Chapter 15
Theory and Application of Multiple Mapping Conditioning for Turbulent Reactive Flows

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Abstract This chapter presents the basic theory and conceptual evolution of the multiple mapping conditioning (MMC) framework, and presents recent applications for turbulent reactive flows. MMC was initially formulated as a method that integrates the probability density function (PDF) and conditional moment closure (CMC) models through a generalisation of mapping closure. MMC models utilise a *reference space*, whose PDF is prescribed a priori or which is simulated by some means such as a Markov diffusion process. The turbulent fluctuations of all scalars in this method are divided into *major* and *minor* groups, and the former are associated with the reference space via a mapping function. The reference space describes a low-dimensional manifold which can fluctuate in any given way, while the fluctuations of the (real) scalars are fully or partially confined relative to that reference space. The dimensionality of the reference space is usually small. For

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example, in non-premixed combustion a reference space emulating the mixture fraction usually suffices. There are both *conditional* and *probabilistic* conceptualisations of MMC and both *deterministic* and *stochastic* mathematical formulations. In the past decade, an extension of probabilistic MMC has emerged that is known as *generalised MMC* that removes some of the formality of the original formulation and extends the type and usage of the reference variables. Generalised MMC is commonly associated, although not exclusively, with large eddy simulations (LES). This chapter reviews the conceptual and theoretical advances in MMC since its original formulation and also reviews some of the recently published applications of MMC in turbulent reactive flows.

Keywords MMC · Reactive flows · RANS · LES · PDF method Mixing model

Nomenclature

r_m	Characteristic scale in physical space
f_m	Characteristic scale in reference space
W_I	Chemical reaction rate
Q_α	Conditional expectation
$\mathbf{U}$	Conditional velocity
D	Diffusion coefficient
B_{kl}	Diffusion coefficient
$d_{x,i}^{p,q}$	Distance between particle in physical space
A_K	Drift coefficient
$\tilde{Z}_{LES}$	Filtered LES mixture fraction
X_I	Mapping function
Z	Mixture fraction
S_I^*	Mixing operator
MW	Molecular weight
n_s	Number of chemical species
n_m	Number of dimensions of manifold
$\mathrm{N_p}$	Number of particles
P_ξ	Pdf of reference space
P	Probability density function (PDF)
$\mathbf{Y}(x, t)$	Reactive scalar space
N_{ij}	Scalar dissipation
Y	Scalar, reactive scalar species mass fraction
T	Temperature
C_{min}	Timescale ratio
v	Velocity vector
w_p	Weight of particle p
w_I^*	Wiener processes

Greek symbols

ρ Density
τ_{min} Minor dissipation timescale
ξ Reference variable
τ_{ϕ} Scalar mixing timescale
ξ'' Subgrid fluctuation

15.1 Introduction

In the past few decades, several turbulent combustion models have been developed and demonstrated for both premixed and non-premixed turbulent flames (Veynante and Vervisch 2002). In most practical combustion systems, these two distinct areas are not encountered and combustion occurs under partially premixed conditions. The probability density function (PDF) method (Pope 1985) is one of the few models which, although initially developed for non-premixed combustion, is general enough in its formulation to be applicable to all combustion regimes (Pei et al. 2015; Brauner et al. 2016; Cao et al. 2007; Lindstedt and Vaos 2006). This is because the reaction rate term appears naturally in closed form, whereas in other combustion models some form of approximation is needed for the average or filtered reaction source. There is a caveat, however. The mixing term in the governing equation for the PDF is unclosed and not all of the mixing models which have been developed are applicable to all combustion regimes. Additionally, a disadvantage of the conventional PDF method is that the cost of computation is relatively large and for realistic systems involving hundreds of species, the application of PDF methods can become impractical. Addressing these issues is a motivation for the ongoing development of the multiple mapping conditioning models (Klimenko and Pope 2003).

Conditional moment closure (CMC) (Klimenko and Bilger 1999) is a well-known turbulent combustion model whereby the reaction rate closure is obtained by formulating the governing equations in terms of the conditional expectations of reactive scalars. In its simplest form, known as first-order CMC, the scalar quantities (species mass fraction and temperature) are assumed to fluctuate jointly with the fluctuation of one key quantity (normally the mixture fraction for non-premixed combustion) and the fluctuations around the conditional means are neglected. This model is computationally efficient relative to the PDF method while it lacks the ability to predict cases where the above assumption is invalid, for example, in partially premixed combustion where parameterisation by the mixture fraction breaks down. To address this extensions have been developed, like conditioning on multiple variables (Kronenburg 2004) or making second-order approximations to the conditional reaction rates (Mastorakos and Bilger 1998),

but these increase complexity by requiring closure of additional terms and they also increase the computational cost.

Since 2003 the multiple mapping conditioning (MMC) framework has emerged (Klimenko and Pope 2003). It may be seen as a logical extension of the conventional PDF method and conditional moment closure (CMC) through the generalisation of the mapping closure concept (Girimaji 1992; Pope 1991). MMC models utilise a *reference space*, whose PDF is either prescribed a priori or which is simulated by some means such as a Markov diffusion process. The turbulent fluctuations of all scalars in this method are divided into *major* and *minor* groups, and the former are associated with the reference space via a mapping function. For model simplicity and computational tractability, the dimensionality of the reference space is usually small. For example, in non-premixed combustion a reference space made of a single variable emulating the mixture fraction usually suffices. The reference space therefore describes a low-dimensional manifold which can fluctuate in any given way, while the fluctuations of the (real) scalars are fully or partially confined relative to that reference space. According to the MMC governing equations, the small-scale (micro) mixing occurs locally in the reference space, and provided that the reference space adequately describes the accessed composition space, the mixing will effectively be local in composition which is a desirable property. There are both *conditional* and *probabilistic* forms of MMC (Klimenko and Pope 2003; Klimenko 2005). The conditional form is associated with either a deterministic or stochastic computational implementation of the model and assumes that the minor scalars can fluctuate only jointly with the major scalars such that their conditional fluctuations are negligibly small. Probabilistic MMC is associated only with the stochastic form and allows the minor scalars to fluctuate relative to the major scalars, although these conditional fluctuations are still expected to be small. In this way, the MMC model becomes a full PDF model with MMC playing the role of a mixing model that is local in a reference space. In the past decade, an extension of probabilistic MMC has emerged that is known as generalised MMC (Klimenko 2005; Cleary and Klimenko 2009; Sundaram et al. 2016). This approach removes some of the formality of original MMC and extends the type and usage of the reference variables to incorporate non-Markov variables and variables that are used for purposes other than localisation of the mixing operation.

MMC adequately integrates the PDF and CMC approaches. It exploits the advantages of both the methods and reduces some of their complications. As a result, it is proving useful for modelling various combustion regimes including non-premixed atmospheric (Devaud et al. 2013; Ge et al. 2013; Straub et al. 2016; Varna et al. 2017; Vogiatzaki et al. 2011, 2015; Wandel and Lindstedt 2013) and high pressure engine-like conditions (Salehi et al. 2017), premixed combustion (Sundaram and Klimenko 2017), partially premixed combustion (Galindo et al. 2017) and aerosol nucleation (Neuber et al. 2017; Vo et al. 2017). This book chapter presents a review of MMC and the evolution in its conceptualisation. In the subsequent sections, a description of the basic concepts and theory will be presented including its different formulations. Results from the recent literature are reviewed. At the end of this chapter, conclusions are drawn. This work may be read

in conjunction with book chapter by Cleary and Klimenko (2011), in which case Sect. 15.2 of the present work may be skipped over, whereas the reviewed applications in Sect. 15.3 contain new research conducted since the earlier book chapter was published. The model derivations are not included here, and readers are directed towards the original publications, especially, those by Klimenko and co-workers (Klimenko and Pope 2003; Sundaram et al. 2016; Klimenko 2005, 2007, 2009a, b; Klimenko and Cleary 2010), if details of the derivations are sought after.

15.2 Concepts and Theory

In this section, we present the concepts underpinning MMC, starting with the governing equations for scalar transport and their joint PDF. We then introduce the idea of a reference space and review the mapping closure concept, which together provides closures to the MMC governing equations which are subsequently presented in both their deterministic and stochastic forms. Finally, the concepts and theory of generalised MMC are explored.

15.2.1 Scalar Transport Equations the MMC Concept

The transport equation for the n_s-dimensional reacting scalar space $Y(x,t) = (Y_1, Y_2, \ldots, Y_I, \ldots, Y_{n_s})$ is given by

$$\frac{\partial \rho Y_I}{\partial t} + \nabla.(\rho v Y_I) - \nabla.(\rho D \nabla Y_I) = w_I, \tag{15.1}$$

where $v = v(x,t)$ is the fluid velocity, D is the diffusion coefficient which for our present purposes is assumed to be equal for all species, ρ is the density, and w_I is the rate of production of species I. Both ρ and w_I are usually known functions of species mass fractions, Y_I, temperature (or enthalpy) and pressure.

In a turbulent flow, the stochastic distribution of the composition can be given by the one-time, one-point Favre joint PDF, $P_Y(y;x,t)$. In the limit of high Reynolds number, the PDF transport equation is

$$\frac{\partial \bar{\rho} P_Y}{\partial t} + \nabla.(\bar{\rho} u P_Y) + \frac{\partial W_I \bar{\rho} P_Y}{\partial y_I} + \frac{\partial^2 N_{IJ} \bar{\rho} P_Y}{\partial y_I y_J} = 0, \tag{15.2}$$

where the conditional expectations of velocity, production term, scalar dissipation and density are

$$u(y;x,t) \equiv \langle \rho v | Y = y \rangle / \rho_Y \tag{15.3}$$

$$W_I(y;x,t) \equiv \langle \rho w_I | Y = y \rangle / \rho_Y \tag{15.4}$$

$$N_{IJ}(y;x,t) \equiv \langle \rho D \frac{\partial Y_I}{\partial x_k} \frac{\partial Y_J}{\partial x_l} | Y = y \rangle / \rho_Y \tag{15.5}$$

and

$$\rho_Y(y;x,t) \equiv \langle \rho | Y = y \rangle \tag{15.6}$$

Here, the upper case subscripts *I, J,* and *K* run over n_s species and the lower case subscripts run over the orthogonal spatial dimensions. The lower case vector $\boldsymbol{y}$ is the sample space for $\boldsymbol{Y}$.

The above PDF is defined for the n_s-dimensional composition space, but in MMC the range of turbulent fluctuations is confined (fully or partially, depending on the interpretation of MMC that is taken) to a reduced n_m-dimensional manifold where $n_m < n_s$ corresponds to number of major species who subset is denoted $\boldsymbol{Y}^m$. The remaining subset of size $n_\alpha = n_s - n_m$ is referred to as the set of minor species denoted $\boldsymbol{Y}^\alpha$. Lower case Roman and Greek symbols are used to denote members of the major and minor species subsets, respectively. Major species are permitted to fluctuate in any physically realisable way, while the minor species are either (i) assumed to fluctuate jointly with the major species so that conditional fluctuations $\langle Y'_\alpha | Y^m = y^m \rangle = 0$, or (ii) have finite but (usually) small conditional fluctuations. In either interpretation the reduced PDF of the major species should satisfy the equation

$$\frac{\partial \bar{\rho} P_{Y_m}}{\partial t} + \nabla.(\bar{\rho} u P_{Y_m}) + \frac{\partial W_i \bar{\rho} P_{Y_m}}{\partial y_i} + \frac{\partial^2 N_{ij} \bar{\rho} P_{Y_m}}{\partial y_i y_j} = 0 \tag{15.7}$$

In the former interpretation, which is known as conditional MMC, the minor species are fully described by their conditional expectations $Q_\alpha(y^m;x,t) = \langle Y_\alpha | Y^m = y^m \rangle$ satisfying

$$\frac{\partial Q_\alpha}{\partial t} + u \nabla Q_\alpha + W_i \frac{\partial Q_\alpha}{\partial y_i} - N_{ij} \frac{\partial^2 Q_\alpha}{\partial y_i y_j} = W_\alpha \tag{15.8}$$

The full PDF is then approximated as

$$P_Y = P_{Y_m}.\delta(Q - y^\alpha) \tag{15.9}$$

In the latter interpretation, which is known as probabilistic MMC, the minor species fluctuations are not formally neglected but advantage is taken of the greater accuracy and lower computational cost that is afforded in the modelling by keeping the fluctuations of the minor species close to those of the major species.

The selection of the major species is nearly always case dependent. If the wrong or too few major species are chosen then the assumption that the conditional fluctuations of the minor species are small may be invalidated. If too many major species are chosen then the computational cost may be high. A broad definition is given to what may constitute a major species. It may be one of the key chemical species such as a product gas like carbon dioxide, or it may be a derived quantity like the mixture fraction which is useful in non-premixed combustion, the reaction progress variable which may be useful in premixed combustion or, even, combinations of the above and scalar dissipation which may be useful in partially premixed combustion (Kronenburg and Cleary 2008).

15.2.2 Reference Variables and Mapping Closure

Equations (15.7) and (15.8) contain conditional velocity $\boldsymbol{u}$ and the conditional scalar dissipation N_{ij} which are unclosed. The closure is achieved in MMC through the use of a reference space. Although the utilisation of a reference space is not a new idea in turbulent combustion modelling (Girimaji 1992, 1993; Pope 1991; Chen et al. 1989), MMC takes it a step further generalising the concept for both homogeneous and inhomogeneous flow conditions. In the original version of MMC formulated by Klimenko and Pope (2003), the reference space is linked to the major scalar space although it is stochastically independent of it to satisfy the independence and linearity principles, that is, required of good PDF mixing models (Subramaniam and Pope 1998). Generalised MMC (Klimenko 2005; Cleary and Klimenko 2009; Sundaram et al. 2016) broadens the concept further and allows additional reference variables that may be separate from the major species space but are useful quantities for emulating the turbulent distributions of the reactive scalars.

Mapping functions, $X_I(\boldsymbol{\xi}; x, t)$, provide a one-to-one transformation between the reference space, $\boldsymbol{\xi} = \left(\xi_1, \xi_2, \ldots, \xi_k, \ldots, \xi_{n_r}\right)$, and the reactive scalars, Y_I. Since mapping functions are the function of stochastic variables they are stochastic quantities themselves. They are characterised by a probability density function, P_X, which is a model for P_Y. The advantage is that, unlike the unclosed transport equation for P_Y given by Eq. (15.2), the transport equation for P_X is in closed form due to the known PDF of the reference space, P_ξ. This is the essence of mapping closure. P_ξ is known either because it is prescribed as in the original derivation of Klimenko and Pope (2003) or simulated independently of $\boldsymbol{Y}$ (Cleary and Klimenko 2009; Varna et al. 2017; Wandel and Lindstedt 2009).

Mapping functions are non-decreasing functions of their arguments at any given time. The general concept of a mapping function is explained by Vogiatzaki (2010) for a single reference variable, ξ, emulating a single major scalar, $Y = Z$ (i.e. the mixture fraction) in a non-premixed jet flame. Figure 15.1a shows the mapping functions (solid lines) in reference space, along with the standard Gaussian PDF of the reference space, P_ξ (dashed line). The black, green and red lines describe the evolution of mapping functions in reference space for rich, lean and shear layer

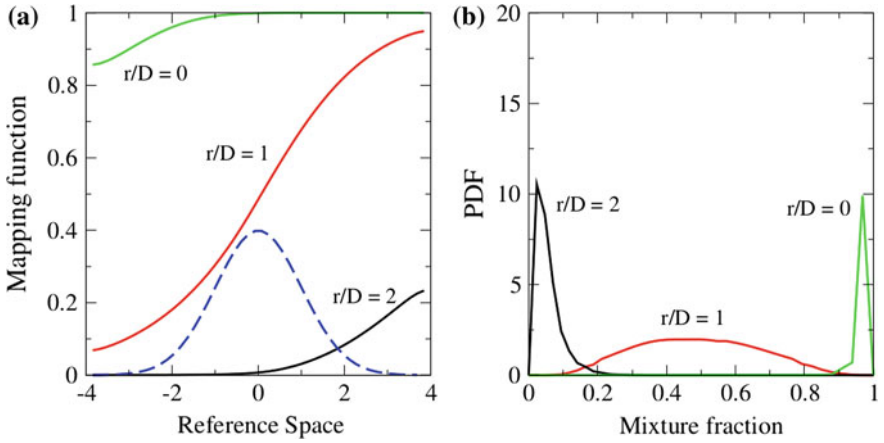

Fig. 15.1 **a** Mapping functions (solid lines) at different radial locations and the (static) reference variable Gaussian distribution (dashed line) over reference space. **b** Corresponding PDF's of mixture. Figure is from Vogiatzaki (2010)

regions, respectively. Figure 15.1b presents the corresponding mixture fraction PDFs, P_Z. In MMC, for each physical location, a mapping function is calculated that has as input the reference space and as output the range of the expected values of the species under consideration. Knowing both the reference space PDF and the values of the mapping function, the PDF of the physical scalar can then be calculated according to the mapping closure methodology.

15.2.3 Deterministic MMC

The deterministic form of the transport equation for the temporal and spatial evolution of the mapping functions $X_I(\boldsymbol{\xi}; x, t)$ is (Klimenko and Pope 2003)

$$\frac{\partial X_I}{\partial t} + U.\nabla X_I + A_k \frac{\partial X_I}{\partial \xi_k} - B_{kl} \frac{\partial^2 X_I}{\partial \xi_k \xi_l} = W_I, \tag{15.10}$$

where the subscript I represents all scalars (both major and minor) while k and l represent the major scalars only. This deterministic version of the model equations is associated only with the conditional perspective of MMC.

The above equation introduces the conditional (on reference space) velocity $U(\boldsymbol{\xi}; x, t)$, a drift coefficient $A_k(\boldsymbol{\xi}; x, t)$, a diffusion coefficient $B_{kl}(\boldsymbol{\xi}; x, t)$ and the conditional reaction rate $W_I = W_I(X(\boldsymbol{\xi}))$. The adjoint transport equation with the one-point, one-time joint PDF of the stochastic reference field is given by

$$\frac{\partial \bar{\rho} P_\xi}{\partial t} + \nabla.(\bar{\rho} U P_\xi) + \frac{\partial A_k \bar{\rho} P_\xi}{\partial \xi_k} + \frac{\partial^2 B_{kl} \bar{\rho} P_\xi}{\partial \xi_k \xi_l} = 0 \tag{15.11}$$

Equations (15.10) and (15.11) combined are formulated for compliance of the MMC model with Eq. (15.8) for the marginal PDF of the major species and Eq. (15.9) for the conditional expectation of minor species. A detailed examination of this compliance may be found in Klimenko and Pope (2003). Depending on the number of reference variables (for the present this is equal to the number of major scalars), MMC can be construed as a PDF or a CMC model. If $n_r = n_s$, then MMC becomes a complete joint PDF model; if $n_r < n_s$ then we have only n_r independent scalars whose evolution maps to the n_r-dimensional marginal PDF of the major scalars, while the remaining $n_s - n_r$ minor scalars are the dependent variables which are tackled through conditioning methods. It is, however, important to note that a single transport equation, Eq. (15.10), exists for all species, both major and minor. In deterministic MMC, the computational cost is directly linked to the number of reference variables. When a single reference variable such as mixture fraction is used, MMC is similar to first-order CMC although, as demonstrated below, it has a closed-form model for conditional scalar dissipation rate and the PDF of the mixture may be derived from the simulations rather than being an input quantity as it is in CMC. Likewise, the computational cost of MMC with a single reference variable will be comparable to that of first-order CMC. Moreover, by virtue of being expressed as a function of the independent joint Gaussian reference space, the deterministic MMC formulation presented above is valid for any number of reference variables, whereas specific CMC models need to be formulated as additional conditioning variables are added.

The coefficients U, A_k and B_{kl} are now described. They have to be specified consistently with the transport equation for P_ξ. Although other formulations are possible, we limit ourselves here to the version described in Klimenko and Pope (2003) corresponding to a jointly standard Gaussian distribution for P_ξ with zero mean and unity variance:

$$P_\xi(\boldsymbol{\xi}) = G(\xi_1)G(\xi_2)G(\xi_3)\ldots G\left(\xi_{n_r}\right), \tag{15.12}$$

$$G(\xi_k) = \frac{1}{\sqrt{2\pi}} exp\left(-\frac{\xi_k^2}{2}\right). \tag{15.13}$$

This distribution complies with Eq. (15.11) provided that (Klimenko and Pope 2003)

$$U(\boldsymbol{\xi}; x, t) = U^{(0)} + U_k^{(1)} \xi_k, \tag{15.14}$$

$$A_k(\boldsymbol{\xi}; x, t) = -\frac{\partial B_{kl}}{\partial \xi_l} + B_{kl}\xi_l + \frac{1}{\bar{\rho}} \nabla.\left(\bar{\rho} U_k^{(1)}\right). \tag{15.15}$$

The conditional velocity is linearly dependent on the reference space which is a common practice in conditional moment methods (Klimenko and Bilger 1999). Following mapping, closure convention B_{kl} is modelled independent of $\boldsymbol{\xi}$ leading to

$$U^{(0)} = \tilde{v} \tag{15.16}$$

$$U_k^{(1)} \langle \xi_k X_i \rangle = \widetilde{v' Y_i'} \tag{15.17}$$

$$B_{kl}(x,t) \left\langle \frac{\partial X_i}{\partial \xi_k} \frac{\partial X_j}{\partial \xi_k} \right\rangle = \tilde{N}_{ij}. \tag{15.18}$$

The quantities in angular brackets are average values obtained by convolution with P_ξ and $\tilde{N}_{ij}$ is the unconditional Favre-averaged scalar dissipation. Herein is the biggest advantage of using the mapping closure concept. Equations (15.16)–(15.18) show that the turbulence-chemistry interactions are closed using unconditional Favre-averaged quantities whereas external models for the conditional quantities are conventionally required to close the transport equation for the joint PDF and CMC.

15.2.4 Stochastic MMC

The solution to the Eq. (15.10) through a finite difference method, while practical for $n_r \sim 1$ (Devaud et al. 2013; Vogiatzaki et al. 2009), becomes computationally expensive for $n_r \gg 1$. The stochastic form of MMC can be derived based on the use of Lagrangian notional particles (Klimenko and Pope 2003):

$$dx^* = U\left(\boldsymbol{\xi}^*, x^*, t\right) dt, \tag{15.19}$$

$$d\xi_k^* = A_k^0\left(\boldsymbol{\xi}^*, x^*, t\right) + b_{kl}\left(\boldsymbol{\xi}^*, x^*, t\right) d\omega_l^*, \tag{15.20}$$

$$dX_I^* = \left(W_I^* + S_I^*\right) dt, \tag{15.21}$$

$$\langle S_I^* | \boldsymbol{\xi}^* = \boldsymbol{\xi}, x^* = x \rangle = 0. \tag{15.22}$$

In the above set of equations,

$$A_k^0 = A_k + \frac{2}{\tilde{P}_\xi} \frac{\partial B_{kl} P_\xi}{\partial \xi_l}, \tag{15.23}$$

$$b_{kl} b_{li} = 2B_{kl}. \tag{15.24}$$

Stochastic quantities that are associated with the evolution of notional particles are denoted by the asterisks. Equation (15.19) accounts for the transport in physical space, where the location of the particle is represented by x^* and $d\omega_i^*$ is the

increment of a Wiener process with zero mean and variance equal to dt. Equations (15.20) and (15.21) govern the transport in the reference space and composition space, respectively. W_I^* is the chemical source term and S_I^* is a mixing operator which simulates the conditional scalar dissipation. As stated in Eq. (15.22), the application of mixing does not alter the conditional expectations. The purpose of S_I^* is to keep the values of X_I^* close to its conditional mean value $\bar{X}_I^* = \langle X_I^* | \boldsymbol{\xi}^* = \boldsymbol{\xi}, x^* = x \rangle$. It is specific to MMC and ensures that mixing is local in both reference and physical spaces. It controls the dissipation of minor fluctuations and for this reason, may be referred to as the minor mixing operator (Sundaram et al. 2016). The dissipation of major fluctuations is simulated through Eq. (15.20) that is closed with Eqs. (15.23) and (15.24) which are linked to Favre mean quantities via Eq. (15.18). Under the conditional MMC perspective, fluctuations of X_I^* relative to $\bar{X}_I^*$ are constrained as much as possible and are treated as stochastic error whose impact on the conditional means diminishes with increasing number of notional particles. Under the conditional perspective, the stochastic formulation is equivalent to the deterministic formulation. The alternative probabilistic perspective treats the fluctuations as modelling quantities that allow P_X obtained by a solution to Eqs. (15.19)–(15.22) to emulate P_Y, even if the number of reference scalars is small. This latter view is especially relevant to the generalised form of MMC discussed below.

Mixing models are needed for the mixing operator, S_I^*. Since it controls only the minor fluctuations the choice of mixing model is not expected to have a significant impact on the results. Here, we present the modified Curl's model (Janicka et al. 1979) version of the minor mixing operator which has been most commonly used in practical stochastic MMC simulations. An overview of other mixing models may be found in Celis and da Silva (2015). The MMC-Curl mixing operator which involves an interaction between particles grouped into pairs (denoted by p and q) that are local in reference space and mixed over a time step duration of Δt (Straub et al. 2016):

$$X^{*,p}(t+\Delta t) = X^{*,p}(t) + \lambda\left(X^{p,q}(t) - X^{*,p}(t)\right)\frac{\Delta t}{\tau_\phi} \tag{15.25}$$

$$X^{*,q}(t+\Delta t) = X^{*,q}(t) + \lambda\left(X^{p,q}(t) - X^{*,q}(t)\right)\frac{\Delta t}{\tau_\phi} \tag{15.26}$$

In the above, $\lambda = 1 - exp\left[-\frac{w_p + w_q}{W}\frac{N}{2}\right] \approx \frac{w_p + w_q}{W}\frac{N}{2}$ where w_p, w_q and W are the weights of particles p and q and their sum, respectively. The number of particles per CFD cell is N. The quantity τ_ϕ is the scalar mixing timescale as found in conventional PDF methods (Pope 1985) and is here termed as the major dissipation timescale. As already stated, the particle pairs in MMC are not randomly selected but rather are selected such that they are local to each other in reference space. Therefore, all particles at a location (typically within one CFD cell) are sorted by their reference value and stored in an array. Two neighbouring particles within this

array are selected as a pair to be mixed. This mixing rule ensures localness in composition space. The mixing operator for the selected particle pair can now be written as

$$S_I^* = \frac{dX^{*,k}}{dt} \approx \lambda \frac{X^{p,q} - X^{*,k}}{\tau_{min}} \tag{15.27}$$

The minor mixing timescale, τ_{min}, controls the conditional fluctuations of scalars around the conditional mean. The timescales have the following relation

$$\tau_{min} = C_{min}.\tau_\phi \tag{15.28}$$

Wandel and Klimenko (2005) used the DNS study of Mitarai et al. (2003) for a homogeneous turbulent reacting flow with one-step irreversible chemistry to demonstrate how the ratio of the minor to major dissipation timescales controls the conditional fluctuations. A ratio of $O(100)$ yields rapid dissipation of the minor fluctuations and the model closely resembles first-order CMC. A ratio of 8 was identified to produce the correct level of conditional fluctuations in their homogeneous turbulence test case and recently Straub et al. (2016) corroborated that finding against data for the Sandia D–F laboratory flame series.

15.2.5 Generalised MMC

The term *generalised MMC* was first coined by Klimenko (2005) to name a form of MMC which relaxed some of the strictness implied by the original MMC model derived by Klimenko and Pope (2003), in particular by the dividing reference space into conditioning variables and non-conditioning variables. Conditioning reference variables emulate certain Lagrangian characteristics of turbulent flows and are used to localise the mixing in the space of the major species manifold. Non-conditioning reference variables assist the emulation of the turbulent quantities but are not used for localisation of mixing. Conditioning variables localise the mixing and imply a significant computational cost, whereas non-conditioning variables assist the simulations only and do not imply a major additional burden. As examples of generalised MMC, Klimenko (2005) suggested: (i) MMC with multiple dissipation-like non-conditioning variables whose purpose is to emulate a stochastic MMC diffusion coefficient, B_{kl}; (ii) MMC with velocity-like non-conditioning variables; and (iii) MMC with mixture fraction and dissipation-like reference variables obtained with the help of LES of the flow field.

Cleary and Kronenburg incorporated multiple dissipation-like reference variables in the deterministic context (Cleary and Kronenburg 2007). However, by its nature, the deterministic form of MMC implies conditioning must occur on all reference variables and that many dissipation-like variables were required to

emulate the spectrum of its fluctuations effectively at substantial computational cost. Generalised MMC is, therefore, best implemented in stochastic form.

Wandel and Lindstedt have developed and validated generalised MMC with velocity-like reference variables obtained from a stochastic binomial Langevin simulation (Wandel and Lindstedt 2013; Wandel and Lindstedt 2009; Wandel 2013). A comprehensive comparison of results for a turbulent mixing layer (Wandel and Lindstedt 2009) and the Sandia Flame E (Wandel and Lindstedt 2013) indicate good performance of the model.

Klimenko's initial model for MMC in the context of LES involved a single conditioning reference variable $\xi = \bar{\xi} + \xi''$, which emulates the stochastic mixture fraction, Z. Here $\bar{\xi} = \tilde{Z}_{LES}$ is the filtered LES mixture fraction field and ξ'' emulates the subfilter fluctuations of that mixture fraction that are modelled using multiple non-conditioning dissipation-like reference variables (similar to option (i) introduced above). This MMC-LES model would be suitable for a conventional stochastic Monte Carlo simulation, where there are many notional particles in each LES grid cell. Such an approach would come at a very large computational cost. An alternative much lower cost method based on a sparse stochastic implementation was subsequently developed (Cleary and Klimenko 2009, 2011; Cleary et al. 2009; Vo et al. 2017). In sparse methods, the number of notional particles to simulate the reacting scalar field is less than the number grid cells for the LES simulation of the flow field. At the larger scale separating mixing particles, the subgrid fluctuations ξ'' now play only a minor role and can be neglected. The model formulation remains much the same as Eqs. (15.19)–(15.22), except that Eq. (15.20) is replaced by.

$$d\xi_k^* = d\tilde{Z}_{LES}^* \tag{15.29}$$

For the mixing operation particles mix in pairs that are selected according to a minimisation of the square distance in an extended space comprised of ξ and x:

$$\hat{d}_{p,q}^2 = \sum_{i=1}^{3} \left(\sqrt{3} \frac{d_{x,i}^{p,q}}{r_m} \right) + \left(\frac{d_f^{p,q}}{f_m} \right) \tag{15.30}$$

Here, $d_{x,i}^{p,q}$ and $d_f^{p,q}$ are the distance between mixing particles in physical space and reference mixture fraction space, respectively, and r_m and f_m are characteristic scales in those spaces.

The advent of sparse methods and the use of non-Markov reference variables (i.e. in sparse MMC-LES the traced filtered mixture fraction from the LES replaces the stochastically modelled reference variable) has resulted in an extended interpretation of what constitutes generalised MMC. Here, we repeat verbatim the statements made in Cleary and Klimenko (2011):

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

- *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 (here, Eq. (15.20) or its replacement Eq. (15.29)) rather than by the surrogate mixing operator, S_I.*

Also to this effect, Sundaram et al. (2016) have list five propositions on the nature of generalised MMC.

15.3 Applications of MMC

Different versions of MMC have been used to simulate conditions ranging from non-premixed to premixed (including partially premixed) combustion regimes within the context of RANS and LES. In these models, a reference variable is used to imitate mixture fraction and/or progress variable. In deterministic MMC models, additional reference variables are used to imitate scalar dissipation and/or sensible enthalpy. A few examples, focusing particularly on the more recent cases, are reviewed in this section.

15.3.1 Deterministic MMC Applications

In deriving MMC for the first time Klimenko and Pope (2003) validated the deterministic version of the model against DNS data for the three stream mixing problem. Kronenburg and Cleary examined MMC for DNS cases of homogeneous, isotropic decaying turbulence using multiple reference variables (Kronenburg and Cleary (2008), Cleary and Kronenburg (2007a, b)); namely mixture fraction, normalised sensible enthalpy and scalar dissipation. The transient flame-phenomena, such as, extinction and reignition are captured to some extent. The first application of the deterministic MMC approach to laboratory jet diffusion flames with complex hydrocarbon chemistry is reported in Vogiatzaki et al. (2009a, b). A single reference variable was used to emulate the mixture fraction, and very good agreement with the experimental data may be observed. The most recent application of deterministic MMC is by Devaud et al. (2013) who implemented it into an LES

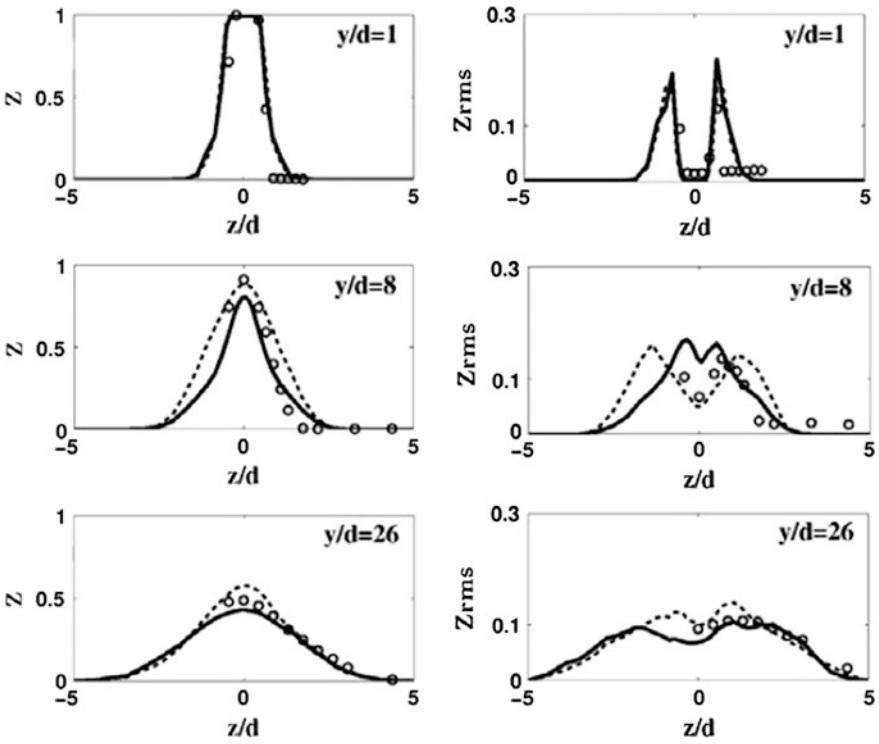

Fig. 15.2 Radial profile of mean mixture fraction and rms. Symbol represents experimental data, dashed lines LES solution and solid lines corresponds to MMC. Figure is from Devaud et al. (2013)

code to simulate a lifted jet diffusion flame in a vitiated coflow. They also used a single reference variable to emulate the subfilter distribution of mixture fraction. Figure 15.2 shows the time-averaged radial profiles of mixture fraction and its rms. There is overall good agreement with the experimental data.

15.3.2 Stochastic MMC Applications

As already mentioned, the first implementation of stochastic MMC was done by Wandel and Klimenko (2005) who validated it against the DNS data of Mitarai et al. (2003) for a homogeneous turbulent reacting flow with one-step irreversible chemistry. The first application to jet diffusion flames is reported in Vogiatzaki et al. (2011). The flame under consideration was the well-known Sandia flame D. In their formulation, they employed a single Markov reference variable mapped to the mixture fraction. Micro-mixing involved the interaction by exchange with the mean

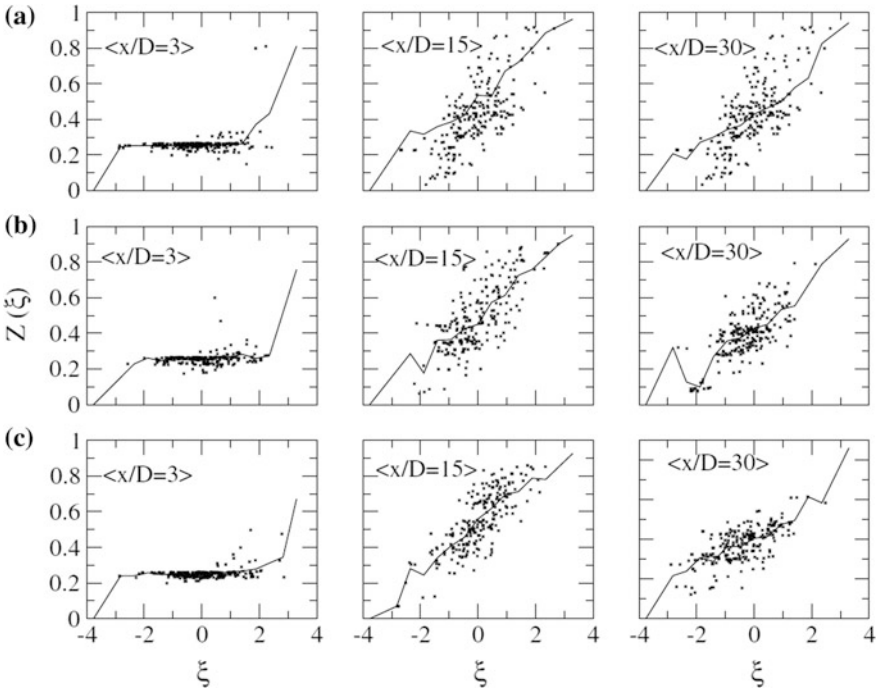

Fig. 15.3 Profiles of the mixture fraction at various axial locations over the reference space. **a** First row $\tau_{min} = \tau_D$ **b** Middle row $\tau_{min} = 0.7\tau_D$ **c** Bottom row $\tau_{min} = 0.5\tau_D$. Figure is from Vogiatzaki et al. (2011)

(IEM) mixing model (Dopazo and Obrien 1974). An additional minor dissipation timescale ($\tau_{\min}$) has been introduced within the MMC formulation that controls the fluctuations of the scalars around the conditional mean. Figure 15.3 shows the mixture fraction profiles in the reference space at different axial locations for three different minor timescales $\tau_{min} = \tau_D, 0.7\tau_D$ and $0.5\tau_D$, where τ_D is the physical dissipation timescale. It is evident that conditional fluctuations decrease with a decrease in the minor timescale. A similar observation can also be made for the reactive scalars, such as temperature and species mass fractions that are shown in Fig. 15.4. The MMC results with the three different values of τ_{min} are also compared with results from a conventional PDF-IEM simulations (i.e. without localisation of mixing in a reference space and, importantly, without the additional controlling parameter τ_{min}). While the MMC with $\tau_{min} = \tau_D$ produces reasonably accurate scatter plots the conventional PDF-IEM yields only very low levels of conditional fluctuations.

Subsequently, Vogiatzaki et al. (2015) investigated the sensitivity of stochastic MMC to different numbers of notional particles per grid cell and to different micro-mixing models. They tested $N_p =$ 20, 50 and 100 and both Curl's and IEM variants of MMC in RANS of Sandia Flame F. Figures 15.5 and 15.6 show scatter

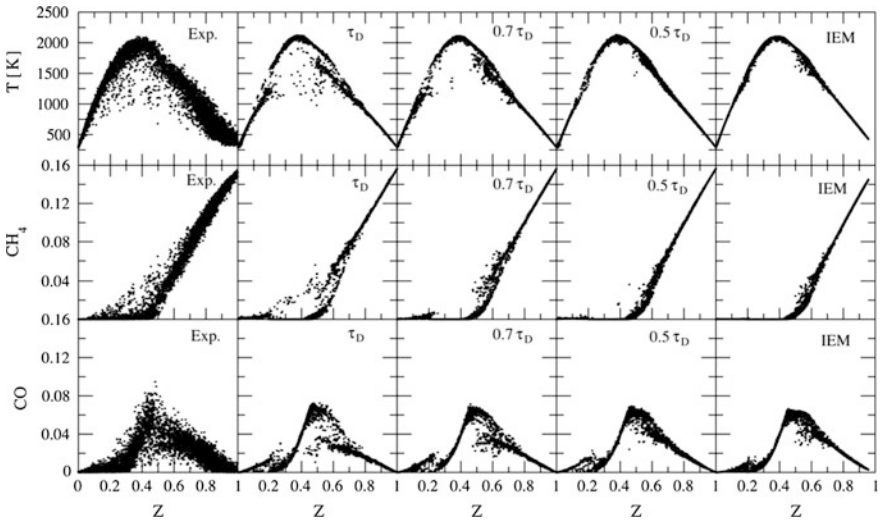

Fig. 15.4 Scatter plots of temperature, mixture fractions of CH_4, CO over the mixture fraction space at $x/D = 15$. Figure is from Vogiatzaki et al. (2011)

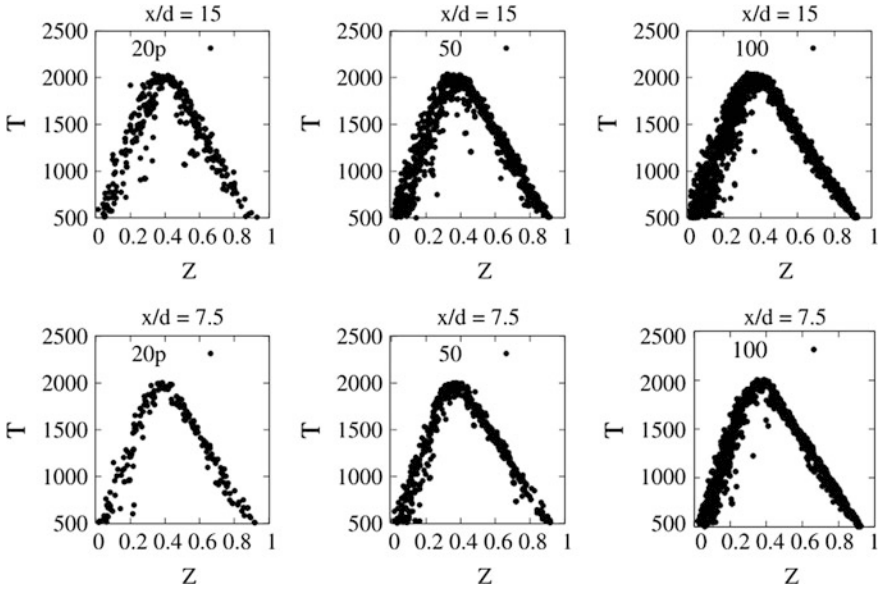

Fig. 15.5 Scatter plots of temperature over the mixture fraction space at $x/D = 7.5$ and 15 for MMC-IEM with three different particle number densities. Figure is from Vogiatzaki et al. (2015)

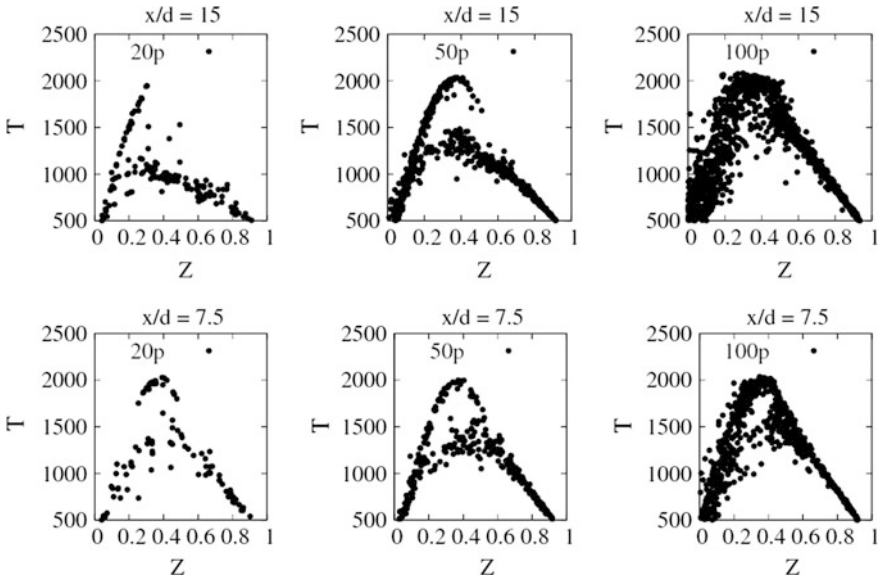

Fig. 15.6 Scatter plots of temperature over the mixture fraction space at $x/D = 7.5$ and 15 for PDF-IEM with three different particle number densities. Figure is from Vogiatzaki et al. (2015)

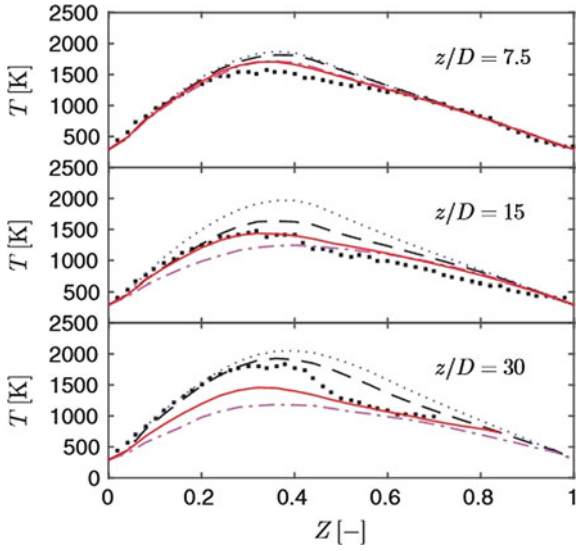

Fig. 15.7 Conditional temperature at different axial locations. Square symbols represent experimental data, red solid lines are PDF-Curls solutions, blue dotted lines are for MMC with $C_{min} = 0.25$, black dashed line for $C_{min} = 0.30$, pink dashed line for $C_{min} = 0.35$. Figure is from Straub et al. (2016)

plots of temperature versus mixture fraction for different N_p in both MMC-IEM and PDF-IEM simulations. The MMC method is noticeably less sensitive to a number of particles used per CFD cell with little difference in the results above $N_p = 50$ and even $N_p = 20$ is not much different.

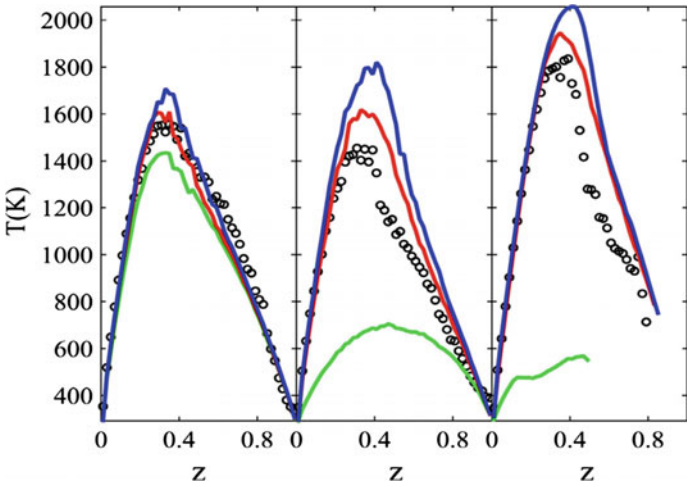

Fig. 15.8 Conditional temperature profiles at $x/D = 7.5$ (left), $x/D = 15$ (centre) and $x/D = 30$ (right). Blue, red and green lines correspond to target correlation parameters of $r_t = 0.948$, 0.935 and 0.912, respectively. Figure is from Varna et al. (2017)

Straub et al. (2016) also conducted stochastic MMC-RANS for Sandia Flame D-F to examine the effect of variation of the minor mixing timescale. Figure 15.7 represents the conditional temperature profiles of Sandia Flame F at three different axial locations. Results from a PDF-modified Curl's simulation are also included. $C_{\min} = 0.30$ gives the best agreement with the experimental data for Sandia Flame F and that value is close to that proposed by Wandel and Klimenko ($C_{\min} = 0.25$) for DNS of a homogenous reacting flow. Other values of $C_{\min}$ clearly show the underprediction ($C_{\min} = 0.35$) and overprediction ($C_{\min} = 0.25$) of conditional temperature (Wandel and Klimenko 2005). Readers should note that different definitions of $C_{\min}$ have been used in Straub et al. (2016) and Wandel and Klimenko (2005). Modified Curl's mixing model, which is known to overpredict the level of conditional fluctuations on account of the non-local nature of its mixing, fails to predict the flame reignition at $z/D = 30$.

Quite recently, Varna et al. (2017a, b) implemented a RANS-based stochastic MMC for the Sandia D–F series, where the static standard Gaussian reference variable proposed by Klimenko and Pope (2003) is replaced by a spatially and temporally evolving reference variable having the same mean and variance as the real mixture fraction while remaining stochastically independent of it. The adapted model is conceptually simpler than the original MMC formulation, but some terms are eliminated and the model does not directly account for the small-scale balance between diffusion and reaction. Consequently, the model overcomes the numerical instabilities found in the original formulation of MMC (Vogiatzaki et al. 2011). Figure 15.8 shows the conditional temperature profiles in Flame F for different values of the target correlation coefficient which corresponds to the correlation

between the reference and real mixture fractions and is linked to the ratio of the minor to major timescales.

15.3.3 Sparse MMC-LES Applications

Sparse MMC-LES is cost-effective in comparison to the conventional intensive stochastic simulations of the filtered density function. Using the Sandia flame series as a benchmark, Ge et al. (2013) demonstrated high-quality MMC-LES predictions are possible with as low as 1 Lagrangian particle per 27 Eulerian cells (1L/27E). Due to the significant reduction in the number of particles relative to intensive methods, sparse MMC-LES appears to be particularly useful in applications involving detailed chemical kinetics of complex fuels. Salehi et al. (2017) applied MMC-LES to the simulation of transient autoignition of n-dodecane under high pressure, engine relevant conditions. Figure 15.9 shows the change in vapour penetration length over time for a non-reacting case at 900 K for two threshold values of mixture fraction. The threshold value of mixture fraction ($Z_{th} = 0.1\%$) prescribed by engine combustion network (ECN) slightly overpredicts the penetration length after 0.5 ms. The other threshold value of mixture fraction used in simulations is more consistent with the experimental data. The ignition delay time and lift-off length for an autoigniting case are plotted in Fig. 15.10 for different values of the chamber ambient temperature and oxygen volume fraction. The ignition delay times and their trends with variations in the ambient conditions are satisfactorily predicted and the observed discrepancies are largely ascribed to the limitations of the available chemical mechanisms. While the results are less accurate, the lift of length trends are also predicted well. The results are comparable with the predictions of other turbulent combustion models as shown in Figs. 15.10d and f.

Sundaram et al. (2016) also tested the sparse MMC-LES method for a lifted flame series, specifically the case of a lifted hydrogen flame in a vitiated coflow and examined the sensitivity to the localisation parameter f_m in Eq. (15.30). The results

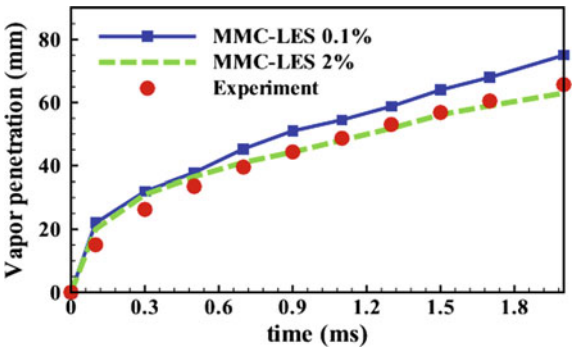

Fig. 15.9 Vapour penetration depth over time for two different definition of the vapour penetration length. Figure is from Salehi et al. (2017)

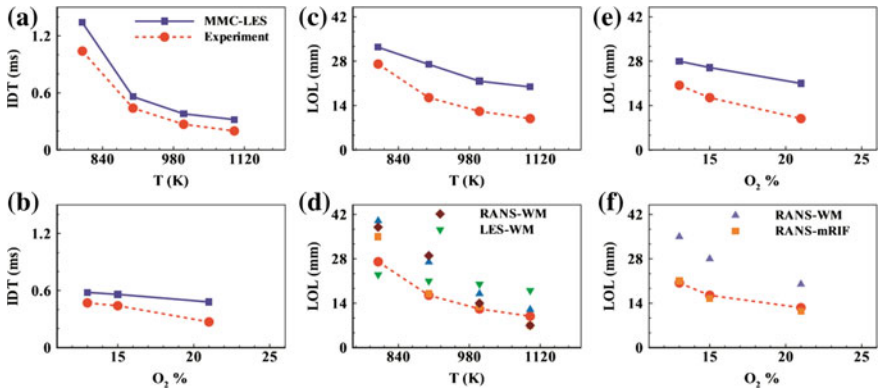

Fig. 15.10 Ignition delay time and lift-off length over ambient temperature and oxygen volume fraction (Salehi et al. 2017)

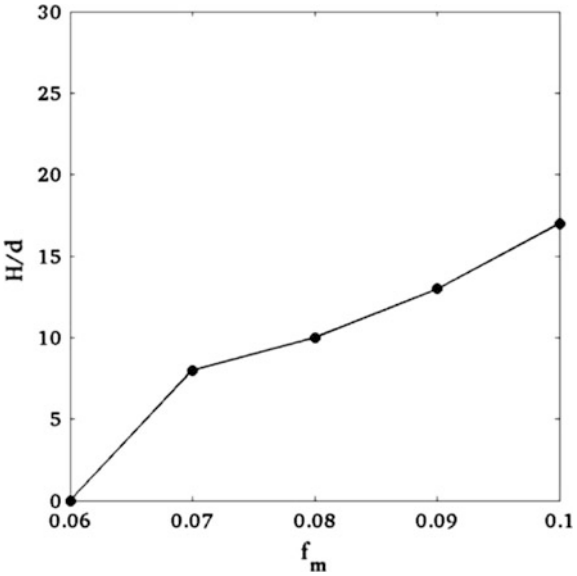

Fig. 15.11 Lift-off height variation with the change in localisation parameter f_m. Figure is from Sundaram et al. (2016)

are shown in Fig. 15.11 indicate that the lift-off height varies almost linearly with f_m and the $f_m = 0.08$ yields a good match with the experimentally observed lift-off value. This value of f_m is somewhat higher than the $f_m = 0.03$ that is suggested by previous studies of piloted jet flames (Ge et al. 2013).

Recently, Galindo et al. (2017) applied sparse MMC-LES to turbulent piloted flames with varying extent of inlet inhomogeneity exhibiting multimode combustion behaviour. The prevailing mode of combustion changes from premixed to non-premixed mode from the nozzle exit to downstream locations and also radially,

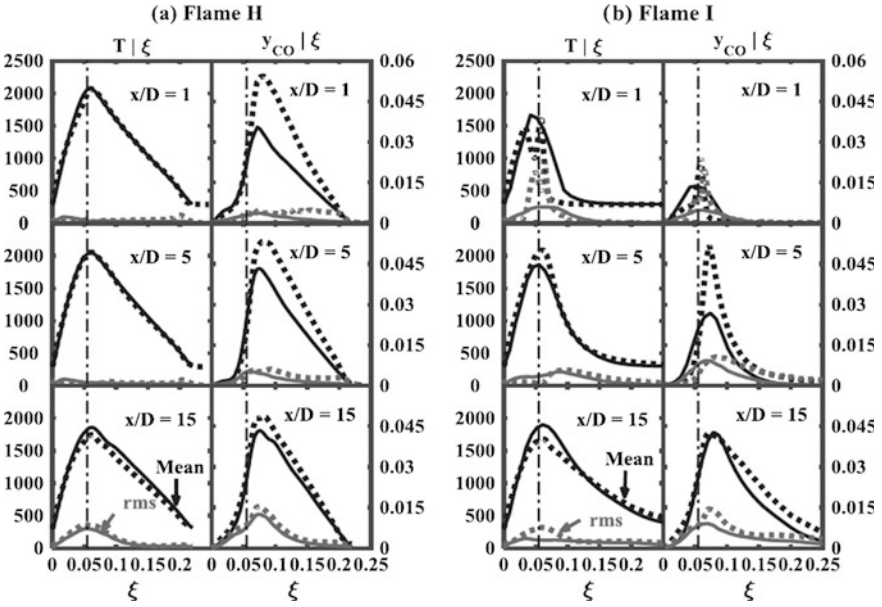

Fig. 15.12 Conditional mean and rms of temperature and CO mass fraction. **a** homogeneous inlet, **b** inhomogeneous inlet. Figure is from Galindo et al. (2017)

where a premixed flame was experimentally observed between the pilot and the main jet with a diffusion flame observed at greater radial locations. Using mixture fraction as the single reference variable, the modelling examined the extent to which the MMC-LES model is applicable to flames displaying the premixed flame-like structure close to the nozzle exit. The conditional profiles of mean and rms of temperature and CO mass fraction for both homogeneous (flame H) and inhomogeneous (flame I) inlet cases are shown below in Fig. 15.12. The conditional temperature statistics are very well predicted for the homogeneous case while the conditional mean of CO mass fractions is significantly underpredicted close to the nozzle exit but improves further downstream where good agreement with the data is observed. For the inhomogeneous inlet case, at $x/D = 1$, the model having only a mixture fraction like reference variable approached but could not completely capture the premixed flame structure. The accuracy of the predictions improves downstream where the combustion mode changes from premixed to non-premixed combustion.

In the past couple of years, some interesting applications of MMC-LES to particle and droplet synthesis processes in turbulent flows have been led by Kronenburg and co-workers (Neuber et al. 2017; Vo et al. 2017). Silica nanoparticle synthesis from silane in a temporal, counter-flowing, double shear layer is modelled using a reduced chemical mechanism of 23 species extending to a single solid state species (Vo et al. 2017). Differential diffusion is modelled in a simplified manner

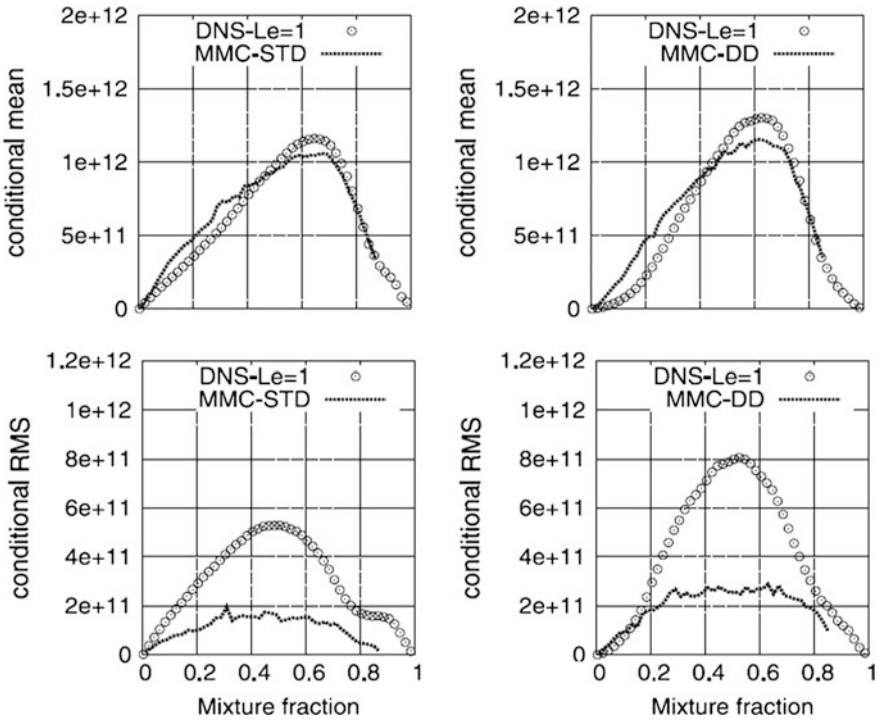

Fig. 15.13 Conditional mean and rms profiles for silica particle number density over mixture fraction. Left side represents results without differential diffusion and right side represents results with differential diffusion. Figure is from Vo et al. (2017)

through a diffusion coefficient weighted scaling of the mixing timescale for the solid silica species. Model predictions are compared to DNS data showing good agreement for the temporal evolution of the mixture fraction and the gaseous chemical species whose reactive timescales are short. The silica is a kinetically limited species with a much longer reaction timescale. As shown in Fig. 15.13 the conditional mean of silica particle number density is predicted quite well while the conditional rms is underpredicted by a large margin. The effects of differential diffusion are evident in both the DNS and MMC-LES with the latter correctly predicting the trend of increasing peak conditional silica number density when the effects of differential diffusion are included. The conditional rms trend is also predicted well when differential diffusion is added, although the quantitative disagreement with the DNS remains large.

Neuber et al. (2017) modelled nucleation and subsequent growth of dibutyl-phthalate (DBP) droplets in a turbulent jet. The droplet size distribution is accounted for by the inclusion of discrete droplet sections in the PDF definition such that the nonlinear interactions between turbulence and nucleation and growth

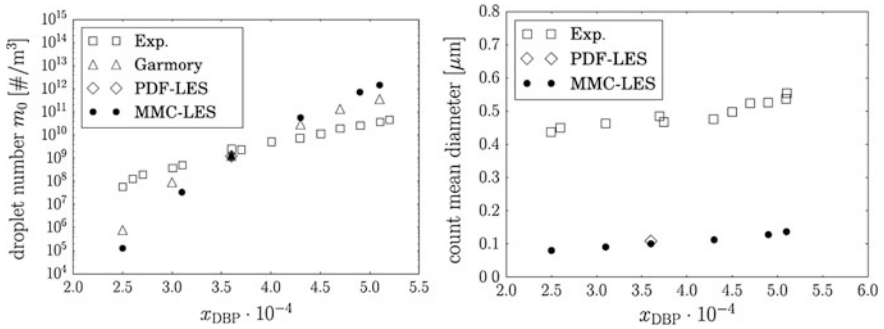

Fig. 15.14 Droplet number and count mean diameter over DBP loading. Exp (Gupta et al. 2011), Garmory and Mastorakos (2008), PDF-LES and MMC-LES (Neuber et al. 2017). Figure is from Neuber et al. (2017)

appear in the governing transport equations in closed form without need of additional filtering or modelling. Both sparse MMC-LES and conventional intensive LES-PDF simulations are compared to experimental data and are shown to produce almost identical results. On account of the sparse distribution of particles that is made possible by the localness of the mixing model, MMC-LES reduces the computational time by a factor of 9 in comparison to the LES-PDF simulations. Figure 15.14 shows the droplet number density and mean diameter at $x/D = 20$ for a range of dibutyl-phthalate (DBP) loadings. The droplet number predictions are quantitatively and qualitatively reasonable in comparison to the experimental data and are also consistent with the previous stochastic fields PDF simulations of Garmory and Mastorakos (2008). The droplet size predictions are significantly underpredicted by all reported models although it is mentioned that there are some reservations about the consistency of the experimental data.

15.3.4 MMC for Premixed Combustion

There are fundamental difficulties that are specific to the modelling of premixed flames using PDF-like methods. These are mainly due to the necessity of avoiding mixing across the flame front. Failure to properly account for localness of mixing in thin premixed flames leads to an inaccurate prediction of the flame propagation speed. Refining the grid in the region of the flame is possible but it comes at a very high-computational cost and consequently, alternative methods based on the artificial thickening of the flame to better match the computational grid have widespread popularity (Kuenne et al. 2011).

Following on from earlier work (Sundaram et al. 2015) on combustor modelling, Sundaram and Klimenko (2017) recently developed a general stochastic MMC approach for the premixed regime and explored the possibility of using different

types of reference variables whose job is to characterise the relative position of stochastic particles with respect to the flame front. These reference variables include the level set variable, a modified shadow position variable and a progress variable. The model which is finally suggested by the authors for further investigation combines the shadow position and progress variable in a two-stage mixing process that involves both intensive particle distributions (for flame front characterisation) and sparse particle distributions (for efficient computation of the detailed reactive species). Their simulation results for an idealised 1-D planar flame in the thin reaction zone regime with single step chemistry are shown in Fig. 15.15, where physical space is denoted by the symbol, x, the reference shadow position is denoted by the symbol, ξ, and the progress variable is denoted by ϕ. Figure 15.15a shows the mapping of the physical space with the reference space and it correctly produces very thin reaction zone in ξ space due to the localness of the first stage of mixing. Figures 15.15b and c show the progress variable in physical and reference spaces, respectively. In the physical space, significant scatter is observed while a thin flamelet-like solution is obtained in the reference space. By design, the model always produces the thin flame structure in reference space, whereas the degree of flame thickening in physical space is controlled in the model by a localisation parameter which can be adjusted to emulate the conditions that are observed in the real flame.

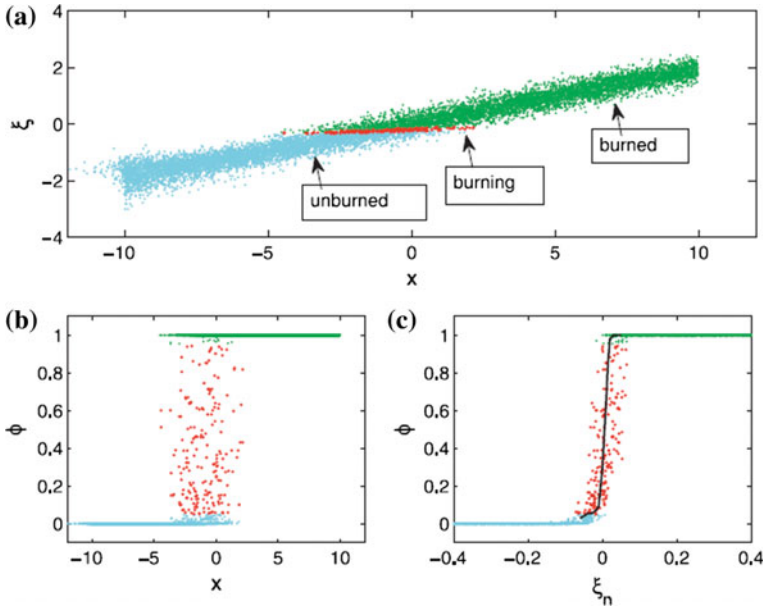

Fig. 15.15 Simulation result for 1-D planer flame with premixed MMC. **a** Mapping of reference space with physical space **b** particle distribution of progress variable in physical space and **c** particle distribution of progress variable in reference space. Figure is from Sundaram and Klimenko (2017)

15.4 Conclusions

This chapter provides an overview on the relatively new MMC approach to turbulent reacting flows. The basic concepts and theory of MMC along with recently published application are presented here in a condensed form. MMC is an attractive approach because it allows the coupling of different existing models into a single methodological framework through the use of a reference space and the concept of mapping functions. This allows the required extensibility for the modelling of certain terms which are otherwise complicated to close. The MMC model may be formulated both in deterministic and stochastic forms. In general, the deterministic framework of MMC is a natural extension of CMC while the stochastic MMC can be a complete joint PDF method. In the LES context, MMC has allowed the use of sparse distributions of notional Lagrangian particles which reduce cost and allow for, among other things, tractable computations of flames with complex chemistry. Within both the RANS and LES contexts, MMC has been demonstrated to be an accurate and computationally affordable approach. Model predictions are found to be sensitive to the minor dissipation timescale, and the literature suggests ways in which it can be formulated for accurate predictions of the conditional fluctuations. MMC is also proving useful for regimes other than non-premixed combustion and some recent applications to flames with inhomogeneous (partially premixed) inlets, premixed flames and particle and droplet synthesis have been reviewed here.

References

Brauner T, Jones WP, Marquis AJ (2016) LES of the cambridge stratified swirl burner using a sub-grid pdf approach. Flow Turbul Combust 96:965–985

Cao RR, Wang HF, Pope SB (2007) The effect of mixing models in PDF calculations of piloted jet flames. Proc Combust Inst 31:1543–1550

Celis C, da Silva LFF (2015) Lagrangian mixing models for turbulent combustion: review and prospects. Flow Turbul Combust 94:643–689

Chen HD, Chen SY, Kraichnan RH (1989) Probability-distribution of a stochastically advected scalar field. Phys Rev Lett 63:2657–2660

Cleary MJ, Klimenko AY (2009) A generalised multiple mapping conditioning approach for turbulent combustion. Flow Turbul Combust 82:477–491

Cleary MJ, Klimenko AY (2011) Multiple mapping conditioning: a new modelling framework for turbulent combustion. In: Echekki T, Mastorakos E (eds) Turbulent combustion modelling. advances, new trends and perspectives. Springer

Cleary M, Klimenko A (2011b) A detailed quantitative analysis of sparse-Lagrangian filtered density function simulations in constant and variable density reacting jet flows. Phys Fluids 23:115102

Cleary MJ, Kronenburg A (2007a) Multiple mapping conditioning. For extinction and reignition in turbulent diffusion flames. Proc Combust Inst 31:1497–1505

Cleary M, Kronenburg A (2007b) 'Hybrid' multiple mapping conditioning on passive and reactive scalars. Combust Flame 151:623–638

Cleary MJ, Klimenko AY, Janicka J, Pfitzner M (2009) A sparse-Lagrangian multiple mapping conditioning model for turbulent diffusion flames. Proc Combust Inst 32:1499–1507

Devaud CB, Stankovic I, Merci B (2013) Deterministic multiple mapping conditioning (MMC) applied to a turbulent flame in large eddy simulation (LES). Proc Combust Inst 34:1213–1221

Dopazo C, Obrien EE (1974) Approach to autoignition of a turbulent mixture. Acta Astronaut 1:1239–1266

Galindo S, Salehi F, Cleary MJ, Masri AR (2017) MMC-LES simulations of turbulent piloted flames with varying levels of inlet inhomogeneity. Proc Combust Inst 36:1759–1766

Garmory A, Mastorakos E (2008) Aerosol nucleation and growth in a turbulent jet using the stochastic fields method. Chem Eng Sci 63:4078–4089

Ge Y, Cleary MJ, Klimenko AY (2013) A comparative study of Sandia flame series (D-F) using sparse-Lagrangian MMC modelling. Proc Combust Inst 34:1325–1332

Girimaji SS (1992) A mapping closure for turbulent scalar mixing using a time-evolving reference field. Phys Fluids a-Fluid Dyn 4:2875–2886

Girimaji SS (1993) A study of multiscalar mixing. Phys Fluids a-Fluid Dyn 5:1802–1809

Gupta A, Ifeacho P, Schulz C, Wiggers H (2011) Synthesis of tailored WO3 and WOx ($2.9 < x < 3$) nanoparticles by adjusting the combustion conditions in a H2/O2/Ar premixed flame reactor. Proc Combust Inst 33:1883–1890

Janicka J, Kolbe W, Kollmann W (1979) Closure of the transport-equation for the probability density-function of turbulent scalar fields. J Non-Equilib Thermodyn 4:47–66

Klimenko AY (2005) Matching conditional moments in PDF modelling of nonpremixed combustion. Combust Flame 143:369–385

Klimenko A (2007) On simulating scalar transport by mixing between Lagrangian particles. Phys Fluids 19:031702

Klimenko A (2009a) Lagrangian particles with mixing. I. Simulating scalar transport. Phys Fluids 21:065101

Klimenko A (2009b) Lagrangian particles with mixing. II. Sparse-Lagrangian methods in application for turbulent reacting flows. Phys Fluids 21:065102

Klimenko AY, Bilger RW (1999) Conditional moment closure for turbulent combustion. Prog Energy Combust Sci 25:595–687

Klimenko A, Cleary MJ (2010) Convergence to a model in sparse-Lagrangian FDF simulations. Flow Turbul Combust 85:567–591

Klimenko AY, Pope SB (2003) The modeling of turbulent reactive flows based on multiple mapping conditioning. Phys Fluids 15:1907–1925

Kronenburg A (2004) Double conditioning of reactive scalar transport equations in turbulent nonpremixed flames. Phys Fluids 16:2640–2648

Kronenburg A, Cleary MJ (2008) Multiple mapping conditioning for flames with partial premixing. Combust Flame 155:215–231

Kuenne G, Ketelheun A, Janicka J (2011) LES modeling of premixed combustion using a thickened flame approach coupled with FGM tabulated chemistry. Combust Flame 158:1750–1767

Lindstedt RP, Vaos EM (2006) Transported PDF modeling of high-reynolds-number premixed turbulent flames. Combust Flame 145:495–511

Mastorakos E, Bilger R (1998) Second-order conditional moment closure for the autoignition of turbulent flows. Phys Fluids 10:1246–1248

Mitarai S, Riley JJ, Kosaly G (2003) A Lagrangian study of scalar diffusion in isotropic turbulence with chemical reaction. Phys Fluids 15:3856–3866

Neuber G, Kronenburg A, Stein OT, Cleary MJ (2017) MMC-LES modelling of droplet nucleation and growth in turbulent jets. Chem Eng Sci 167:204–218

Pei YJ, Hawkes ER, Kook S, Goldin GM, Lu TF (2015) Modelling n-dodecane spray and combustion with the transported probability density function method. Combust Flame 162:2006–2019

Pope SB (1985) Pdf methods for turbulent reactive flows. Prog Energy Combust Sci 11:119–192

Pope SB (1991) Mapping closures for turbulent mixing and reaction. Theoret Comput Fluid Dyn 2:255–270

Salehi F, Cleary MJ, Masri AR, Ge Y, Klimenko AY (2017) Sparse-Lagrangian MMC simulations of an n-dodecane jet at engine-relevant conditions. Proc Combust Inst 36:3577–3585

Straub C, De S, Kronenburg A, Vogiatzaki K (2016) The effect of timescale variation in multiple mapping conditioning mixing of PDF calculations for Sandia Flame series D–F. Combust Theory Modell, 1–19. https://doi.org/10.1080/13647830.2016.1191677

Subramaniam S, Pope SB (1998) A mixing model for turbulent reactive flows based on Euclidean minimum spanning trees. Combust Flame 115:487–514

Sundaram B, Klimenko AY (2017) A PDF approach to thin premixed flamelets using multiple mapping conditioning. Proc Combust Inst 36:1937–1945

Sundaram B, Klimenko A, Cleary M, Maas U (2015) Prediction of NO x in premixed high-pressure lean methane flames with a MMC-partially stirred reactor. Proc Combust Inst 35:1517–1525

Sundaram B, Klimenko AY, Cleary MJ, Ge YP (2016) A direct approach to generalised multiple mapping conditioning for selected turbulent diffusion flame cases. Combust Theor Model 20:735–764

Varna A, Cleary MJ, Hawkes ER (2017a) A multiple mapping conditioning mixing model with a mixture-fraction like reference variable. Part 2: RANS implementation and validation against a turbulent jet flame. Combustion and Flame (2017). https://doi.org/10.1016/j.combustflame.2017.03.017

Varna A, Cleary MJ, Hawkes ER (2017b) A multiple mapping conditioning mixing model with a mixture-fraction like reference variable. Part 1: Model derivation and ideal flow test cases. Combust Flame. https://doi.org/10.1016/j.combustflame.2017.03.016

Veynante D, Vervisch L (2002) Turbulent combustion modeling. Prog Energy Combust Sci 28:193–266

Vo S, Kronenburg A, Stein OT, Cleary MJ (2017a) Multiple mapping conditioning for silica nanoparticle nucleation in turbulent flows. Proc Combust Inst 36:1089–1097

Vo S, Stein OT, Kronenburg A, Cleary MJ (2017b) Assessment of mixing time scales for a sparse particle method. Combust Flame 179:280–299

Vogiatzaki K (2010) Stochastic and deterministic multiple mapping conditioning for jet flames, Imperial College London

Vogiatzaki K, Kronenburg A, Cleary MJ, Kent JH (2009a) Multiple mapping conditioning of turbulent jet diffusion flames. Proc Combust Inst 32:1679–1685

Vogiatzaki K, Cleary MJ, Kronenburg A, Kent JH (2009b) Modeling of scalar mixing in turbulent jet flames by multiple mapping conditioning. Phys Fluids 21

Vogiatzaki K, Kronenburg A, Navarro-Martinez S, Jones WP (2011) Stochastic multiple mapping conditioning for a piloted, turbulent jet diffusion flame. Proc Combust Inst 33:1523–1531

Vogiatzaki K, Navarro-Martinez S, De S, Kronenburg A (2015) Mixing modelling framework based on multiple mapping conditioning for the prediction of turbulent flame extinction. Flow Turbul Combust 95:501–517

Wandel AP (2013) Conditional dissipation of scalars in homogeneous turbulence: closure for MMC modelling. Combust Theor Model 17:707–748

Wandel AP, Klimenko AY (2005) Testing multiple mapping conditioning mixing for Monte Carlo probability density function simulations. Phys Fluids 17

Wandel AP, Lindstedt RP (2009) Hybrid binomial Langevin-multiple mapping conditioning modeling of a reacting mixing layer. Phys Fluids 21

Wandel AP, Lindstedt RP (2013) Hybrid multiple mapping conditioning modeling of local extinction. Proc Combust Inst 34:1365–1372