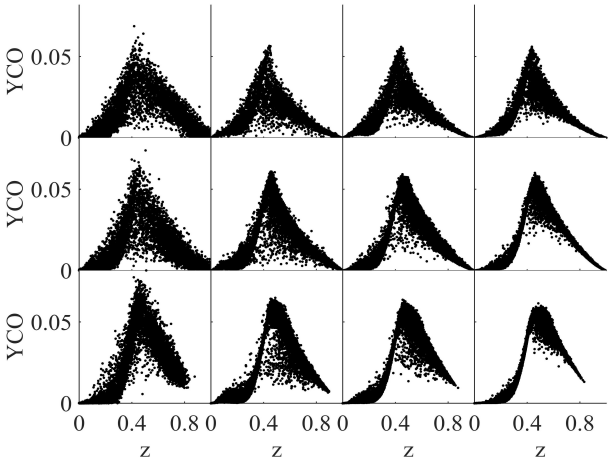

Figure 5: Sensitivity of the scatter plot of Y_{CO} to b_o at $x/d = 7.5$ (top), $x/d = 15$ (centre) and $x/d = 30$ (bottom). Legends same as in Fig. 4.

of Sandia flame E. It is seen that the variance of the mixture fraction and the reference variable decay at unequal rates when $b_o \neq 0.71$: the mixture fraction variance decays slower than the reference variable variance when $b_o < 0.71$ and faster when $b_o > 0.71$, in accordance with the theory. For a given value of C_ξ and C_{min}, higher the value of b_o greater the localness of mixing model. When $b_o = 0.71$, C_ξ and C_{min} can be determined using DNS and experimental data without any ambiguity and hence is recommended. The MMC mixing model calculates the conditional and unconditional statistics of flame E satisfactorily with $b_o = 0.71$, $C_\xi = 2$ and $C_{min} = 8$.

Acknowledgements

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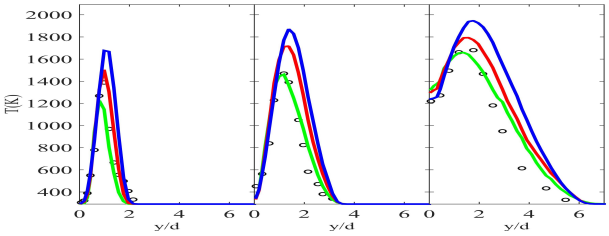

Figure 6: Sensitivity of the unconditional mean of T to b_o at $x/d = 7.5$ (left), $x/d = 15$ (centre) and $x/d = 30$ (right). Symbols: experiments; green line: $b_o = 0.3$; red line: $b_o = 0.71$; blue line: $b_o = 0.9$.

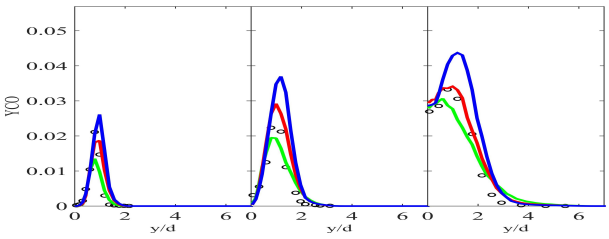

Figure 7: Sensitivity of the unconditional mean of Y_{CO} to b_o at $x/d = 7.5$ (left), $x/d = 15$ (centre) and $x/d = 30$ (right). Symbols and lines same as in Fig. 6.

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