Recent Developments of the Multiple Mapping Conditioning Mixing Model

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1 Introduction

Multiple Mapping Conditioning (MMC) [1] is a mixing model for turbulent combustion which effectively unifies the features of Probability Density Function (PDF) and Conditional Moment Closure (CMC).

The PDF method is a statistical approach for solving a modelled transport equation for the one-point, one-time Eulerian joint PDF for velocity and reactive scalars. PDF methods are applicable for premixed, nonpremixed and partially premixed combustion. Dopazo and O'Brien [2] consider a composition joint PDF to model mixing and chemical reactions in turbulent flows. Since Pope [3] established the relationship between particle models and PDF methods, particle methods have emerged as a powerful approach for solving PDF transport equations. A compelling feature of PDF models is the exact evaluation of reaction rates. In reality, the hundreds of species involved in realistic chemical processes generate stiff differential equations and invoke a high computational cost.

CMC is a modelling perspective for nonpremixed combustion which arose from measurements in jet diffusion flames and in reactive mixing layers [4,5], where fluctuations in temperature and composition were observed to correlate to fluctuations in key variables. MMC unites the PDF and CMC approaches, allowing the generality of PDF methods while exploiting the properties of CMC.

In its initial deterministic form, MMC represented a version of CMC subsisted by a consistent PDF methods for the mixture fraction(s) [1]. A stochastic formulation was also introduced in [1] as a full-scale PDF method and a computationally efficient form of the deterministic model. Further evolution from stochastic to generalised MMC occurred by removal of restrictions on Markov reference variables to include traced Lagrangian quantities in Eulerian DNS or LES [6]. Reference variables can be obtained by other simulation methods and used to enforce desired properties by conditioning or localisation in mixture fraction space and emulation of scalar dissipation fluctuations. Early development and application of MMC in homogeneous and inhomogeneous turbulent combustion was performed by the Combustion and Multiscale Modelling group at the University of Queensland, in Imperial College and other institutions [7, 8].

In this paper, the concept of a reference variable is used in a non-reacting homogeneous flow to demonstrate the possibility of simulating and controlling differential diffusion. LES is also used to provide a reference variable in laboratory scale methane and hydrogen flame cases. The possibility of

using a sparse distribution of Lagrangian particles to model reactive scalars for a reduction in cost of three orders of magnitude is demonstrated.

2 Applications

2.1 Laboratory Flame Cases

The sparse-Lagrangian method with generalised MMC has been applied to the Sandia flame series D-F of methane [9] and a lifted hydrogen flame [10]. For these non-premixed cases, an Eulerian LES generates filtered turbulent flow field data including velocity, pressure and mixture fraction while a sparse ensemble of Pope particles solves a Filtered Density Function (FDF) [11] for reactive scalars. A gradient-fractal model is used to control the distance in reference mixture fraction space between mixing particles to be the same as the more sparse simulation [12]. The possibility of obtaining good results while reducing the number of Pope particles used in simulations has been demonstrated. The MMC model has two key parameters: the parameter f_m, which balances localisation in *f*-space with localisation in the physical space, and the parameter C_L, which controls the mixing timescale constant (i.e. the minor dissipation time) that can be used to control the degree of localisation.

For the Sandia flame series D-F, f_m is set to 0.03 and C_L is set to unity. One Lagrangian particle is used per 27 Eulerian cells (1L/27E). For these constants, the predicted conditional and unconditional reactive scalars are in very good agreement with experimental data for flames D and E at all locations in the flow [13]. For flame F, which is close to blow-off, results are qualitatively correct and the bimodal nature of the extinction is captured, but there is an early prediction of re-ignition. The increased level of extinction arising from the increasing jet velocity is successfully captured by the model with a single value of f_m.

The Cabra lifted flame is formed by a high velocity jet of cold hydrogen fuel and a hot coflowing oxidizer. The lift-off height is known to increase with decreasing coflow temperature. The Cabra flame exhibits sensitivity to both physical and numerical parameters. The most influential parameters are coflow temperature, mixing timescale and localisation. For a constant f_m, the flame tended towards attachment for increasing coflow temperatures. The degree of sensitivity towards temperature exhibited in our simulations is in line with experimental data [14, 15]. It is possible to match the conditional and unconditional scalars by varying C_L and f_m.

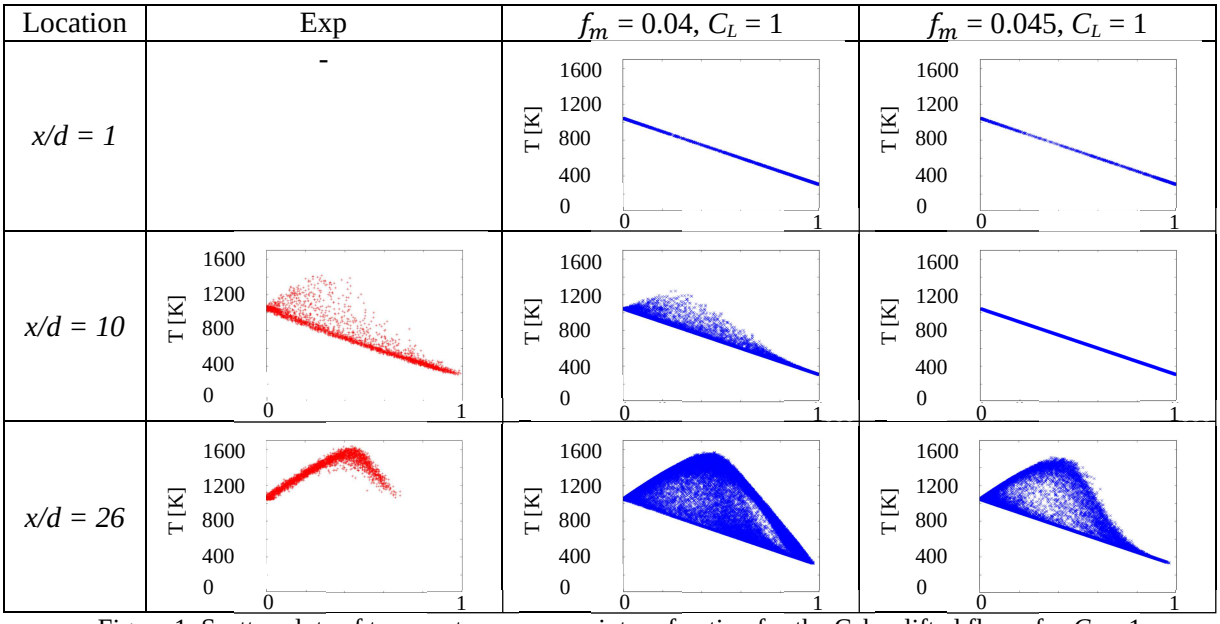

Figure 1. Scatter plots of temperature versus mixture fraction for the Cabra lifted flame for C_L = 1.

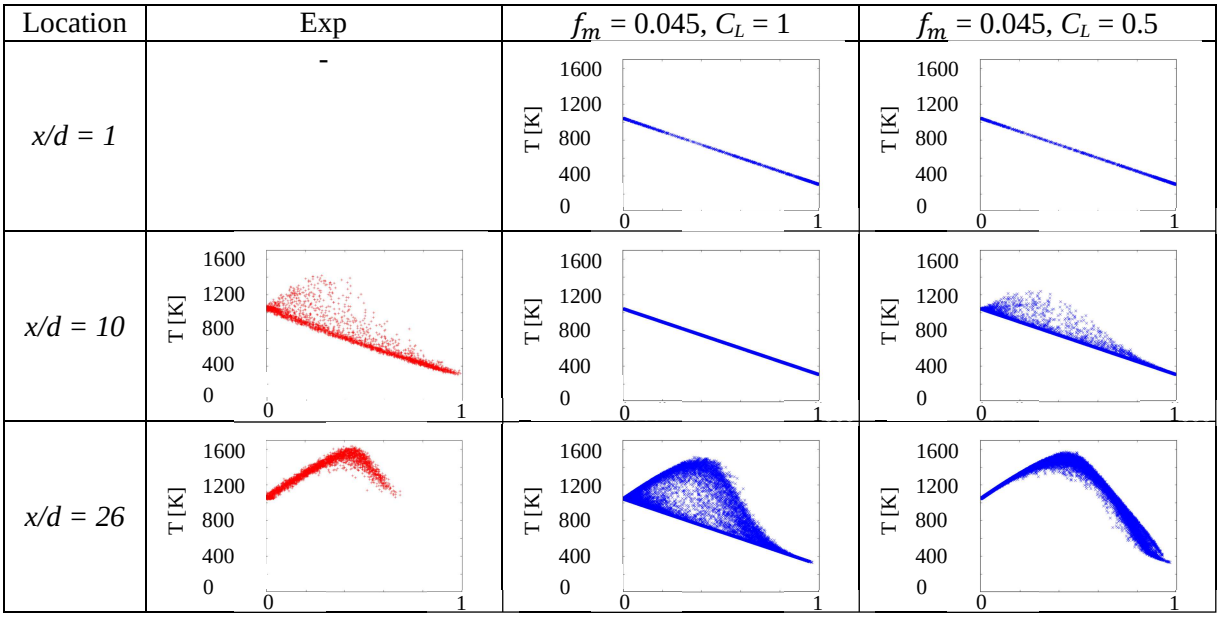

Figure 2. Scatter plots of temperature versus mixture fraction for the Cabra lifted flame for f_m = 0.045

Based on MMC simulations of the Sandia flame series [13], where localisation of particle pairs is 0.03, f_m values ranging from 0.03 to 0.05 are tested for the Cabra flame. It is noted that the gradient-fractal model proposed in [12] can ensure consistent mixing in spite of different Pope particle densities. Each localisation value produced significantly different results. Enforcing excessive localisation in mixing by increasing f_m resulted in global extinction. The optimum value of f_m for this case is approximately 0.04, as shown in Figure 1, close to f_m for the Sandia flame series, indicating some consistency in localisation for different configurations and fuels. C_L values of 1 and 0.5 were also considered. Modification of C_L influences the dissipation of mixture fraction and scalars. A reduction in C_L allows stabilises the flame closer to the nozzle inlet, as shown in Figure 2.

One Lagrangian particle is used per eight Eulerian cells (1L/8E), over three times as many particles as those used in the Sandia flame simulations (1L/27E). This degree of particle intensity is required for the lifted flame as numerical diffusion effects tend to dominate in less intensive simulations. Differential diffusion has not been modelled in these simulations of the Cabra hydrogen-air flame and it is possible that its effects have influenced results here. Section 2.2 proposes a modified version of MMC which accounts for different diffusivities of scalars.

2.2 Differential Diffusion

In turbulent flames, molecular heat and mass diffusivities of inert or reacting chemical species are usually different, so that each scalar diffuses at a different rate. Despite this, most theoretical models of turbulent flames effectively ignore differential diffusion, by assuming the same molecular diffusivities of all species and of heat (the unity Lewis number assumption) and neglecting the effects of molecular diffusion compared to turbulent diffusion. These assumptions are attractive because they lead to great modelling simplifications but there are ample experimental and numerical evidences [16, 17, 18] that unequal molecular diffusion often influences species compositions. While the MMC mixing model was originally developed for the equal diffusivity condition, it can be modified to account for differential diffusivity.

Two passive scalars Y_I and Y_{II} are introduced in a homogeneous, isotropic turbulent field each having a different molecular diffusivity denoted by D_I and D_{II} respectively. In the absence of spatial advection

and diffusion, the scalars Y_I and Y_{II} evolve according to the mixing operation with the mixing extent α which is a random number bounded between 0 and 1 that is independent of the particle scalar values. Defining β=1-α , γ=1-β^2 and Δt the duration of the mixing step, Equation 1 indicates a link between the mean value of γ and the minor dissipation time of the flow, τ_D ,which is defined as the average value of scalar variances over the dissipation rate [19]:

$$\tau_D = \frac{4\Delta t}{\langle \gamma \rangle} \qquad (1)$$

Two methods for treating differential diffusion are introduced: a) two reference variable method and b) one reference variable method. Both methods demonstrate the ability of MMC to predict the different rates of decay of the scalar variances due to differential diffusion. The two reference variable model can also control and emulate rate of decorrelation of the scalars at the same time.
An Ornstein-Uhlenbeck (OU) processes which is a stationary, Gaussian and Markovian diffusion processes is used in modeling our reference variables. The stochastic differential equation for above process has the following form:

$$d\xi_i^* = -\frac{\xi_i^*(t)}{\tau_i}dt + \left(\frac{2}{\tau_i}\right)^{1/2} dW_i(t) \quad \text{i=I,II} \qquad (2)$$

Where *W(t)* is a Weiner process (random walk) and time scale τ is selected so that the statistics of $\xi^*(t)$ match the statistics of real turbulence.
For both models simulations are performed using 10,000 Pope particles (i.e. Lagrangian particles with properties and mixing) which are initialised by $Y_I^* = Y_{II}^*$.

a) Two reference variable method

With the use of two reference variables, MMC can be modified to account for the loss of correlation of two scalars due to differential diffusion. In particular, for two scalars with the same initial values and equal diffusivities the scalars would remain to be fully correlated at all times. However, when the diffusivities are not equal, the scalars become progressively decorrelated from each other. By introducing two stochastically independent reference variables ξ_I and ξ_{II} , which are modeled with the use of two independent Ornstein-Uhlenbeck (OU) processes, each of two scalars Y_I and Y_{II} are progressively modulated by independent stochastic processes and lose the correlation. Hence, by enforcing the required decorrelation rate on our reference variables, we control the rate of decorrelation of the differentially diffusing scalars without interference with the proper mixing process.

b) One reference variable method

In this model we used MMC to emulate difference in scalar variance decay rates due to differential diffusion which is the prime problem that needs to be addressed in practical simulations. There is only one reference variable ξ_I for localising mixing of both scalars Y_I and Y_{II}. ξ_I evolves according to two timescales; τ_I is selected independently and linked to τ_D by defining the constant r_1 while τ_{II} is a side stepping timescale linked to τ_I and a constant r_0 according to Equation 3. ξ_I changes according to τ_I, producing ξ_I^*, and mixing for scalar Y_I is localised in this reference variable space. Mixing of scalar Y_{II} is performed with ξ_I^* after it has evolved according to that side stepping time scale τ_{II}. So we have two model parameters $r_1$and r_0.

$$r_1 = \frac{\tau_I}{\tau_D}, r_0 = \frac{\tau_{II}}{\tau_I} \qquad (3)$$

Figure 3 shows decay of scalar variances versus time for this model. The figure is indicative of exponential decay of the variances in time represented by approximately straight lines of constant

slopes on the log-linear plot. As can be seen the dissipation of scalar fluctuations by mixing occurs at different rates for two scalars due to their different diffusivities.

Equation 4 indicates the relationship between the physical time scales of two scalars Y_I and Y_{II} which are defined as t_1 *and* t_2 respectively with model parameter r_0. α can be selected in advance to determine r_0 in this model.

$$\frac{t_2}{t_1} = 1 + \frac{\alpha}{r_0} \qquad (4)$$

As can be seen in Figure 3, a reasonable match between the MMC predicted decay rate and the DNS data is obtained by setting the appropriate model parameters. These results obtain for the mixing extent of α = 0.02 and parameters r_1 = 8 and r_0 = 1.3.

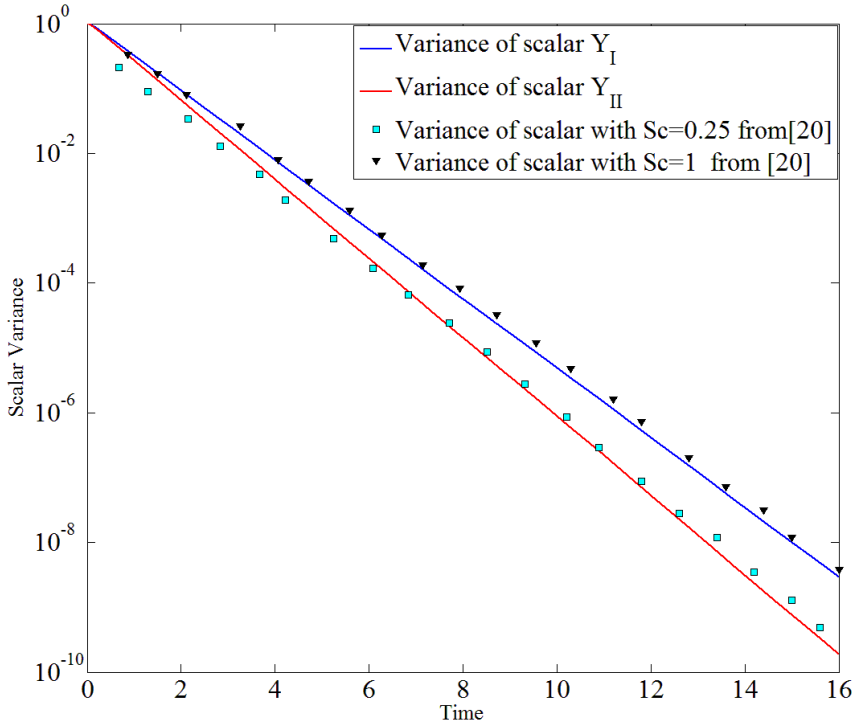

Figure 3. Scalar variances versus time

3 Conclusion

The concept of independent reference variables in the Multiple Mapping Conditioning framework can be used to simulate various phenomena in combustion. Two modified forms of MMC to predict differential diffusion effects are developed and the ability of these models to emulate variance decays and decorrelation between passive scalars is demonstrated. Further work on differential diffusion will investigate dependence of model parameters on Lewis and Reynolds numbers and introduce single step and complex chemical kinetics. Additionally, further sparse-Lagrangian MMC simulations of complex fuels and burner configurations are required to determine the universality of the localisation parameter.

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