Application of Hybrid Binomial Langevin-Multiple Mapping Conditioning Method to Reacting Jet Flow

Andrew P. Wandel[1,*] and R. Peter Lindstedt[2]
[1]Computational Engineering and Science Research Centre
Faculty of Engineering and Surveying
University of Southern Queensland, Qld, 4350, Australia
[2]Department of Mechanical Engineering
Imperial College of Science, Technology and Medicine, London, SW7 2BX, UK

Abstract

The hybrid binomial Langevin-MMC (Multiple Mapping Conditioning) method combines the advantages of the binomial Langevin and MMC models in a consistent manner to overcome difficulties in each. The binomial Langevin method provides joint velocity-scalar statistics, but the treatment of scalars is complex since specification of the bounds is not trivial. The MMC method is capable of dealing with the mixing of any number of scalars, but it can be difficult to specify coefficients involving averages of the scalars and the introduced reference space. The difficulties are overcome by using the velocity statistics from the binomial Langevin model to obtain the reference variable for MMC and, subsequently, the mixing of MMC scalars is performed in a manner that minimises the difference between the mixture fractions for each submodel. The current work expands past studies of NO conversion in a mixing layer to include a study of the Sandia D Flame in preparation for the application to more complex combustion phenomena. Results compare favourably with experimental data and other models.

Keywords: binomial Langevin model, Multiple Mapping Conditioning model, Sandia flame

1. Introduction

With the pressure to reduce emissions becoming a key factor in the design process of modern combustion systems, engineers are moving closer to the combustion limits. This results in finite-rate chemistry effects (such as extinction/reignition) becoming important and such phenomena are increasingly examined through computational methods [1,2]. Because simple models generally cannot completely describe these effects, transport probability density function (PDF) models are often required [3]. Extinction and reignition processes amplify the sensitivity of the results to different closure elements, including molecular mixing [4], so developments continue to be made in this area. A hybrid model [5] was recently proposed that used the Multiple Mapping Conditioning (MMC) [6] and binomial Langevin [7] models as its basis. The proposal was to use the binomial Langevin model to solve joint velocity-scalar statistics with one scalar (a mixture fraction), while the MMC model was used to solve for all scalars (including the mixture fraction). The goal was to overcome the implementation difficulties inherent in solving bounded scalars in the binomial Langevin model, while simultaneously overcoming difficulties with specifying certain coefficients in the MMC model. This was achieved by forcing the mixture fraction in the MMC component of the model to approach the binomial Langevin value, while using the dominant velocity component from the binomial Langevin solution as a basis for the MMC reference variable. The approach is consistent with the methodology proposed in that another variable can be used to define the reference quantity rather than solving explicit transport equations for the latter [8]. Following the success achieved with the method for a reacting mixing layer [5], the authors here apply the method to a reacting jet (Sandia Flame D [9]). The Reynolds number is too low to cause significant local extinction/reignition events. However, by verifying the model for this case, subsequent studies of higher Reynolds number flames (Sandia Flames E and F) can be attempted in the knowledge that only the extinction/reignition phenomena are independent quantities in the sensitivity analysis.

2. Model Formulation

The hybrid binomial Langevin–MMC model [5] is described in this section. First the binomial Langevin model is outlined, then the MMC model and, finally, the link used in the hybrid model is described.

2.1 Binomial Langevin model

A generalized form of the binomial Langevin model for the joint-PDF (Probability Density Function) of velocity and multiple scalars was developed by Hůlek and Lindstedt [10]. The stochastic differential equation for velocity component u_i is:

$$du_i^p = \left(\alpha_1\delta_{ij} + \alpha_2\beta_{ij}\right)\left(u_j^p - \langle u_j\rangle\right)\frac{dt}{\tau_u} + \left(C_0\langle\varepsilon\rangle\right)^{1/2} dw_i \qquad (1)$$

* Corresponding author:
Phone: (+61) 7 4631 2230
Email: andrew.wandel@usq.edu.au

where p denotes the pth particle, $\tau_u = \langle k \rangle / \langle \varepsilon \rangle$ is the turbulent timescale, k the turbulent kinetic energy, ε the turbulent dissipation rate, $\langle \varepsilon \rangle$ its average, dw_i a Wiener process, and β_{ij} the Reynolds stress anisotropy tensor:

$$\beta_{ij} = \left\langle u_i' u_j' \right\rangle \Big/ \left\langle u_k' u_k' \right\rangle - \tfrac{1}{3}\delta_{ij} . \qquad (2)$$

The remaining coefficients are $C_0 = 2.1$, $\alpha_2 = 3.7$ and $\alpha_1 = -(\tfrac{1}{2} + \tfrac{3}{4}C_0) - \alpha_2(\beta_{ll})^2$. The corresponding stochastic differential equation for any scalar η is:

$$d\eta^p = G_\eta\left(\eta^p - \langle \eta \rangle\right)\frac{dt}{\tau_\eta} + \left(B_\eta \left\langle \varepsilon_\eta \right\rangle\right)^{1/2} dw_{\text{bin}} . \qquad (3)$$

The mean scalar dissipation rate is $\langle \varepsilon_\eta \rangle = \langle \eta'^2 \rangle / \tau_\eta$, the scalar timescale was modelled as $\tau_\eta = \tau_u / C_\phi$ ($C_\phi = 2.3$ was chosen [3]) and dw_{bin} is a binomial Wiener process [7]. The drift coefficient G_η is

$$G_\eta = -\left\{ K_\eta \left[1 - \left\langle \left(\frac{\eta'^p}{\eta_*'} \right)^2 \right\rangle \right] + 1 \right\} \qquad (4)$$

while the diffusion coefficient B_η is

$$B_\eta = K_\eta \left[1 - \left(\frac{\eta'^p}{\eta_*'} \right)^2 \right] \qquad (5)$$

where

$$K_\eta = K_0 \left(1 - \frac{\theta_\eta}{|\theta_\eta| + 1} \right)$$

$$\theta_\eta = C_K \frac{\left[\left(\eta^p - \langle \eta \rangle\right)\left(u_i^p - \langle u_i \rangle\right) - \langle \eta' u_i' \rangle \right] \langle \eta' u_i' \rangle}{\frac{2}{3}\langle k \rangle \langle \eta'^2 \rangle}$$

with $K_0 = 2.1$ and $C_K = 0.76$. The other quantities are:

$$\eta'^p = \eta^p - \langle \eta \rangle^p$$

$$\eta_*' = \begin{cases} \eta_{\max}'^p, & \eta'^p > 0 \\ \eta_{\min}'^p, & \eta'^p < 0 \end{cases}$$

$$\langle \eta \rangle^p = \eta_{\min}\big|_{c=c^p} + \left(\langle \eta \rangle - \eta_{\min}\big|_{c=c^p} \right) \frac{\eta_{\max}\big|_{c=c^p} - \eta_{\min}\big|_{c=c^p}}{\eta_{\max}\big|_{c=\langle c \rangle} - \eta_{\min}\big|_{c=\langle c \rangle}}$$

where c is a basis scalar; usually the mixture fraction.

This models many physical processes well [10]. However, a practical difficulty arises with the definition of the max and min values used to define η_*' and $\langle \eta \rangle^p$ for reactive scalars. The total mass fraction is one and some compositions are impossible, so the possible range for a particular scalar depends on the values taken by all other scalars. For the hybrid model [5], only the mixture fraction is modelled so the problem is avoided.

2.2 MMC model

The MMC concept is that all the scalars Z_I can be transported in a mathematical space, called the reference space, thereby making the transport simpler because the reference space can be defined to take any properties. The simplest reference space ξ is one-dimensional and is conventionally related to the mixture fraction. For this one-dimensional reference space, the deterministic form of the conditional MMC transport equation is [6]:

$$\frac{\partial \overline{Z}_I}{\partial t} + \mathbf{U} \cdot \nabla \overline{Z}_I + A \frac{\partial \overline{Z}_I}{\partial \xi} - B \frac{\partial^2 \overline{Z}_I}{\partial \xi^2} = W_I\left(\overline{Z}\right) \qquad (6)$$

where Z_I represents each scalar I, $\overline{Z}_I \equiv \left\langle Z_I \,\middle|\, \xi \right\rangle$ is the conditional average of Z_I given the value of the reference variable ξ, A and B are the drift and diffusion coefficients respectively and W_I is the chemical source term for specie I and is a function of all scalars. Because ξ and the velocity $\mathbf{U}$ are both taken to have Gaussian distributions, they are modelled to be linearly related to each other (Z_0 is the mixture fraction):

$$\mathbf{U} = \langle \mathbf{u} \rangle + \left(\langle \mathbf{u}' Z_0' \rangle \big/ \langle \xi' Z_0' \rangle \right) \xi \qquad (7)$$

In the current implementation, the scalars are transported stochastically:

$$dZ_I^p = \left(S + W_I\right) dt , \qquad (8)$$

where S represents the mixing process, for which the Modified Curl's model [11, 12] was used. To enforce locality in the mixing process, particle pairs p and q were chosen so that the following was satisfied:

$$\left| \xi^p - \xi^q \right| \le \left(B \Delta t \right)^{1/2} . \qquad (9)$$

This process mimics the diffusive term of a stochastic differential equation (SDE). Note that (9) is not a minimisation: the specification is that particles p and q are close to each other, not the closest possible pairing. In practice, the inequality may be violated by outliers, but this does not pose any numerical difficulty.

2.3 Hybrid model

It is a necessary condition for the consistency of the model that the velocity $\mathbf{U}$ described in (7) is identical to the velocity u_i described in (1). Assuming that there is a velocity component that is most important for the mixing process (the radial velocity here), and that (7) satisfies the variance of that component [thereby eliminating the covariances in (7)], the following model for ξ is obtained:

$$\xi^p = \left(u_2^p - \langle u_2 \rangle \right) \Big/ \left\langle u_2'^2 \right\rangle^{1/2} . \qquad (10)$$

Equation (10) obviates the need to solve an SDE for ξ directly since an SDE is solved for u_2, (1), whose coefficients are well-defined.

The diffusion coefficient used in (9) is modelled by

$$B \approx \tfrac{1}{2}\left\langle \varepsilon_\eta \right\rangle \left\langle \left(\partial \overline{Z}_0 / \partial \xi\right)^2 \right\rangle^{-1}, \qquad (11)$$

where $\langle \varepsilon_\eta \rangle$ is defined after (3) and the derivative of the conditional average mixture fraction is used instead of the ill-defined instantaneous derivative. Since B is solely used in (9), which only provides an approximate limit, any error has a negligible impact on the results.

The amount of mixing used to define S in (8) is designed to minimise the following:

$$\left|Z_0^p - \eta^p\right| + \left|Z_0^q - \eta^q\right| \qquad (12)$$

where Z_0 is the MMC mixture fraction, transported by (8), and η is the binomial Langevin mixture fraction, transported by (3). A relaxation factor b was also used in the Modified Curl's mixing so that if $b = 0$, no mixing occurred and if $b = 1$, (12) was satisfied. This parameter is designed to control the level of conditional fluctuations as the criterion given in (12) can lead to excessive mixing. (The unconditional fluctuations are less sensitive to b but more sensitive to B.) The initial estimate of the required amount of mixing was reduced by the factor b. For the current simulations $b = 0.12$ was used. It is well known that scalar results are sensitive to the parameter $C_\phi = \tau_u / \tau_\eta$ [13, 14]. However, away from the selected value of $b = 0.12$, the current results were independent of C_ϕ, which suggests that sensitivity to C_ϕ could be a test for the correct value of b.

3. Results

The Sandia Flame D set of experiments [9] was chosen for further testing of the hybrid binomial Langevin–MMC model. While Flame D itself does not display significant extinction/reignition phenomena, successful modelling of this moderate Reynolds number case is a good step towards the verification of the implementation. Subsequently, results from the modelling of more complex phenomena can be analysed with an understanding of any inherent bias in the model.

The simulation performed here had, on average, 100 particles per cell, with 70 cells in the radial direction. The width of the domain increased in line with the entrainment of fluid. The simulation was performed with a parabolic code, with approximately 1600 axial steps to reach $x/D = 80$. The results are compared with the EMST (Euclidean Minimal Spanning Tree) approach [15] implemented into an elliptical code using 61 × 61 cells and also 100 particles per cell on average [16]. The domain extended to larger radial locations, but was considered sufficiently resolved [16]. To isolate the implementation effect, the EMST subroutines [17] were applied to the same program as the hybrid model.

Figure 1 shows the Favre-averaged mixture fraction $\langle Z \rangle$ profiles across the jet at various stations downstream of the outlet. There are negligible differences between the models from the same program. Near the centreline, the new results predict the experimental results quite accurately, while the previous EMST results generally over-predict the amount of mixing. The radial location of $\langle Z \rangle = 0.5$ tends to be over-predicted by the new results and under-predicted by the previous results, while the total spread of the jet tends to be under-predicted by the new results and over-predicted by the old results.

The accurate prediction of $\langle Z \rangle$ appears to be critical in the prediction of the mean temperature $\langle T \rangle$ (Fig. 2). Where $\langle Z \rangle$ was predicted more accurately, so was $\langle T \rangle$, with both EMST implementations performing better on the lean side of the peak $\langle T \rangle$. The new results tended to predict the cold radial location ($\langle T \rangle = 300$ K) better.

The rms mixture fraction is shown in Fig. 3, with the hybrid model producing somewhat better results in the upstream locations, while the previous EMST results performed best at the downstream station. The new EMST results were always larger than the hybrid model and increased with decreasing C_ϕ. The prediction of the peak rms location was similar for all implementations and similar to the experimental results.

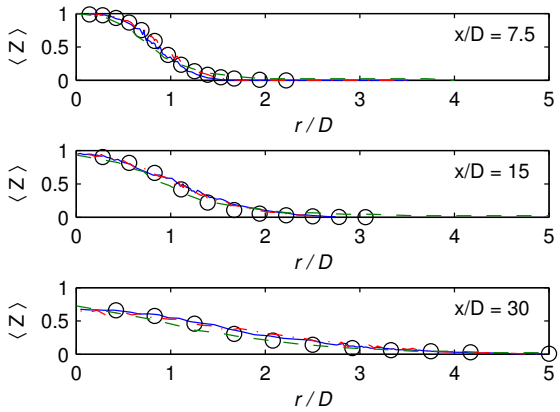

Figure 1: Favre-averaged mixture fraction profiles at various stations. Hybrid binomial Langevin–MMC, —; EMST ($C_\phi = 2.0$) (current), – ·; EMST ($C_\phi = 2.0$) [16], – –; Experiment [9], ○.

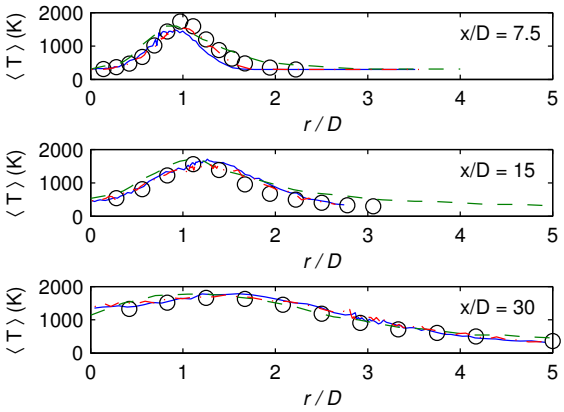

Figure 2: Favre-averaged temperature profiles at various stations. As per Fig. 1.

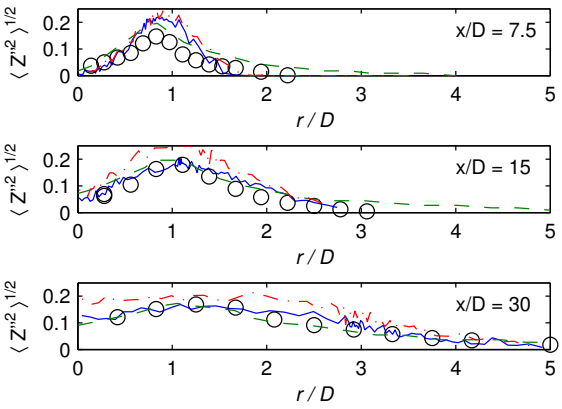

Figure 3: Favre-averaged rms mixture fraction profiles at various stations. As per Fig. 1.

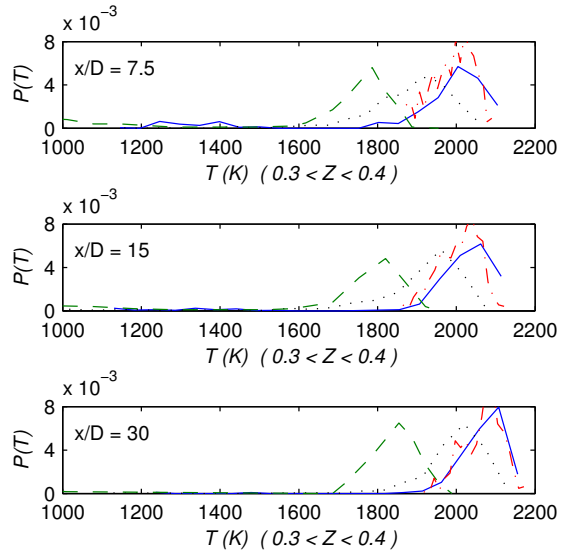

Figure 4: Conditional PDFs of temperature, conditioned on mixture fraction. Hybrid binomial Langevin–MMC, —; EMST (C_ϕ = 2.0) (current), – ·; EMST (C_ϕ = 1.5) [16], – –; Experiment [9], ···.

Figure 4 shows the PDFs of temperature, with data selected based on the mixture fraction being in the range (0.3, 0.4). The previous EMST results burned colder than the experiment, while the new results burned hotter than the experiment. This explains why the peak mean temperature for the previous EMST results was located closer to the centreline, while for the new results, it was located further from the centreline. The most significant difference between the new EMST results and the hybrid model is that the new EMST results predict complete burning, while the hybrid model predicts a small amount of local extinction, in line with the experimental results.

It is apparent that many of the differences between the models are due to the specific implementation (parabolic versus elliptic, chemistry calculations, etc). While the three numerical results produce similar mean results, the prediction of higher moments (standard deviation, PDFs) is variable, with none of the implementations able to be categorised as "best". However, the hybrid binomial Langevin–MMC model seems to perform better for the higher moments than the equivalent EMST results, encouraging further testing.

4. Conclusions

The hybrid binomial Langevin–MMC model has been applied to a reacting round jet, with results matching the experimental results with a reasonable level of accuracy and, arguably, comparing favourably with alternative closure models. The results encourage an extension to higher Reynolds number cases and further evaluation under conditions that display significant local extinction/re-ignition phenomena.

5. Acknowledgments

This work was largely carried out at Imperial College London, with funding from the EPSRC Grant No. GR/T22766 and ONR Award N000140710993. The authors also wish to thank Dr. Gabriel Roy and Dr. Andreas Kronenburg for helpful comments.

6. References

[1] S.T. Smith and R.O. Fox, Phys. Fluids **19** (2007), p. 085102.

[2] B. Merci, B. Naud and D. Roekaerts, Flow, Turbul. Combust. **79** (2007), p. 41.

[3] R.P. Lindstedt, S.A. Louloudi, J.J. Driscoll and V. Sick, Flow, Turbul. Combust. **72** (2004), p. 407.

[4] Z. Ren and S.B. Pope, Combust. Flame **136** (2004), p. 208.

[5] A.P. Wandel and R.P. Lindstedt, Phys. Fluids, **21** (1) (2009), p. 015103.

[6] A.Y. Klimenko and S.B. Pope, Phys. Fluids, **15** (7) (2003), pp. 1907–1925.

[7] L. Valiño and C. Dopazo, Phys. Fluids A, **3** (12) (1991), pp. 3034–3037.

[8] M.J. Cleary and A.Y. Klimenko, Flow, Turbul. Combust., **82** (2009), pp. 477–491.

[9] R.S. Barlow and J.H. Frank, Proc. Comb. Inst., **27** (1998), p. 1087.

[10] T. Hůlek, and R.P. Lindstedt, Comb. Sci. Tech., **136** (1998), pp. 303–331.

[11] C. Dopazo, Phys. Fluids **22** (1979), p. 20.

[12] J. Janicka, W. Kolbe and W. Kollmann, J. Non-Equilib. Thermodyn., **4** (1979), p. 47.

[13] C. Béguier, I. Dekeyser and B. E. Launder, Phys. Fluids, **21** (3) (1978), pp. 307–310.

[14] Z. Warhaft and J. L. Lumley, J. Fluid Mech., **88** (4) (1978), pp. 659–684.

[15] S. Subramaniam and S.B. Pope, Combust. Flame, **115** (1998), pp. 487–514.

[16] J. Xu and S.B. Pope, Combust. Flame, **123** (2000), pp. 281–307.

[17] Z. Ren, S. Subramaniam and S.B. Pope, (2002), http://eccentric.mae.cornell.edu/~tcg/emst