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Mixture-Fraction Based Hybrid Binomial-Langevin–MMC Modelling Applied to Auto-ignition in Vitiated Flow

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Abstract

A new hybrid binomial Langevin–MMC (Multiple Mapping Conditioning) modelling approach is proposed. The mixture fraction derived from the binomial Langevin model is used to specify the reference variable for MMC. The modified Curl's model is used to close the stochastic MMC mixing term. The new model is applied to a jet burner with a vitiated co-flow (the "Cabra burner") with methane as the fuel. The first- and second-order statistics show good agreement with experimental data.

1 Introduction

With the pressure to reduce emissions becoming a key factor in the design of modern combustion systems, engineers are moving closer to the combustion limits. This results in finite-rate chemistry effects (e.g. extinction and 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 [5,6] was recently proposed that used the Multiple Mapping Conditioning (MMC) [7] and binomial Langevin (BL) [8] 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 BL 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 BL value, while using the dominant velocity component from the BL solution as a basis for the MMC reference variable. The current approach is consistent with this methodology. However, it is simplified with the mixture fraction derived from the BL solution used directly to define the reference quantity rather than via an explicit transport equation [9].

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2 Theory

The hybrid binomial Langevin–MMC model is described below. First the BL model is outlined, then the MMC model, both of which are common to previous work [5,6]. Finally, the new link between the BL and MMC models is described.

2.1 Binomial Langevin Model

A generalised 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:

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

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:

$$\beta_{ij} = \langle u_i'u_j'\rangle / \langle u_k'u_k'\rangle - \tfrac{1}{3}\delta_{ij} \quad (2)$$

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

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

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

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

while the diffusion coefficient B_η is

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

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

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

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

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

where c is a basis scalar; usually the mixture fraction or a reaction progress variable.

The above approach reproduces 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 unity and compositions are further constrained by the mass of each element (e.g. C, O and H). Accordingly, the permissible range for a particular scalar depends on the values of all other scalars. By contrast, for the hybrid model [5,6], only the mixture fraction is required and the problem is avoided.

2.2 MMC model

The MMC concept is that all scalars Z_I can be transported in a mathematical space (i.e. 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 [7]:

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

where Z_I represents each scalar I, $\overline{Z}_I \equiv \langle Z_I \,|\, \xi\rangle$ 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 species I and is a function of all scalars. Because ξ and the velocity U are both taken to have Gaussian distributions, they are modelled to be linearly related to each other (Z_0 is the mixture fraction):

$$\mathbf{U} = \langle\mathbf{u}\rangle + \left(\langle\mathbf{u}'Z'_0\rangle/\langle\xi'Z'_0\rangle\right)\xi \qquad (7)$$

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, not the closest possible pairing. In practice, the inequality may be violated by outliers, but this does not pose any numerical difficulty.

2.3 Mixture-fraction–based hybrid model

All the details up to this point are identical to the previous, velocity-based hybrid model [5,6]. The key difference with the current approach is that the reference variable ξ is defined to be the BL mixture fraction η. Following the approach of Wandel [13], mixing proceeds via the Modified Curl's model with the exchange between selected paired particles specified as 50% of full mixing. The fraction of particles to be mixed is treated as a parameter that can be specified independently. Work is underway to determine a relationship between the fraction of particles to be mixed and scalar statistics to enable *a priori* determination.

3 Results

The Cabra burner in Fig. 1 and with methane as the primary fuel [14] was used as the test case with base conditions specified. A parabolic code [3] was used for a single realisation with 1865 streamwise locations and 80 cross-stream cells (the width of the domain expanded with the entrainment width); and 400 particles/cell. The fraction of particles mixed each time step was 6%; this is at least 10 times as many particles as Modified Curl's model would mix for the same mixing parameters.

The mean mixture fraction is presented is quantitatively similar to results [15] using the same code but with the Modified Curl's mixing model. The similarity is essentially due to the fluid mechanics of the solver. The mixture fraction rms (Fig. 2) has its peak in the correct location, but tends to be significantly under-predicted for most of the domain.

The mean temperature results (Fig. 3) are arguably excellent and again similar to previous results [15]. The temperature rms results (Fig. 4) appear outstanding. The authors could not find any other RANS-based approach that correctly predicts the locations of both the rise at $z/d = 40$ and the decrease at $z/d = 60$. Of those LES simulations which report the temperature rms, some cannot simultaneously predict both these locations [16,17]; the remainder do not predict a local maxima in the radial profile of mean temperature at $z/d = 40$ [18,19]. The current results appear unique.

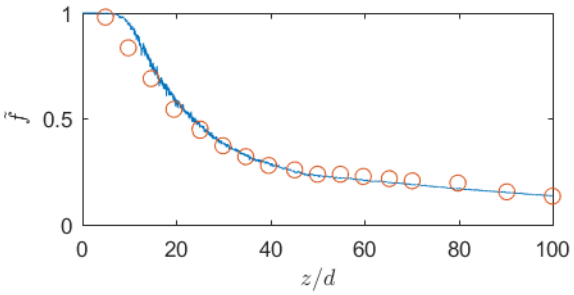

Figure 1: Centreline mean mixture fraction profile. MMC, line; experiment, symbol [14].

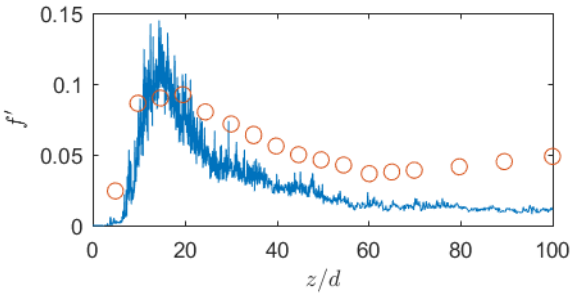

Figure 2: Centreline mixture fraction rms profile. As per Fig. 1.

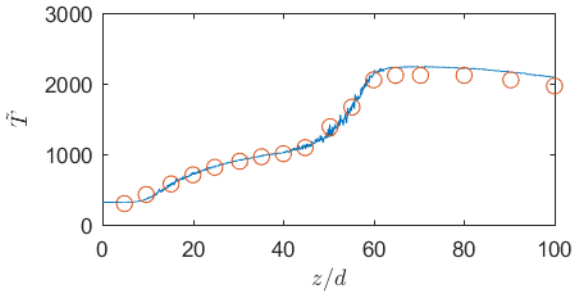

Figure 3: Centreline mean temperature profile. Symbols as per Fig. 1.

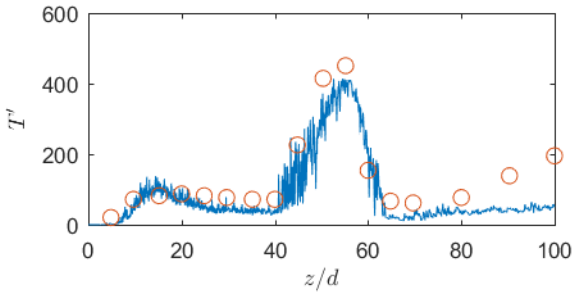

Figure 4: Centreline temperature rms profile. Symbols as per Fig. 1.

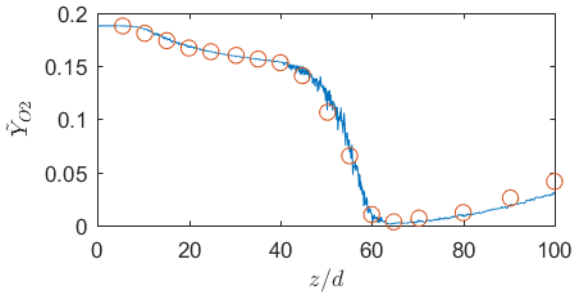

Figure 5: Centreline O_2 mean mass fraction profile. Symbols as per Fig. 1.

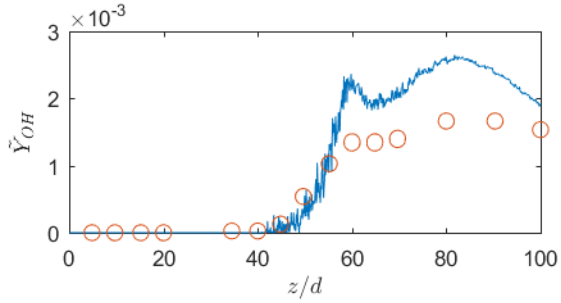

Figure 6: Centreline OH mean mass fraction profile. Symbols as per Fig. 1.

The prediction of the O_2 profile (Fig. 5) is very satisfactory and quantiatively similar to previous results [15]. The OH profile (Fig. 6) shows accurate predictions of the trend, but with a clear over-prediction for $z/d > 60$.

The radial profiles of mixture fraction (Fig. 7) show good agreement with experimental data with the trends matches the centreline results in Figs. 1 and 2. Similarly, the radial profiles of temperature (Fig. 8) show good agreement with experimental data. The results are essentially similar to the Modified Curl's results [15]. However, the rms temperature profile at $z/d = 70$ is substantially over-predicted by the Modified Curl's model for $r/d < 3$, while the current results are substantially improved.

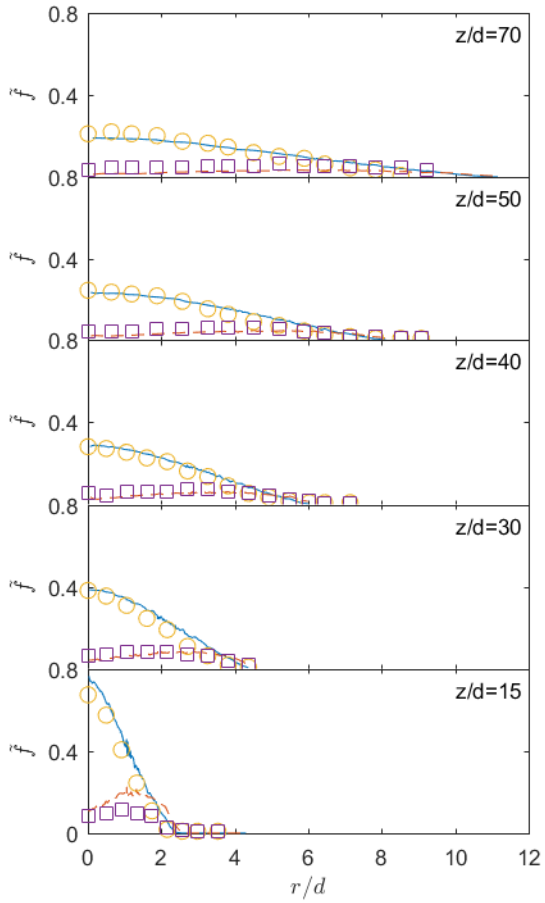

Figure 7: Radial mixture fraction profiles. Mean: MMC, line; expt, circles [14]. rms: MMC, dashed line; expt, squares [14].

The procedure to determine the liftoff height follows the methodology of [14]: it is the average of the axial locations where C_2H_4 is 100 ppm and C_2H_2 is 2 ppm. For the current simulation, this was found to be 42 diameters, as opposed to the experimental value of 35 [14]. Other measurements of this configuration [20] indicate that the value could be closer to 50. Because this variable is highly sensitive to the boundary conditions of velocity and temperature, a parametric study will be performed in the future.

4 Conclusions

A new hybrid binomial Langevin–MMC model is proposed. The linkage between the models is by virtue of the BL mixture fraction being used as the MMC reference variable. The model is closed by using the Modified Curl's model with the amount of mixing half the original Curl's model [13]. To close the model, the fraction of particles mixed each time step is an input parameter; ongoing efforts are investigating a relationship which can be used to govern this value.

A jet burner with vitiated co-flow [14] was simulated to test the model. The first-order statistics of mixture fraction, temperature and species mass fraction were matched very well, which is fundamentally due to the fluid mechanics, since similar results were obtained using the Modified Curl's model [15]. The location of the peak in centreline mixture fraction rms was predicted well, but the value far downstream was severely under-predicted. However, the centreline temperature rms was

predicted extraordinarily well, which is largely due to the performance of the mixing model, since the directly comparable Modified Curl's model did not predict the location of the significant decrease at $z/d = 60$. The authors have not found another RANS simulation which is able to predict the shape of this quantity. Some LES models are also incapable of predicting this shape [16,17]; those which are able to predict the shape of this quantity fail to predict the radial profiles correctly by not producing the local maxima in mean temperature at $z/d = 40$ [18,19]. The liftoff height was predicted within accepted uncertainties associated with the burner exit boundary conditions. The behaviour of the flame is known to be highly sensitive to the inflow conditions; future work will assess the model for this parametric study.

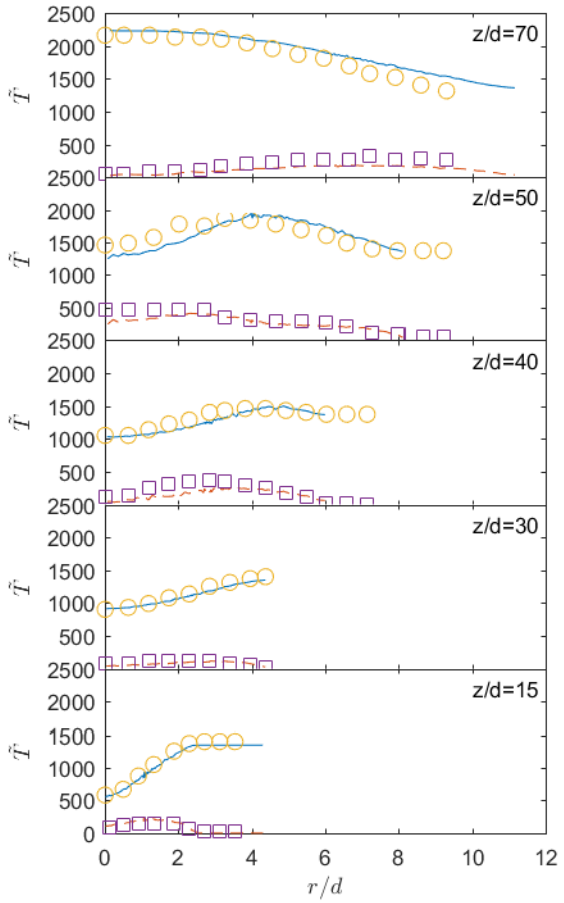

Figure 8: Radial temperature profiles. Symbols as per Fig. 7.

5 Acknowledgment

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