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MMC MODELLING AND FLUCTUATIONS OF THE SCALAR DISSIPATION

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ABSTRACT
The fluctuating properties of the scalar dissipation, that are known to significantly affect turbulent combustion processes, are modelled on the basis of the Multiple Mapping Conditioning (MMC) method.

INTRODUCTION
The Multiple Mapping Conditioning (MMC) approach [1] to turbulent non-premixed combustion is characterised by dividing all fluctuations of the reactive species into major and minor. The major fluctuations are treated with assistance of the stochastic reference variables while the minor fluctuations are either neglected (conditional MMC) or treated by conventional mixing models (probabilistic MMC) [1, 2]. In its treatment of the major fluctuations, the MMC approach is compliant with all mixing criteria (such as linearity, independence, localness, boundness, etc). The major fluctuations are restricted to a certain manifold whose dimension is determined by the dimension of the reference space[3]. Generally, the concept of MMC can be characterised as a combination of Conditional Moment Closure (CMC) [4] and the PDF (Probability Density Function) models [5, 6]. The PDF models and closures involve Mapping Closure (MP) [7, 8, 9], EMST [10], IECM or IEM (stands for Interactions by Exchange with the Mean or with the Conditional Mean) [6], Curl's [11] and other PDF models.

The MMC reference variables may represent turbulent fluctuations of different physical nature. In simplified versions of MMC, the reference variables simulate the mixture-fraction-type fluctuations (although it should be noted that the reference variables are not identical to the actual variables that represent the simulated mixture fractions). The two-stream mixing has a single mixture fraction and a single mixture-fraction-like reference variable; the three-stream mixing problem involves two independent mixture fractions and two independent mixture-fraction-like reference variables and so on [1]. In order to distinguish various versions of MMC models, we can specify the version of the model as "arguments" of MMC. The symbol "Z" is used to emphasise the use of the mixture-fraction-like reference variables (while "2Z" indicates the use of two mixture-fraction-like reference variables and the bold "$\mathbf{Z}$" can be used to indicate an unspecified number of multiple mixture-fraction-like reference variables). In probabilistic MMC [2], a conventional mixing model is used to treat minor fluctuations and the type of the model can also be added to the acronym MMC. Neglecting the minor fluctuations (that is in line with the conditional methods) is logical to indicate by the "CMC" argument. For example, performance MMC(2Z) is evaluated in [1] for three-stream mixing; asymptotic analysis of MMC(Z,IECM) is conducted in [12]. Performance of MMC(Z,CMC) in a self-similar mixing layer is investigated in [13].

In the present work, we consider the two-stream (1Z) problem but explicitly introduce additional reference variables that simulate the fluctuations generated by the scalar dissipation (the idea of using the scalar dissipation as a conditioning variable in CMC equations was pioneered in [14]). This version of MMC can be denoted by MMC(Z,$\mathbf{N}$,CMC) or MMC(Z,$\boldsymbol{\chi}$,CMC) depending on which variable is used to denote the scalar dissipation but, in the rest of the paper we abbreviate this notation to MMC($\mathbf{N}$). Although this model is compliant with the general MMC principles, a specific analysis is needed to ensure compliance of the model with the known properties of mixing and to determine the unknown parameters of the model related to the additional reference variables.

GENERAL MMC FORMULATION
Deterministic Formulation
The conditional MMC is specified by the following equations [1]

$$\frac{\partial \bar{Y}_I}{\partial t} + \mathbf{U}\cdot\boldsymbol{\nabla}\bar{Y}_I + A_k\frac{\partial \bar{Y}_I}{\partial \xi_k} - B_{kl}\frac{\partial^2 \bar{Y}_I}{\partial \xi_k \partial \xi_l} = \bar{W}_I, \tag{1}$$

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

where sums are taken over repeated indices; the small indices $i, j, k, ... = 0, 1, ..., n_r$ run over the reference variables $\xi_0, \xi_1, ...$; the capital indices $I, J, ... = 0, 1, ..., n_s$ run over the variables modelling the reactive species $\bar{Y}_0, \bar{Y}_1, ...$; $\bar{\rho}$ models the average density and the joint PDF $P_\xi = P(\boldsymbol{\xi}; \mathbf{x}, t)$ of the stochastic reference variables $\xi_0^*, \xi_1^*, ...$ is required to satisfy equation (2). Equation (1) is solved for $\bar{Y}_I = \bar{Y}_I(\boldsymbol{\xi}; \mathbf{x}, t)$ while the stochastic values $\bar{Y}_I^* = \bar{Y}_I(\boldsymbol{\xi}^*; \mathbf{x}, t)$ represent a model for physical reactive scalars whose joint PDF $P_Y = P(\mathbf{Y}; \mathbf{x}, t)$ is shown to satisfy the conventional scalar PDF equation [1]

$$\frac{\partial \bar{\rho} P_Y}{\partial t} + \nabla \cdot (\mathbf{u}_Y \bar{\rho} P_Y) + \frac{\partial \bar{W}_I \bar{\rho} P_Y}{\partial Y_I} +$$

$$+ \frac{\partial^2 N_{IJ} \bar{\rho} P_Y}{\partial Y_I \partial Y_J} = 0 \tag{3}$$

with

$$N_{ij} \equiv \left\langle N_{ij}^\circ (\boldsymbol{\xi}^*, \mathbf{x}, t) \, | \mathbf{Y} \right\rangle, \; N_{IJ}^\circ \equiv B_{kl} \frac{\partial \bar{Y}_I}{\partial \xi_k} \frac{\partial \bar{Y}_J}{\partial \xi_l}$$

$$\mathbf{u}_Y \equiv \langle \mathbf{U} (\boldsymbol{\xi}^*, \mathbf{x}, t) \, | \mathbf{Y} \rangle, \; \bar{W}_I \equiv W_I(\bar{\mathbf{Y}}) \tag{4}$$

defining a consistent model for the conditional scalar dissipation N_{ij} tensor, the conditional velocity $\mathbf{u}_Y$ and the chemical reaction rate. The MMC methodology allows for the PDF P_ξ to be selected as standard Gaussian provided the MMC coefficients are given by

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

$$A_k = -\frac{\partial B_{kl}}{\partial \xi_l} + B_{kl} \xi_l + a_k \tag{5}$$

where $a_k(\mathbf{x}, t) \equiv \bar{\rho}^{-1} \boldsymbol{\nabla} \cdot \left(\bar{\rho} \mathbf{U}_k^{(1)} \right)$.

Equations (1) and (2) allow for the conservative formulation of the MMC equations given by

$$\frac{\partial \bar{\rho} P_\xi \bar{Y}_I}{\partial t} + \boldsymbol{\nabla} \cdot \left(\mathbf{U} \bar{\rho} P_\xi \bar{Y}_I \right) + \frac{\partial A_k^\circ \bar{\rho} P_\xi \bar{Y}_I}{\partial \xi_k} -$$

$$- \frac{\partial^2 B_{kl} \bar{\rho} P_\xi \bar{Y}_I}{\partial \xi_k \partial \xi_l} = \bar{W}_I P_\xi \tag{6}$$

Stochastic Formulation

The MMC model can be equivalently formulated in terms of the stochastic Ito equations

$$d\mathbf{x}^* = \mathbf{U} (\boldsymbol{\xi}^*, \mathbf{x}^*, t) \, dt, \tag{7}$$

$$d\xi_k^* = A_k^\circ (\boldsymbol{\xi}^*, \mathbf{x}^*, t) \, dt + b_{kl} (\boldsymbol{\xi}^*, \mathbf{x}^*, t) \, dw_l^*, \tag{8}$$

$$dY_I^* = (W_I^* + S_I^*) \, dt, \tag{9}$$

where

$$\langle S_I^* | \boldsymbol{\xi}, \mathbf{x} \rangle = 0 \tag{10}$$

$$A_k^\circ \equiv A_k + \frac{2}{P_\xi} \frac{\partial B_{kl} P_\xi}{\partial \xi_l}, \; 2B_{kl} = b_{ki} b_{li} \tag{11}$$

The link between the stochastic and deterministic versions of the models is given by the relationship $\bar{Y}_I(\boldsymbol{\xi}, \mathbf{x}, t) \equiv \langle Y_I^* | \boldsymbol{\xi}, \mathbf{x} \rangle$. It should be noted that in conditional MMC (which is mainly considered in the present work) $\bar{Y}_I$ is treated as a model for the scalars while, in probabilistic MMC, Y_I^* simulates the scalar values [1, 2]. The operator S_I is an arbitrary operator that must satisfy $\langle S_I^* | \boldsymbol{\xi}, \mathbf{x} \rangle = 0$ and some other conditions [1]. The purpose of this operator is to keep Y_I^* close to $\bar{Y}_I^*$.

Replacement of the Variables

The reference variables $\boldsymbol{\xi}^*$ can be replaced by a new set of reference variables $\tilde{\boldsymbol{\xi}}^* = \tilde{\boldsymbol{\xi}}(\boldsymbol{\xi}^*, \mathbf{x}, t)$ and the MMC equations remain valid with the use of new variables but the coefficients in the equations have to take the new values [2]

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

$$\tilde{B}_{ij} = B_{kl} \frac{\partial \tilde{\xi}_i}{\partial \xi_k} \frac{\partial \tilde{\xi}_j}{\partial \xi_l} \tag{12}$$

$$\tilde{A}_k^\circ \equiv \tilde{A}_k + \frac{2}{P_{\tilde{\xi}}} \frac{\partial \tilde{B}_{kl} P_{\tilde{\xi}}}{\partial \tilde{\xi}_l}, \; 2\tilde{B}_{kl} = \tilde{b}_{ki} \tilde{b}_{li}$$

$$P_{\tilde{\xi}} = P_\xi \det \left(\frac{\partial \tilde{\xi}_i}{\partial \xi_k} \right)^{-1}, \; \tilde{U} = U \tag{13}$$

The replacement of the variables represents a mathematically equivalent transformation that does not alter the actual closure: P_Y, N_{ij} and equation (3) remain the same.

DISSIPATION-LIKE REFERENCE VARIABLES

Modelling of the fluctuating properties of the scalar dissipation can be performed within the MMC framework. In this version of the model, MMC($\mathbf{N}$), we assume that ξ_0 is a mixture-fraction-like variable and specify the diffusion coefficients by

$$B_{00} = \bar{B}_{00}(\mathbf{x}, t) \Phi(\breve{\boldsymbol{\xi}}; \mathbf{x}, t), \; B_{0\alpha} = B_{\alpha 0} = 0$$

$$\Phi = \exp(\phi), \quad \phi = c_\alpha \xi_\alpha + c_0 \tag{14}$$

where $B_{\alpha\beta} = B_{\alpha\beta}(\mathbf{x}, t)$ and the reference variables $\breve{\boldsymbol{\xi}} = \{\xi_1, ..., \xi_{n_r}\}$ are used to simulate the fluctuations of the scalar dissipation ($\breve{\boldsymbol{\xi}}$ does not include ξ_0 which is used as a mixture-fraction-like variable). The Greek indices run only over $1, 2, ..., n_r$ (while $i, j, k, ...$ run over $0, 1, 2, ..., n_r$). The variables $\breve{\boldsymbol{\xi}}^*$ are assumed to be Gaussian to ensure that the distribution of Φ^* is log-normal. Without restricting the generality of our consideration, we can require that $\breve{\boldsymbol{\xi}}^*$ are standard Gaussian (uncorrelated with zero mean and unit dispersion) since the new standard Gaussian variables can be always introduced by replacing $\breve{\boldsymbol{\xi}}$ by their linear combinations and adjusting coefficients c_α in $\phi = c_\alpha \xi_\alpha + c_0$. We select $c_0 = -c_\alpha c_\alpha / 2$ and normalise Φ so that the mean value of $\Phi^* \equiv \Phi(\breve{\boldsymbol{\xi}}^*; \mathbf{x}, t)$ is unity:

$$\langle \Phi^* \rangle = \exp\left(c_0 + \frac{c_\alpha c_\alpha}{2}\right) = 1, \tag{15}$$

$$\left\langle (\Phi^*)^2 \right\rangle = \exp(2c_0 + 2c_\alpha c_\alpha) = \exp(c_\alpha c_\alpha) \tag{16}$$

With unitary transformations of ξ_α, we can always transform $B_{\alpha\beta}$ into a diagonal form $B_{\alpha\beta} = \delta_{\alpha\beta}/\tau_\beta$ and preserve the standard Gaussian distribution for ξ_α. Here, we introduce characteristic times τ_β for the inverses of the diagonal values of $B_{\alpha\beta}$ and also denote $\tau_0 \equiv 1/B_{00}$ and $\bar{\tau}_0 \equiv 1/\bar{B}_{00}$. With the use of (5) we obtain

$$A_\alpha = \xi_\alpha \delta_{\alpha\beta}/\tau_\beta + a_\alpha \tag{17}$$

Each of the variables ξ_α represents a distinctive mode of the scalar dissipation fluctuations characterised by its characteristic time τ_α. Note that the term $A^-_{\alpha\beta}\xi_\beta$ with an arbitrary antisymmetric matrix $A^-_{\alpha\beta} = -A^-_{\beta\alpha}$ can be added to (17). This matrix can be responsible for interactions of the modes and for complex and repeated roots. Although we neglect $A^-_{\alpha\beta}$ in the present consideration, $A^-_{\alpha\beta}$ can be potentially useful for more accurate modelling of the scalar dissipation properties.

In order to investigate the major properties of MMC($\mathbf{N}$), it is convenient to introduce the new reference variables $\tilde{\xi}_0 = \bar{Y}_0 = Z$ and $\tilde{\xi}_\alpha = \xi_\alpha$. Here and further in the paper the zeroth scalar Y_0 is denoted by Z and assumed to represent the mixture fraction: $W_0 = 0$. The new diffusion and drift coefficients are determined by (12)

$$\tilde{B}_{00} = \frac{1}{\tau_i}\frac{\partial Z}{\partial \xi_i}\frac{\partial Z}{\partial \xi_i} = N^\circ_{00}, \; \tilde{B}_{0\alpha} = \tilde{B}_{\alpha 0} = \frac{\delta_{\alpha\beta}}{\tau_\alpha}\frac{\partial Z}{\partial \xi_\beta},$$

$$\tilde{A}_0 = \bar{W}_0 = 0, \; \tilde{A}_\alpha = A_\alpha, \; \tilde{B}_{\alpha\beta} = B_{\alpha\beta} \tag{18}$$

The MMC equation takes the form

$$\frac{\partial \bar{Y}_I}{\partial t} + \mathbf{U}\cdot\boldsymbol{\nabla}\bar{Y}_I - N^\circ_{00}\frac{\partial^2 \bar{Y}_I}{\partial Z^2} - 2\tilde{B}_{0\alpha}\frac{\partial^2 \bar{Y}_I}{\partial Z \partial \xi_\alpha} +$$

$$+\frac{1}{\tau_\alpha}\left(\xi_\alpha \frac{\partial \bar{Y}_I}{\partial \xi_\alpha} - \frac{\partial^2 \bar{Y}_I}{\partial \xi_\alpha^2}\right) = \bar{W}_I \tag{19}$$

where the equation coefficients should be expressed as functions of Z, $\breve{\boldsymbol{\xi}}$, $\mathbf{x}$ and t. The value $N^*_{00} = N^\circ_{00}(\boldsymbol{\xi}^*; \mathbf{x}^*, t)$ models the instantaneous Lagrangian properties of the scalar dissipation while N°_{00} is specified by

$$N^\circ_{00} = \tilde{B}_{00} = B_{kl}\frac{\partial Z}{\partial \xi_k}\frac{\partial Z}{\partial \xi_l} = N_0 + N_1 \tag{20}$$

where $N_0 = \bar{N}_0 \Phi(\breve{\boldsymbol{\xi}}; \mathbf{x}, t)$ and

$$\bar{N}_0 \equiv \bar{B}_{00}\frac{\partial Z}{\partial \xi_0}\frac{\partial Z}{\partial \xi_0}, \quad N_1 \equiv B_{\alpha\beta}\frac{\partial Z}{\partial \xi_\alpha}\frac{\partial Z}{\partial \xi_\beta} \tag{21}$$

COMPLIANCE WITH THE MAJOR LIMITS

In this section, we examine compliance of the model with the fast chemistry [15] and the flamelet [16] limits.

Fast Chemistry Limit

Assuming that the characteristic reaction time scale τ_W is much smaller than all of τ_i (including, of course, the characteristic dissipation time τ_0), we note that, to the leading order of the analysis, $Y_I = Y_I(Z)$ represents the chemical equilibrium state for Y_I. Substitution of $Y_I = Y_I(Z)$ into (19) results in

$$-N^\circ_{00}\frac{\partial^2 \bar{Y}_I}{\partial Z^2} = \bar{W}_I \tag{22}$$

Flamelet Limit

Derivation of the flamelet equation from (19) is also not difficult. We assume that the width ΔZ of the reaction zone is so small that the characteristic time $\tau_Z = \Delta Z^2 / N^\circ_{00}$ is much smaller than any of τ_i: $\tau_Z/\tau_i \sim \varepsilon^2 \ll 1$. Following [16], we can use $z = (Z - Z_{\rm st})/\varepsilon$ in the reaction zone and retain the unsteady term in the flamelet equation by introducing a very fast time $\tilde{t} = t/\tau_Z$. The leading terms result in

$$\frac{\partial \bar{Y}_I}{\partial t} - N^\circ_{00}\frac{\partial^2 \bar{Y}_I}{\partial Z^2} = \bar{W}_I \tag{23}$$

COMPLIANCE WITH CMC

In the previous section, we demonstrated the consistency of the MMC model with fast or small-scale asymptotes – the fast chemistry and flamelet limits. In this section, our goal is to examine the performance of the model in the opposite case when the characteristic observation time τ_c is much longer compared to the time scales τ_α characterising the scalar dissipation. This case is studied in CMC and its analysis is more difficult compared to the derivations of the previous section. We assume that all of the times τ_α are small and can be represented by $\tau_\alpha = \varepsilon\tilde{\tau}_\alpha$ where ε is a small parameter.

Asymptotic Evaluation of the Scalar Dissipation

In this section we analyse the equation for the simulated mixture fraction and obtain a simplified asymptotic expression for the simulated mixture fraction dissipation N_{00}°. The equation for the mixture fraction takes the form

$$\frac{\partial Z}{\partial t} + \mathbf{U}\cdot\boldsymbol{\nabla} Z + A_0\frac{\partial Z}{\partial \xi_0} - B_{00}\frac{\partial^2 Z}{\partial \xi_0^2} +$$

$$+\frac{1}{\varepsilon\tilde{\tau}_\alpha}\left(\xi_\alpha\frac{\partial Z}{\partial \xi_\alpha} - \frac{\partial^2 Z}{\partial \xi_\alpha^2}\right) = 0 \qquad (24)$$

This equation is obtained from (1) and, with $\bar{W}_I$ on its right-hand side, is valid for any Y_I. The solution of this equation is given by

$$Z = Z(\xi_0, \mathbf{x}, t) + O(\varepsilon) \qquad (25)$$

Equations (20) and (20) specify the simulated dissipation of the mixture fraction. The value of $N_1 \sim \varepsilon^2/\tau_\alpha \sim \varepsilon$ can be neglected in comparison with $N_0 \sim 1$ while N_0 is given by $N_0 = \bar{N}_0\Phi(\breve{\boldsymbol{\xi}};\mathbf{x},t)$ where $\bar{N}_0 = \bar{N}_0(\xi_0, \breve{\boldsymbol{\xi}};\mathbf{x},t)$. If we take into account (25), we can write $\bar{N}_0 = \bar{N}_0(\xi_0;\mathbf{x},t) + O(\varepsilon)$ or substitute $\xi_0 = \xi_0(Z;\mathbf{x},t)$ and obtain $\bar{N}_0 = \bar{N}_0(Z;\mathbf{x},t)$ to the leading order. Hence,

$$N_{00}^{\circ} = \bar{N}_0(Z;\mathbf{x},t)\Phi(\breve{\boldsymbol{\xi}};\mathbf{x},t) + O(\varepsilon) \qquad (26)$$

and the leading order approximations (25) & (26) are implied in the other equations presented below. Now we need to assess the conditional mean and variance of the scalar dissipation $N_0^* = N_0(Z^*, \breve{\boldsymbol{\xi}}^*;\mathbf{x},t)$ where $Z^* = Z(\xi_0^*, \mathbf{x}, t)$ is stochastically independent of ξ_α^*. The averages of N_0^* over all $\breve{\boldsymbol{\xi}}^*$ conditioned on $Z^* = Z(\xi_0^*, \mathbf{x}, t) = Z$ are given by

$$\langle N_0^* | Z\rangle = \bar{N}_0(Z, \mathbf{x}, t) \qquad (27)$$

$$\left\langle (N_0^*)^2 | Z\right\rangle = \bar{N}_0^2(Z,\mathbf{x},t)\exp\left(c_\alpha c_\alpha\right) \qquad (28)$$

Thus, the sum $c_\alpha c_\alpha$ is determined by the level of fluctuations of the scalar dissipation and depends on the Reynolds number.

Asymptotic Expansions

In this subsection, we examine the equations for the other species which are convenient to write in the form of (19)

$$\frac{\partial \bar{Y}}{\partial t} + \mathbf{U}\cdot\boldsymbol{\nabla}\bar{Y} - N_0\frac{\partial^2 \bar{Y}}{\partial Z^2} - 2\tilde{B}_{0\alpha}\frac{\partial^2 \bar{Y}}{\partial Z\partial \xi_\alpha} +$$

$$+\frac{1}{\varepsilon\tilde{\tau}_\alpha}\left(\xi_\alpha\frac{\partial \bar{Y}}{\partial \xi_\alpha} - \frac{\partial^2 \bar{Y}}{\partial \xi_\alpha^2}\right) = \bar{W} \qquad (29)$$

Note that $\tilde{B}_{0\alpha} \sim 1$ due to (18) and $\partial Z/\partial\xi_\alpha \sim \varepsilon$. Since the equations for all species $\bar{Y}_I$ are the same we omit the index "I" and represent solution in the form of the asymptotic expansion $\bar{Y} = Y_0 + \varepsilon Y_1 + \ldots$. The leading order term satisfies

$$\frac{1}{\tilde{\tau}_\alpha}\left(\xi_\alpha\frac{\partial Y_0}{\partial \xi_\alpha} - \frac{\partial^2 Y_0}{\partial \xi_\alpha^2}\right) = 0 \qquad (30)$$

and has a solution given by $Y_0 = Y_0(Z, \mathbf{x}, t)$. Note that the PDF $P_{\breve{\xi}}$ — the standard Gaussian joint PDF of $\xi_1, ..., \xi_{n_r}$ — satisfies the equation

$$\frac{1}{\tilde{\tau}_\alpha}\left(-\frac{\partial \xi_\alpha P_{\breve{\xi}}}{\partial \xi_\alpha} - \frac{\partial^2 P_{\breve{\xi}}}{\partial \xi_\alpha^2}\right) = 0 \qquad (31)$$

The next order equation takes the form

$$\frac{1}{\tilde{\tau}_\alpha}\left(\xi_\alpha\frac{\partial Y_1}{\partial \xi_\alpha} - \frac{\partial^2 Y_1}{\partial \xi_\alpha^2}\right) = \Psi \qquad (32)$$

where

$$-\Psi \equiv \frac{\partial \bar{Y}_0}{\partial t} + \mathbf{U}\cdot\boldsymbol{\nabla}\bar{Y}_0 - N_0\frac{\partial^2 Y_0}{\partial Z^2} - \bar{W}$$

By adding up equation (32) multiplied by $P_{\breve{\xi}}$ and equation (31) multiplied by Y_1 we obtain

$$\frac{1}{\tilde{\tau}_\alpha}\left(-\frac{\partial \xi_\alpha Y_1 P_{\breve{\xi}}}{\partial \xi_\alpha} - \frac{\partial^2 Y_1 P_{\breve{\xi}}}{\partial \xi_\alpha^2}\right) = \Psi P_{\breve{\xi}} \qquad (33)$$

Integrating the last equation over all ξ_α yields the solvability condition

$$\int_\infty \Psi P_{\breve{\xi}} d\breve{\boldsymbol{\xi}} = \mathbf{0} \qquad (34)$$

that results in

$$\frac{\partial \bar{Y}_0}{\partial t} + \mathbf{U}\cdot\boldsymbol{\nabla}\bar{Y}_0 - \bar{N}_0\frac{\partial^2 Y_0}{\partial Z^2} - \bar{W} = 0 \qquad (35)$$

and

$$\Psi = \Theta\left(\exp\left(c_\alpha\xi_\alpha + c_0\right) - 1\right), \quad \Theta \equiv \bar{N}_0\frac{\partial^2 Y_0}{\partial Z^2} \qquad (36)$$

Here we assume that $U = U(\xi_0, x, t)$ and $a_\alpha = 0$. If U is dependent on ξ_α then another term with $U_\alpha^{(1)}\xi_\alpha$, should be added to Ψ. The analysis of this term is not conducted in the present work but it is clear that, since MMC is a fully PDF compliant method, the velocity/scalar correlations should be modelled correctly provided $\mathbf{u}_Y$ represents an adequate model for the physical velocity conditioned on all scalars. Equation (35) indicates consistency with the first order CMC equation that is, generally, expected in MMC but determining the coefficients of the model would need examining the conditional variance.

Asymptotic Solution

The solution of (33) with Ψ specified by (36) is given by

$$\frac{Y_1 P_{\breve{\xi}}}{\Theta} = f(\breve{\boldsymbol{\xi}}) \equiv \int_0^\infty \left(\psi(\breve{\boldsymbol{\xi}}, \tilde{t}^\circ) - \psi(\breve{\boldsymbol{\xi}}, \infty)\right) dt^\circ \tag{37}$$

where

$$\psi(\breve{\boldsymbol{\xi}}, \tilde{t}^\circ) \equiv P_{\breve{\xi}}(\breve{\boldsymbol{\xi}} - \breve{\boldsymbol{\xi}}^\circ(\tilde{t}^\circ))$$

represents a standard Gaussian distribution shifted to the point $\xi^\circ_\alpha(\tilde{t}^\circ) \equiv c_\alpha \exp(-\tilde{t}^\circ/\tilde{\tau}_a)$ (no sum is taken over α). The location of the point depends on the time-like parameter $\tilde{t}^\circ$ that should not be confused with the time t. The solution f is written as $f(\breve{\boldsymbol{\xi}})$, although f may depend on Z, $\mathbf{x}$ or t through the parameters of (33). We note that

$$\xi_\alpha(\breve{\boldsymbol{\xi}}, \tilde{t}^\circ) + \frac{\partial \psi(\breve{\boldsymbol{\xi}}, \tilde{t}^\circ)}{\partial \xi_\alpha} = \xi^\circ_\alpha(\tilde{t}^\circ)\psi(\breve{\boldsymbol{\xi}}, \tilde{t}^\circ)$$

and that $d\xi^\circ_\alpha = -(\xi^\circ_\alpha/\tilde{\tau}_\alpha)dt^\circ$ with no sum taken over α. Evaluation of the line integral between the points O (given by $\xi_\alpha = 0$) and C (given by $\xi_\alpha = c_\alpha$)

$$\frac{1}{\tilde{\tau}_\alpha}\left(\frac{\partial f}{\partial \xi_\alpha} + \frac{\partial^2 f}{\partial \xi_\alpha^2}\right) = \int_0^\infty \frac{\xi^\circ_\alpha(\tilde{t}^\circ)}{\tilde{\tau}_\alpha} \frac{\partial \psi(\breve{\boldsymbol{\xi}}, \tilde{t}^\circ)}{\partial \xi_\alpha} dt^\circ =$$

$$= \int_{\mathrm{O}}^{\mathrm{C}} \frac{\partial P_{\breve{\xi}}(\xi_\alpha - \xi^\circ_\alpha)}{\partial \xi_\alpha} d\xi^\circ_\alpha = P_{\breve{\xi}}(\breve{\boldsymbol{\xi}}) - P_{\breve{\xi}}(\breve{\boldsymbol{\xi}} - \mathbf{c}) =$$

$$= \left(1 - \exp\left(c_\alpha \xi_\alpha + c_0\right)\right) P_{\breve{\xi}}(\breve{\boldsymbol{\xi}}) = -\frac{\Psi}{\Theta} P_{\breve{\xi}}(\breve{\boldsymbol{\xi}}) \tag{38}$$

proves that $\Theta f(\breve{\boldsymbol{\xi}})$ represents a solution for $Y_1 P_{\breve{\xi}}$. Although the term $\psi(\breve{\boldsymbol{\xi}}, \infty) = P_{\breve{\xi}}(\breve{\boldsymbol{\xi}})$ disappears in this sequence of transformations, it is needed to ensure convergence of the integral in (37) at $\tilde{t}^\circ \to \infty$. Note that an arbitrary constant can be added to Y_1. We determine this constant by the condition that $\langle Y_1^* | Z \rangle = 0$, where $\langle Y_1^* | Z \rangle = \left\langle Y_1(Z, \breve{\boldsymbol{\xi}}^*, \mathbf{x}, t) \right\rangle$. Integration of (37) over all $\breve{\boldsymbol{\xi}}$ demonstrates that this conditions is satisfied by $Y_1 = \Theta f(\breve{\boldsymbol{\xi}})/P_{\breve{\xi}}$.

Evaluating the Generation Term

Since $Y_0 = Y_0(Z, \mathbf{x}, t)$ and $\langle Y_1^* | Z \rangle = 0$, we note that $Q = Y_0$ and $Y' = \varepsilon Y_1$ in the decomposition $Y = Q + Y'$ where $Q = \langle Y^* | Z \rangle$ ("prime" denotes the fluctuations with respect to the conditional means). Since MMC is a fully PDF compliant method, the conditional variance equation for $K \equiv \left\langle (Y')^2 | Z \right\rangle$ should involve the generation terms $G_W = 2\langle Y'W' | Z \rangle$, $G_U = -2\langle Y'\mathbf{U}' | Z \rangle \cdot \boldsymbol{\nabla} Q$ and $G_N = 2\langle N_0' Y' | Z \rangle \partial^2 Q/\partial Z^2$ and the dissipation term (see [4, 17, 18, 19] for details). Here, we focus on the term G_N whose analysis is most difficult. With asymptotic representations obtained in the previous subsections, this term can be approximated by

$$G_N \approx 2\int_\infty \Psi Y' P_{\breve{\xi}} d\breve{\boldsymbol{\xi}} = 2\Theta \int_\infty \Psi f(\breve{\boldsymbol{\xi}}) d\breve{\boldsymbol{\xi}} =$$

$$= 2\Theta \int_0^\infty \int_\infty \psi(\breve{\boldsymbol{\xi}}, \tilde{t}^\circ) \Psi d\breve{\boldsymbol{\xi}} d\tilde{t}^\circ = 2\Theta^2 \tau_N \tag{39}$$

where

$$\tau_N \equiv \int_0^\infty \left(\exp\left(c_\alpha^2 \exp\left(-\frac{t^\circ}{\tau_\alpha}\right)\right) - 1\right) dt^\circ \tag{40}$$

the sum is taken over repeated α and a new time-like variable $t^\circ = \varepsilon \tilde{t}^\circ$ is introduced. Since $\phi^*(t) = c_\alpha \xi^*_\alpha(t) + c_0$ represents a Gaussian process (while $\Phi^* = \exp(\phi^*)$ in (14) is log-normal), the correlation function of $\Phi^*(t)$ given by

$$R(\Delta t) = \langle \Phi^{*\prime}(t) \Phi^{*\prime}(t + \Delta t) \rangle = \tag{41}$$

$$\langle \exp\left(\phi^*(t) + \phi^*(t + \Delta t)\right) \rangle - 1 = \exp(r(\Delta t)) - 1$$

where $\Phi^{*\prime}(t) \equiv \Phi^*(t) - 1$ and another "logarithmic" correlation function $r(\Delta t) \equiv \left\langle \phi^{*\prime}(t) \phi^{*\prime}(t + \Delta t) \right\rangle$, $\phi^{*\prime}(t) \equiv c_\alpha \xi^*_\alpha(t)$ are used in the equation. The correlation $r(\Delta t)$ can be easily evaluated since $\xi^*_\alpha(t)$ represents a superposition of independent Orstein-Ulhenbeck stochastic processes with the characteristic times τ_α: $r(t) = c_\alpha^2 \exp(-t/\tau_\alpha)$. The equation for the generation term G_N takes the form

$$G_N = 2\bar{N}_0^2 \left(\frac{\partial^2 Q}{\partial Z^2}\right)^2 \tau_N \tag{42}$$

where

$$\tau_N \equiv \int_0^\infty \langle \Phi^{*\prime}(0) \Phi^{*\prime}(t^\circ) \rangle \, dt^\circ \tag{43}$$

and $\Phi^*(t) = N_0^*/\bar{N}_0$. Note that this value for G_N coincides with the CMC theoretical prediction for this term [17] obtained on the basis of the "corrected" Kolmogorov theory of turbulence.

SELECTING THE MMC(N) PARAMETERS

The parameters $\bar{N}_0$, c_α and τ_α of the MMC($\mathbf{N}$) model are to be selected to match the mean values of the mixture fraction dissipation and its fluctuating properties. The proper choice for the coefficients c_α and τ_α should match not only the variance of the dissipation but also the Lagrangian correlations of the dissipation. More reference dissipation-like variables would allow for a better match of the required characteristics. Note that the fluctuating properties of the dissipation are Reynolds-dependent.

Although consistency with CMC conditional fluctuations generations can be achieved by matching only a single parameter, τ_N, we can consider mixing processes whose characteristic scales are τ_m are within the range of τ_α. With respect to the fast dissipation fluctuations $\tau_\beta \ll \tau_m$ the MMC($\mathbf{N}$) model would act as a CMC-like model while for the slow fluctuations $\tau_\gamma \gg \tau_m$ the MMC($\mathbf{N}$) model would behave more like the Fast Chemistry or Flamelet models. Thus the consistency of the integral τ_N should also be provided for any selected group of the fast modes. In other words, we require that the whole Lagrangian correlation function should be matched as closely as it possible for the given number of the reference variables.

CONCLUSIONS

The present work introduces a more complex version of MMC: MMC($\mathbf{N}$). In addition to the standard MMC mixture-fraction-like reference variable(s), this version of the model has several dissipation-like reference variables used to simulate the Lagrangian stochastic properties of the scalar dissipation. In addition to the general properties of MMC models, the model is shown to be consistent with the Fast Chemistry and Flamelet limits as well as the major features of the first and second order CMC equations. The model can be expected to simulate regimes with intermediate time scales laying between the areas of CMC and Flamelet applicability.

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