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Multiple mapping conditioning in homogeneous reacting flows

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Abstract

Multiple mapping conditioning (MMC) is used to model local extinction and reignition phenomena in homogeneous, isotropic decaying turbulence. It is recognized that mixture fraction alone is not sufficient to account for turbulent scalar fluctuations and that more than one reference variable needs to be introduced. We introduce a second reference variable with a dual character: the second variable is a dissipation-like variable that emulates the intermittent behaviour of scalar dissipation and it is therefore the cause for local extinction in our modelling. However,the second variable is also used to match the scalar variance of a reaction progress variable to ensure consistency in temperature flucutations of the MMC model and Direct Numerical Simulations. The resulting model provides a (fully) closed formulation for the modelling of local extinction and re-ignition events and predictions of the joint probability distribution of mixture fraction and sensible enthalpy, of reactive species and of the global conversion rates are good and clear improvments over conventional mixture fraction based methods that use mixture fraction as the only conditioning paramenter.

Introduction

One of the major challenges for turbulent combustion modelling is the accurate description of the turbulence-chemistry interactions that can determine chemical conversion rates and flame stability. The chemical source term may be strongly affected by turbulence, but usually appears in unclosed form in the averaged scalar transport equations and needs modelling. Computational methods for non-premixed combustion can be based on the mixture fraction concept where turbulent fluctuations of the reactive scalars are linked to the turbulent fluctuations of mixture fraction. The conditional moment closure (CMC) model [12] is one of these approaches. Here, transport equations for the reactive species conditionally averaged on the mixture fraction, Z, are solved. Often, the fluctuations around the conditional means are small and the reaction term can easily be closed using first moments. CMC has been applied to a variety of flames [21, 8, 6, 18] with some success.

The applicability of first order closures is, however, limited to flames where fluctuations around the conditional mean are small. This is certainly not given in flames with local extinction and re-ignition where a strong dependence on mixture fraction ceases to exist and the flame structure would need to be described by at least two variables and their joint PDF: the mixture fraction and a suitably defined reaction progress variable. Kronenburg [14] showed that fluctuations of reactive scalars correlate well with fluctuations of mixture fraction and normalised sensible enthalpy, $\hat{h}_s$, in flames with moderate to significant extinction and re-ignition and that double conditioning leads to accurate first order closures of the chemical source term. Double conditioning approaches have, however, a major shortcoming: the closures of the doubly conditioned dissipation terms and of the joint PDF of sensible enthalpy and mixture fraction. Presumed β-PDFs for the conditional sensible enthalpy, $P(\hat{h}_s|Z)$, may be acceptable approximations, however, the computation of the conditional variance of sensible enthalpy,$\langle \hat{h}_s''^2 \mid Z\rangle$, suffers from inacurate modelling often based on laminar flamelet assumptions. In addition, accurate models for doubly conditioned scalar dissipation do not exist.

Klimenko and Pope [13] suggested multiple mapping conditioning (MMC) for turbulent reacting flows. MMC is a generalized mapping closure that shares some characteristics with joint PDF [19] and CMC methods and both, stochastic and deterministic implementations are possible [11]. Turbulent fluctuations (and species) are divided into "major" and "minor" groupings. The fluctuations of the major scalars are not restricted and they are modelled using a set of stochastic reference variables. In deterministic MMC minor fluctuations are not permitted and the minor scalars can therefore fluctuate only jointly with the major scalars which is equivalent to a low-dimensional manifold in scalar space that is allowed to vary with time and space. Therefore, deterministic MMC(Z), where mixture fraction is the only major scalar, is equivalent to CMC(Z) when the latter is combined with generalised mapping closure to ensure consistency between the PDF for Z and its dissipation. Here and in the remainder of the paper, the terms in the brackets following the acronyms MMC or CMC indicate the conditioning scalars. In MMC, functional dependencies between a reference space with a known turbulence distribution and the physical composition space are sought and the number of the major scalars, $n_{\rm maj}$, therefore determines the dimension of the reference space.

Different implementations of MMC have been applied to cases of extinction and reignition in homogeneous, isotropic, decaying turbulence [24, 3, 2]. Wandel and Klimenko [24] used probabilistic MMC with one-step chemistry and a single reference variable with some success. Cleary and Kronenburg [3] use a single mixture-fraction-like reference variable with four-step chemistry and scalar dissipation fluctuations that cause local extinction were modelled via up to three dissipation-like reference variables [11]. Unfortunately, agreement with DNS data was far from being perfect, and the complexity and computational demands due to the introduction of four conditioning variables may not be justified. Crucial for the failure to predict extinction and re-ignition events accurately is -as in the case of CMC(Z,N), see reference [1]- the weak correlation between the chemical source term (or temperature) and scalar dissipation during re-ignition. In contrast to MMC(Z,N), MMC with reference variables for mixture fraction and sensible enthalpy, MMC($Z,\hat{h}_s$), gives excellent predictions of all major species and captures the degree and timing of extinction and re-ignition rather well. However, MMC($Z,\hat{h}_s$) does not account for the physical mechanism that is the driving force for extinction to occur: the scalar dissipation fluctuations. MMC($Z,\hat{h}_s$) does not generate fluctuations around the conditional mean and conditional fluctuations must be imposed. In other words, if all reactive scalars are initialized as function of mixture fraction, the

reactive scalars will remain functions of mixture fraction. These functions can vary with time and space, but no conditional fluctuations will be generated and MMC would therefore be equivalent to first order CMC(Z). This led to a hybrid approach where a shape for the conditional PDF was presumed and an additional transport equation for the conditional variance of sensible enthalpy needed to be solved [2]. The major advantage of 'hybrid' MMC($Z,\hat{h}_s$) over CMC($Z,\hat{h}_s$) is therefore the implicit closure of the doubly conditioned dissipation terms, however, uncertainties with respect to the modelling of the joint PDF remain.

The introduction of an MMC model with reference variables for mixture fraction, scalar dissipation and sensible enthalpy might be considered as the next logical step, but this approach will still fail in generating fluctuations in sensible enthalpy space. Instead, it needs to be recognised that scalar dissipation fluctuations and the generation of fluctuations in sensible enthalpy space are linked and need to be correlated. In the next section we will present a modification of MMC($Z,\hat{h}_s$) where fluctuations with respect to means conditioned on the mixture fraction are generated within the model by attributing a 'dual' character to a reference variable. The second reference variable is dissipation-like, it however represents sensible enthalpy. We then give a brief description of the DNS database that is used for the validation of the model. Finally, the performance of the implicit closures for the joint PDF, for the doubly conditioned dissipation of mixture fraction and sensible enthalpy and for the conditional variances are assessed.

Multiple mapping conditioning

The MMC transport equation for the evolution of the mapping function, $\mathbf{X}(\xi)$, is given by [13]

$$\frac{\partial X_I}{\partial t}+\mathbf{U}\cdot\nabla X_I+A_k\frac{\partial X_I}{\partial \xi_k}-B_{kl}\frac{\partial^2 X_I}{\partial \xi_k\partial \xi_l}=W_I. \qquad (1)$$

The upper case subscript I denotes all scalars (major and minor), the lower case subscripts k and l are for the major scalars only and the vector ξ represents the reference space. We emphasise that a single equation governs the evolution of mapping functions for all scalars of interest and no differentiation is made for major or minor scalars. The solution of equation (1) ensures that the joint PDF of $\mathbf{X}(\xi)$ satisfies the PDF transport equation of the joint PDF of all scalars, P_ϕ. Note that minor fluctuations are omitted, minor scalars are therefore conditionally averaged on major scalars and Klimenko and Pope [13] showed that the solution of equation (1) satisfies the joint PDF transport equation for the major scalars and the CMC transport equations for the minor scalars.

First order closure of the conditionally averaged chemical reaction term, $W_I=W_I(\xi)$, follows from the omission of the minor fluctuations and closures for the MMC coefficients of velocity, drift and diffusion ($\mathbf{U}$, A_k and B_{kl}) are obtained through necessary consistency with the joint reference space PDF transport equation

$$\frac{\partial\bar{\rho}\bar{P}_\xi}{\partial t}+\nabla\cdot\left(\mathbf{U}\bar{\rho}\bar{P}_\xi\right)+\frac{\partial A_k\bar{\rho}\bar{P}_\xi}{\partial\xi_k}+\frac{\partial^2 B_{kl}\bar{\rho}\bar{P}_\xi}{\partial\xi_k\partial\xi_l}=0. \qquad (2)$$

The coefficients can be determined for any assumed form of the reference PDF. For simplicity, we use stationary Gaussian PDFs with zero mean and unity variance and the coefficients can then be obtained from

$$\mathbf{U}=\mathbf{U}(\xi;\mathbf{x},t)=\mathbf{U}^{(0)}+\mathbf{U}_k^{(1)}\xi_k \qquad (3)$$

$$A_k=-\frac{\partial B_{kl}}{\partial\xi_l}+B_{kl}\xi_l+\frac{1}{\bar{\rho}}\nabla\cdot\left(\bar{\rho}\mathbf{U}_k^{(1)}\right) \qquad (4)$$

$$\mathbf{U}^{(0)}=\widetilde{\mathbf{v}} \qquad (5)$$

$$\mathbf{U}_k^{(1)}\langle\xi_k^* X_i^*\rangle=\widetilde{\mathbf{v}'\phi_i'}. \qquad (6)$$

In the above $\mathbf{v}$ is the flow velocity, the asterisk denotes stochastic quantities and the term in angular brackets is the ensemble mean. The reader is referred to Klimenko and Pope [13] for more details on the derivation of equation (1) and on the constraints that govern the form of the MMC coefficients.

The key to successful MMC modelling is the correct selection of the diffusion coefficients B_{kl} and $\mathbf{U}_k^{(1)}$. In homogeneous turbulence $\mathbf{U}_k^{(1)}\equiv 0$, and B_{kl} is the only parameter that can be chosen in the present study to match scalar statistics with DNS. The diffusion coefficients in equation (1) are related to the Favre averaged scalar dissipation tensor by

$$\left\langle B_{kl}\frac{\partial X_i}{\partial\xi_k}\frac{\partial X_j}{\partial\xi_l}\right\rangle=\widetilde{N}_{ij}. \qquad (7)$$

Klimenko [9, 11] suggested the use of dissipation-like variables to emulate the effects of scalar dissipation fluctuations that are crucial for the modelling of extinction and re-ignition events. Scalar dissipation fluctuations are expected to have a log-normal distribution and their effect on the evolution of scalar quantities can be approximated by modelling the diffusion coefficient of the mixture fraction reference variable as

$$B_{11}=\bar{B}_{11}\varphi(\xi_2;\mathbf{x},t). \qquad (8)$$

Here, ξ_1 represents mixture fraction space and ξ_2 represents the dissipation-like variable. The function

$$\varphi=exp(c_\alpha\xi_2-c_\alpha^2/2) \qquad (9)$$

describes the fluctuations of B_{11} around its mean value $\bar{B}_{11}$. Since the reference variable ξ_2 is normally distributed, B_{11} will have a log-normal distribution with the mean $\bar{B}_{11}$. The second moment of φ is

$$\langle(\varphi)'^2\rangle=exp(c_\alpha c_\alpha)-1. \qquad (10)$$

Following Klimenko [9], the instantaneous mixture fraction scalar dissipation is related to its conditional mean by $N_{11}\approx\langle N_{11}\mid\eta\rangle\varphi$ which gives

$$c_\alpha c_\alpha=\ln\left(\frac{\langle N_{11}'^2\mid\eta\rangle}{\langle N_{11}\mid\eta\rangle^2}+1\right). \qquad (11)$$

It has been pointed out above that the validity of the source term closure in equation (1) requires small fluctuations of the minor scalars with respect to the n_{maj}-dimensional manifold. It has been shown previously [14] that fluctuations around the conditional averages are small if the conditioning scalars are mixture fraction and sensible enthalpy while they are relatively large if reactive species are conditioned on mixture fraction and scalar dissipation. The dilemma is clear: it is desirable to have ξ_2 represent sensible enthalpy, while we would also need ξ_2 to represent a dissipation-like variable to generate fluctuations around the (singly) conditioned mean. These two requirements do not have to be exclusive. It is important to realize that equation (7)

determines which quantity is represented by the reference variable. Matching of the diffusion coefficient B_{kl} with the dissipation $\widetilde{N}_{ij}$ ensures the correct level of (unconditional) scalar fluctuations of scalars i and j. Any reference variable ξ_2 may adopt the character of a dissipation-like variable if B_{11} is modelled by equation (8). The physical quantity that is represented by ξ_2 is irrelevant. We can now exploit the strong negative correlation between conditional temperature fluctuations and fluctuations in scalar dissipation during the extinction process. Large values for N will lead to low temperatures due to the large strain imposed on the burning flamelet. We therefore propose the following modelling for the diffusion coefficients B_{kl}:

$$B_{11} = \overline{B}_{11}\exp(c_\alpha\xi_2 - c_\alpha^2/2) \quad (12)$$

$$B_{12} = \overline{B}_{12} \quad (13)$$

$$B_{22} = \overline{B}_{22}, \quad (14)$$

where the overbar denotes averaged values that can be obtained from equation (7). Note that the averaged values are by definition independent of ξ_i while the exponential dependency affects the averages for the gradients in ξ_1-space that need to be computed for equation (7). The correlation between dissipation and temperature fluctuations decreases with increasing degree of extinction and $c_\alpha \to 0$ for complete extinction. A simple correlation function, f_{corr}, that describes the degree of extinction can be based on the mean sensible enthalpy (or temperature) at stoichiometric and we employ $f_{corr} = -\langle\hat{h_s} \mid \eta = Z_{st}\rangle$. The parameter c_α is therefore modelled as

$$c_\alpha = f_{corr}\ln\left(\frac{\langle N_{11}'^2 \mid \eta\rangle}{\langle N_{11} \mid \eta\rangle^2} + 1\right)^{1/2}. \quad (15)$$

As in reference [2], the scalar field for this specific MMC model is $\phi = \{Z, \hat{h}_s, Y_1, Y_2, ..., Y_{n_s}\}$ where $\hat{h}_s = \int_{T_o}^{T} c_p dT / h_{s,\max}$ is the normalized sensible enthalpy and n_s is the number of chemical species considered. The sample space is $\psi = \{\eta, \zeta, y_1, y_2, ..., y_{n_s}\}$ where η and ζ are the sample space variables for the two major species Z and $\hat{h}_s$ and lower-case y_α are used for the minor scalars. The reference space has two dimensions with ξ_1 and ξ_2 emulating the turbulent fluctuations of Z and $\hat{h}_s$ respectively. All scalars are initialized in $\xi_1 - \xi_2$-space as described in [2].

Numerical simulations

Modelling results are compared to DNS of hydrocarbon combustion in homogeneous, isotropic, decaying turbulence. The DNS database is identical to DNS described in Kronenburg and Papoutsakis [16] and used for validation in references [3, 2]. The velocity and scalar fields are solved using a pseudo-spectral method implemented by Kerr [5] and the turbulence field can be characterised by an initial Taylor Reynolds number of $Re_\lambda^0 = 54$, an initial integral length scale of $l_0 = 1.11$ and a corresponding time scale of $\tau_0 = 1.08$. All quantities are non-dimensionalized. Non-premixed combustion where fuel and oxidizer are segregated initially, will be simulated. The mixture fraction field is initialized following Mell *et al.* [17], and all reactive scalars are then initialized as functions of mixture fraction where the functional dependence is obtained from independent flamelet computations with a scalar dissipation rate that is representative for the initial conditions of the mixture fraction field. Following Swaminathan and Bilger [22] the fuel and air composition (by weight) are 15%/34%/51% CH_4/N_2/Ar and 30%/70% O_2 and N_2, respectively. The stoichiometric mixture fraction is 1/3 and all simulations are performed on 256^3 grid nodes.

We use a four-step mechanism to approximate the combustion of methane with air and the simplified kinetics scheme by Jones and Lindstedt [4] allows for simulating finite rate chemistry with local extinction and re-ignition. Transport equations need to be solved for Z, CH_4, CO, H_2 and $\hat{h}_s$. The Prandtl number is set to $Pr = 0.7$ and unity Lewis numbers are assumed. All other species (O_2, CO_2, H_2O, Ar, N_2) can then be determined from the element mass balances. The minimum sensible enthalpy is equal in the fuel and oxidizer streams and a maximum sensible enthalpy can be obtained from the product of the methane mass fraction in the fuel stream and the enthalpy of combustion as $h_{s,\max} = h_{\text{comb}} Y_{CH_4,F}$. The normalized sensible enthalpy, $\hat{h}_s$ is then given by $\hat{h}_s = (h_s - h_{s,\min})/(h_{s,\max} - h_{s,\min})$. Please note that this is equivalent to the definition of reduced temperature $\Theta = (T - T_0)/(T_{\max} - T_0)$ for a constant property flow and the initial conditions for $\hat{h}_s$ can be obtained from the flamelet solution.

Local extinction will only be present if the turbulence time scales are of the same order as the chemical time scales, i.e. Damköhler number, $Da = \tau_0/\tau_c$ must be relatively low. However, typical three dimensional DNS calculations do not have Reynolds numbers large enough to yield sufficiently low turbulence time scales. Here we follow the technique used in references [7, 22] where the pre-exponential factors of the four-step chemical kinetics scheme are adjusted to increase the chemical time scales and thus, to reduce the Damköler number. This method ensures relatively low computational cost while the key parameter that controls extinction and re-ignition can be adjusted. Three cases are investigated here with different pre-exponential scaling factors f and approximate scalar dissipation rates at quenching:

- Case A with moderate local extinction; $f = 0.10 \times 10^{-2}$ and $N_q = 0.30s^{-1}$,
- Case B with significant local extinction; $f = 0.45 \times 10^{-3}$ and $N_q = 0.090s^{-1}$ and
- Case C with global extinction; $f = 0.22 \times 10^{-3}$ and $N_q = 0.045s^{-1}$.

The variation in pre-exponential factors and the corresponding quenching values for scalar dissipation ensures a variable degree of extinction for the three cases. Turbulent mixing increases scalar gradients at the beginning of the computations while turbulence decay and an advanced mixing state lead to smaller dissipation values at later times. The smaller dissipation values then allow reignition in Cases A and B at $t^* > 1.2$.

The MMC equations are solved for the same scalars simulated in the DNS. The convective term in equation (1) can be neglected due to the homogeneity of flow and scalar fields. The diffusion and drift terms are modelled according to equations (12) and (4), respectively. A semi-implicit scheme using second-order differencing in reference spaces and first-order temporal discretisation is used. Conditional reaction rates are treated explicitly. For the reference variables there are 50 cells in the range $-4 < \xi < 4$ with clustering near $\xi = 0$. Computations using increased grid resolution do not produce significant changes in the results.

The joint PDF of the major scalars (which in MMC approximates the joint PDF of all scalars) is generally known at the initial time. The joint PDF is related to the mapping functions of the major scalars through an equality of the cumulative distribution functions in scalar and reference spaces. For multi-dimensional spaces an ordering of the major scalars is re-

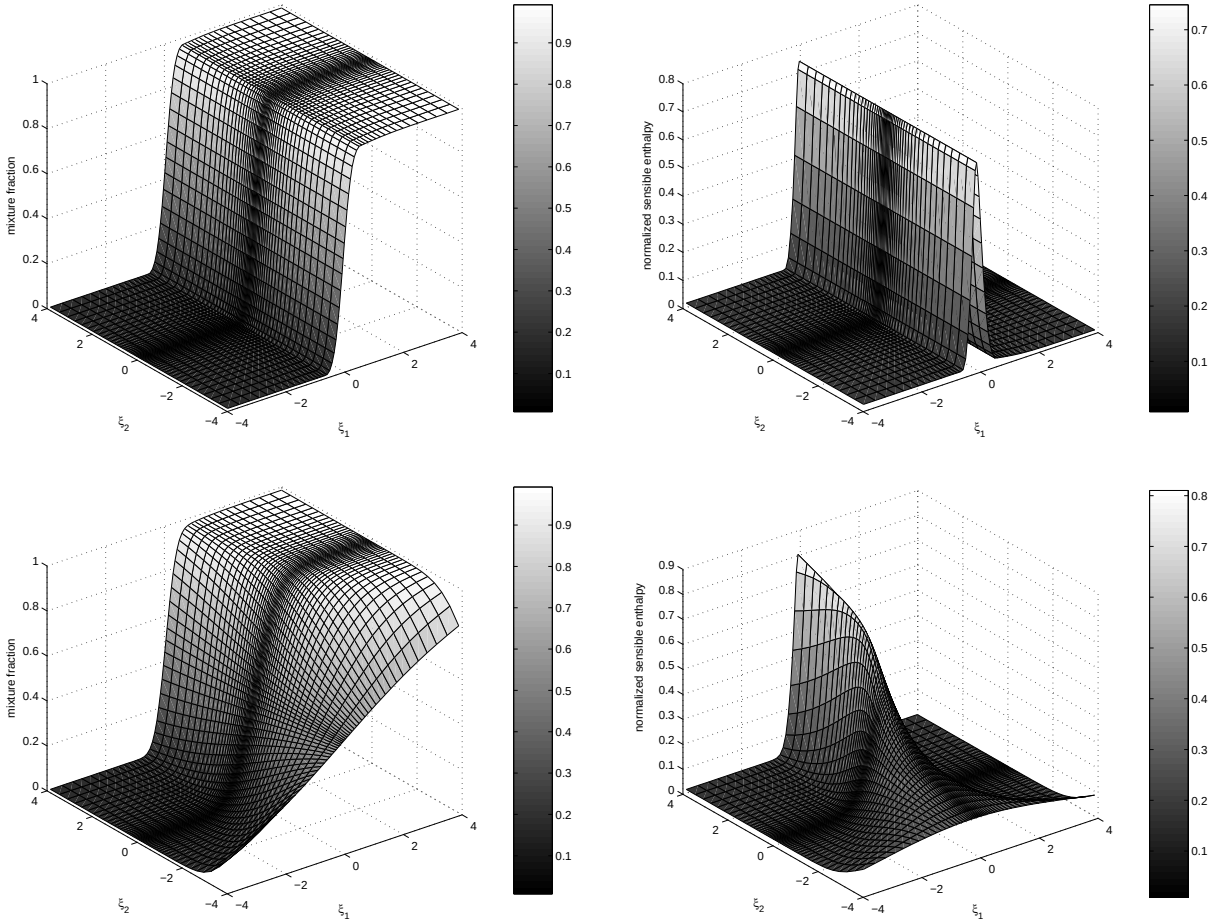

Figure 1: Mixture fraction and normalized sensible enthalpy in reference space at $t^* = 0.0$ (top) and $t^* = 1.0$ (bottom).

quired [13, 20]. As the primary dependence in turbulent diffusion flames is on the mixture fraction we order the variables with mixture fraction first and normalised sensible enthalpy second. The mapping function for mixture fraction is initially a function of ξ_1 only and is determined by solving the following integral equation for X_1:

$$\int_0^{X_1(\xi_1)} P(\eta) d\eta = \int_{-\infty}^{\xi_1} P(\xi_1) d\xi_1. \qquad (16)$$

Here $P_Z(\eta)$ is the marginal PDF for mixture fraction. Subsequently the mapping function X_2 for normalised sensible enthalpy is made at each ξ_1 via

$$\int_0^{X_1(\xi_1,\xi_2)} P(\zeta \mid \eta) d\zeta = \int_{-\infty}^{\xi_2} P(\xi_2) d\xi_2. \qquad (17)$$

where $P(\zeta \mid \eta)$ is the PDF in ζ conditioned on η. The mapping functions for the minor scalars are deterministic functions of X_1 and X_2. We use stretched laminar flamelet initial conditions.

Model results

Further Closures

First, further closure assumptions are introduced. Full MMC closure requires the unconditional dissipation $\widetilde{N}_{11}$, $\widetilde{N}_{12}$, $\widetilde{N}_{22}$ and the conditional scalar dissipation fluctuations $\langle N_{11}'^2 \mid \eta \rangle / \langle N_{11} \mid \eta \rangle$. While models for the passive and reactive scalar dissipation exist [23], we are not aware of any model for the cross-correlation $\widetilde{N}_{12}$. Usually, $\widetilde{N}_{12} \ll \widetilde{N}_{11}$ due to its change in sign around stoichiometric and we suggest $\widetilde{N}_{12} = 0$ and neglect cross-correlations in equation (1) by setting $\overline{B}_{12} = \overline{B}_{21} = 0$. $\overline{B}_{11}$ and $\overline{B}_{22}$ can then be computed from a reduced 2×2 matrix deduced from equation (7). A final assumption refers to the modelling of the scalar dissipation fluctuations. They can be estimated having a lognormal variance of one leading to $c_\alpha = -1$ following equation (15). DNS data shows that the mixture fraction dependence of c_α is small and that $c_\alpha \approx -0.3$ initially before increasing to approximately $c_\alpha \approx -1.1$ at the end of the simulation. Slightly faster extinction can therefore be observed for constant $c_\alpha = -1$, but differences are small since the correlation function $f_{corr} = -\langle \hat{h}_s \mid \eta = Z_{st} \rangle$ decreases with increasing degree of extinction and this reduces the effective coefficient in the exponential function, equation (12), quickly. The joint PDF, the mean mass fractions of the reactive species and their variances are hardly affected by the introduction of the additional closure assumptions and a comparison is therefore not shown here. It is noted that the new MMC(Z, h_s) implementation now requires merely the unconditional dissipations of mixture fraction and sensible enthalpy as input for the modelling of the effects of homogeneous turbulence on the reaction process and the modelling of the evolution in mixture fraction-sensible enthalpy space is thus fully closed.

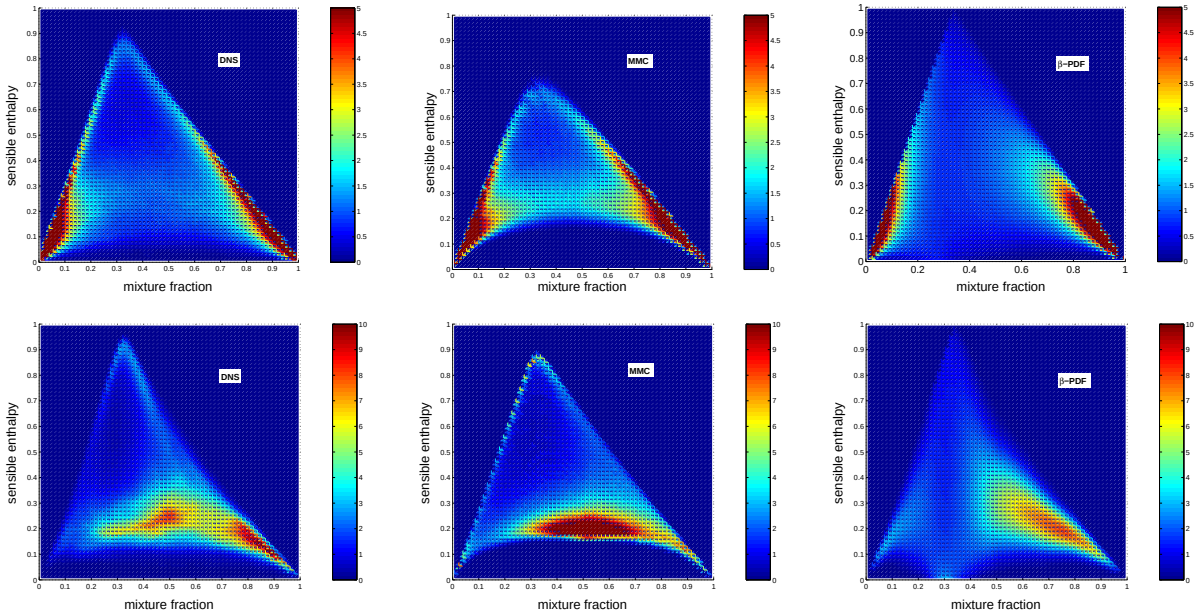

Figure 2: Comparison of the joint mixture fraction-sensible enthalpy PDF from DNS with modelling results at different times ($t^* = 1.0$ (top) and $t^* = 2.5$ (bottom)).

Prediction of the major scalars

MMC models the evolution of all scalars in reference space and the distribution of the major scalars gives their joint PDF in real space. In this subsection we will analyze the modelling of the major scalars only. For a better illustration of the method, we show in figure 1 the mapping functions of mixture fraction and sensible enthalpy at the start of the simulation and at $t^* = 1.0$. As described above, Z is initialized as function of ξ_1 only, and the Heaveside function in ξ_1-space results from a double δ-PDF in real space. The ξ_1 location of the step determines the average mixture fraction, $\langle Z \rangle$. The normalized sensible enthalpy is initialized as a function of Z and peaks where $Z(\xi_1, \xi_2) = Z_{st} = 1/3$. Note that $\hat{h}_s$ is independent of ξ_2 initially. The exponential dependence of B_{11} on ξ_2 (cf. equation (12)) leads to higher diffusion for low ξ_2 and causes more mixing and a noticeable reduction in temperature. It is therefore responsible for local extinction. To facilitate the analysis of MMC, all results are now transformed into $\eta - \zeta-$space using the expression

$$P_{Z,\hat{h}_s} = P_\xi \cdot \det\left(\frac{\partial X_j}{\partial \xi_k}\right)^{-1} \tag{18}$$

that relates the presumed PDF in reference space, P_ξ, with the modelled PDF, $P_{Z,\hat{h}_s}$, in physical space. The resulting joint PDF, $P_{Z,\hat{h}_s}(\eta, \zeta)$, can now directly be compared with DNS data.

Figure 2 demonstrates good qualitative agreement between MMC and DNS at different times, in particular around stoichiometric. The key characteristic of the modelled joint PDF is the capability to capture the location of the extrema correctly. For better quantitative comparison, the joint PDFs are plotted along ζ for constant mixture fraction values in figure 3. The bimodal character of the conditional PDF is well captured around stoichiometric and the location of the maxima is well approximated. A somewhat wider distribution is noted in the DNS data and the qualitative agreement between MMC and DNS is similar at all times. Of major influence is an artefact of the model. A large diffusion coefficient at low ξ_2 leads to enhanced mixing not only of temperature and species but also of mixture fraction. This leads to low gradients of Z for negative ξ_2 as can be seen in figure 1 and to the relatively high probability for low temperatures around the mean value of mixture fraction, $\langle Z \rangle$. The current implementation of MMC fixes high dissipation values to certain regions in ξ_1-ξ_2-space while in real space the intermittent behaviour of scalar dissipation does not lead to specific regions of low mixture fraction gradients. A stochastic implementation of MMC may alleviate these shortcomings, but this coupling cannot be avoided in deterministic MMC. In the current study, the low gradients of Z at low ξ_2 do not unduly affect the average concentrations and modelling errors seem acceptable.

For better comparison with previous modelling attempts [15, 2], a presumed β-distribution of the joint PDF is also included in figures 2 (right column) and 3 (dashed lines). The presumed joint PDF can be modelled by $P^\beta_{Z,\hat{h}_s}(\eta, \zeta) = P^\beta(\zeta \mid \eta) \cdot P^\beta(\eta)$ where the superscript $\cdot^\beta$ indicates the presumed $\beta-$probability distribution. MMC shows clear improvements over a $\beta-$PDF distribution, in particular around stoichiometric. The conditional β-PDF cannot capture the bi-modal distribution with extrema away from the bounds, it exhibits an almost constant slope in ζ-space in figure 3 and is thus qualitatively wrong. The conditional $\beta-$PDF performs better away from stoichiometric where only one extremum exists (see figure 3) but it shall be noted that the conditional variance of sensible enthalpy has been taken from DNS to construct the conditional β-PDF, P($\zeta \mid \eta$). Large uncertainties in the modelling of the conditional variance equation will almost certainly lead to further deviations of the β-PDF from DNS data even away from stoichiometric. MMC avoids many of the issues associated with the modelling of the conditional variance equation and the conditional variance is solved implicitly.

A more common measure for the level of extinction is the conditional temperature of sensible enthalpy at stoichiometric. All three cases are included in figure 4 and agreement between MMC and DNS is excellent for cases B and C. The level of ex-

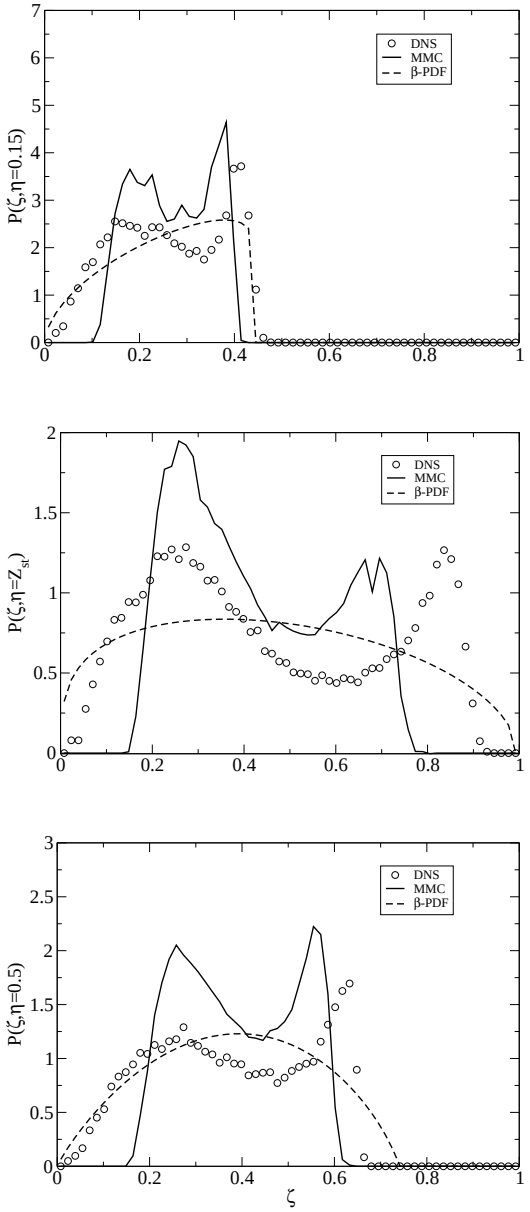

Figure 3: Joint PDF as function of ζ for different constant mixture fraction values at $t^* = 1.0$.

tinction and the onset of reignition in case B are modelled well. Results from MMC(Z) are included here for comparison with conventional single conditioning methods such as singly conditioned CMC and to re-iterate the need for doubly-conditioned approaches. Unfortunately, predictions for case A are less satisfactory. The level of extinction is not well predicted and this is in line with earlier studies [3, 2]. The lack of local extinction is due to an underprediction of the variance. This is primarily caused by enforcing positive B_{22} which is a necessary condition for numerical stability. Klimenko [10] suggests that matching of the *conditional* fluctuations is important for accurate MMC predictions. This is certainly correct, however, even the imposition of the correct fluctuations in sensible enthalpy space [2] did not lead to improved modelling results due to the constraint of $B_{22} \geq 0$. Possible improvements of the present implementation of MMC(Z, h_s) include ξ_1 dependence of B_{11} to ensure independence of B_{11} from η and lognormality for constant η that is violated in the results presented here at later times due to the evolution of Z in $\xi_1 - \xi_2$-space. However, we carried

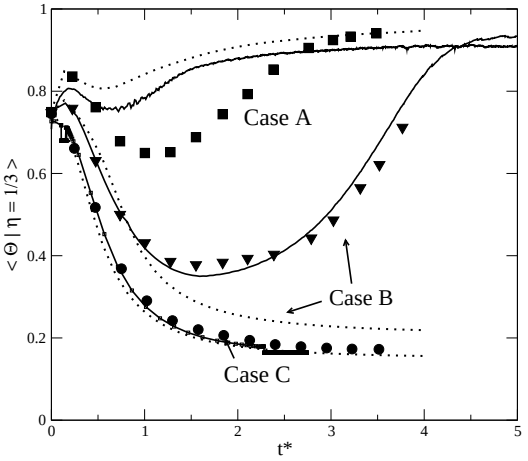

Figure 4: Conditionally averaged sensible enthalpy as a function of time for $\eta = Z_{st}$. Symbols denote DNS data, the solid lines are results from MMC(Z,$\hat{h}_s$) and the dashed lines are from MMC(Z).

out computations with these modifications, but improvements are marginal, they do not justify the added complexity and are therefore not shown here.

The averaged temperature is a global measure for the performance of the simulation methods. Figure 5 compares the evolution of the mean temperature from MMC(Z,$\hat{h}_s$) predictions with DNS and MMC(Z). MMC(Z,$\hat{h}_s$) predictions are good at all times and the somewhat narrow distribution in ζ-space that

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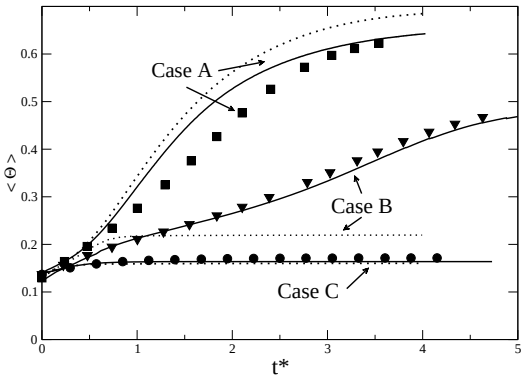

Figure 5: Comparison of mean temperature as function of time.

Prediction of the minor scalars

Predictions of all reactive (minor) species are good at all times. Figure 6 compares doubly conditioned mass fractions of CO from DNS and MMC as function of ζ for $\eta = Z_{st}$ and $\eta = 0.5$. The cut-off that can be observed for MMC for high and low ζ-values results from the predicted zero probability in this region. Good agreement of the doubly conditioned quantities with DNS data implies that mixture fraction and normalized sensible enthalpy describe turbulent scalar fluctuations well and that the chemical source term can be modelled with first order closure based on these doubly conditioned mass fractions. This can be expected since earlier studies on doubly conditioned moment closure [16, 15] demonstrated that the two major (or conditioning) scalars Z and $\hat{h}_s$ parameterize the composition space well

and that fluctuations around the doubly conditioned means are small. Agreement with DNS is satisfactory for the volume averaged quantities that are shown in figure 7 for all solved minor species as function of time for all three cases. It is apparent that the quality of the prediction for the volume averages follows the trends in the predictions of the joint PDF. Good agreement can be achieved for cases B and C, however, the underpredition of the level of extinction for case A leads to clear deviations of the MMC simulations from the DNS for all species mass fractions and

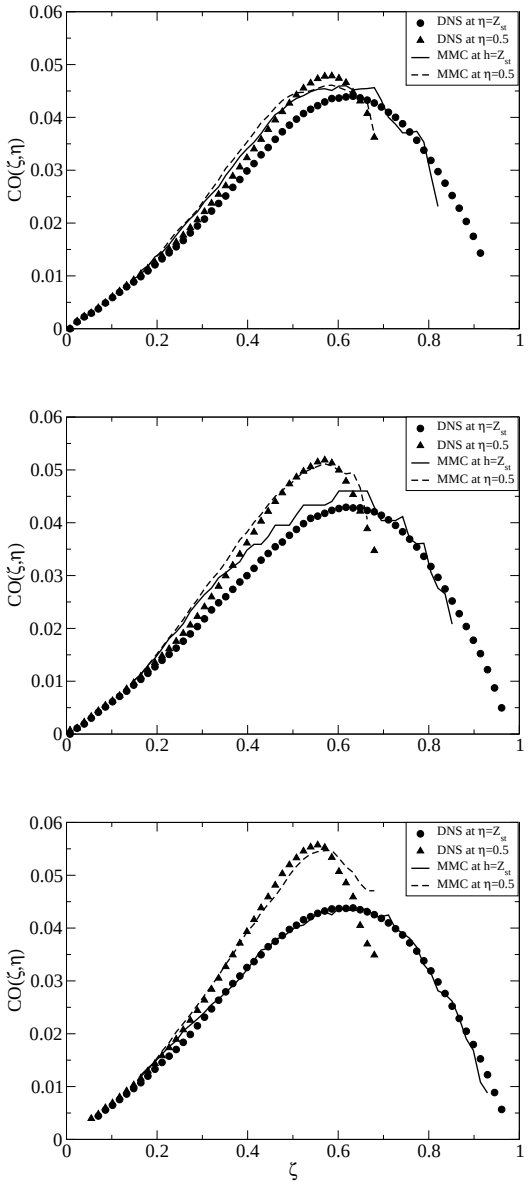

Figure 6: Comparison of doubly conditioned CO mass fraction for fixed mixture fraction values at $t^* = 1.0$ (top), $t^* = 2.0$ (centre) and $t^* = 3.0$ (bottom).

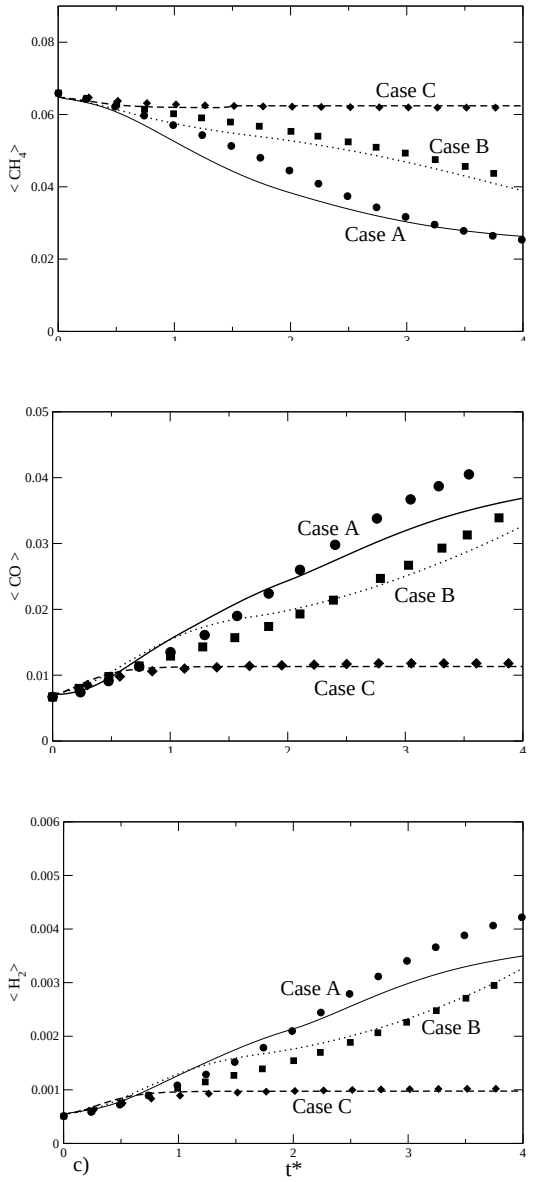

Figure 7: Comparison of mean mass fractions of minor species as function of time.

Conclusion

Multiple Mapping Conditioning has been used to model hydrocarbon combustion with local extinction and reignition due to turbulent strain. In the current implementation, the two reference variables represent mixture fraction and normalized sensible enthalpy, however, the strong correlation between sensible enthalpy and scalar dissipation fluctuations during the extinction process is exploited. The second reference variable is therefore implemented as a dissipation-like variable and a correlation coefficient is introduced to characterize the correlation between dissipation fluctuations and sensible enthalpy. This allows for matching the scalar fluctuations of mixture fraction and sensible enthalpy and for generating conditional fluctuations of the temperature field about its mean. The evolution of mixture fraction and sensible enthalpy in reference space model their joint distribution well and results are a clear improvement over previous modelling approaches using conditional presumed β-distributions. Further modelling assumption of negligible cross-correlations and of a lognormal distribution of dissipation in reference space with a variance of unity do not markedly affect the quality of the predictions and a fully closed deterministic model that is capable of predicting extinction and re-ignition has been presented. Predictions of major and minor species is good and qualitatively comparable to earlier preditions using a 'hybrid' model [2] where conditional sensible enthalpy fluctuations had to be taken from DNS and were imposed on the MMC computations to ensure the correct evolution of conditional temperature

fluctuations and the occurence of extinction.

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