Chapter 7
Multiple Mapping Conditioning: A New Modelling Framework for Turbulent Combustion

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Abstract Multiple mapping conditioning (MMC) is a relatively new addition to the list of models for turbulent combustion that unifies the features of the probability density function, conditional moment closure and mapping closure models. This chapter presents the major concepts and theory of MMC without the detailed derivations which can be found in the cited literature. While the fundamental basis remains the same, MMC ideas have undergone considerable evolution since they were first proposed and the result is a generalised combustion modelling framework which can more transparently and simply incorporate the major turbulence models which have been developed over the past decades including LES. A significant part of this chapter is devoted to a review of the published MMC applications comparing model predictions with DNS and experimental flame databases. Finally, the chapter concludes with a list of some of the advances in MMC methodology that we can expect to see in the coming years.

7.1 Introduction

Multiple Mapping Conditioning (MMC), introduced by Klimenko and Pope in 2003 [21], is a theoretically rigorous combination of the Probability Density Function (PDF) [17, 40] and Conditional Moment Closure (CMC) [20] models incorporating a generalisation of mapping closure [7, 41]. The mapping closure is generalised in the sense that assumptions are not made about the type of flow being modelled, whereas conventional mapping closures for combustion (e.g. amplitude mapping closure [7]) are formally valid in homogeneous turbulence only. Rather than being a specific turbulent combustion model, MMC can be viewed more as a framework for turbulent combustion modelling. This framework contains a gen-

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eral set of principles and equations from which specific MMC based models can be formulated to suit a particular turbulent combustion problem.

Of all the models available, the PDF models (reviewed in Chapter 6) provide the most detailed information about the stochastic characteristics of all species involved in a combustion process, and, most importantly, they permit an exact evaluation of the reaction rates. However, realistic chemical processes involve hundreds of species, n_s, and the differential equations which describe those realistic kinetics are always stiff. Therefore a direct evaluation of the joint composition PDF is expensive as it requires the solution of equations in that n_s-dimensional composition space. While the complete composition space in a turbulent flow is indeed highly dimensional, it is not necessary in a practical model to allow all species to fluctuate in all ways. There are constraints due to conservation of elements and other conservation principles, there are fast reactions of some species forcing them to be close to their partial equilibrium states, and (simply stated) fluctuations of some species are unimportant to the major combustion processes [21]. This concept has lead to the notion of an n_m-dimensional reduced manifold ($n_m < n_s$) onto which the full n_s-dimensional composition space is projected. The dimension of the manifold should be commensurate with the effective dimension of the accessed region in composition space for the flow under consideration and this can be expected to increase with flow complexity [45]. From this manifold notion alternative modelling approaches have evolved. One approach, of which the intrinsic low-dimensional manifold (ILDM) method [32] is the prime example, involves dimension reduction by systematically reducing the number of species in the chemical kinetics scheme. This reduced number of species then defines the low-dimensional manifold to which the eliminated species have a functional relationship. In a numerical implementation the source terms for the manifold species are determined from the reduced kinetics and the eliminated species may be tabulated. While a deficiency of ILDM is that it neglects turbulent mixing effects in obtaining the low-dimensional manifold, related kinetics reduction methods such as the reaction-diffusion manifold method (REDIM) [5] explicitly address chemistry-transport coupling. Ren and Pope [46] review ILDM, REDIM and related methods.

A second modelling approach to evolve from the notion of reduced manifolds is to retain arbitrarily detailed chemical kinetics schemes (i.e. with n_s species) but derive transport equations which effectively restrict the compositions to a certain manifold. The primary example of such models in the recent literature is CMC [20] (reviewed in Chapter 5) which is founded on the hypothesis that, in non-premixed combustion, there is a strong correlation between turbulent fluctuations of reactive scalars and the fluctuations of the mixture fraction. Flamelet models [39] (reviewed in Chapter 3) exploit this correlation also and often include parameterisation by the scalar dissipation effectively creating a two-dimensional manifold. In CMC, the mass fractions of the reactive scalars are conditionally averaged on the mixture fraction leaving an equation which has only a single composition dimension (i.e. mixture fraction space) in addition to the dimensions of time and space. Simple first-order closures can be found for the conditional chemical reaction rates by making the assumption that the conditional fluctuations (i.e. the fluctuations of reactive

species concentrations relative to mean concentrations conditioned on the mixture fraction) are negligibly small. As a result of its low dimensionality and the simplicity of the source term closure, the cost of first-order CMC computations is much lower than the cost of PDF computations. In partially- or fully-premixed combustion, or in non-premixed combustion with strong local extinction, the first-order CMC closure of chemical source terms is less accurate and CMC models with higher order reaction rate closures [26, 33] and CMC models with an additional temperature related conditioning variable [27] have proven successful in some of these cases but they also introduce additional terms which are difficult to model.

MMC effectively unifies the PDF and CMC approaches and allows for all of the generality of PDF methods while also exploiting some of the advantages of CMC. Both deterministic and stochastic MMC formulations exist. Deterministic MMC is the natural extension of CMC and the stochastic MMC is in fact a complete joint PDF method with MMC playing the role of a mixing model which enforces localness within a defined manifold. Since the basic MMC framework was first proposed [21] a number of specific MMC models have been developed and tested [8, 10, 11, 29, 54–57]. The key feature common to all is the use of reference variables which are related to the physical quantities in turbulent combustion (e.g. mixture fraction, sensible enthalpy, velocity and scalar dissipation). In the original form of MMC [21] the reference variables are used as conditioning variables which form a manifold constraining the computed compositions. Fluctuations around quantities conditionally averaged on that reference space are considered to be small and in the basic form of MMC they are neglected for the purposes of calculating reaction rates. These fluctuations are specific to MMC and are called minor fluctuations. Later a more generalised interpretation of reference variables in stochastic MMC emerged [23], whereby reference variables can take other roles in addition to conditioning such as emulating scalar dissipation fluctuations. This generalised interpretation allows fluctuations relative to the reference manifold to be exploited (rather than minimised) so as to better model the physical conditional fluctuations while keeping computational cost small.

The remainder of this review chapter is organised as follows. Section 7.2 presents the basic MMC as it was first proposed [21]. It includes a description of the context and concepts of MMC, a brief explanation of mapping closures, a presentation of the deterministic and stochastic model equations, a discussion of the qualitative properties of the model and a brief discussion on the replacement of reference variables resulting in equivalent MMC models with alternatively distributed and physically meaningful reference spaces. Section 7.3 deals with the generalised interpretations of MMC. Here we discuss MMC with conditioning and non-conditioning reference variables and in the context of large eddy simulations. Section 7.4 reviews the published MMC applications for a range of homogeneous and inhomogeneous reacting flows. Finally in Section 7.5 we summarise the major features of MMC and the different forms the model can take and suggest areas of research which we believe could dominate the coming decade of research in the field.

7.2 The Basic MMC Framework

7.2.1 Context and Concepts

The multidimensional reacting scalar space $\boldsymbol{Y}(\boldsymbol{x},t) = (Y_1,\ldots,Y_I,\ldots,Y_{n_s})$ is governed by the well known transport equation

$$\frac{\partial \rho Y_I}{\partial t} + \boldsymbol{\nabla}\cdot(\rho \mathbf{v} Y_I) - \boldsymbol{\nabla}\cdot(\rho D \boldsymbol{\nabla} Y_I) = w_I. \tag{7.1}$$

Here $\mathbf{v} = \mathbf{v}(\boldsymbol{x},t)$ is the fluid velocity, D is the diffusivity which is assumed to be the same for all species, ρ is the density, and w_I is the rate of creation of species I due to chemical reactions. In turbulent flows the stochastic distribution of compositions can be represented by the Favre one-time, one-point joint PDF, $\widetilde{P}_Y(\boldsymbol{y};\boldsymbol{x},t) = \prod_{I=1}^{n_s} \rho(\boldsymbol{y})\delta(y_I - Y_I)/\overline{\rho}$ where the lower case $\boldsymbol{y}$ denotes the sample space for $\boldsymbol{Y}$, and the tilde and overline denote Favre and conventional averages, respectively. In high Reynolds number flows the transport equation for $\widetilde{P}_Y$ derived from (7.1) is given by [40]

$$\frac{\partial \overline{\rho}\widetilde{P}_Y}{\partial t} + \boldsymbol{\nabla}\cdot(\overline{\rho}\mathbf{u}\widetilde{P}_Y) + \frac{\partial \overline{\rho} W_I \widetilde{P}_Y}{\partial y_I} + \frac{\partial^2 \overline{\rho} N_{IJ} \widetilde{P}_Y}{\partial y_I \partial y_J} = 0 \tag{7.2}$$

where

$$\mathbf{u}(\boldsymbol{y};\boldsymbol{x},t) \equiv \langle \rho \mathbf{v} | \boldsymbol{Y} = \boldsymbol{y}\rangle / \rho_Y \tag{7.3}$$

$$W_I(\boldsymbol{y};\boldsymbol{x},t) \equiv \langle \rho w_I | \boldsymbol{Y} = \boldsymbol{y}\rangle / \rho_Y. \tag{7.4}$$

$$N_{IJ}(\boldsymbol{y};\boldsymbol{x},t) \equiv \langle \rho D \frac{\partial Y_I}{\partial x_k}\frac{\partial Y_J}{\partial x_l} | \boldsymbol{Y} = \boldsymbol{y}\rangle / \rho_Y \tag{7.5}$$

$$\rho_Y(\boldsymbol{y};\boldsymbol{x},t) \equiv \langle \rho | \boldsymbol{Y} = \boldsymbol{y}\rangle. \tag{7.6}$$

The fundamental assumption of MMC is that the compositions which occur in the different realisations of the flow are confined to an n_m-dimensional manifold within the n_s-dimensional composition space where $n_m < n_s$. The n_m species in this manifold are called "major species" and their turbulent fluctuations are called "major fluctuations" while the term "minor species" refers to the remaining set of $n_\alpha = n_s - n_m$ species. The word "species" is interpreted to include chemical species and also other quantities related to the composition such as mixture fraction and enthalpy. Furthermore, our terminology of major and minor species does not imply that those species are present in large and small concentrations. A major species is denoted by Y_i (lower case Roman subscript) and Y_α (lower case Greek subscript) is used to denote a minor species. The set of all major species is denoted as $\boldsymbol{Y}^m$ and

the set of minor species is $\boldsymbol{Y}^{\alpha}$. As will be seen when the transport equations are presented, MMC does not discriminate in its treatment of major and minor species and this demarcation has been introduced as a conceptual aid only. Major species are those which are permitted in the model to fluctuate in any physically realisable way whereas minor species are restricted to fluctuate only jointly with the major species and can be fully characterised by mean values conditionally averaged on the major species. Provided that the major species are properly selected then the joint PDF of all species can be effectively replaced by the marginal PDF of major species, $\widetilde{P}_{Y^m}(\boldsymbol{y}^m;\boldsymbol{x},t)$, supplemented by the conditional means of the minor species $Q_{\alpha}(\boldsymbol{y}^m;\boldsymbol{x},t) = \langle Y_{\alpha}|\boldsymbol{Y}^m = \boldsymbol{y}^m\rangle$ such that

$$\widetilde{P}_Y = \widetilde{P}_{Y^m} \cdot \delta(\boldsymbol{Q} - \boldsymbol{y}^{\alpha}). \tag{7.7}$$

The reduced PDF of major species and conditional expectations of minor species are governed by

$$\frac{\partial \overline{\rho}\widetilde{P}_{Y^m}}{\partial t} + \boldsymbol{\nabla} \cdot (\overline{\rho}\mathbf{u}\widetilde{P}_{Y^m}) + \frac{\partial \overline{\rho} W_i \widetilde{P}_{Y^m}}{\partial y_i} + \frac{\partial^2 \overline{\rho} N_{ij} \widetilde{P}_{Y^m}}{\partial y_i \partial y_j} = 0 \tag{7.8}$$

and

$$\frac{\partial Q_{\alpha}}{\partial t} + \mathbf{u}\boldsymbol{\nabla} Q_{\alpha} + W_i \frac{\partial Q_{\alpha}}{\partial y_i} - N_{ij} \frac{\partial^2 Q_{\alpha}}{\partial y_i \partial y_j} = W_{\alpha}. \tag{7.9}$$

From the assumption that the n_m-dimensional major species manifold effectively describes the accessed region in the n_s-dimensional composition space, terms of the form of $\widetilde{P}_{Y^m}^{-1} \boldsymbol{\nabla} \cdot (\langle \mathbf{u}'' Y_{\alpha}'' | \boldsymbol{Y}^m = \boldsymbol{y}^m \rangle \widetilde{P}_{Y^m})$, which would normally appear in CMC, have been omitted from (7.9). The double prime denotes conditional fluctuations.

Like any model for the joint scalar PDF, (7.8) and (7.9) contain two unclosed terms – the conditional velocity, $\mathbf{u}$, and the conditional scalar dissipation, N_{ij}. The development of good closure models, particularly models for N_{ij}, is an ongoing area of research in both the joint PDF and CMC communities [17, 50]. As described in the next section MMC employs an indirect approach based on a generalisation of mapping closure to solve the above equations consistently and in a numerically stable manner.

7.2.2 Mapping Functions

The mapping closure concept was first introduced by Chen et al. [7] and a detailed description of mapping closures for turbulent combustion is provided by Pope [41]. Only the main concepts are repeated here. We introduce the n_r-dimensional set of random variables $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_i, \ldots, \xi_{n_r})$ called the reference space whose distribution is prescribed and represented by the joint reference PDF, $\widetilde{P}_{\xi}(\boldsymbol{\xi};\boldsymbol{x},t)$. The aim is to find a set of mapping functions $\boldsymbol{X}(\boldsymbol{\xi};\boldsymbol{x},t) = (X_1, \ldots, X_I, \ldots, X_{n_s})$ such that $\boldsymbol{X}$ is statistically equivalent to $\boldsymbol{Y}$. In basic MMC a reference variable is assigned to em-

ulate the turbulence of each of the major species and therefore $n_r = n_m$. The word "emulate" implies that reference variables do not model the physical scalars directly, but that there is statistical equivalence between the mapping functions in that reference space and the physical scalar field. Statistical information about $\boldsymbol{Y}$ is then obtained simply from the modelled mapping functions and the prescribed reference space joint PDF:

$$\begin{aligned}
\widetilde{Y}_I(\boldsymbol{x},t) &= \int_{\boldsymbol{\xi}} X_I \widetilde{P}_\xi d\boldsymbol{\xi} \\
\widetilde{Y_I'^2}(\boldsymbol{x},t) &= \int_{\boldsymbol{\xi}} (X_I - \widetilde{Y}_I)^2 \widetilde{P}_\xi d\boldsymbol{\xi} \\
&\vdots \\
\widetilde{P}_Y(\boldsymbol{y};\boldsymbol{x},t) &= \int_{\boldsymbol{\xi}} \delta(\boldsymbol{X}-\boldsymbol{y}) \widetilde{P}_\xi d\boldsymbol{\xi}.
\end{aligned} \tag{7.10}$$

The concept of mapping functions may be more readily understood by examining the case of a single inert major scalar $Y_Z(t)$ (the mixture fraction) whose mapping $X_Z(\xi,t)$ is the function of a single standard Gaussian distributed reference variable with mean $\langle\xi\rangle = 0$ and variance $\langle\xi'^2\rangle = 1$. Figure 7.1 shows the time evolution of the mixture fraction PDF, $\widetilde{P}_Z(\eta;t)$ (where η is the sample space variable for Y_Z) and the corresponding mapping function X_Z in a homogeneous field with decaying turbulence [8]. The field is initialised at $t^* = 0$ (t^* is a normalised time) so that fuel ($Y_Z = 1$) and air ($Y_Z = 0$) are mostly segregated with only a small amount of smoothing between the two components. This corresponds to $\widetilde{P}_Z$ being close to two delta functions and X_Z is close to a Heaviside function in reference space with $X_Z = 0$ for $\xi < 0$ and $X_Z = 1$ for $= \xi > 0$. As time evolves $\widetilde{P}_Z$ approaches a Gaussian distribution with a mean of $\widetilde{Y}_Z = 0.5$ and with decaying variance. As there is always a linear mapping between any two Gaussian distributed fields X_Z approaches a straight line with a decreasing gradient.

7.2.3 The Deterministic MMC Model

The MMC model equation governing the evolution of mapping functions in time, and physical and reference spaces is [21]

$$\frac{\partial X_I}{\partial t} + \mathbf{U}\cdot\boldsymbol{\nabla} X_I + A_k \frac{\partial X_I}{\partial \xi_k} - B_{kl}\frac{\partial^2 X_I}{\partial \xi_k \partial \xi_l} = W_I. \tag{7.11}$$

This equation is valid for general inhomogeneous flows. From the assumption that minor fluctuations are negligibly small a first-order closure of the conditional reaction rate is applied such that $W_I = W_I(\boldsymbol{X})$. Equation (7.11) introduces the condi-

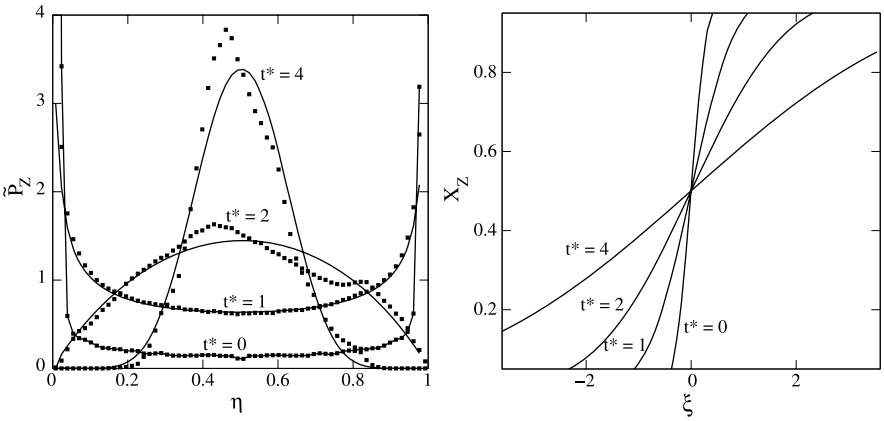

Fig. 7.1: Mixture fraction PDF, $P_Z(\eta)$ (left) and mixture fraction mapping function, $X_Z(\xi)$ (right) in homogeneous decaying turbulence at various normalised times. Symbols are DNS data and lines are MMC model results. Figures adapted from [8].

tional velocity, drift and diffusion coefficients $\mathbf{U}(\boldsymbol{\xi};\boldsymbol{x},t)$, $A_k(\boldsymbol{\xi};\boldsymbol{x},t)$, and $B_{kl}(\boldsymbol{\xi};\boldsymbol{x},t)$, respectively, whose closures are discussed below. We remind readers that the upper case Roman subscript I represents all scalars (both major and minor) while the lower case Roman subscripts k and l are for the major scalars only. An elegant aspect of MMC is that, despite the conceptual division into major and minor species, a single equation governs the transport of all species without discrimination. Mapping functions which satisfy the deterministic model equation (7.11) are themselves deterministic functions and the stochasticity of the modelled scalar field results from the stochasticity of the reference field, $\boldsymbol{\xi}$, whose one-point, one-time joint PDF must satisfy the equation [21]

$$\frac{\partial \overline{\rho}\widetilde{P}_\xi}{\partial t} + \boldsymbol{\nabla}\cdot(\overline{\rho}\mathbf{U}\widetilde{P}_\xi) + \frac{\partial \rho A_k \widetilde{P}_\xi}{\partial \xi_k} + \frac{\partial^2 \rho B_{kl}\widetilde{P}_\xi}{\partial \xi_k \partial \xi_l} = 0. \tag{7.12}$$

There is not space in this review to demonstrate the compliance of the MMC model equations (7.11) and (7.12) with equations (7.8) and (7.9) for $\widetilde{P}_{Y^m}$ and Q_α. However it is explicitly demonstrated by Klimenko and Pope [21]. We note that this compliance is not restrictive on the dimensions involved except the trivial requirement that $n_r \leq n_s$. If $n_r = n_s$ is selected then MMC is a full joint PDF model with a generalised mapping closure for the conditional scalar dissipation. Note that solution of (7.11) for $n_r >> 1$ via finite difference methods is likely to be computationally intractable and the efficient stochastic form of the equations presented in Section 7.2.4 is recommended. MMC reference variables can be selected to emulate fluctuations induced by variations of the mixture fraction and other scalars, dissipation, velocity and, in principle, any other useful quantity [21]. Although a poor selection of reference variables does not render MMC invalid it brings addi-

tional complexity without improving the quality of the modelling. From its roots in CMC, practical MMC tends to focus on mixture fraction conditioning and then on conditioning by other quantities. The CMC limit of MMC is achieved when a single reference variable ($n_r = 1$) is chosen to emulate the mixture fraction. Under these conditions MMC is effectively first-order CMC plus a consistent closure of the mixture fraction PDF and conditional mean scalar dissipation.

The MMC velocity, drift and diffusion coefficients are selected so that (7.12) is satisfied for a prescribed (or independently determined) distribution of the joint reference PDF, P_ξ. It is possible to determine the coefficients for any reasonable distribution, however, following the mapping closure convention the reference variables are given standard Gaussian distributions (i.e. zero mean and unit variance):

$$\widetilde{P}_\xi(\boldsymbol{\xi};\boldsymbol{x},t) = \widetilde{P}_\xi(\boldsymbol{\xi}) = G(\xi_1)G(\xi_2)\ldots G(\xi_{n_r})$$
$$G(\xi_k) = \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{\xi_k^2}{2}\right). \tag{7.13}$$

For this reference PDF distribution, it can be shown [21] that (7.12) is satisfied when the velocity and drift coefficients are selected to take the following forms:

$$\mathbf{U}(\boldsymbol{\xi};\boldsymbol{x},t) = \mathbf{U}^{(0)} + \mathbf{U}_k^{(1)}\xi_k \tag{7.14}$$

$$A_k(\boldsymbol{\xi};\boldsymbol{x},t) = -\frac{\partial B_{kl}}{\partial \xi_l} + B_{kl}\xi_l + \frac{1}{\overline{\rho}}\boldsymbol{\nabla}\cdot(\overline{\rho}\boldsymbol{U}_k^{(1)}). \tag{7.15}$$

A linear conditional velocity model is commonly used in CMC models [20] and is also suggested for MMC. There is further discussion on this matter below. The last term in (7.15) is particular to MMC and does not appear in conventional mapping closures [41]. Because of that term, MMC as a PDF model is a generalised mapping closure method that makes no assumption about the homogeneity of the flow. In addition, of course, MMC is a CMC model for the minor species.

The velocity terms $\mathbf{U}^{(0)}$ and $\mathbf{U}_k^{(1)}$ depend on the model employed for the drift coefficient, B_{kl}. Selecting B_{kl} to be independent of ξ gives

$$\mathbf{U}^{(0)}(\boldsymbol{x},t) = \widetilde{\mathbf{v}} \tag{7.16}$$

$$\mathbf{U}_k^{(1)}(\boldsymbol{x},t)\langle\xi_k X_i\rangle = \widetilde{\mathbf{v}'Y_i'} \tag{7.17}$$

$$B_{kl}(\boldsymbol{x},t)\left\langle\frac{\partial X_i}{\partial \xi_k}\frac{\partial X_j}{\partial \xi_l}\right\rangle = \widetilde{N}_{ij}. \tag{7.18}$$

In the above the averages in angular brackets are determined by integration weighted by the reference PDF and $\widetilde{N}_{ij}$ is the unconditional Favre-averaged scalar dissipa-

tion. Note that these relations are the interactions between the turbulence and reacting scalar fields. The great advantage of employing mapping closure is that the turbulence-chemistry interactions are closed using the unconditional Favre-averaged velocity, turbulent scalar flux and scalar dissipation rather than the more difficult to model conditional averages required to close joint PDF and CMC equations (7.8) and (7.9).

Compliance with the reference PDF does not imply that the MMC coefficients are unique and multiple different forms are possible. The velocity $\boldsymbol{U}$, expressed in (7.14) in terms of $\boldsymbol{\xi}$, $\boldsymbol{x}$ and t, represents a model for conditional velocity $\langle \mathbf{v}|\boldsymbol{Y}\rangle$, which can conventionally be approximated by $\langle \mathbf{v}|Y_Z\rangle$ where Y_Z is the mixture fraction. The simplest, linear approximation of the conditional velocity $\langle \mathbf{v}|Y_Z\rangle = \widetilde{\mathbf{v}} + \beta Y_Z$, where the coefficient β is linked to the turbulent scalar flux as in (7.17), is commonly used in CMC [20]. Kuznetsov and Sabelnikov [30] introduced this approximation and found that the joint Gaussian distribution of the velocity-scalar fluctuations implied by the linear model may be too strong an assumption at the tails of the mixture fraction PDF and may cause convergence difficulties. A clipped version whose shape is an "erf-like" function is more stable and agrees with experiments since larger scalar and velocity fluctuations tend to be less correlated than smaller fluctuations. The same authors [30] note that the linear approximation does not yield the same turbulent diffusivity for the first and the second moment of the mixture fraction ($D_{t2} \neq D_{t1}$). While Kuznetsov and Sabelnikov [30] believed that the different moments should have different turbulent diffusivities, the most common approach in RANS involves assuming the same diffusivities for both moments (i.e. $D_{t2} = D_{t1}$). Mortensen [37] correctly pointed out that using the linear approximation of the conditional velocity in CMC simulations is inconsistent with using the assumption $D_{t2} = D_{t1}$ in the scalar variance equation. This, of course, should not be interpreted as a general inconsistency of the PDF and second moment equations since a consistent equation for any scalar moment is a consequence of, and can be derived from, the PDF equation. The problem of consistency in the common assumption $D_{t2} = D_{t1}$ can be resolved by using Pope's gradient approximation [40] which, as was repeatedly noted [30, 37], yields the same turbulent diffusivities for all moments. This approximation, however, tends to have a shape which is a "tan-like" function and may overestimate velocity-scalar correlations at the tails. On one hand, linear dependence between velocity, whose distribution is close to Gaussian, and the reference variables, which is also Gaussian, can be expected. On the other hand, Gaussian distributions of each of the stochastic variables does not guarantee a joint distribution, which is needed for linear dependence of the conditional expectations. Due to boundedness of the mixture fraction and unboundedness of the Gaussian reference variable, the dependence of $\langle \mathbf{v}|Y_Z\rangle$ on Y_Z determined by (7.14) tends to be "tan"-like. This overestimates dependence at the tails and may cause difficulties in MMC simulations. Recently, Vaishnavi and Kronenburg [53] have suggested a method that can make MMC consistent with any adopted approximation for $\langle \mathbf{v}|Y_Z\rangle$. It seems that this method may become important for inhomogeneous MMC simulations.

7.2.4 The Stochastic MMC Model

Following the methods described by Pope [40] a stochastic form of MMC can be derived which is equivalent to the deterministic model given by Eqs. 7.11 and 7.12. The stochastic formulation is based on the use of Lagrangian particles. In addition to conventional scalar properties, stochastic MMC assigns reference values to those stochastic particles. The equivalent stochastic formulation of MMC is given by [21]

$$d\boldsymbol{x}^{*(p)} = \mathbf{U}(\boldsymbol{\xi}^{*(p)};\boldsymbol{x}^{*(p)},t)dt \tag{7.19}$$

$$d\xi_k^{*(p)} = A_k^0(\boldsymbol{\xi}^{*(p)};\boldsymbol{x}^{*(p)},t)dt + b_{kl}(\boldsymbol{\xi}^{*(p)};\boldsymbol{x}^{*(p)},t)d\omega_l^{*(p)} \tag{7.20}$$

$$dX_I^{*(p)} = (W_I^{*(p)} + S_I^{*(p)})dt \tag{7.21}$$

$$\langle S_I^* | \boldsymbol{\xi}^* = \boldsymbol{\xi}, \boldsymbol{x}^* = \boldsymbol{x}\rangle = 0 \tag{7.22}$$

where

$$A_k^0 = A_k + \frac{2}{\widetilde{P}_\xi}\frac{\partial B_{kl}\widetilde{P}_\xi}{\partial \xi_l} \tag{7.23}$$

$$b_{ki}b_{li} = 2B_{kl}. \tag{7.24}$$

In the above asterisks indicate stochastic quantities, the bracket index (p) indicates a value associated with an individual particle and ω_I^* are Wiener processes. As for the deterministic model, the reference PDF, $\widetilde{P}_\xi$, is prescribed and (7.20) is solved to model the turbulent diffusion of scalars in the reference space.

Equation (7.21) governs transport in scalar space due to chemical reaction, W_I, and a mixing operation, S_I. The latter is not specified beyond the requirement in (7.22) that it not alter the conditional expectations. The treatment of W_I and S_I depends on one's interpretation of stochastic MMC. The first interpretation is that equations (7.19) through (7.22) are an efficient stochastic numerical scheme for solving the deterministic mapping equation (7.11). For $n_r \gg 1$ the stochastic form will be cheaper to compute than a finite difference method applied to the deterministic equations. The goal is to find $\overline{X}_I^* = \langle X_I^* | \boldsymbol{\xi}^* = \boldsymbol{\xi}, \boldsymbol{x}^* = \boldsymbol{x}\rangle$ which can be shown to satisfy (7.11) [21] and we therefore refer to this approach as the conditional interpretation of MMC. We set $W_I^{*(p)} = W_I(\overline{\boldsymbol{X}}^*)$ and the job of the mixing operator is to keep the minor fluctuations $X_I'^{(p)} = X_I^{*(p)} - \overline{X}_I^*$ small. Inevitably there will be some scattering around $\overline{X}_I^*$ and this is treated as stochastic error to be minimised by using a large number of particles.

The alternative, probabilistic interpretation of MMC, is to consider the stochastic values $X_I^{*(p)}$ as models for the turbulent realisations of the composition; that is the PDF $\widetilde{P}_X = P(\boldsymbol{X}^*|\boldsymbol{x}^* = \boldsymbol{x})$ is the model for $\tilde{P}_Y$. Practically, stochastic MMC is almost always used as a probabilistic (PDF) model and the recent trend is to imply "probabilistic" when the term "stochastic MMC" is used. In general, the minor fluctuations are still expected to be small when MMC conditioning is effective but deviations from the reference space manifold are now permitted. We set $W_I^{*(p)} = W_I(\boldsymbol{X}^{*(p)})$ and S_I is used to dissipate the usually small but not-negligible minor fluctuations. Note that in conventional joint PDF methods the surrogate mixing models account for the dissipation of all fluctuations, whereas in MMC the mixing operator dissipates only the minor fluctuations and the dissipation of major fluctuations is modelled by diffusion in reference space (see Eq. 7.20). Therefore MMC results are expected to have a lower sensitivity than conventional PDF models to the form of the surrogate mixing model.

In practice, the dissipation of minor fluctuations can occur only if mixing is between particles which are close in ξ-space as demanded by (7.22) and this gives MMC its localness. This localness effectively enforces a CMC-type closure on the mixing model. Here the term CMC is quite general and refers to any method for obtaining conditional means according to (7.9). The probabilistic MMC is a full joint PDF method which, through the mixing model, incorporates the ideas of CMC. Specific surrogate mixing models to dissipate the minor fluctuations can be formulated in a variety of ways but the simplest models are those based on the conventional PDF mixing models such as IEM (interaction by exchange with the mean) [15], IECM (interaction by exchange with the conditional mean) [42] and Curl's model [13] and its modifications [19]. The IECM model can be seen as a special version of MMC-IEM that involves conditioning only on velocity. Traditional MMC pays more attention to conditioning on scalars than to conditioning on velocity and it is not clear whether the true MMC regime can be achieved by IECM [23].

Here we present two alternatives, MMC-IEM and MMC-Curls. MMC-IEM is represented by the mixing operator

$$S_I^{*(p)} = \frac{\overline{X}_I^* - X_I^{*(p)}}{\tau_s}. \tag{7.25}$$

Minor fluctuations are dissipated through adjustments of the relaxation timescale, τ_s, and $\overline{X}_I^*$ is calculated within narrow (i.e. local) ξ bins. This model requires that the number of particles is large so that $\overline{X}_I^*$ can be calculated accurately. In MMC-Curl's model particles p and q are paired on the basis that they are close to each other in ξ-space. During each interaction they have their values reset to the two-particle average $X_I^{*(p)\text{new}} = X_I^{*(q)\text{new}} = (X_I^{*(p)} + X_I^{*(q)})/2$. As particles move randomly in ξ-space new particle pairs are formed as needed to maintain localness in that space. Other two-particle interaction schemes, more sophisticated than the scheme shown above, are possible and practical implementations (e.g. Refs [11, 56] tend to use modified versions of Curl's model [19].

7.2.5 Qualitative Properties of MMC

Being both joint PDF and CMC compliant, MMC inherits the qualitative properties of both. The reaction rates can be modelled by conditional means or by instantaneous stochastic quantities. In the PDF limit convective transport is treated exactly [40] while the convective transport of conditional quantities is modelled by the local properties of the flow (see the ξ dependence of the velocity in (7.14)). An important outcome of MMC is that the PDF of the major scalars and the conditional scalar dissipation are modelled consistently. Lists of desirable properties of conditional scalar dissipation and surrogate mixing models have been suggested and expanded by various authors [16, 44, 51]. MMC adheres to the most essential of these properties [21, 22]: conservation of means, boundedness of scalars and their linear combinations, linearity and independence, localness, equal treatment of all scalars, decay of variances and relaxation to a Gaussian PDF distribution in homogeneous turbulence. Additionally, as MMC in its stochastic form does not specify the form of the surrogate mixing model, the option remains to develop mixing schemes which also include, among other phenomena, the effects of Reynolds number, turbulence length scales and reactions.

A key reason for the observed quality of MMC is the independence of the reference variables and the composition variables ensuring linearity of MMC mixing. This independence does not, of course, imply that $\boldsymbol{\xi}$ and $\boldsymbol{Y}$ are uncorrelated. In fact, correlation is necessary for localisation in reference variables to be a useful constraint. The independence does, however, imply that $\boldsymbol{\xi}$ should be able to fluctuate without taking the local and instantaneous value of $\boldsymbol{Y}$ into account. Practically, a reasonable degree of independence of reference and composition scalar fields is achieved when those fields are modelled by different processes or equations (e.g. $\boldsymbol{\xi}$ can be modelled by the Markov process (7.20) which is independent of the transport of $\boldsymbol{Y}$). Note that this interpretation of independence allows for some quantities, such as density, to be common to both equations.

7.2.6 Replacement of Reference Variables

The velocity, drift and diffusion coefficient closures in Sections 7.2.3 and 7.2.4 are consistent with the reference PDF transport equation when that PDF is a joint standard Gaussian. This is convenient from a mathematical perspective but a better physical understanding of MMC can be gained by replacement of these standard Gaussian reference variables with random variables which more closely resemble the physical major scalars that they emulate.

A reference space transformation from $\boldsymbol{\xi}$ to $\hat{\boldsymbol{\xi}} = \hat{\boldsymbol{\xi}}(\boldsymbol{\xi};\boldsymbol{x},t)$ is achieved by replacing the velocity, drift and diffusion coefficients by [22]

$$\hat{A}_i = \frac{\partial \hat{\xi}_i}{\partial t} + \boldsymbol{U} \cdot \nabla \hat{\xi}_i + A_k \frac{\partial \hat{\xi}_i}{\partial \xi_k} - B_{kl} \frac{\partial^2 \hat{\xi}_i}{\partial \xi_k \partial \xi_l} \tag{7.26}$$

$$\hat{B}_{ij} = B_{kl} \frac{\partial \hat{\xi}_i}{\partial \xi_k} \frac{\partial \hat{\xi}_j}{\partial \xi_l} \tag{7.27}$$

$$\hat{\boldsymbol{U}} = \boldsymbol{U}. \tag{7.28}$$

Although the transformed velocity coefficient in (7.28) is unchanged this does not imply the linear functional form in $\boldsymbol{\xi}$-space corresponds to a linear form in $\hat{\boldsymbol{\xi}}$-space. The new reference space PDF is given by

$$\widetilde{P}_{\hat{\xi}} = \widetilde{P}_{\xi} \det \left(\frac{\partial \hat{\xi}_i}{\partial \xi_k} \right)^{-1}. \tag{7.29}$$

Note that the replacement of variables is simply a mathematically equivalent transformation that does not alter the physical nature of the MMC closures.

An obvious case is the replacement of a single standard Gaussian variable that emulates mixture fraction, ξ, with a new random variable $\hat{\xi} = \eta$ that has the same distribution as the actual mixture fraction (i.e. $\widetilde{P}_{\eta} = \widetilde{P}_Z$). It is important to remember that the mixture fraction reference variable is not the actual mixture fraction, Y_Z, which is modelled by the mapping X_Z. To preserve the independence of the reference variables, η is a mixture-fraction-like variable with equivalent (or topologically similar) statistics to Y_Z. For this special case the transformed coefficients $\hat{A}_i$ and $\hat{B}_{ij}$ are

$$\hat{A} = 0 \tag{7.30}$$

$$\hat{B} = B \left(\frac{\partial X_Z}{\partial \xi} \right)^2. \tag{7.31}$$

It can be readily seen that replacement of ξ by η and substitution of the new coefficients into the mapping equation (7.11) yields the conditional moment equation (7.9) with conditioning on the mixture fraction. The coefficient $\hat{B}$ appears in the place of, and is therefore a model for, the conditional scalar dissipation

$$\langle N | \eta \rangle = \hat{B} = B \left(\frac{\partial X_Z}{\partial \xi} \right)^2. \tag{7.32}$$

Generally speaking, a higher quality emulation of the mixture fraction by the reference variable η makes modelling of the mixture fraction Y_Z easier.

A detailed application of the replacement of reference variables for a multidimensional reference space emulating mixture fraction and sensible enthalpy is contained

in Refs [9, 29]. With such transformations the similarities and differences between the MMC and EMST [51] models are quite obvious. Both models treat conditional scalar dissipation locally in composition space and use mapping closures to achieve this. Where they differ is that EMST uses the stochastic compositions to determine localness, but in so doing violates principles of independence and linearity. MMC, on the other hand, uses reference variables which are formally independent of the stochastic compositions to determine localness and thus it adheres to those principles. However, MMC requires a model for the reference variables and finding a suitable model may not be trivial, especially for reacting quantities.

7.3 Generalised MMC

The basic MMC framework presented in the preceding section is a rather formal model. It assumes that the major species manifold is known and that minor fluctuations are negligibly small. (The probabilistic MMC allows minor fluctuations but until now they have been assumed to be small). The use of standard Gaussian reference variables is conventional and mathematically convenient, but it also removes some physical transparency from the model equations. In this section we present a generalised MMC which, as the name suggests, generalises the concepts of MMC and makes them more amenable to practical implementation. Generalised MMC concepts were first proposed in Ref. [23] to expand the purpose of reference variables beyond conditioning or localisation. A series of subsequent papers [10, 11, 24, 25] developed generalised MMC for the DNS/LES regime and replaced Markov reference variables with Lagrangian variables traced within an Eulerian field. Although the main generalised MMC concepts are presented below, readers interested in a detailed analysis should consult the published articles cited above.

7.3.1 Reference Variables in Generalised MMC

The basic MMC model uses $n_r = n_m$ independent reference variables to emulate each of the major species. In the stochastic form of the model mixing is localised in the reference space effectively linking the modelled composition with the species concentrations conditionally averaged on that space. In the conditional interpretation of MMC minor fluctuations are neglected and therefore the composition is modelled as the conditional mean. In probabilistic MMC, in which minor fluctuations are permitted, the fluctuations are dissipated towards the conditional means by the minor dissipation operator, S_I. The probabilistic MMC interpretation is assumed for the remainder of this section. Reference variables which perform a localisation role (this is the only role we have considered until now) are now called conditioning reference variables to distinguish them from other sorts of reference variables to be discussed below. As before the total number of reference variables is labelled as n_r

and the number of conditioning reference variables is n_c with $n_c \leq n_r$. The set of conditioning variables $\boldsymbol{\eta} = (\eta_1, \eta_2, \ldots, \eta_{n_c})$ forms a subset of $\boldsymbol{\xi}$.

From a practical perspective it may not always be possible or desirable to have a conditioning reference variable to emulate each of the major species. Limiting computational cost is the major reason for this – a greater number of conditioning reference variables requires a larger number of particles to ensure adequate localisation in the space of each of those reference variables. If $n_c < n_m$ then, in general, minor fluctuations are not negligibly small and their variances should be controlled to so that the model predicts the physical conditional variances accurately.

By accepting minor fluctuations in the model we also create the possibility of including reference variables which assist the modelling but which are not used for conditioning purposes. Practically this means that mixing is localised only in the space of the n_c conditioning reference variables, while the non-conditioning reference variables complement the conditioning reference variables and improve the emulation of the physical quantities.

Until now we have only considered reference variables modelled by Markov processes as in (7.20). However, once we allow for the possibility that $n_c < n_r$ or even for $n_c \ll n_r$, any physically relevant process can be used. For example, reference variables can be Lagrangian quantities obtained with the use of DNS or LES. Indeed a non-Markov process can be approximated well by a Markov process of much higher dimension. Motions of Brownian or fluid particles in a turbulent flow are deemed to be non-Markovian while DNS simulations tracing these particles represent a Markov process of a large dimension.

7.3.2 Features of Generalised MMC Models

The generalised MMC model equations were initially proposed in Ref. [23] in the same form as the basic stochastic MMC equations (7.19) through (7.21) and with (7.22) replaced by

$$\langle S_I^* | \boldsymbol{\eta}^* = \boldsymbol{\eta}, \boldsymbol{x}^* = \boldsymbol{x} \rangle = 0. \tag{7.33}$$

while $\langle S_I^* | \boldsymbol{\xi}^* = \boldsymbol{\xi}, \boldsymbol{x}^* = \boldsymbol{x} \rangle$ may be non-zero. It is possible to demonstrate that a failure to satisfy condition (7.22) under the conditional interpretation of MMC will generate a spurious term in the modelled PDF transport equation (the effect of mixing in the direction of non-conditioning reference variables can be interpreted as a mixing-generated diffusion). Hence, using a conditional interpretation of generalized MMC is not recommended. Note that generalized MMC is a stochastic model and it does not generally have a deterministic version. However, with a probabilistic interpretation, generalised MMC remains compliant with the PDF transport equation. Indeed, complying with the PDF equation requires that $\langle S_I^* | \boldsymbol{x}^* = \boldsymbol{x} \rangle = 0$ to allow for representation of the mixing operator in terms of the divergence of dissipation, N_{IJ}°:

$$\widetilde{P}_X \langle S_I^* | \boldsymbol{X}^* = \boldsymbol{X}, \boldsymbol{x}^* = \boldsymbol{x} \rangle = \frac{\partial N_{IJ}^{\circ} \widetilde{P}_X}{\partial X_J}. \tag{7.34}$$

In Ref. [21], this was shown using with the use of (7.22), which represents a sufficient but not necessary condition. A weaker condition, $\langle S_I^* | \boldsymbol{x}^* = \boldsymbol{x} \rangle = 0$, which can be obtained from (7.33), is sufficient for compliance with the PDF equation. Due condition (7.33) generalised MMC mixing does not alter the values of $\overline{X}_I = \langle X_I^* | \boldsymbol{\eta}^* = \boldsymbol{\eta}, \boldsymbol{x}^* = \boldsymbol{x} \rangle$ and hence, in the absence of non-linear reacting terms, $\overline{X}_I^*$ is determined by the properties of the stochastic trajectories of $\boldsymbol{\eta}^*$ and not by the form or quality of the surrogate mixing operator. In other words, MMC enforces the desired conditional properties, through the stochastic properties of the reference variables, on any reasonable surrogate mixing operator. This, however, does not apply to higher conditional moments which are determined by the form and quality of that mixing.

Since stochastic models aim to produce statistically equivalent fields their model equations are not unique and alternative forms can be derived. MMC with Gaussian reference variables is mathematically convenient but some physical transparency of the model is lost. It is, of course, possible to transform the equations for alternatively distributed reference variables according the methods described in Section 7.2.6 and although this improves the physical transparency of the model the transformed drift and diffusion coefficients are complex. An alternative option is to apply the generalised MMC principles within other existing models for turbulent combustion (e.g. any of the various formulations and closures of the joint PDF models). In the broadest sense, then, generalised MMC can be interpreted as the application of the conditioning/localisation condition (7.33) within an existing (or maybe yet to be developed) stochastic combustion model. This interpretation has been taken in practical hybrid binomial Langevin-MMC [57] and MMC-LES applications [10, 11].

The following three points summarise the essential features of a good generalised MMC model [23]:

- The conditioning reference variables should emulate as closely as possible the Lagrangian properties of the key major species to ensure accurate evaluation of conditional species expectations without compromising the independence of the reference space. This can be done with the assistance of non-conditioning reference variables.
- The surrogate mixing operator, S_I, should set the dissipation of minor fluctuations to correspond to the dissipation of physical conditional fluctuations. (Due to the independence of reference and composition scalar fields, minor fluctuations and conditional fluctuations are not the same thing but they are linked).
- The conditioning reference variables should be selected so that minor fluctuations are not too large. This ensures that scalar dissipation is predominantly modelled by diffusion in reference space (e.g. Eq. 7.20) rather than by the surrogate mixing operator, S_I.

7.3.3 MMC with Dissipation-like Reference Variables

We consider an MMC model governed by (7.19) through (7.21) and (7.33) with a single conditioning reference variable η emulating the physical mixture fraction, Y_Z, via the mapping function X_Z. If η does not have a standard Gaussian PDF then the coefficients are modified as described in Section 7.2.6. Conditional fluctuations $Y_I'' = Y_I - \langle Y_I'' | Y_Z \rangle$ are modelled indirectly via the minor fluctuations $X_I'''^{(p)} = X_I^{*(p)} - \overline{X}_I^*$. As it is, the model does not explicitly generate minor fluctuations and they are present only if they appear in the boundary conditions or if generated by the surrogate mixing model [23]. Although generation of minor fluctuations by the mixing model can in principle be used to model the conditional fluctuations [10] it may be difficult to control. An alternative model is to introduce additional non-conditioning reference variables to emulate the scalar dissipation fluctuations which are physically responsible for the appearance of conditional fluctuations. The reference space is defined as $\boldsymbol{\xi} = (\eta, \xi_{d_1}, \xi_{d_2}, \ldots)$ where ξ_{d_i} are called dissipation-like reference variables. The MMC model with dissipation-like variables has the modified diffusion coefficients [23]

$$B_{\eta\eta} = \overline{B}_{\eta\eta}\Phi, \quad B_{\eta d_i} = B_{d_i\eta} = 0, \quad B_{d_i d_j} = \frac{\delta_{d_i d_j}}{\tau_{d_i}} \tag{7.35}$$

$$\Phi(\xi_{d_i}; \boldsymbol{x}, t) = \exp(c_{d_i}\xi_{d_i} - \frac{c_{d_i}c_{d_i}}{2}) \tag{7.36}$$

$$c_{d_i}c_{d_i} = \ln\left(\frac{\langle N_{\eta\eta}'^2 | Y_Z \rangle}{\langle N_{\eta\eta} | Y_Z \rangle} + 1\right) \tag{7.37}$$

In the above, $\overline{B}_{\eta\eta}$ is the value of the diffusion coefficient without inclusion of the dissipation fluctuations. Each dissipation-like reference variable emulates scalar dissipation fluctuations of a certain frequency, $1/\tau_{d_i}$, where τ_{d_i} spans between the Kolmogorov and macro time scales of the flow. Giving each ξ_{d_i} a standard Gaussian distribution ensures that the conditional scalar dissipation $\langle N_{\eta\eta} | \eta \rangle$ has a lognormal distribution. For modelling where the ratio $\tau_{d_{i-1}}/\tau_{d_i}$ is selected to be the same for all dissipation-like variables it can be shown that the constants c_{d_i} are also equal [23]. In basic MMC, all reference variables $\boldsymbol{\xi}$ must be used for conditioning while generalised MMC may involve conditioning only on η, or η and Φ, which seems to be more practical.

7.3.4 DNS/LES Simulated Reference Variables

The computational tractability of Markov processes such as the random walk given by (7.20) have led to them being widely used in stochastic turbulence models [43]. However, the great advances in computing power mean that LES and maybe even DNS are becoming more viable means of modelling non-reacting stochastic diffusion processes and velocity fields. The cost of performing reacting DNS is still prohibitive while LES does not resolve the thin reaction zones. Therefore hybrid methods such as the LES/joint scalar FDF (filtered density function) model [12, 18] have been developed whereby velocity and passive scalar fields are simulated by conventional Eulerian LES and the reactive scalar field is simulated by a stochastic particle scheme.

As noted in Section 7.3.1, the Markov reference variables can be replaced in generalised MMC by traced Lagrangian values within an Eulerian DNS or LES simulated field (i.e. particle reference variable values are the Eulerian values observed at the particle locations). One can note that the highest quality reference variable is the actual physical variable simulated by a fully resolved DNS. The Eulerian reference field is simulated according to

$$\frac{\partial \rho \xi_i}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{v} \xi_i) - \boldsymbol{\nabla} \cdot (\rho D \boldsymbol{\nabla} \xi_i) = w_{\xi_i}. \tag{7.38}$$

For passive scalars the source term $w_{\xi_i} = 0$. The mixture fraction is the most obvious reference variable to be modelled in this way for non-premixed combustion but, in principle, other passive or reactive reference variables could also be selected. In the LES version, the filtered form of (7.38) is solved and a closure is required for the source term of any reactive reference variables. If LES subgrid fluctuations are filtered out a Markov process similar to (7.20) can be used to emulate the subgrid distribution such that $\xi_i = \xi_i^{\mathrm{LES}} + \xi_i'^{\mathrm{RW}}$; (RW = random walk) [23]. Practical applications [10, 11] of MMC in LES tend to have far fewer Lagrangian particles for the stochastic reacting species field than there are Eulerian LES grid cells (see Section 7.4.4). Therefore the explicit inclusion of subgrid fluctuations in the formulation of the reference variables is unlikely to have a significant effect on the determination of localness in reference space. Of course the subgrid component of ξ_i may have a significant effect on conditional velocity (according to the linear closure given by (7.14)) or if some of the reference variables represent velocity components. If the random walk component of ξ_i is neglected (as has been done in practical applications) the subgrid conditional velocity can instead be closed by the alternative gradient model [12, 40] which manifests in the stochastic equation for the spatial transport:

$$d\boldsymbol{x}^{*(p)} = \left(\mathbf{U}^{(0)} + \frac{1}{\overline{\rho}} \nabla (\overline{\rho} D_{\mathrm{eff}}) \right) dt + \sqrt{2 D_{\mathrm{eff}}}\, d\boldsymbol{\omega}^{*(p)} \tag{7.39}$$

where D_{eff} is the sum of subgrid and (if needed) molecular diffusivities.

7.4 Examples

In the past five years an impressive list of publications have proposed and tested specific deterministic and stochastic MMC (including generalised MMC) models in a range of idealised, homogeneous combustion conditions [8, 9, 29, 56] and inhomogeneous, laboratory non-premixed and partially premixed flame conditions [10, 11, 54, 55, 57]. Each of these specific MMC models has a reference variable to emulate mixture fraction while a few of the deterministic models have additional reference variables to emulate scalar dissipation and/or sensible enthalpy [8, 9, 29]. In the inhomogeneous cases MMC has been coupled with RANS based turbulence models [54, 55], with the binomial Langevin model to model the joint velocity-scalar PDF [57] and LES to simulate the joint scalar FDF [10, 11]. The key features of these applications are summarised below.

7.4.1 MMC in Homogeneous Turbulence

7.4.1.1 Stochastic MMC

The first application of MMC to reacting flow conditions was the stochastic MMC reported by Wandel and Klimenko [56]. Results are compared against DNS data [35] in homogeneous turbulence with finite-rate, one-step chemistry and significant local extinction. A single reference variable emulates the mixture fraction and, as the probabilistic MMC interpretation is used, minor fluctuations of the single reactive scalar, normalised temperature, are present. An MMC-Curl's surrogate mixing model dissipates the minor fluctuations and the mixing timescale, $\tau_{\min}$, is set proportional to the macro-mixing timescale, denoted by τ_{maj}. Despite the simplicity of the flow and chemistry this modelling demonstrates the ability of stochastic MMC to capture heavy local extinction and subsequent reignition events more accurately than other commonly used models such as CMC, fast chemistry, Curl's, IEM and EMST. The performance of IEM, Curl's and EMST models is investigated in detail in Mitarai et al. [36] for the same test conditions. It is instructive to compare the scatter plots of temperature versus mixture fraction for those models and DNS in Ref. [36] with the MMC scatter plots in Ref. [56]. IEM fails to produce the correct physical behaviour as it cannot change the shape of the joint PDF from its initial conditions and nor can it generate conditional fluctuations of temperature with respect to mixture fraction. Curl's model produces physically plausible compositions for this case but as mixing is not local in composition space it significantly overpredicts conditional fluctuations and the reignition is very slow compared to the DNS. While EMST is local in composition space it violates the principles of independence and linearity and in its basic form EMST can lead to "stranding" [51] or mixing along certain preferential lines leading to non-physical behaviour. For the test case described MMC produces physically realistic and accurate results.

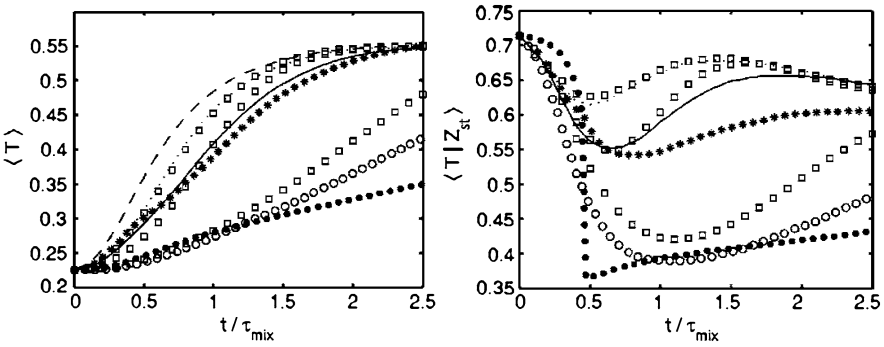

Fig. 7.2: Mean (left) and conditional mean at stoichiometry (right) of temperature. MMC (lowest to highest: $\tau_{\min}/\tau_{\text{maj}} = 1/1.04$, $1/8$ and $1/100$), $\square$; DNS data, $-$; EMST, $*$; CMC, $\cdots$; Curl's model, $\circ$; IEM $\bullet$; fast chemistry, $---$. Figures adapted from [56].

Figure 7.2 below shows the mean temperature (left) and the conditional mean temperature at stoichiometry (right) as a functions of time for the DNS and the various models. It can be seen that both EMST and MMC with $\tau_{\min}/\tau_{\text{maj}} = 1/8$ predict mean temperature very well while the other models either significantly overpredict the rate of temperature rise (CMC and fast-chemistry) or significantly under predict it (IEM and Curl's). For the conditional temperature MMC with $\tau_{\min}/\tau_{\text{maj}} = 1/8$ is the most accurate model. The MMC results are, however, qualitatively and quantitatively sensitive to the parameter $\tau_{\min}/\tau_{\text{maj}}$. By setting $\tau_{\min}/\tau_{\text{maj}} = 1/100$ the model rapidly dissipates any minor fluctuations, and hence conditional fluctuations, of temperature which may be generated. Thus this MMC result closely resembles those for first-order CMC. Alternatively by setting $\tau_{\min}/\tau_{\text{maj}} = 1/1.05$ the model does not dissipate minor fluctuations, and hence conditional fluctuations, fast enough and produces results similar to Curl's model. Although more research is required to determine the best values $\tau_{\min}/\tau_{\text{maj}}$ for a range of practical combustion conditions, the timescale ratio parameter appears to provide a useful mechanism for controlling the level of conditional fluctuations which is not available in many other mixing models. The authors [56] caution that the correct value of $\tau_{\min}/\tau_{\text{maj}}$ is unlikely to be universal or constant with time. The variability with time is illustrated in the results for $\tau_{\min}/\tau_{\text{maj}} = 1/8$ which slightly underpredicts the rate of reignition (see conditional temperature rise in Fig. 7.2). Attempts to reduce that timescale ratio (for all time steps) in order to more rapidly dissipate conditional fluctuations in the later stages of the evolution inadvertently leads to inaccuracy during the initial extinction phase. The creation of a model for $\tau_{\min}/\tau_{\text{maj}}$ would be advantageous but is not trivial. Any such model would need to account for the rate of dissipation and generation of conditional variance by the surrogate mixing model as analysed in Ref. [23].

7.4.1.2 Deterministic MMC

The first application of deterministic MMC is, in fact, contained alongside the original MMC derivation [21]. A three-stream, non-reactive, homogeneous mixing field is modelled with the use of two reference variables emulating two independent mixture fractions. It is shown that the joint PDF of the two mixture fractions is modelled in a very realistic manner and results are in excellent agreement with the analytical solution.

The first applications of deterministic MMC for reactive fields are found in a series of three papers by Cleary and Kronenburg [8, 9, 29]. They propose and test various deterministic MMC models against DNS [28] of homogeneous, decaying turbulence with varying levels of local extinction (up to global extinction). It had previously been established [28] that CMC with conditioning on the mixture fraction alone was inappropriate for these flame conditions due to the importance of conditional fluctuations which are neglected in first-order CMC. A number of previous CMC studies [6, 27, 28] identified scalar dissipation and normalised sensible enthalpy as possible choices for a second conditioning variable for flames with significant local extinction. In fact both quantities have an important role in the physics of local extinction and subsequent reignition. While fluctuating scalar dissipation is the primary instability which causes conditional fluctuations, those conditional fluctuations tend to correlate better with temperature related quantities such as sensible enthalpy, than with scalar dissipation.

The three MMC papers progress incrementally. The first [8] has reference variables emulating mixture fraction and multiple scalar dissipation-like quantities each of which is associated with a certain dissipation timescale (see (7.35) through (7.37)). As expected from the earlier CMC results [6], while conditioning on mixture fraction and a single scalar dissipation variable is able to model the extinction phase well, it cannot accurately predict the subsequent reignition phase which occurs after the turbulence has sufficiently decayed. Any deterministic MMC inevitably forces reference variables to be conditioning variables but at low temperatures there is decorrelation of reactive species and scalar dissipation fluctuations [27] and hence the assumption of negligible conditional/minor fluctuations and first-order reaction rate closures are inappropriate. Although the MMC results improve modestly with additional dissipation-like reference variables the model is illustrated to be unsuitable for a deterministic formulation. Note that dissipation-like reference variables were initially suggested as non-conditioning reference variables in the stochastic formulation of MMC (see Section 7.3).

The second paper [9] proposes an MMC model with reference variables emulating mixture fraction and normalised sensible enthalpy. Like previous CMC calculations with the same conditioning variables [28] results for reactive species are impressive. This is because the manifold comprising of only mixture fraction and sensible enthalpy adequately describes the accessed region in composition space. However, the model does not have a mechanism for introducing the physical instabilities (i.e. fluctuations in scalar dissipation) that cause extinctions to occur in the first place. To overcome this deficiency the fluctuations are imposed on the model

using DNS data for the conditional PDF of normalised sensible enthalpy. The result is a hybrid MMC / presumed PDF model which accurately describes the evolution of minor scalars but which does not predict the joint PDF of the major scalars.

The third paper [29] describes an MMC model which is a novel combination of the previous two. There is a reference variable emulating mixture fraction and a second reference variable which emulates normalised sensible enthalpy but that is also a dissipation-like variable which can generate the fluctuations leading to local extinctions. It is explained that any reference variable may adopt the character of a dissipation-like variable and that the physical quantity it emulates is irrelevant. Through the dual-nature of the second reference variable the model exploits the strong negative correlation between sensible enthalpy fluctuations and fluctuations in scalar dissipation during the extinction process. Specifically (7.37) is replaced by

$$c_{d_1} = f_{\text{corr}} \ln \left(\frac{\langle N''^2_{\eta\eta} | \eta \rangle}{\langle N_{\eta\eta} | \eta \rangle} + 1 \right)^{1/2} \tag{7.40}$$

where the correlation function is simply the conditional normalised sensible enthalpy at stoichiometry $f_{\text{corr}} = -\langle \hat{h}_s | \eta = Y_{Z\text{st}} \rangle$. While this third model is complete and follows the physics of the problem better than the previous two models on which it is based, the quality of the results is mixed. For the flame case with heavy local extinction followed by reignition and another case with global extinction, predictions of major and minor species are in very good agreement with DNS data. A particularly impressive outcome is the model's ability to accurately predict the bimodal distribution of sensible enthalpy in near stoichiometric mixtures as shown in Fig. 7.3. This is in contrast to an assumed β-PDF which cannot give a bimodal distribution between arbitrary minimum and maximum sample space limits. Interestingly, for a third test case exhibiting only moderate local extinction the model performs poorly and noticeably underpredicts the extent of that mild extinction. This is blamed on a realizability constraint which artificially restricts some of the diffusion coefficients to positive values to ensure numerical stability.

7.4.2 MMC with RANS

Two papers by Vogiatzaki et al. document the implementation of deterministic MMC into a RANS computer code and report on model performance for two laboratory jet diffusion flames with complex hydrocarbon chemistry. The first paper [54] reports on modelling of the DLR A and B $CH_4/H_2/N_2$ flames [2, 34] and the second paper [55] presents results and an expanded analysis for the Sandia $CH_4/O_2/N_2$ Flame D [1, 49]. In each case a single Gaussian reference variable emulates the mixture fraction. As the flame cases exhibit low levels of local extinction, conditioning on mixture fraction alone is appropriate as is established by many past accurate CMC and flamelet computations. Figure 7.4 (from

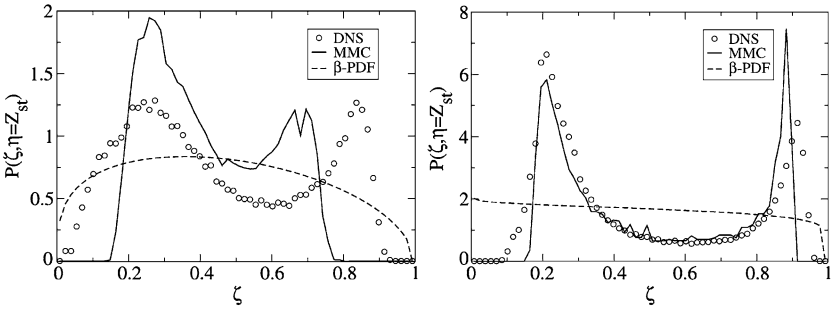

Fig. 7.3: Conditional PDF of normalised sensible enthalpy at stoichiometry at two different times. Figures adapted from [29].

Ref. [55]) shows that MMC predictions of the mixture fraction PDF for Sandia Flame D closely resemble a β-PDF. Close to the nozzle agreement with experimental data is excellent while the downstream discrepancies are linked to the commonly observed underprediction of the mixture fraction variance by the $k-\varepsilon$ turbulence closure. Conditional scalar dissipation does not appear explicitly in MMC but can be determined by (7.32) following a replacement of reference variables from ξ to η. Figure 7.5 shows conditional scalar dissipation profiles for Sandia Flame D conditions by MMC and two alternative closures based on integration of the mixture fraction PDF transport equation [14] and amplitude mapping closure (AMC) [7]. MMC reproduces the profile shapes and the location of the peak value better than the integrated PDF method and is an improvement over AMC which always gives the peak conditional scalar dissipation at mixture fraction equal to 0.5. MMC compares quite well to the 1D experimental data but is unable to capture the slightly bimodal shape which is even more apparent in the more accurate 3D experimental data. Although the obvious qualities of MMC do not make a significant difference to reactive scalar predictions in these simple flames (results are of similar good accuracy to those for CMC with standard PDF and conditional scalar dissipation closures) the MMC computations represent an important first step prior to application to more difficult flame cases which require additional conditioning variables and for which simple PDF shape presumptions and conditional scalar dissipation closures are not available.

7.4.3 MMC with the Binomial Langevin Model

A novel, hybrid model combining the binomial Langevin model [52] and stochastic MMC was introduced by Wandel and Lindstedt [57] to model the joint velocity-

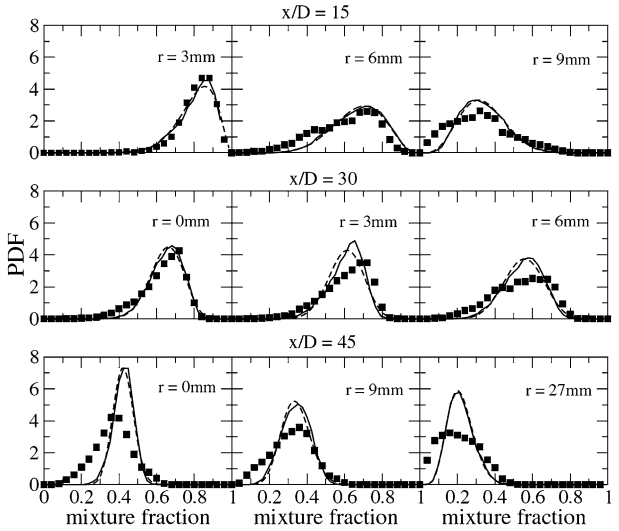

Fig. 7.4: Mixture fraction PDF at various locations for Sandia Flame D. Squares are experimental data, solid lines are MMC predictions, and dashed lines are β-PDFs. Figure adapted from [55].

scalar statistics in an inhomogeneous, reacting scalar mixing layer that was investigated experimentally by Saetran et al. [48] and Bilger and co-workers [3, 31]. The hybrid approach overcomes implementation difficulties associated with producing a bounded scalar field in the binomial Langevin context, while providing a simple and accurate means for obtaining the MMC coefficients (calculation of terms involving the gradient $\partial X/\partial\xi$ can be difficult in stochastic MMC when there is a lot of scatter). The hybrid model employs the principles of a generalised MMC closure. In the MMC part of the hybrid model, rather than solving (7.20), the single conditioning reference variable is instead modelled by inverting (7.14) and some other manipulation to give

$$\eta^{*(p)} = \frac{u_2^{*(p)} - \widetilde{u}_2}{\sqrt{\widetilde{u_2'^2}}}. \tag{7.41}$$

Here u_2 is the dominant velocity component (in this case the transverse component) and it is modelled by the binomial Langevin model. Note that (7.41) has the advantage that it does not contain the diffusion coefficient B and thus it is not necessary to calculate the gradients $\partial X/\partial\xi$. The model also has an additional *pseudo* mixture fraction that is solved according to the binomial Langevin model. The pseudo mixture fraction is a non-conditioning reference variable used only to calculate the extent of mixing between particle pairs while mixing localisation is in η-space

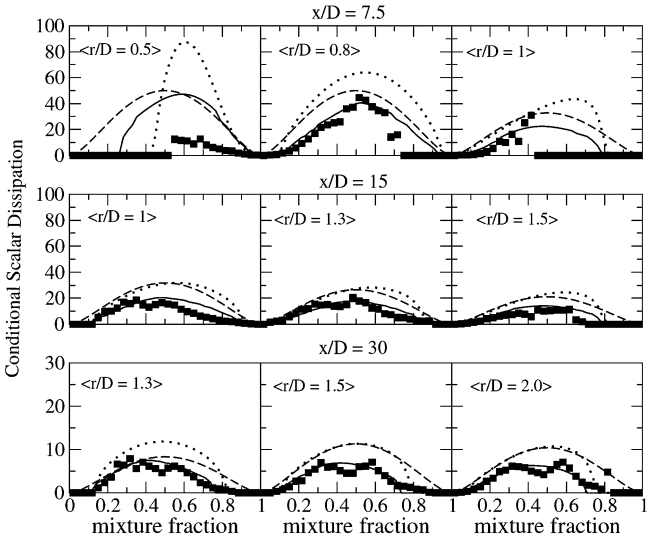

Fig. 7.5: Profiles of local conditional scalar dissipation in mixture fraction space for Sandia Flame D. Squares are 1D experimental data, solid lines are the MMC model, dotted lines are the integrated PDF model, and dashed lines are the AMC model. Figure adapted from [55].

only. (We caution that the notation used in this chapter for conditioning and non-conditioning reference variables is different to that used by Wandel and Lindstedt.)

The paper contains a detailed analysis of the model and makes extensive comparisons with experimental data. These indicate that the model is robust and provides a similar level of accuracy to the binomial Langevin model by itself. While results for mean quantities are in very good agreement with experimental data, the second moments are generally underpredicted signifying a need for future improvements such as better control of the dissipation of minor fluctuations by the surrogate mixing model. Due to the aforementioned elimination of implementation difficulties associated with the binomial Langevin and stochastic MMC models the hybrid model is reported to have a relatively modest computational cost. Application of this model to inhomogeneous flows is underway and preliminary results are encouraging.

7.4.4 MMC with LES

Two recent papers have documented the application of MMC with LES [10, 11] for the Sandia $CH_4/O_2/N_2$ Flame D [1, 49]. The model is a generalised MMC with the reference variable given by the LES filtered mixture fraction. The most compelling

aspect is the demonstration of a new very low-cost, sparse-Lagrangian scheme for simulation of the joint scalar FDF, made possible due to the high quality of the MMC mixing closure. Conventional FDF simulations employ an "intensive-Lagrangian" particle scheme with many particles per Eulerian LES grid cell, and the terminology of "sparse-Lagrangian" is introduced to refer to simulations with significantly fewer Lagrangian particles for the joint scalar FDF than there are Eulerian grid cells. The simulations of Flame D are performed for (on average) one particle for every 10 to 12 LES cells culminating in as few as 35,000 particles over the 70 jet-nozzle diameter flow domain. This represents a two or three order of magnitude reduction in particle numbers and computational cost relative to conventional intensive-Lagrangian FDF simulations of the same or similar flame conditions. As a result of the very low cost the sparse-Lagrangian simulations are able to use detailed 219-step chemistry, whereas previous FDF simulations of hydrocarbon flames have required reduced or tabulated chemistry. (A list of recent FDF computations is compiled by Haworth [17].)

The theoretical basis for sparse-Lagrangian simulations is established in two papers [24, 25] while Ref. [10] elaborates on the physical reasoning in support of sparse methods and the reasons for the success of generalised MMC under such conditions. Modelling aside, if it is assumed that a particle within the ensemble representing the one-point, one-time FDF is statistically independent of all other particles, then all those other particles can be removed while the one remaining particle continues to represent that FDF. That probability distribution exists whether we have sufficient numbers of particles to determine it locally or not. From a modelling perspective the problem of using very few particles is that numerical diffusion (i.e. numerical bias in the Lagrangian fields) can become larger than is justified or needed if that diffusion performs a modelling role. Therefore modelling the FDF with very few particles requires a high quality mixing model which specifically minimises numerical diffusion. MMC does this by enforcing localness in the reference space. Whereas non-local mixing models such as IEM are successful in intensive-Lagrangian FDF simulations by virtue of the high spatial resolution of LES, it seems that only models (such as MMC), which enforce localness and adhere to the other desirable qualities of mixing models, are capable when particle numbers are significantly reduced. It should be stressed that the finest details of the fields are not available with so few particles but the published works [10, 11] demonstrate that the major stationary statistics of the reacting scalar fields (i.e. conditional and unconditional means and variances) are in good agreement with experimental data. Figure 7.6 (taken from Ref. [11]) shows radial profiles of unconditional means and variances of temperature and mass fraction of carbon monoxide and the hydroxyl radical. Results are in good agreement with the experimental data and furthermore have a low sensitivity to a five-fold increase in the number of particles.

The model contains two tuneable parameters: a mixing timescale constant and a localness parameter which determines the relative degree of localisation in reference (filtered mixture fraction) and physical spaces. These parameters are adjusted to control the small but not insignificant conditional fluctuations. More work is neces-

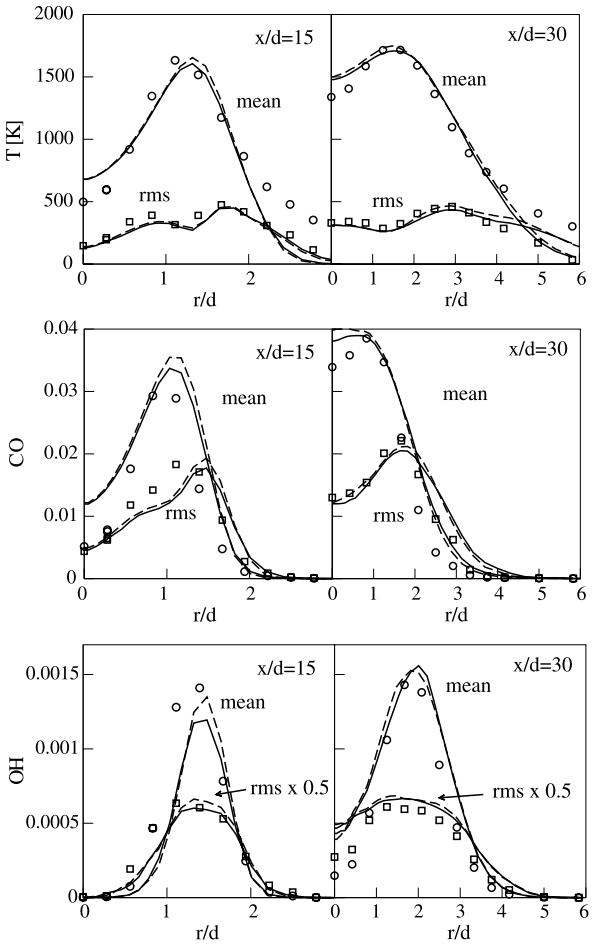

Fig. 7.6: Unconditional mean and rms for temperature, CO and OH at two downstream locations. Open symbols - experimental data, solid lines - MMC with nominally 35,000 particles, broken lines - MMC with nominally 175,000 particles. Figure adapted from [11].

sary to determine the selection of such parameters for a wide range of conditions including those with significant local extinction phenomena. For some complex flame regimes, where conditional fluctuations relative to mean values conditioned on the mixture fraction are very large, additional reference variables (e.g. to emulate sensible enthalpy or other related quantities) may be necessary. However, the need for a filtered source term closure for reacting reference variables could pose a significant challenge if this is attempted.

A principal problem of sparse-Lagrangian methods is related to the evaluation of density which must be obtained from a small number of particles and coupled to the more highly resolved LES flow field. The existing MMC publications do not address this but rather have a tabulated density. Thus there is no coupling or consistency between the Eulerian LES and Lagrangian FDF fields. Ongoing but as yet unpublished research at The University of Queensland has successfully treated the density coupling issue through a conditionally averaged form of the equivalent enthalpy method of Muradoglu et al. [38] which ensures numerical stability and consistency.

7.5 Summary and Future Directions

This chapter has reviewed the MMC concepts and theory, and their evolution, along with the key specific MMC model applications since it was first proposed in 2003. In its most basic deterministic form MMC represents a closed and consistent combination of joint PDF modelling for a set of major species which describe the accessed region in composition space and conditional moment closure for the set of minor species which fluctuate jointly with the major scalars. The closure and consistency is facilitated by mapping closure which is generalised for inhomogeneous flows. MMC has evolved from a deterministic to a stochastic method. Although an equivalent stochastic formulation was introduced initially as a computationally efficient form of the deterministic model it also allows a generalised interpretation where fluctuations of minor species relative to the major species manifold may be exploited and where the reference variables are used to enforce desired properties by conditioning/localisation in mixture fraction space (i.e. a CMC-type mixing model closure) and emulation of scalar dissipation fluctuations. Further evolution of generalised MMC has occurred with the replacement of Markov reference variables by traced Lagrangian quantities in Eulerian DNS or LES. The possibility also exists to obtain reference variables by other simulation or modelling methods.

From the perspective of MMC the use of LES to provide reference variables is expensive but this is more than compensated for through the demonstrated possibility of using a sparse distribution of particles to model the Lagrangian FDF. While a PDF must describe the distributions of all turbulent scales an FDF need only describe the subgrid distributions while the large scale turbulence is resolved by the LES. Therefore from the perspective of LES simulations, generalised MMC allows high-quality, efficient simulations that are dramatically less expensive than conventional intensive-Lagrangian FDF simulations or even LES with chemical source terms modelled using the resolved quantities at the Eulerian grid centres. The concept of sparse-Lagrangian simulations is associated with the FDF method and is not coincident with the concepts of MMC, per se. Sparse simulations with closures other than generalised MMC are certainly possible, however only generalised MMC closures are currently known to work for sparse simulations.

The advances and challenges of MMC research in the coming years will include (but are certainly not restricted to):

- the application of various specific MMC models to a wide range of laboratory combustion conditions and flame regimes to establish the best choice of model parameters;
- the application in inhomogeneous flows of MMC with multiple reference variables emulating more complex accessed composition spaces;
- the expanded testing and development of hybrid MMC methods which borrow ideas from other established models;
- the establishment of criteria for assessing the optimal compromise between quality and economy in current and new sparse-Lagrangian MMC closures;
- the establishment of consistent and stable density coupling methods in sparse-Lagrangian simulations; and
- the application of MMC to conditions of greater engineering and practical interest.

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