Chapter 5
The Conditional Moment Closure Model

A. Kronenburg and E. Mastorakos

Abstract The relatively recent Conditional Moment Closure methods for turbulent reacting flows have advanced from application to relatively well behaved, simple laboratory flames to complex flow geometries and flame conditions with intense turbulence-chemistry interactions. The progress on second order closures, double conditioning approaches, two-phase and premixed CMC is reviewed in the first part of this chapter, while the second part is largely dedicated to numerical methods to solve the CMC equations and to the model's capability to address questions of direct engineering interest such as the modelling of diesel engine combustion and the analysis of flame stabilization mechanisms.

5.1 Introduction

More than ten years ago, the first and - to date - last comprehensive review of the Conditional Moment Closure (CMC) method was published by Klimenko and Bilger [35]. Yet, great strides have been made in advancing the method from its rather typical application to relatively simple and "well behaved" diffusion flames to more complex flow geometries and flame conditions.

The development of the Conditional Moment Closure (CMC) method was motivated by the need to provide accurate closures for the average of the non-linear turbulent reactive source term. It was conceptually derived as a mixture fraction based approach for non-premixed turbulent combustion and has as such some similarities with laminar flamelet methods. The basic idea is to exploit a strong correlation be-

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tween reactive scalar species and the mixture fraction and hence fluctuations in reactive scalar space can be associated with fluctuations in mixture fraction space. Conditioning of the reactive species on mixture fraction then leads to relatively small fluctuations around the conditional mean, and a simple first order closure for the chemical source can be found. Hence, transport equations for the reactive species mass fractions conditioned on mixture fraction have been derived, and some unclosed terms such as the conditional velocity and the conditionally averaged scalar dissipation need to be modelled. Relatively simple models for these terms suffice and the solution of the temporal and spatial evolution of the conditional moments gives relatively good predictions of finite-rate chemistry effects for a wide range of turbulent diffusion flames [25, 31, 66, 67, 69].

During the last decade, the majority of CMC-related theoretical development has focused on the modelling of flame regimes where local correlations between reactive scalars and mixture fraction are weakened. This decorrelation will for example occur in flames with local extinction, in lifted flames where fuel and oxidizer mix without combustion before the stabilization point and more generally, in any flow with regions of partial or complete premixing prior to ignition. Here, fluctuations around the conditional mean will start to become significant, but it is very important to realize that CMC is not rendered invalid if conditioned and conditioning quantities are not well correlated. The CMC transport equations can be derived without making assumptions on the degree of correlation. However, closures of unclosed terms, and in particular of the conditionally averaged chemical source term, need improvements to account for the effects of fluctuations on the evolution of the conditioned moments.

The second major focus of CMC research has been on the application of the method to more complex flow geometries and flame conditions with technical relevance such as engine and gas turbine related environments. The two foci of work determine the structure of the remainder of this chapter which is largely split into two major sections. The next section is called “methodological developments” where we will briefly review the standard formulation of the conditional moment closure method and then elaborate on techniques that account for flame conditions where reactive scalars do not correlate well with mixture fraction, namely the second order closures and double conditioning. Further, specific subsections are dedicated to the discussion of the first steps in CMC related premixed flame modelling and advances in two-phase flow CMC. The second major section (Section 5.3) is dedicated to applications of CMC to problems of engineering interest. Several research groups have worked on CMC for diesel engine combustion, auto-ignition studies, flame stabilization, CMC as combustion sub-model for Large-Eddy Simulations (LES) for improved flow field modelling in complex geometries, and more generally, on pollutant predictions where finite rate effects dominate. While the theoretical framework for the application of CMC is well established, some implementation and modelling issues arise. Section 5.3 will provide an up-to-date assessment of CMC and its capabilities, but improvements to the technique are certainly needed to allow application to all flow and flame regimes. We will attempt to outline future steps in CMC de-

velopment in the final part of Section 5.3 that should serve as encouragement and guideline to new researchers in the field of CMC modelling.

5.2 Methodological Developments in CMC

The CMC transport equations for turbulent reacting flows were derived by Klimenko [33] and Bilger [4] using somewhat different methodologies and primary closure assumptions. Details on the differences are discussed in [35], and we limit ourselves here to present one approach only that is called "the decomposition method". Its derivation requires little knowledge of combustion, it is based on the well known instantaneous transport equations for reactive and passive scalars and only standard mathematical techniques need to be used. The derivation in the next subsection will be quite general and standard closures will be introduced. The further subsections discuss more advanced closures such as second order and double conditioning approaches, but also outline CMC's potential for the modelling of premixed flames. Modifications that need to be made for multiphase combustion are described in Section 5.2.5.

5.2.1 The CMC Equations

We will first define the conditional mean, $Q_k(\mathbf{Z}^c,\mathbf{x},t)$, of a scalar $Y_k(\mathbf{x},t)$ as

$$Q_k(\mathbf{Z},\mathbf{x},t) = \langle Y_k(\mathbf{x},t) \mid \mathbf{Y}^c = \mathbf{Z}^c \rangle. \tag{5.1}$$

The angular brackets denote ensemble averages of Y_k, conditioned on $\mathbf{Y}^c = \mathbf{Z}^c$, where $\mathbf{Y}$ is a multidimensional scalar space, and $\mathbf{Z}$ is its sample space. The choice whether a specific scalar is a conditioned or a conditioning quantity is problem dependent, however, the sets of conditioned and conditioning quantities are mutually exclusive and no scalar should be part of both sets. The arrays to the right of the vertical bar in Eq. 5.1 should be understood to represent a (usually small) subset of the entire scalar space, $\mathbf{Y}^c = (Y_1, Y_2, \ldots, Y_{n_c})$ and $\mathbf{Z}^c = (Z_1, Z_2, \ldots, Z_{n_c})$, where the number of conditioning scalars, n_c, should be much smaller than the number of scalars, n_{sc}. The scalar space of the conditioned quantities is then given by $\mathbf{Y}^q = (Y_{n_c+1}, \ldots, Y_k, \ldots, Y_{n_{sc}})$, and the superscripts 'c' and 'q' are used here to indicate scalar arrays with conditioning and conditioned quantities, respectively. Note that the scalar array may include mixture fraction, scalar dissipation and an energy related scalar such as enthalpy or temperature. The conditional mean - or conditional expectation - is related to the joint probability density function through

$$\langle Y_k \mid \mathbf{Y}^c = \mathbf{Z}^c \rangle = \int_{-\infty}^{+\infty} Z_k P(Z_k \mid \mathbf{Y}^c = \mathbf{Z}^c) dZ_k = \frac{\int_{-\infty}^{+\infty} Z_k P(Z_k, \mathbf{Z}^c) dZ_k}{P(\mathbf{Z}^c)}, \tag{5.2}$$

where spatial and temporal dependencies have been omitted for clarity of presentation, and the unconditional mean can be obtained from the conditional mean by integration across the entire sample space of the conditioning variables,

$$\langle Y_k \rangle = \int_{-\infty}^{+\infty} \langle Y_k \mid \mathbf{Y}^c = \mathbf{Z}^c \rangle P(\mathbf{Z}^c) d\mathbf{Z}^c. \tag{5.3}$$

The starting point for the derivation of the CMC equations is the well known transport equation for chemically reactive species, discussed in Chapter 2, which is repeated here for the reader's convenience,

$$\rho \frac{\partial Y_k}{\partial t} + \rho u_i \frac{\partial Y_k}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\rho D_k \frac{\partial Y_k}{\partial x_i}\right) = w_k. \tag{5.4}$$

In Eq. 5.4 we have used Fick's law for the diffusive flux. The instantaneous mass fraction Y_k can now be decomposed into the conditional mean and the fluctuation around the conditional mean,

$$Y_k(\mathbf{x},t) = Q_k(\mathbf{Z},\mathbf{x},t) + Y_k''(\mathbf{x},t) \tag{5.5}$$

and be inserted into Eq. 5.4. The chain rule of differentiation is applied to all temporal and spatial derivatives of Q_k. Note, for example, the application of the chain rule to the time derivative,

$$\frac{\partial Y_k}{\partial t} = \frac{\partial Q_k}{\partial t} + \frac{\partial Q_k}{\partial Z_j}\frac{\partial Z_j}{\partial t} + \frac{\partial Y_k''}{\partial t}, \qquad j = 1,\ldots,n_c \tag{5.6}$$

and its application to the spatial derivatives - or repeated applications for the diffusion term - obeys identical rules. The entire resulting equation needs to be conditionally averaged again, and the final CMC equation results in

$$\begin{aligned} \langle \rho \mid \mathbf{Z}^c \rangle \frac{\partial Q_k}{\partial t} = &- \langle \rho u_i \mid \mathbf{Z}^c \rangle \frac{\partial Q_k}{\partial x_i} + \langle w_k \mid \mathbf{Z}^c \rangle - \langle w_j \mid \mathbf{Z}^c \rangle \frac{\partial Q_k}{\partial Z_j} \\ &+ \langle \rho D_k \frac{\partial Y_j}{\partial x_i}\frac{\partial Y_j}{\partial x_i} \mid \mathbf{Z}^c \rangle \frac{\partial^2 Q_k}{\partial Z_j \partial Z_j} + \langle \rho D_k \frac{\partial Y_j}{\partial x_i}\frac{\partial Y_l}{\partial x_i} \mid \mathbf{Z}^c \rangle \frac{\partial^2 Q_k}{\partial Z_j \partial Z_l} \\ &+ e_q + e_y \end{aligned} \tag{5.7}$$

with

$$\begin{aligned} e_q &\equiv \langle \frac{\partial}{\partial x_i}\left(\rho D_k \frac{\partial Q_k}{\partial x_i}\right) + \rho D_k \frac{\partial Y_j}{\partial x_i}\frac{\partial^2 Q_k}{\partial x_i \partial Z_j} + \frac{\partial}{\partial x_i}\left[\rho (D_k - D_j)\frac{\partial Y_j}{\partial x_i}\right]\frac{\partial Q_k}{\partial Z_j} \mid \mathbf{Z}^c \rangle \\ e_y &\equiv -\langle \rho \frac{\partial Y_k''}{\partial t} + \rho u_i \frac{\partial Y_k''}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\rho D_k \frac{\partial Y_k''}{\partial x_i}\right) \mid \mathbf{Z}^c \rangle. \end{aligned}$$

All terms on the RHS need closure. The e_q-term can usually be neglected under high Reynolds number assumptions [35], but needs to be modeled if differential diffusion effects are to be included [37, 38]. Similarly, the e_y-term that involves all the

fluctuations around the conditional mean, must not be omitted in the presence of significant differential diffusion effects, but can be set to zero in the absence of differential diffusion and if a "good" set of conditioning variables is selected. The term "good" refers to the correlation of the (unconditional) fluctuations of the conditioned scalars with the (unconditioned) fluctuations of the conditioning scalars. A perfect correlation would lead to $Y_k'' \approx 0$, however, correlations are hardly ever perfect, and based on the primary closure hypothesis employed in the decomposition method [35], $e_y P(\mathbf{Z}^c) = -\nabla \cdot \left[\langle \rho \mid \mathbf{Z}^c \rangle \langle \mathbf{u}'' Y_k'' \mid \mathbf{Z}^c \rangle P(\mathbf{Z}^c)\right]$, we may propose a gradient diffusion approximation for e_y. The validity of the gradient diffusion model has been corroborated by Richardson et al. [63] for relatively high turbulence levels. Deviations between the model and DNS data at low turbulence levels are due to countergradient transport present in the studied expanding flames that involved propagating fronts; such phenomena may be absent in attached non-premixed flames. The importance of e_y, and therefore the importance of the accuracy of its closure, strongly depends on flow and flame conditions. It is of paramount importance for flame stabilization in lifted flames where flame propagation is the dominating stabilization mechanism [15, 24].

The best modeling approaches for the conditional velocity, $\langle \rho u_i \mid \mathbf{Z}^c \rangle$, dissipation, $N_{jj} \equiv \langle D \nabla Y_j \nabla Y_j \mid \mathbf{Z}^c \rangle$ and cross-dissipation, $N_{jl} \equiv \langle D \nabla Y_j \nabla Y_l \mid \mathbf{Z}^c \rangle$, have not yet been established for multidimensional conditioning spaces. Ample experience exists, however, for simple, single conditioning ($n_c = 1$), where $Y_1 = \xi$ and $Z_1 = \eta$ with ξ being mixture fraction and η its sample space. Single conditioning on mixture fraction leads to the standard CMC equations,

$$\rho_\eta \frac{\partial Q_k}{\partial t} + \langle \rho u_i \mid \eta \rangle \frac{\partial Q_k}{\partial x_i} = \rho_\eta N_\eta \frac{\partial^2 Q_k}{\partial \eta^2} + \langle w_k \mid \eta \rangle - \frac{1}{P_\eta} \frac{\partial}{\partial x_i} \left[\rho_\eta \langle u_i'' Y_k'' \mid \eta \rangle P_\eta\right] \quad (5.8)$$

with scalar dissipation $N \equiv D \nabla \xi \nabla \xi$ and subscript η indicating dependence on mixture fraction.

Sreedhara et al. [71] assessed different standard closures for the conditional velocity, $\langle \mathbf{u} \mid \eta \rangle$ and the conditional scalar dissipation, $\langle N \mid \eta \rangle$. The different models for $\langle \mathbf{u} \mid \eta \rangle$ were termed (1) "conditional independence", (2) "linear in terms of unconditional flux" and (3) "gradient diffusion in terms of local PDF". Only minor differences between the models could be observed for the jet flames studied; such comparison is not available for more complicated flows.

Standard models for conditionally averaged scalar dissipation have been termed (1) "AMC"-, (2) "Girimaji's"- and (3) "double integration of the PDF transport equation"-model [71]. Theoretically, the AMC-model [57] requires the presence of unmixed fluid, a condition that will not be satisfied in regions downstream of the potential core of a jet. Girimaji's model [20] has been derived for homogeneous flows and - strictly speaking - may not hold in regions with strong mean gradients. In contrast, the integration of the PDF transport equation ensures consistency between conditionally averaged dissipation and the scalar's probability distribution in all regions of the flow [40] and as such, should be the modeller's choice. However, the PDF transport equation requires a "good" model for the conditionally averaged

velocity, and accurate numerical integration of the equation is difficult in regions of low probability. Practically, all three models provide qualitatively similar results for conditionally averaged scalar dissipation in Sandia Flame D [2], with the AMC-model being symmetric in η-space and the PDF-model deviating most from symmetry. 3-D measurements [2] show some asymmetry, but it would be difficult to decide on the superiority of one specific model. Notable differences exist in a bluff body flame, but lack of experimental data makes judgment on the quality of the different models impossible.

Further models with great promise have been developed by Devaud et al. [14], Cha et al. [8] and Mortensen and de Bruyn Kops [51], however, none of the models has been validated by comparison with experimental data, and they are therefore not discussed further in the present review.

The key to successful CMC modelling is the accuracy of the closure of the conditionally averaged chemical source term, $\langle w_k \mid \eta \rangle$. The assumption of relatively small fluctuations around the conditional mean allows for simple first order closure of the reaction rate term, i.e.

$$\langle w_k \mid \eta \rangle = w_k(\mathbf{Q}, \eta). \tag{5.9}$$

This closure has proven adequate for many applications, but more complex closures may become necessary if fluctuations become significant. It is repeated here that the CMC equation (Eq. 5.8) remains valid even if fluctuations are large, however, the accuracy of above closures will suffer and different modelling strategies will need to be employed. Rather unexpectedly, improved closures of the e_y-term may not be necessary, however, accurate modelling of the chemical source term is crucial [36, 43]. The latter can be achieved by multiple conditioning (see Section 5.2.3) or by second order closures that are discussed next.

5.2.2 Advances in Second Order Closures

The reasons for fluctuations around the conditional mean are diverse. Mixture fraction is a good conditioning scalar for all non-premixed flames, however, relatively strong fluctuations in scalar dissipation due to turbulence directly affect the flame structure, this leads locally to deviations from the conditional mean and induces fluctuations. If scalar dissipation fluctuations are large, local extinction can occur and conditional fluctuations are significant as shown in Fig. 5.1. Similar conditional fluctuations can be observed in turbulent flows where fuel and oxidizer partially premix before ignition occurs. In addition, relatively large variations of ignition location can exist even in statistically stationary cases, e.g. Gordon et al. [21] reported fluctuations of lift-off height of around 10 jet diameters in experiments with jets issued into hot vitiated air. Mastorakos [47] reviewed the spatial fluctuations of autoignition spots in detail and found that the fluctuations of the scalar dissipation rate are crucial for generating conditional reaction rate fluctuations.

It seems obvious that the influence of these fluctuations cannot be ignored. However, advanced closures do not necessarily aim at improved modelling of the term that involves the fluctuations, but seek an improvement to the existing closures for the chemical source term. The second order closures presented in this Subsection therefore focus on a second order correction of the conditionally averaged source term only.

The forward reaction rate of any bi-molecular elementary reaction, m, $[C_k] + [C_l] \rightleftharpoons [C_r] + [C_s]$ can be expressed in Arrhenius form,

$$w^m(\rho, \mathbf{Y}, T) = A_m \rho^2 \frac{Y_k Y_l}{M_k M_l} T^{b_m} exp(-T_{a,m}/T) \tag{5.10}$$

and a Taylor expansion around the conditionally averaged first order approximation yields

$$\begin{aligned} \langle w^m \mid \eta \rangle &= w^m(\rho_\eta, \mathbf{Q}, \eta) \cdot \left(1 + \frac{\langle Y_k'' Y_l'' \mid \eta \rangle}{Q_k Q_l} + T_1 + T_2\right) \\ T_1 &\equiv \left(b_m + \frac{T_{a,m}}{Q_T}\right) \left(\frac{\langle Y_k'' T'' \mid \eta \rangle}{Q_k Q_T} + \frac{\langle Y_l'' T'' \mid \eta \rangle}{Q_l Q_T}\right) \\ T_2 &\equiv \frac{1}{2} \left(b_m(b_m - 1) + \frac{2(b_m - 1) T_{a,m}}{Q_T} + \frac{T_{a,m}^2}{Q_T^2}\right) \cdot \frac{\langle T''^2 \mid \eta \rangle}{Q_T^2}. \end{aligned} \tag{5.11}$$

The second term in the brackets in Eq. 5.11 accounts for the correlation between species k and l, T_1 approximates the correlations between species and temperature and T_2 results from higher moments of temperature. These higher order corrections can be significant and easily exceed the first order approximation, in particular for reactions with high activation energies (due to the dependence of T_2 on squared $T_{a,m}$) as can be found in the first Zel'dovich step of NO formation. Closure of Eq. 5.11 requires knowledge of the conditionally averaged correlations between all chemically reactive species, $G_{kl} = \langle Y_k'' Y_l'' \mid \eta \rangle$ and between species and temperature

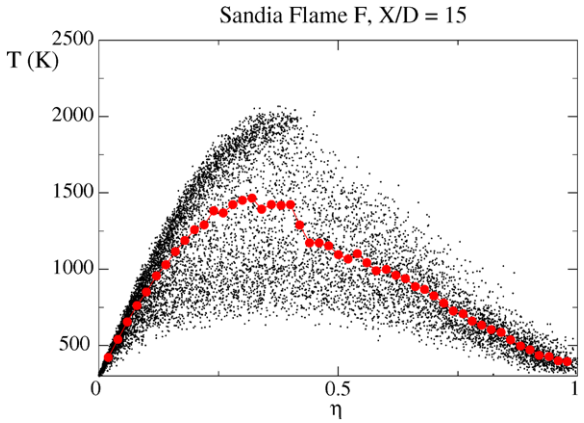

Fig. 5.1: Measurements of temperature as function of mixture fraction in a piloted methane-air jet diffusion flame with significant local extinction and re-ignition (Sandia Flame F). The filled symbols indicate the conditional mean of temperature, $Q_T = \langle T \mid \eta \rangle$. Reprinted from [19] with permission from the Combustion Institute.

$G_{kT} = \langle Y_k'' T'' \mid \eta \rangle$. A major issue is apparent: second order closure requires the solution of $n_{sc}(n_{sc}+1)/2$ additional transport equations for the conditional variance and co-variance, a task hardly feasible when using detailed chemical kinetics for hydrocarbon combustion. Early attempts by Mastorakos and Bilger [48] and Kronenburg et al. [39] used global mechanisms that could be parameterized by two variables, however, extension was not straightforward, and these methods therefore lacked generality. Kim and Huh [29] introduced the idea that second order corrections need to be applied to rate limiting steps only. They identified four rate limiting elementary reactions in a detailed methane-air mechanism (GRI 2.11 with 49 species and 277 reactions) that control the radical pool, the CO-CO_2 conversion, initialization and chain termination. These reactions involve 9 species (and temperature), and the resultant reduction from 1250 to 45 additional equations renders the problem trackable. The conditionally averaged variance and co-variance equations as such can easily be derived using the PDF or decomposition method [26],

$$\begin{aligned}
\frac{\partial G_{kl}}{\partial t} &+ \langle u_i \mid \eta \rangle \frac{\partial G_{kl}}{\partial x_i} - N_\eta \frac{\partial^2 G_{kl}}{\partial \eta^2} + \frac{1}{\rho_\eta P_\eta} \frac{\partial}{\partial x_i} \left[\rho_\eta \langle u_i'' Y_k'' Y_l'' \mid \eta \rangle P_\eta \right] \\
&+ \frac{\partial Q_k}{\partial x_i} \cdot \langle Y_l'' u_i'' \mid \eta \rangle - \frac{\partial Q_l}{\partial x_i} \cdot \langle Y_k'' u_i'' \mid \eta \rangle \\
= \quad & \langle w_k'' Y_l'' + w_l'' Y_k'' \mid \eta \rangle - 2 \langle D \left(\frac{\partial Y_k''}{\partial x_i} \frac{\partial Y_l''}{\partial x_i} \right) \mid \eta \rangle \\
& + \langle N'' Y_k'' \mid \eta \rangle \frac{\partial^2 Q_l}{\partial \eta^2} + \langle N'' Y_l'' \mid \eta \rangle \frac{\partial^2 Q_k}{\partial \eta^2} + \frac{1}{\rho_\eta P_\eta} \frac{\partial J_{gkl}}{\partial \eta}
\end{aligned} \tag{5.12}$$

with the transport equation for G_{kT} being identical in form. Primary closure assumptions have been invoked (i.e. e_q-terms and differential diffusion effects are neglected) and all terms on the LHS are closed or can be closed with standard closures. However, all terms on the RHS require additional models. Closures have been mainly suggested by the Sydney [45, 72] and Pohang [26, 27, 29] research groups. A set of relatively simple closures is given by

$$\langle w_k'' Y_l'' \mid \eta \rangle = \frac{\partial w_k}{\partial Y_\alpha} \mid_{Y=Q} G_{l\alpha} \tag{5.13}$$

$$2 \langle D \left(\frac{\partial Y_k''}{\partial x_i} \frac{\partial Y_l''}{\partial x_i} \right) \mid \eta \rangle = 2 \sqrt{C_k C_l} \frac{\varepsilon}{k} G_{kl} \tag{5.14}$$

$$\langle N'' Y_k'' \mid \eta \rangle = R_k N_\eta \langle G_{kk} \mid \eta \rangle^{1/2} \tag{5.15}$$

$$J_{gkl} = C_g \rho_\eta N_\eta P_\eta \frac{\partial G_{kl}}{\partial \eta} \tag{5.16}$$

Equation 5.13 is a first order approximation of the correlation between the chemical source term and the species and can be easily obtained from a Taylor expansion of w_k around $w_k(\mathbf{Q})$, multiplication with Y_l'' and subsequent conditional averaging [17]. The dissipation terms (Eq. 5.14) are modelled by an equivalence of the scalar fluctuation and turbulence time scales, C_k and C_l are constants to be discussed below,

and successful modelling of the dissipation-scalar correlations (Eq. 5.15) relies on a "good" choice of $R_k = R_{N''Y_k''} N_{rms}/N_\eta$ with $R_{N''Y_k''}$ being the correlation coefficient between N'' and Y_k''. The turbulent transport in conserved scalar space, J_{gkl}, is modelled assuming gradient transport [26].

A second set of alternative closures can be based on laminar flamelet assumptions [29, 72] where scalar fluctuations around their conditional means can be associated with fluctuations in scalar dissipation. The laminar flamelet solution can be parameterized by the value of scalar dissipation at stoichiometric and further assumptions of independence of $P(\eta)$ and $P(N_{st})$ and log-normality of $P(N_{st})$ lead to a closed form of the equations

$$\langle w_k'' Y_l'' \mid \eta \rangle = \frac{G_{ll}^{1/2}}{\sigma_l} \times A$$

$$A = \left(\int w_k^S Y_l^S P_N(N_{st}) dN_{st} - \int w_k^S P_N(N_{st}) dN_{st} \int Y_j^S P_N(N_{st}) dN_{st} \right) \quad (5.17)$$

$$2\langle D \left(\frac{\partial Y_k''}{\partial x_i} \frac{\partial Y_l''}{\partial x_i} \right) \mid \eta \rangle = 2D \int \frac{\partial ln Y_k''^S}{\partial \eta} \frac{\partial ln Y_l''^S}{\partial \eta} P_N(N_{st}) dN_{st} \quad (5.18)$$

$$\langle N'' Y_k'' \mid \eta \rangle = \frac{N_\eta G_{kk}^{1/2}}{N_{\eta,st} \sigma_i} \times B$$

$$B = \left(\int N_{st} Y_k^S P_N(N_{st}) dN_{st} - \int N_{st} P_N(N_{st}) dN_{st} \int Y_k^S P_N(N_{st}) dN_{st} \right) \quad (5.19)$$

where superscript 'S' indicates laminar flamelet solutions and σ_k is the RMS of Y_k^S. No alternative closure is suggested for J_{gkl}.

Data for *a priori* closure validation is scarce, the accuracy of some approximations has not yet been established (e.g. Eq. 5.13), and all existing studies rely on DNS of reactive mixtures in homogeneous, isotropic turbulence for the assessment of Eqs. 5.13-5.19. Sreedhara et al. [71] reported good qualitative and quantitative agreement between DNS and models based on the flamelet assumption with one notable exception: the flamelet model performed poorly for the closure of the dissipation term (Eq. 5.18). This is in contrast to the findings of Swaminathan and Bilger [72], but -in general- good performance of Eq. 5.18 cannot be expected in flames with local extinction since the flamelet approximation imposes certain gradients in mixture fraction space. This can best be illustrated by analysing conditionally averaged temperature or mass fractions of product species such as CO_2 and H_2O: their maxima around stoichiometric impose zero gradients while extinction and re-ignition events lead to a decorrelation of these scalars and mixture fraction resulting in the disappearance of the local minimum of dissipation around stoichiometry. It further needs to be emphasized that good quantitative agreement could only be established with additional scaling factors in Eqs. 5.17 and 5.19 that account for the "mismatch between mean scalar dissipation and mean reaction rate" [71]. Dissipation and temperature (and therefore reaction rate) are well correlated during extinction, however, they are rather uncorrelated during re-ignition leading to the need of

the additional parameter. These scaling factors need to be taken from DNS. Omitting these additional factors, Eqs. 5.17 and 5.19 introduce modelling errors of up to 100% and 30%, respectively. Furthermore, it should be noted that flamelet assumptions for the closure of the conditional variance equation lead to inconsistencies with the transport equation for the conditional mean: they could also be used to model $\langle w_k \mid \eta \rangle$.

Equations 5.15-5.16 provide decent agreement between models and DNS, but errors in peak values of up to 50% may occur. Sreedhara et al. [71] assessed different constants for C_k in Eq. 5.14. Standard values of $C_k = 1$ for major species and temperature and $C_k = 2$ for radicals tend to underpredict dissipation rates while order of magnitude estimates, exploiting proportionality of the gradient of radicals with $C_k = 1/\xi_{st}$ and of major species with $C_k = 1/\sqrt{\xi_{st}(1-\xi_{st})}$, lead to overpredictions. In terms of qualitative behaviour, this model represents the counterpart to the flamelet based model: it always predicts local maxima around stoichiometric and fails to predict local minima that occur while scalar and mixture fraction are well correlated. Last, Eq. 5.15 allows for similar freedom in choosing modelling constants. The correlation coefficient is unknown, and DNS data show large variations between -1 and +1 [48, 72]. Fortunately, $R_{N''Y_k''}$ is approximately constant in mixture fraction regions where the second derivative of Q_l is large, and the modelling of the third and fourth RHS terms in Eq. 5.12 with constant $R_{N''Y_k''} = O(1)$ is adequate.

Even though *a priori* analysis of all suggested closures is not quite satisfactory, predictions of the conditional variance and co-variances are promising. "Good" agreement has been achieved for conditionally averaged temperature and species RMS in several jet diffusion flames [29, 39]. However, second order closures have had limited impact on predictions of major scalars and temperature. Peak temperatures and O_2 mass fractions could markedly be improved in flames with local extinction and re-ignition (Sandia Flames D, E and F) [17, 29], however, leaving room for improvement. Temperature predictions in bluff body flames (flames HM1 and HM3) were hardly affected by changes to the modelling of the chemical source term [70], but effects on minor species are significant. All studies show clear improvements of predicted OH, NO and even CO levels and examples are presented in Fig. 5.2.

In contrast to the above where the second-order correction has been applied to only one or just a few reacting scalars, De Paola et al. [58] used second-order closure without any reduction in the dimensionality of the second-order correlation matrix, i.e. they solved transport equations for all $\langle Y_k'' Y_l'' | \eta \rangle$ and $\langle Y_k'' T'' | \eta \rangle$. The application to autoignition problems with a 32-species chemical mechanism that included low temperature autoignition was successful. The validity of some closures in the second-order CMC equation has also been explored by comparison with DNS of autoigniting jets [64].

It seems that some effects cannot be captured by second order closures, it is unclear why temperature predictions in bluff body flames are rather unimpressed by improved source term modelling and corrections to the chemical source term may not suffice here. It is unlikely that any - yet to be demonstrated - inaccuracy of closures for the variance equations can be blamed; variance and co-variances are reasonably well predicted but no sign of better temperature predictions in HM1 and

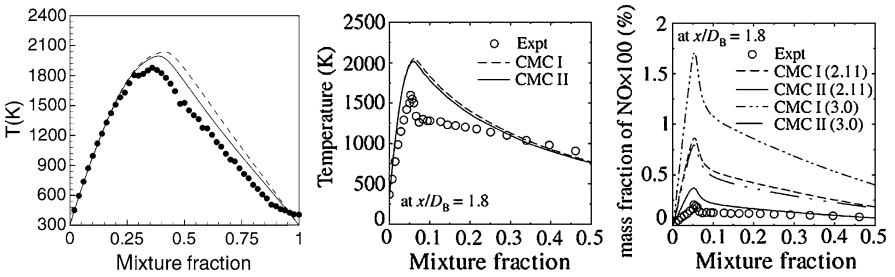

Fig. 5.2: CMC computations of temperature in Sandia Flame E (left), of temperature in the Sydney bluff body flame HM3 (centre) and of NO in HM3 (right). Computations (solid lines denote second order closure and dashed lines are results from first order closure) are from [29, 70] and measurements (symbols) are from [13, 19]. The numbers 2.11 and 3.0 in the right figure refer to GRI mechanisms used for the computations. Reprinted from [29, 70] with permission from the Combustion Institute.

HM3 can be detected. It is possible that the fluctuation terms themselves should not be neglected - after all Kronenburg and co-workers [42, 43] based their statement on the importance of e_y on DNS of reacting flows in homogeneous, isotropic turbulence. The strategy that is pursued in the next Section therefore aims at a reduction of the fluctuations themselves and problems may be avoided.

5.2.3 Advances in Doubly Conditioned Moment Closures

Large fluctuations around the conditional mean indicate that the conditioning variable does not sufficiently parameterize the combustion process. The introduction of further conditioning variables should reduce the fluctuations if a strong dependence of the reactive species on the new conditioning variables can be established, and suitable choices for these variables, their implementation and modelling issues are discussed next.

5.2.3.1 Basics of Double Conditioning

Traditionally, the flamelet equations suggest two quantities that parameterize the composition field: mixture fraction and scalar dissipation. We have seen above in Eqs. 5.17-5.19 that laminar flamelet assumptions can be invoked and instantaneous composition fields can be parameterized by mixture fraction and scalar dissipation if mixture fraction alone ceases to suffice as conditioning scalar. The introduction of scalar dissipation as second conditioning variable seems a particularly adequate choice in flames with flame extinction since large values of scalar dissipation are the cause of extinction and lead to flame quenching. Cha et al. [9] therefore intro-

duced scalar dissipation as second conditioning variable and formulated a closed set of equations for the computation of the evolution of the reactive scalars doubly conditioned on mixture fraction and scalar dissipation at $\eta = 0.5$. Their DNS of reactive scalars in homogeneous turbulence used 1-step chemistry and showed varying degrees of extinction and re-ignition. The results show that doubly conditioned CMC predicts extinction well, but unfortunately, the onset of re-ignition is predicted much too early. Scalar dissipation may be a good indicator of extinction events, however, scalar dissipation does not correlate well with species composition after flame extinction occurred. In addition, conditioning on instantaneous values of scalar dissipation neglect the importance of relevant chemical time scales on the flame. Very short events of very large dissipation values will not necessarily lead to extinction due to a finite response time needed by the flame. Similarly, events of low dissipation values (let them be long or short) will not automatically lead to re-ignition since re-ignition requires heat flux to the mixture.

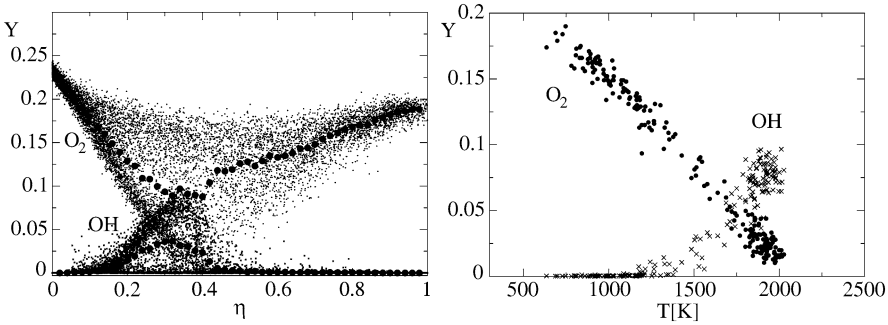

Fig. 5.3: Measurements of O_2 and OH mass fractions in a piloted jet diffusion flame (Sandia Flame F) at X/D=15. (a) O_2 and OH as function of mixture fraction, where filled symbols indicate the conditional means, and (b) O_2 and OH as function of mixture fraction ($\xi \approx \eta_{st}$) and temperature. Measurements are from [1]. Reprinted from [42] with permission from the Combustion Institute.

The key issue here is the lack of correlation of the chemical source term with scalar dissipation, and this results in the flamelet assumptions losing their validity. Now, we may want to remember our original goal of finding an accurate closure for the chemical source term. The chemical source term is largely dependent on the provision of fuel and oxidizer and on temperature. Therefore, Bilger [3] proposed conditioning on mixture fraction and sensible enthalpy and experimental data from a piloted jet diffusion flame with significant extinction provide support. Figure 5.3 (left) shows instantaneous mass fractions of O_2 and OH as function of mixture fraction at a downstream distance of X/D=15. Apparently, mixture fraction alone does not parameterize the flame well, and large scatter around the conditional mean can be observed. Figure 5.3 (right) shows the same data with mixture fraction values around $\xi = 0.351$ (the stoichiometric mixture fraction) as function of temperature.

Now the fluctuations have been greatly reduced, and we may be able to find fits through the data that correspond to the doubly conditioned means.

The governing equations for the doubly conditioned scalars result directly from Eq. 5.7 with $\mathbf{Z}^c = (\eta, \zeta)^T$, where ζ represents the sample space of normalized sensible enthalpy, $\hat{h}_s = \int_{T_0}^{T} c_p dT / \int_{T_0}^{T_{ad}} c_p dT$, and can then be written as

$$\frac{\partial Q_k}{\partial t} + \langle u_i \mid \eta, \zeta \rangle \frac{\partial Q_k}{\partial x_i} = \langle w_k \mid \eta, \zeta \rangle - \langle w_{h_s} \mid \eta, \zeta \rangle \frac{\partial Q_k}{\partial \zeta} + N_{11} \frac{\partial^2 Q_k}{\partial \eta^2} + N_{22} \frac{\partial^2 Q_k}{\partial \zeta^2} + 2N_{12} \frac{\partial^2 Q_k}{\partial \eta \partial \zeta} - \frac{1}{\rho_{\eta,\zeta} P(\eta, \zeta)} \frac{\partial \left[\rho_{\eta,\zeta} \langle u_i'' Y_k'' \mid \eta, \zeta \rangle P(\eta, \zeta) \right]}{\partial x_i} \tag{5.20}$$

As above, high Reynolds numbers have been assumed, differential diffusion effects are neglected and the doubly conditioned dissipation terms are defined as $N_{11} \equiv \langle D \nabla \xi \nabla \xi \mid \eta, \zeta \rangle$, $N_{22} \equiv \langle D \nabla \hat{h}_s \nabla \hat{h}_s \mid \eta, \zeta \rangle$ and $N_{12} \equiv \langle D \nabla \xi \nabla \hat{h}_s \mid \eta, \zeta \rangle$. The last RHS term may approximate zero due to the expected reduction in fluctuations around the mean. In principle, the number of conditioning scalars can be increased arbitrarily up to $n_c = n_{sc}$, but every addition of a conditioning variable increases the dimension of $\mathbf{Q}$, and more than two conditioning variables may not be feasible for the computation of combustion in 2- or 3-dimensional geometries. Two conditioning variables should suffice to characterize a wide range of flame regimes: mixture fraction is the key quantity for non-premixed combustion while sensible enthalpy constitutes a kind of a progress variable that characterizes species compositions in premixed flames. Realizations of species compositions should therefore be close to a two-dimensional space parameterized by mixture fraction and sensible enthalpy.

5.2.3.2 Modelling Partially Premixed Flames

An approach that employs conditioning on mixture fraction and sensible enthalpy should be ideally suited for the modelling of partially premixed flames where both the degree of mixing and the reaction progress determine fuel conversion and flame structure. A number of studies have dealt with reactive flows where significant local extinction leads to unburnt, partially premixed regions that later re-ignite due to turbulent and/or molecular diffusion of heat towards the premixed mixture. As indicated above Cha et al. [9] used DNS of flames with extinction and reignition in homogeneous turbulence to establish the lack of correlation between scalar dissipation and a reactive mixture during re-ignition, and in similar studies, Kronenburg [36, 43] assessed the suitability of mixture fraction and sensible enthalpy as conditioning variables. The latter studies demonstrate the potential of the doubly conditioned moment closure approach: the reactive species concentrations correlate well with ξ and $\hat{h}_s$ at all times, fluctuations around the doubly conditioned mean are very small, and CMC predictions agree very well with DNS data. The timing of extinction and the onset of re-ignition are captured accurately and the closure of chemical conversion rates can be based on doubly conditioned values. However, it shall not be

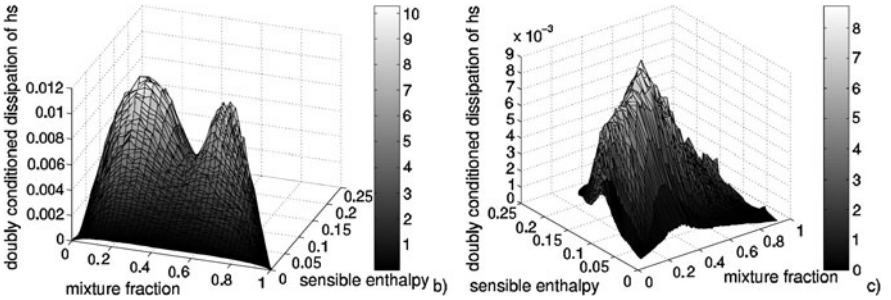

Fig. 5.4: DNS data of doubly conditioned dissipation of normalized sensible enthalpy at two different times: $t^* = 0.8$ (left) and $t^* = 2.5$ (right) where t^* denotes time normalized by the initial eddy turnover time. Reprinted from [36] with permission. Copyright © 2004, American Institute of Physics.

forgotten that double conditioning brings a whole host of new issues that need to be addressed. The doubly conditioned dissipation terms, N_{11} and N_{22}, and their cross-correlation, N_{12}, are not closed and need modelling. Hasse and Peters [22] suggest independence of the scalar dissipation of the respective second conditioning scalar. This may hold if - as in their case - both conditioning scalars are passive, mixture fraction-like. In a similar context, Nguyen et al. [56] parameterize the composition space by mixture fraction and a progress variable. They suggest independence of N_{11} of the progress variable and impose a functional dependence of N_{22} on mixture fraction such that local maxima occur at stoichiometric. This may hold when progress variable and mixture fraction are not well correlated, but should lead to gross overpredictions of the dissipation rate in regions where flamelet solutions exist. This is demonstrated in Fig. 5.4 for N_{22} with the help of DNS data [36]. Initially, temperature - and therefore sensible enthalpy - is a strong function of mixture fraction, temperature maxima exist where $\xi = \eta_{st}$, and N_{22} therefore tends to zero at locations with stoichiometric mixture. Local extinction destroys this correlation and the minimum of N_{22} at η_{st} disappears.

Accurate closures of the dissipation terms thus seem difficult and so far only been attempted as part of DNS related studies where the mean dissipation rates of mixture fraction and sensible enthalpy could be extracted from the DNS. In addition, the joint PDF of mixture fraction and sensible enthalpy and the conditionally averaged velocity do not result from the CMC equations and must be separately modelled. The modelling of the doubly conditioned dissipation rates can be avoided, if we solely focus on the modelling of the chemical source term. Bradley et al. [6] based their closure of the chemical source term on tabulated scalar fields that were obtained from flamelet solutions and parameterized by mixture fraction and temperature. Kronenburg and Kostka [42] improved the method slightly, and the assumption of a β-distribution of the conditional probability density function $P_{\xi,\hat{h}_s}(\zeta \mid \eta)$

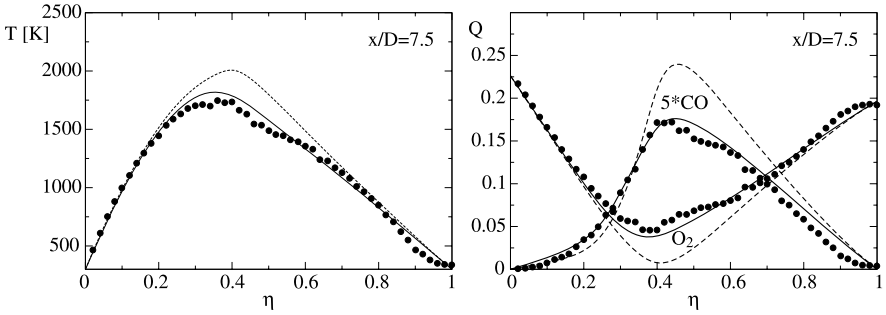

Fig. 5.5: Conditionally averaged temperature (left) and CO and O_2 mass fractions (right) at X/D=7.5 in Sandia Flame E. Symbols represent experimental data from [19], solid lines are CMC predictions with source term closure based on doubly conditioned moments and dashed lines are CMC predictions using a standard first order closure for $\langle w_k \mid \eta \rangle$. Reprinted from [42] with permission from the Combustion Institute.

proved accurate enough to achieve very good agreement of predicted temperature, major species and even CO and NO with measurements of the Sandia Flame series with progressive levels of extinction (Sandia Flames D, E and F). Examples of the results are shown in Fig. 5.5.

Here, we would like to remind the reader that source term modelling by second order closure has not quite led to the expected success with respect to temperature predictions in particular in bluff body flames, but also in flames with significant extinction. This may indicate the importance of the fluctuation terms and/or diffusion in progress variable space that is omitted in singly conditioned approaches. The very good results achieved in [42] may therefore be rather fortunate and accurate modelling of flame regimes with partial premixing may require the solution of the full doubly conditioned moment equations.

We should also mention that such approaches may be used for problems involving autoignition, where locally an autoignition spot is developed and flames propagate around it. The speed of such flames is larger than the conventional flame propagation in unburnt reactants due to the fact that the region away from the autoignition has also been reacting, albeit slowly, and is hence easier to jump to fully-fledged combustion through the action of diffusion of species and heat from the burning region; see Mastorakos [47] for a discussion and Wright et al. [80] for a demonstration of the importance of this quick propagation phase in diesel engines. Double-conditioning may also be used in flame expansion problems in multiple-injection diesel engines or following spark ignition in non-premixed systems; at present such phenomena are captured in single-conditioned CMC (often with acceptable accuracy) through the e_y-term [63, 76].

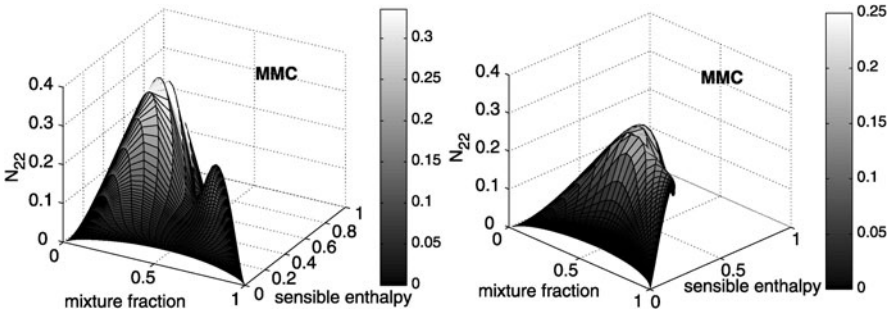

Fig. 5.6: Dissipation of sensible enthalpy predicted by MMC at times $t^* = 1.0$ (left) and $t^* = 2.0$ (right). Reprinted from [41] with permission from the Combustion Institute.

5.2.3.3 Possible Closures Using Multiple Mapping Conditioning

At this point we may want to anticipate Chapter 7 on Multiple Mapping Conditioning (MMC) without giving much detail on the method. We limit ourselves here to state that MMC is *PDF*- and *CMC-consistent*, i.e. the solution of the MMC equation for the conditioning scalars provides their joint probability distribution, and the MMC equations for the conditioned scalars are simple transformations of the CMC equations and therefore provide identical solutions. In this subsection it shall suffice to say that MMC implicitly provides a mapping closure for the conditionally averaged dissipation terms, it succeeds in capturing the evolution of the local minimum of N_{22} as shown in Fig. 5.6. In addition, the evolution of the joint probability of mixture fraction and sensible enthalpy is quite well approximated. MMC correctly predicts a conditional PDF of sensible enthalpy conditioned on mixture fraction with one peak at fully burning conditions and a second peak around $\hat{h}_s = 0.2$. A conventional (conditional) β-PDF would never predict the location of the second peak away from the bounds, and MMC is clearly superior to approaches using presumed PDFs, especially around stoichiometric.

MMC may appear as the solution to the closure issues addressed in the previous sections, but it shall not be forgotten that all the MMC studies presented in this subsection refer to a comparison of MMC with DNS data of reacting flows with reduced chemistry in homogeneous, isotropic turbulence. The feasibility of the method for laboratory flames needs to be assessed, and we may anticipate that extension to complex flow geometries may not be as simple as it first seems. Alternative stochastic implementations of MMC may be more favourable, and this is discussed in much more detail in Chapter 7.

5.2.4 Premixed Combustion

The conditional moment closure method has been derived for non-premixed combustion where mixture fraction makes for an ideal quantity that describes flame structure. We have seen above that the CMC method can be extended to partially premixed flames and further application to premixed flames is straightforward. Chemistry will be strongly linked to a progress variable, and simple first order closure of the chemical source term conditioned on this progress variable can be expected to yield accurate source term closures and pollutant predictions. Martin et al. [46] applied premixed CMC to a flame stabilized on a backward-facing step. This configuration shall mimic the flame stabilization mechanisms in a typical lean premixed gas turbine combustor where high mixing intensities justify the assumption of distributed reaction regimes and therefore spatial homogeneity of the conditional moments. The qualitative agreement between CMC predictions and experiments is good, and CMC with a detailed methane-air mechanism gives a much better match with the measurements than the reduced global mechanisms that are conventionally used in industrial CFD work.

Martin et al. [46] have demonstrated that CMC provides a suitable source term closure, however, CMC itself does not quite address some of the major issues associated with modelling premixed turbulent combustion: the evolution of the progress variable, in particular the temporal and spatial evolution of its probability distribution is one of the major research areas in turbulent combustion modelling (Chapters 4 and 6). Presumed probability distributions may suffice, but the solution of the transport equations for mean and variance require modelling of the mean scalar dissipation and the turbulent scalar flux, two quantities that involve some uncertainty in their modelling. Since the probability distribution $P(\zeta)$ is needed for full closure and the conditionally averaged scalar dissipation of the progress variable and the conditionally averaged turbulent scalar flux appear explicitly in the CMC equations, a series of CMC related studies were dedicated to the analysis of these terms [73, 74]. One of the key issues is the effect of reaction on the scalar dissipation of a reactive scalar. Often, these effects are neglected and dissipations of reactive and passive scalars are modelled equally. Swaminathan and Bray [74] however showed, that the dilatation effects need to be included in the modelling of N_ζ, and they suggested a simple algebraic closure for this quantity. The derivation of conditionally averaged dissipation rates is currently under way, but accurate modelling of the conditionally averaged turbulent flux seems a bit further off.

The two extremes of very fast and very slow chemistry shall be mentioned here, but will not be discussed further. Lee and Huh [44] proposed a zone conditional modelling of premixed flames which corresponds to a CMC approach where the PDF is approximated by two δ-functions at the extremes, and Bilger [5] introduced markers fields for the mapping of the progress variable that may be limited to low Damköhler numbers only. The reader is referred to the above references for more detail on these methods.

5.2.5 Liquid Fuel Combustion

A further area of CMC research that has been enjoying increasing attention recently is the modelling of reacting two-phase flows. It is postulated that liquid fuel combustion is largely determined by the evaporation rate and the mixing between fuel and oxidizer. Conditioning on mixture fraction appears as a promising concept for the accurate closure of the chemical source term. It is well established that in the presence of fuel evaporation, mixture fraction is no longer conserved and additional source terms appear in its transport equations of mean and variance [65]. Mortensen and Bilger [50] derived the fully consistent conditional moment closure equations for spray combustion. The derivation is based on the instantaneous single phase transport equations and a level set/indicator function technique is used to account for the interfaces. The final form of the singly conditioned moment closure equation for two phase flow can be written as

$$\begin{aligned}\frac{\partial Q_k}{\partial t}+\langle u_i \mid \eta\rangle\frac{\partial Q_k}{\partial x_i} &= N_\eta\frac{\partial^2 Q_k}{\partial \eta^2}+\langle w_k \mid \eta\rangle-\frac{1}{\langle\theta\rangle\rho_\eta P_\eta}\frac{\partial}{\partial x_i}\left[\langle\theta\rangle\rho_\eta\langle u_i'' Y_k'' \mid \eta\rangle P_\eta\right]\\ &+\left[Q_{1,k}-Q_k-(1-\eta)\frac{\partial Q_k}{\partial \eta}\right]\frac{\langle \Pi \mid \eta\rangle}{\langle\theta\rangle}\\ &-\frac{1}{\langle\theta\rangle\rho_\eta P_\eta}\frac{\partial}{\partial \eta}\left[(1-\eta)\rho_\eta\langle \Pi'' Y_k'' \mid \eta\rangle P_\eta\right] \qquad (5.21)\end{aligned}$$

where $Q_{1,k}$ denotes the conditionally averaged mass fraction of species k in the liquid droplet. Several new terms that involve the evaporation rate, Π, and its fluctuation appear in the final CMC formulation, and they require closure. The potential of these new equations has not yet been evaluated and closures have not yet been developed.

A simplified form of the CMC equations that neglected spray interactions was applied to studies of spray autoignition under engine-like conditions with some success. Kim and Huh [32] reported no influence of different models for the conditionally averaged evaporation rate on ignition delay times, and even the effects of different models for the closure of the mixture fraction variance equation are within 5%. The latter finding must be contrasted with the DNS studies by Réveillon and Vervisch [62] who analysed the mixing field and showed that droplet evaporation needs to be considered for the computation of the mixture fraction and its variance; it seems that the extra terms in the mixture fraction variance equation made a small contribution in the flow studied by Kim and Huh [32]. Similarly, Wright et al. [80] confirmed good agreement with measurements of ignition delay times and spray penetration lengths in high pressure chambers using CMC and neglecting the evaporation terms in the CMC and mixture fraction variance transport equations. However, it seems premature to arrive at any conclusions from the above engine-related studies on the importance of the modelling of the evaporation terms. The modelling by Kim and Huh [32] was based on a simplistic model for the conditionally averaged evaporation and compared with no closure. Equally, Wright et al. [80]

used zero closures for the variance and CMC equations. These studies simply show that auto-ignition delay times are not extremely sensitive to the correlations between evaporation and mixture fraction, but sufficient experimental data simply does not exist to allow any assessment of their importance on species predictions and flame structure.

Schroll et al. [77] have corroborated the adequacy of CMC for the modelling of droplet combustion. DNS of droplet evaporation and ignition with three different initial droplet diameters shows the lowest conditionally averaged dissipation at the most reactive mixture composition for the smallest droplets and CMC would therefore correctly predict the shortest ignition times for these smallest droplets. However, multiplication with the mixture fraction PDF and integration across mixture fraction space yields the highest unconditionally averaged dissipation for the smallest droplets that would lead - incorrectly - to the longest predicted ignition delay times for these droplets if estimates were based on unconditional values. The CMC concept is therefore ideally suited for the prediction of droplet combustion but some key issues, such as the modelling of the conditionally averaged evaporation rate and its correlation with species mass fractions and mixture fraction need to be addressed. The mixture fraction PDF and the modelling of the scalar dissipation in the presence of spray evaporation are also important to consider. It is fair to say that CMC of two phase flows is in its infancy, and thorough investigations will be needed for a better assessment of the viability of the method in real applications.

5.3 Application to Flows of Engineering Interest

As time progressed from the mid-90's when the first papers on CMC begun to appear, CMC simulations have developed from spatially-integrated formulations to fully three-dimensional applications with strong temporal and spatial variations of the conditional averages, thereby revealing the true strengths of the method. In addition, a shift from RANS to LES has begun to materialise, as well as the application to large furnaces with important radiation effects and to new fuels such as syngas. Some aspects of these simulations and numerical developments are discussed in this Section.

5.3.1 Dimensionality of the CMC Equation

When using the CMC method for realistic problems, first-order CMC, with single conditioning, is the virtually ubiquitous choice today. The key decision to be taken by the user is the spatial dimensionality of the CMC equation, which should reflect the physical nature of the problem, but also may be influenced by the available computational resources. The spatial resolution needed in the CMC equation should not be confused with the resolution needed in the calculation for the velocity or

mixture fraction fields. For statistically-steady attached flames in jets, for example, experiment has suggested that the conditional averages are weak functions of the radial coordinate. Therefore, ignoring streamwise turbulent diffusion and integrating the full CMC equation (Eq. 5.8) across the jet results in:

$$\langle \rho u_i \mid \eta \rangle^* \frac{\partial Q_k}{\partial x_i} = \rho_\eta N_\eta^* \frac{\partial^2 Q_k}{\partial \eta^2} + \langle w_k \mid \eta \rangle \tag{5.22}$$

with the starred quantity being a PDF-weighted integral:

$$\langle \phi \mid \eta \rangle^* = \frac{\int_V \langle \phi \mid \eta \rangle P_\eta dV}{\int_V P_\eta dV} \tag{5.23}$$

with V being the region of integration (line, plane or even volume). For transient problems, such as in diesel engines, volume integration may be performed to result in the time derivative $\partial Q_k / \partial t$ replacing the convective term on the LHS of Eq. 5.22.

The computational requirements for the numerical solution of the resulting parabolic equations is modest, even with quite detailed chemical mechanisms. This approach has provided results of very good accuracy for many problems, especially for jets. The similarity with transient flamelet modelling is evident, although the modelling of $\langle N|\eta \rangle$ and the exact way the volume integration is done tends to differ. Let us denote this simplification to the full multi-dimensional CMC equation as "0DCMC", implying the lack of spatial diffusion.

For some problems, there is little or no direct experimental evidence that the conditional averages are weak functions of space. In lifted jet flames, significant variations of Q_k have been measured [10]. In compression-ignition engines, experimental evidence points to a quite localised first emergence of ignition. Heat losses to engine walls and multiple injections also lead to variations in Q_k [59]. In spark ignition of non-premixed combustors [47], the conditional distributions switch from unburnt to burnt in different regions in space at different times. Such problems necessitate a multi-dimensional CMC formulation, which we will denote as "3DCMC". Numerical solution of the 3DCMC model has been attempted by various research groups and some details are given next.

5.3.2 Numerical Methods

The three-dimensional CMC equation (Eq. 5.8), after modelling the spatial diffusion term, can be written in more generic form as

$$\frac{\partial Q_k}{\partial t} + C(\mathbf{x},t,\eta)\nabla Q_k = N(\mathbf{x},t,\eta)\frac{\partial^2 Q_k}{\partial \eta^2} + \nabla \cdot (D(\mathbf{x},t,\eta)\nabla Q_k) + w_k(\eta, Q_2, \ldots, Q_{n_{sc}}) \tag{5.24}$$

where the coefficients C, N, D are, in general, functions of time, space $\mathbf{x}$, and mixture fraction η and contain information from the fluid mechanical field. Equation 5.24 is a 5-dimensional partial differential equation with a stiff chemical source

term, making its solution at least as challenging as the numerical simulation of a multi-dimensional laminar flame. The user of the elliptic CMC method must decide: (i) whether to solve this equation in its full 3D form or whether to perform some averaging across one of the spatial directions; (ii) the resolution to be used (i.e. the number of grid nodes in each spatial direction); (iii) the size of the chemical mechanism; (iv) the numerical method. Some compromises between the conflicting requirements of having very fine resolution in physical space with the wish to employ a very detailed chemical scheme may have to be made. Typically, central differences are used for discretizing the diffusion in mixture fraction space and for the second-order derivative in physical space, while upwind schemes have been used for the convective term. An alternative strategy to solve the CMC equation before dividing by the mixture fraction PDF, i.e. to solve for $P_\eta Q_k$, has also been proposed [11], but the comments below and the discretization issues apply to that formulation as well.

Assuming a detailed chemical mechanism with, say, $N_s = 50$ species, a discretization in mixture fraction space with $N_\eta = 100$ points, and a physical-space grid of, say, $N_x = N_y = N_z = 25$, and assuming that such a system were to be solved by the Method of Lines, which transforms the partial differential equation into a system of $N_s \times N_\eta \times N_x \times N_y \times N_z$ ordinary differential equations, we would arrive at a system of 75×10^6 o.d.e's. Considering the stiffness involved, which necessitates implicit schemes, the size of this system is just too large for present day solvers. Despite this, in two physical-space coordinates ($N_z = 0, N_x = N_y = 20$), this solution method has been used successfully with the GRI3.0 chemical mechanism and the VODPK solver [24, 25].

An alternative is to solve the CMC p.d.e. by a fractional step (operator splitting) method [16, 18, 23, 31, 59, 60, 80]. In such a scheme, one would solve the sequence

$$\frac{\partial Q_k}{\partial t} + C(\mathbf{x},t,\eta)\nabla Q_k = \nabla \cdot (D(\mathbf{x},t,\eta)\nabla Q_k) \tag{5.25}$$

$$\frac{\partial Q_k}{\partial t} = N(\mathbf{x},t,\eta)\frac{\partial^2 Q_k}{\partial \eta^2} \tag{5.26}$$

$$\frac{\partial Q_k}{\partial t} = w_k(\eta, Q_2, \ldots, Q_{n_{sc}}) \tag{5.27}$$

with each fractional step picking-up the solution from where the previous step left it and advancing it for a given timestep. The chemistry fractional step is the one that takes the most computational time; it will require separate solution of $N_\eta \times N_x \times N_y \times N_z$ stiff ordinary differential equations of the type $dQ_k/dt = w_k$. This is now more affordable, since the stiff solver will have to deal with a smaller system, but the solver used will need to be able to deal effectively with the "restart costs" when solving the chemical step while sweeping across the physical and mixture fraction grid nodes. Splitting the various phenomena incurs an error; this has been assessed [59, 80] and it is not negligible, but it can be controlled by a small enough timestep. The Method of Lines is of course more accurate, but as the size of the

chemical mechanism increases, the operator splitting approach is the only one that is practical.

It is evident that the numerical cost of solving the three-dimensional CMC equation is formidable, and experience shows that it is typically 50-90% of the total computational cost of the whole simulation. The computational burden of a well-resolved CMC simulation is not far from that of a low Reynolds number DNS.

For established flames, the discretization in mixture fraction space must follow the usual practice of clustering the grid nodes around stoichiometry; 50-100 grid nodes are the usual practice. For autoignition problems, the grid must be fine enough across the whole mixture fraction range to resolve the reaction fronts that will propagate across mixture fraction space following ignition [80]. For attached flames, the physical-space gradients are small and hence relatively coarse physical-space grids may be sufficient. Typical values are 10-20 grid nodes. For lifted jet flames, especially in the axial direction, a higher resolution is necessary. Note also the dangers of numerical diffusion associated with upwind differencing and coarse grids when having to resolve sharp transitions from Q_k corresponding to unburnt fluid to Q_k corresponding to burnt fluid.

Recently, Large-Eddy Simulations have begun to appear with CMC as the combustion sub-model. The CMC equation in LES is virtually identical to the RANS formulation discussed above [55]. Various specific choices concerning the sub-models for the conditional velocity and scalar dissipation must be made, especially since it must be recognized from the outset that the physical-space CMC grid will be coarser than the LES grid; this necessitates to develop a strategy concerning how can the fine-grid fluid mechanical quantities be provided to the coarse grid used to solve the CMC equation. Various options exist and are discussed in detail in [75]. The LES/CMC model has been applied to attached jet flames [55], bluff-body flames [52], autoigniting jets [53] and spark ignition problems [76]. The numerical cost here is very high. From a model development point of view, many of the sub-models that are being used have not been properly validated yet for LES.

5.3.3 Applications and Outlook

The CMC model has been used for gaseous statistically-steady flames. Some examples include non-premixed attached jet flames [66, 67, 69], attached bluff-body flames [28, 52, 70, 76], lifted jet flames [15, 24], autoigniting jets [53, 60, 61], and soot formation [78, 79]. It has also been used for transient methane jets [30, 68], heptane sprays [32, 80], and spark-ignition problems [76]. All these simulations have focused on simple geometries and have, in general, produced good results compared to experimental data. In addition to the DNS-based validation, these simulations have also provided more detailed assessment of specific sub-models. The CMC model has also been examined for reacting flows in porous media [34], chemical engineering [49] and atmospheric flows [7], demonstrating thus the wide applicability and usefulness of the method.

CMC is an attractive tool to model complicated geometries and problems. Multi-dimensional CMC has been used for diesel engines [59] and compartment fires [11, 12] and furnaces [23, 65] that have important radiation effects or low-oxygen combustion. The analysis of the results provides very useful insights on the flame structure and brings CMC to the point of practical calculations for design. First-order CMC with single conditioning and proper chemistry seems sufficient for many engineering problems (except for pollutant production, which may necessitate second-order corrections). For problems with significant variations of the conditional averages, such as extinctions, ignitions or quenching due to radiation or convective heat transfer to walls, the current practice is to use refined elliptic CMC.

However, future applications should not be limited to first-order CMC. Second order CMC provides a useful extension to first-order closures. Second-order CMC has been applied to various laboratory flames with decent results; the theoretical framework is well known, but a wider range of applicability would need to be established, and future efforts should be directed towards improved modelling of the conditional variance and co-variance equations, Eq. 5.12. Future progress in the application of double-conditioning approaches may be more challenging. Double conditioning is certainly attractive for (1) flames with partial premixing, for (2) flames with local extinction in the vicinity of the walls where the second conditioning variable could be a wall distance parameter or for (3) engine calculations with multiple injections. The latter has been attempted in a somewhat different framework by Hasse and Peters [22] with multiple conditioning on two different mixture fractions, however, all applications would require the closure of the doubly (or multiply) conditioned dissipation terms which is far from being trivial. Simplification as suggested by Hasse and Peters [22] are certainly not applicable to configurations with a reactive species as second conditioning scalar, and other alternative methods for closure would need to be applied. MMC might offer one possible solution, but modelling suggestions as brought forward by Nguyen et al. [56] should equally be pursued.

Double conditioning could also be applied to liquid fuel combustion where the second conditioning scalar describes the inter-droplet space. However, some more fundamental issues should be assessed in CMC of multiphase flows first, such as the effects of droplet evaporation and of the correlations between evaporation rate and reactive scalar field on conditional moments and on mixture fraction variance. Existing DNS studies and RANS calculations do not give a clear picture on the importance of these terms, and we would need to know under which conditions they become important and how they could be modelled.

But all these exciting new developments with respect to improvements of the chemical source term closure and two-phase flow modelling should not distract from implementation issues as addressed in Sections 5.3.1 and 5.3.2. In particular the dimensionality and also the CMC cell size need to be chosen carefully. Small CMC cells lead to cells with zero probability for some of the mixture fraction bins. In case of non-zero probability of these CMC bins in the neighbouring cells, it is not clear yet how to model convective and diffusive flux into a cell where a certain mixture fraction bin has zero probability. Standard practice is to neglect fluxes below a cer-

tain threshold value of the PDF, however, this may be inaccurate as new simulations for the determination of blow-out limits of lifted flames show [54]. This example simply illustrates that implementation can strongly affect the quality of the predictions, and much more work is needed to understand the correct treatment of zero- (or low) probability moments, in particular in LES-CMC.

5.4 Conclusion

It is of course not possible to give a complete and detailed review on all research activities of the last ten years related to the development and application of novel CMC techniques. The majority of research efforts had been directed towards improvements to the modelling of the conditioned chemical source term and towards CMC applications to flows of practical interest. We have therefore focused in this chapter on rather detailed summaries of second order closures, double conditioning and issues related to CMC in more complex flow geometries. The CMC methodology has advanced within the last ten years, and this chapter should be therefore viewed as complementary to Klimenko and Bilger's review [35]. We hope that it offers some stimuli to new researchers in the field for continued work on the conditional moment closure method.

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