Computations of turbulent lean premixed combustion using conditional moment closure

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Conditional Moment Closure (CMC) is a suitable method for predicting scalars such as carbon monoxide with slow chemical time scales in turbulent combustion. Although this method has been successfully applied to non-premixed combustion, its application to lean premixed combustion is rare. In this study the CMC method is used to compute piloted lean premixed combustion in a distributed combustion regime. The conditional scalar dissipation rate of the conditioning scalar, the progress variable, is closed using an algebraic model and turbulence is modelled using the standard $k$–$\varepsilon$ model. The conditional mean reaction rate is closed using a first order CMC closure with the GRI-3.0 chemical mechanism to represent the chemical kinetics of methane oxidation. The PDF of the progress variable is obtained using a presumed shape with the Beta function. The computed results are compared with the experimental measurements and earlier computations using the transported PDF approach. The results show reasonable agreement with the experimental measurements and are consistent with the transported PDF computations. When the compounded effects of shear-turbulence and flame are strong, second order closures may be required for the CMC.

Keywords: lean premixed flames; conditional moment closure (CMC); conditional scalar dissipation rate

Nomenclature

- $c$: progress variable
- $\bar{c}$: Reynolds averaged $c$
- $\tilde{c}$: Favre averaged $c$
- $c''$: Favre fluctuation of $c$
- $c_p$: specific heat capacity at constant pressure
- $C_{e1}$: constant in the $k$–$\varepsilon$ model
- $C_3$, $C_4$: model parameters in Equation (12)
- $D$: jet port diameter
- $Da$: Damköhler number
- $D_\alpha$: molecular diffusivity of species $\alpha$
- $h$: total enthalpy
- $h^i$: sensible enthalpy
- $\Delta h_{f,\alpha}^i$: enthalpy of formation of species $\alpha$
- $\tilde{k}$: Favre average turbulent kinetic energy (TKE)

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1. Introduction

The combustion of fossil fuels can significantly disturb the natural carbon cycle on our planet [1] leading to global warming [2]. This is mainly because of increased CO₂ levels in the atmosphere resulting from the combustion of hydrocarbons. Also, pollutants such as oxides of sulphur and nitrogen produced by the combustion of fossil fuels often reach the upper atmosphere and drift into regions where natural rain clouds are regularly formed. These pollutants will ultimately fall to the ground in the form of acid rain causing severe damage to our environment, cultural heritage and life in general [3]. Despite these effects,
the use of fossil fuels, especially for high power density applications like transport, will remain imminent until a paradigm shift in transport technology is achieved. Thus, emission legislation is becoming more stringent in order to curtail these detrimental effects, which forces us to develop highly efficient and less polluting combustion systems.

Fuel-lean premixed combustion has the potential to meet these two demands simultaneously, but it is susceptible to combustion oscillation and stability issues, as has been identified in many earlier studies [4–11]. Instability, which is an undesirable aspect of lean premixed combustion, can reduce the life, emission characteristics and efficiency of systems significantly [12]. This combustion mode involves strong interactions between turbulence, chemical reactions and molecular diffusion, and thus its modelling is challenging. However, combustion models capturing these interactions accurately with the ability to predict emissions are required in the design and development of the next generation of lean combustion systems. This requirement provides the impetus for this study.

Flamelet based methods such as the flame surface density method, the $G$-equation method, and the BML (Bray–Moss–Libby) approach and its derivatives are widely used for turbulent premixed flames [11, 13]. These methods consider the turbulent flame as a collection of laminar flames, which is acceptable if the flame scales are much smaller than the turbulence scales and thus the laminar flame structure is undisturbed by the turbulence. Even if the turbulence scales become smaller than the laminar flame scale, the flamelet concept can be used if the reaction zone thickness is smaller than the small-scale turbulent (Kolmogorov) eddies. However, if the reaction time scale for a scalar becomes larger than the typical time scale for small-scale turbulent eddies then the use of flamelet based ideas to compute that particular scalar becomes an issue [14, 15]. Pollutants such as carbon monoxide and nitric oxides are good examples of this. Alternative methods such as Conditional Moment Closure (CMC) [16–18] and transported Probability Density Function (transported PDF) [19] can be employed. The transported PDF approach has been used in many past studies [20–24] for turbulent premixed flames. The CMC method has been developed and validated for non-premixed flames and a brief survey of such work can be found in [25]. An application of this methodology to a turbulent premixed flame behind a backward facing step demonstrated its potential [26]. However, as we shall see in the next section, central issues concerning modelling of the conditional dissipation rate, turbulent transport of conditional fluxes, differential diffusion effects, etc. have yet to be investigated thoroughly. Amzin et al. [27] addressed some of these issues and used the CMC to compute the piloted turbulent stoichiometric methane–air premixed Bunsen flame of Chen et al. [28]. The aim of this work is to test the CMC methodology for premixed flames further by computing piloted premixed jet flames with strong finite rate chemistry effects. These flames were investigated in earlier studies both experimentally [29–31] and numerically [32, 33] and posses good challenges for combustion modelling. The reason for this will become evident while describing the flame conditions and configuration in Section 3.

The outline of this paper is as follows. In the next section, the CMC method for premixed combustion is discussed. The test flames and their attributes relevant for this study are described briefly in Section 3. The computational details are discussed in Section 4 followed by the results and a discussion in Section 5. The conclusion of this study is summarised in the final section.

2. Conditional Moment Closure method

The CMC method is based on the hypothesis that the fluctuations of species mass fractions, temperature and enthalpy in turbulent flames are associated with the fluctuation of a key
scalar \[18\], which is the mixture fraction, \(Z\), for non-premixed combustion and the progress variable, \(c\), for premixed combustion. The mixture fraction is a passive scalar that describes the stoichiometry of the reacting mixture and measures the fuel–oxidiser ratio. It is defined such that \(Z = 0\) in the oxidiser stream and \(Z = 1\) in the fuel stream. The progress variable is a reactive scalar and it can be defined based on temperature or using the fuel mass fraction \[11\]. An alternative definition using the sensible enthalpy is also possible \[18\]. Here, it is defined as
\[
c = 1 - \frac{Y_f}{Y_u} f,
\]
using the fuel mass fraction, where \(Y_u\) is the unburnt fuel mass fraction value, which is used as the conditioning variable in this study. A governing equation for this quantity can be obtained using the transport equation for \(Y_f\) and the instantaneous equation for \(c\) is
\[
\frac{\rho}{c} \frac{\partial c}{\partial t} + \rho u_i \frac{\partial c}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D_c \frac{\partial c}{\partial x_i} \right) + \rho \dot{\omega}_c,
\]
with a Fickian diffusion. The reaction rate is given by \(\dot{\omega}_c = -\dot{\omega}_f / Y_u\).

In CMC, the conditional average of scalar \(\alpha\) is defined as \(Q_\alpha(\zeta; x, t) \equiv \langle Y_\alpha(x, t) | c = \zeta(x, t) \rangle\), with the angle brackets denoting the ensemble averaging of samples satisfying the condition to the right of the vertical bar. The symbol \(\zeta\) is the sample space variable for \(c\).

Transport equations for the conditional mean scalar values, \(Q_\alpha\), are derived by substituting \(Y_\alpha(x, t) = Q_\alpha(\zeta; x, t) + y_\alpha(x, t)\) in the transport equation for the instantaneous scalar value \(Y_\alpha\) \[18\]. The symbol \(y_\alpha\) denotes the conditional fluctuation of scalar \(\alpha\). It is to be noted that density weighted conditional averaging \[18\] must be used. An alternative approach using the velocity–scalar joint probability density function (PDF) is also possible \[18\]. Both of these approaches essentially yield the same transport equation for the conditional mean, \(Q_\alpha\), which is written as \[18, 34\]
\[
\langle \rho | \zeta \rangle \frac{\partial Q_\alpha}{\partial t} + \langle \rho u_i | \zeta \rangle \frac{\partial Q_\alpha}{\partial x_i} - \frac{Le_\alpha}{Le_c} \langle \rho N_c | \zeta \rangle \frac{\partial^2 Q_\alpha}{\partial \zeta^2} =
\]
\[
\langle \dot{\omega}_\alpha | \zeta \rangle - \langle \dot{\omega}_c | \zeta \rangle \frac{\partial Q_\alpha}{\partial \zeta} - \frac{1}{\bar{p}(\zeta)} \frac{\partial}{\partial x_i} \left[ \langle \rho u_i' y_\alpha(x, t) \bar{p}(\zeta) \rangle \right] + e_{Q_\alpha},
\]
where \(Le_\alpha\) is the Lewis number for species \(\alpha\) and \(\bar{p}\) is the Favre PDF of \(c\). The physical meaning of the various terms in Equation (2) is as follows. The first and second terms of Equation (2) denote, respectively, the unsteady and convective changes of \(Q_\alpha\). The third term represents the diffusion of the conditional average in the sample space \(\zeta\). The fourth term is the chemical reaction rate for species \(\alpha\). Since \(c\) is a reactive scalar, see Equation (1), the influence of the conditioning variable on the evolution of \(Q_\alpha\) is given by the fifth term in Equation (2). The sixth term represents the contribution of conditional fluctuation, \(y_\alpha\), to \(Q_\alpha\) evolution. The last term represents the contributions of the molecular diffusion of \(Q_\alpha\) in physical space and the differential diffusion of mass and heat, is given by
\[
e_{Q_\alpha} = \left\{ \frac{\partial}{\partial x_i} \left( \rho D_{\alpha} \frac{\partial Q_\alpha}{\partial x_i} \right) + \rho D_{\alpha} \frac{\partial \zeta}{\partial x_i} \frac{\partial}{\partial x_i} \left( \frac{\partial Q_\alpha}{\partial \zeta} \right) + \frac{\partial Q_\alpha}{\partial \zeta} \frac{\partial}{\partial x_i} \left[ \left( 1 - \frac{Le_\alpha}{Le_c} \right) \rho D_{\alpha} \frac{\partial \zeta}{\partial x_i} \right] \right\} | \zeta |,
\]
where \(Le_\alpha\) is the Lewis number for species \(\alpha\). The molecular diffusion, the first term in Equation (3), is negligible for high Reynolds number flows, and the differential diffusion,
the last term of Equation (3), remains as the dominant term, which can be written as [34]

\[ e_{Q_\alpha} \approx \frac{1}{\tilde{\rho}(\zeta)} \left( 1 - \frac{\text{Le}_\alpha}{\text{Le}_c} \right) \frac{\partial Q_\alpha}{\partial \zeta} \frac{\partial N_c \tilde{p}}{\partial \xi}. \]  

(4)

This term depends on \( \text{Le}_\alpha \). If \( \text{Le}_\alpha / \text{Le}_c = 1 \) this term is zero, which indicates that there are no differential diffusion effects. For this study, \( \text{Le}_c \approx 1 \) and the values of \( \text{Le} \) for the various species involved in a given chemical mechanism are specified using the values in [35]. However, an earlier study [27] showed that the magnitude of \( e_{Q_\alpha} \) is very small for major species compared with minor species. Also, the contribution of this term to various unconditional averages was shown to be negligible [27] and thus this particular term will be ignored for this study. This, however, does not imply that the molecular diffusivity is the same for various species and this effect comes through the diffusive flux of \( Q_\alpha \) represented by the third term of Equation (2). Since the conditional dissipation rate is multiplied by the ratio of Lewis numbers as in Equation (2), the effective diffusivity will be different for different species; the conditional average of lighter species is expected to diffuse quicker. It is known that the balance between reaction, diffusion and convection is delicate for premixed flames and thus the above effect must be retained in their CMC calculation on physical grounds. This essentially implies that the assumption of \( \text{Le}_\alpha = \text{Le}_c \) is unacceptable on physical grounds for premixed flames although it is attractive for computations. Thus, \( \text{Le}_\alpha \neq \text{Le}_c \) and the contribution of \( e_{Q_\alpha} \) to Equation (2) is neglected for this study.

The quantities \( \langle \rho u_\gamma y_\alpha | \zeta \rangle \), \( \tilde{p} \), \( \langle \rho u_i | \zeta \rangle \), \( \langle \dot{\omega}_\alpha | \xi \rangle \) and \( \langle N_c | \zeta \rangle \) require suitable models and appropriate initial and boundary conditions to solve Equation (2). The turbulent flux term is modelled using the gradient transport hypothesis as

\[ \langle u''_i y_\alpha | \eta \rangle = -\mu_t \frac{\partial Q_\alpha}{\partial x_i}, \]  

(5)

where \( \text{Sc}_\alpha \) is the turbulent Schmidt number for scalar \( \alpha \). Theoretical analysis [36], experimental [37, 38] and DNS [39, 40] studies pointed out the existence of both gradient and counter gradient unconditional scalar fluxes in premixed flames. The possibility of having a counter gradient conditional scalar flux has been noted [41] and this can be included in the CMC through a second order approach by solving a transport equation for \( \langle u''_i y_\alpha | \eta \rangle \). This approach will be studied in a future work, however the gradient transport model is used in the current work for simplicity.

The PDF of the progress variable is modelled using a presumed shape given by the beta function as

\[ \tilde{p}(\zeta) = C \xi^{a-1} (1 - \zeta)^{b-1}, \]  

(6)

where

\[ C = \frac{1}{\beta(a, b)}, \quad a = \tilde{c} \left( \frac{1 - g}{g} \right), \quad b = (1 - \tilde{c}) \left( \frac{1 - g}{g} \right), \]  

(7)

with \( g = \tilde{c}^{\alpha \xi} / \tilde{c}(1 - \tilde{c}) \) as the variance parameter and \( \beta(a, b) = \int_0^1 \xi^{a-1} (1 - \xi)^{b-1} \text{d}\xi \). The conditional velocity is modelled using a linear model which showed good agreement with DNS results while other modelling approaches are also available [34]. This linear model is
given by

\[ \langle u_i | \xi \rangle = \tilde{u}_i + \frac{u''_i c''}{c''^2} (\xi - \tilde{c}), \quad (8) \]

where \( \tilde{u}_i \) is the unconditional mean velocity and \( \frac{u''_i c''}{c''^2} \) is the correlation between the velocity fluctuations and the progress variable fluctuations. The velocity–scalar fluctuation correlation is modelled using the gradient flux approximation, which also influences the conditional velocity values. Since \( c''^2 \) is zero in the unburnt and burnt mixtures, the conditional velocities \( \langle u_i | \xi \rangle \) must be equal to the respective unconditional values.

The conditional mean reaction rate is closed using a first order CMC closure [18] as

\[ \langle \dot{\omega}_\alpha (\rho, Y_\alpha, T) | \xi \rangle = \dot{\omega}_\alpha (\langle \rho | \xi \rangle, Q_\alpha, Q_T), \quad (9) \]

where \( Q_T \) is the conditional temperature. The conditional density is obtained using the equation of state and \( Q_T \) through

\[ P = R Q_T \langle \rho | \xi \rangle, \quad (10) \]

where \( R \) is the gas constant.

The conditional mean scalar dissipation rate \( \langle N_c | \xi \rangle \) appearing in Equation (2) is related to the unconditional mean scalar dissipation rate, \( \bar{\rho} \bar{\varepsilon}_c = \bar{\rho} D_c (\partial c''/\partial x_i)(\partial c''/\partial x_i) \) through \( \bar{\varepsilon}_c = \int_0^1 \langle N_c | \xi \rangle \bar{p} \, d\xi \). This relationship can be used to obtain a simple model for the conditional dissipation rate as noted in earlier studies [42, 27] and this model is given by

\[ \langle N_c | \xi \rangle = \frac{\bar{\varepsilon}_c \, f(c)}{\int_0^1 f(c) \bar{p}(c) \, dc}, \quad (11) \]

where \( f(c) \) is a known function obtained from an unstrained laminar flame calculation [42]. The Favre mean scalar dissipation rate, \( \tilde{\varepsilon}_c \), is modelled using a simple algebraic model developed in [43] and it is given by

\[ \tilde{\varepsilon}_c = \frac{1}{\beta'} \left[ (2K_c^* - \tau C_4) \frac{S_0}{\delta_I} + C_3 \bar{k} \right] \tilde{c'', \quad (12)} \]

where \( \beta' = 6.7, \, K_c^* = 0.85 \tau \) for hydrocarbon–air flames, \( C_4 = 1.1/(1 + Ka)^{0.4} \) and \( C_3 = 1.5 \sqrt{Ka}/(1 + \sqrt{Ka}) \). The Karlovitz number is \( Ka = [(2(1 + \tau)^{0.7} \tau (u'/S_\eta)^3 (\delta_{II}/\Lambda))^{0.5} \]

using the turbulence rms velocity \( u' \) and its integral length scale \( \Lambda \). The unstrained laminar flame speed is \( S_0^* \), its thermal thickness is \( \delta_I^* \) and the heat release parameter is \( \tau = (T_b - T_u)/T_u \), where the subscripts \( b \) and \( u \) denote the burnt and unburnt mixtures, respectively. The Favre averaged turbulent kinetic energy and its dissipation are denoted by \( \tilde{k} \) and \( \tilde{\varepsilon} \), respectively. The strong coupling between molecular diffusion and reaction in premixed combustion recognised in earlier studies [21, 22] and the consistency between \( \tilde{\varepsilon}_c \) and \( \langle N_c | \xi \rangle \) are maintained in this approach [27].

The unconditional means are obtained using

\[ \bar{Y}_\alpha = \int_0^1 Q_\alpha \bar{p}(\xi) \, d\xi. \quad (13) \]
An arbitrarily complex chemistry can be used in the CMC to obtain $\langle \dot{\omega}_u | \zeta \rangle$ and $\langle \dot{\omega}_c | \zeta \rangle$ appearing in Equation (2).

All the aforementioned unclosed terms are common for both the CMC and transported PDF approaches. In the transported PDF approach, nevertheless, the reaction rate appears in closed form and thus no modelling is required for it. The conditional dissipation rate and velocities require modelling in both approaches.

3. Test flames

The test flames used in this study are the piloted lean premixed flames of Dunn et al. [30]. The Piloted Premixed Jet Burner (PPJB) used in the experimental study [30], shown in Figure 1, consists of a central jet of a lean premixed methane–air mixture with an equivalence ratio of 0.5 and temperature of 300 K, and a pilot issuing stoichiometric premixed methane–air products. The central jet and the pilot have diameters of 4 and 23.5 mm, respectively. These two streams are surrounded by a hot co-flow from lean premixed laminar H$_2$–air flames with an equivalence ratio of 0.43. The diameter for this hot co-flow is 197 mm. The pilot and the hot co-flow streams flow with small uniform velocities of 0.8 and 0.7 m/s.

![Figure 1. Schematic diagram of the premixed Bunsen burner from [29,30].](image)
Table 1. Properties of the streams of PM1-50 and PM1-200 flames.

| Stream    | D (mm) | $U_0$ (m/s) | $T$ (K) | $\phi$ | Mixture               |
|-----------|--------|-------------|---------|--------|-----------------------|
| Jet       | 4      | 50, 200     | 300     | 0.5    | CH$_4$–air (reactant) |
| Pilot     | 23.5   | 0.8         | 2280    | 1      | CH$_4$–air (products) |
| Co-flow   | 197    | 0.7         | 1500    | 0.43   | H$_2$–air (products)  |

respectively [30]. Four flames are considered in the experimental study and are designated as PM1-50, PM1-100, PM1-150 and PM1-200 with central jet bulk mean velocities, $U_o$, of 50, 100, 150 and 200, respectively [30]. The Reynolds numbers, Re, based on the central jet velocity, diameter $D$, are 12,500, 25,000, 37,000 and 50,000, respectively. The PM1-50 and PM1-200 flames, which have the lowest and highest bulk mean velocities, are considered for this computational investigation. A uniform velocity of 0.2 m/s is specified to account for ambient air entrainment. The characteristics of these streams are summarised in Table 1 for the PM1-50 and PM1-200 flames.

The conditions of these four lean flames are shown in a turbulent combustion regime diagram depicted in Figure 2. These flames are located in the distributed combustion regime based on the turbulence conditions measured at location $x/D = 15$ and $r/D = 0.53$ using laser Doppler velocimetry [31]. The chemical length and time scales are larger than the turbulence scales in this regime. Hence, applying flamelet based methods to these flames may be inappropriate. Note that the values of $\Lambda/\delta_{\theta o}$ for the PM1-50 and PM1-200 flames are 2.4 and 1.8, respectively, and the values of $u'/S_{\theta o}$ are 47 and 443, respectively [44]. The unstrained planar laminar flame speed computed using the PREMIX code of CHEMKIN [45] and the GRI-3.0 chemical mechanism is $S_{\theta o} = 0.051$ m/s and this value is about 6% larger than the value reported by Dunn et al. [31]. Of the four flames investigated experimentally [31], the two extreme cases, summarised in Table 1, are chosen to test the CMC methodology.

Figure 2 also shows the combustion conditions of the stoichiometric flames F1 to F3 of Chen et al. [28] investigated by Amzin et al. [27] using CMC. These flames are located in the thin reaction zones and near the corrugated flamelets regimes. The combustion

![Figure 2](image-url). Premixed combustion regime diagram showing the PM-flames of [31] and F-flames of [28].
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conditions of the lean flames of Dunn et al. [30, 31, 44] are markedly different from those of the stoichiometric flames. Turbulent eddies are expected to penetrate the reaction zones in lean flames causing local extinction. As noted earlier, the \( u' / S^* \) values are so large that they yield Damköhler numbers, \( Da \), very much smaller than unity, i.e. 0.05 and 0.004 for PM1-50 and PM1-200 flames, respectively. These are significantly smaller than the \( Da \) values of the stoichiometric flames in [28]. Thus, the finite rate chemistry effects are expected to be stronger in the lean flames, especially in PM1-200 considered here. As remarked by Klimenko and Bilger [18], the contribution of CMC for premixed combustion is expected to be in capturing the finite rate chemistry effects and thereby predicting species such as CO with slow chemical time scales. Furthermore, it has been noted by Amzin et al. [27] that the CMC methodology holds in all regimes of premixed combustion as it does not invoke any explicit assumption of the influence of turbulent eddies on the flame front structure while deriving Equation (2). However, its accuracy and validity are determined by the assumptions used to obtain sub-models. The capability of RANS-CMC was tested for the thin reaction zones regime in an earlier study [27] and its prediction was observed to be similar to those by other combustion modelling approaches such as flamelets and joint scalar PDFs. The predictive ability of the CMC in the distributed combustion regime is tested in this study by simulating turbulent lean premixed flames. These flames have been used in earlier studies to validate premixed turbulent combustion models such as transported PDF models [31, 32] and large eddy simulation with laminar chemistry [33].

4. Computational details

The computational tool used in this study has been validated in previous CMC studies for stoichiometric premixed flames F1 to F3 marked in Figure 2 [27] and non-premixed combustion [46]. This computer code includes transport equations for the Favre averaged mass, momentum, total enthalpy, progress variable and its variance, mixture fraction and turbulence kinetic energy and its dissipation rate. Models for the source/sink terms in the CMC equations, see Equation (2), are also included. The implementations of these equations and models are discussed in [27].

The Favre averaged continuity, momentum, total enthalpy and turbulence \((k–\varepsilon)\) equations are solved on the physical grid along with transport equations for \( \tilde{c}, c''^2 \) and three fluid markers to be described later in this section. Since three streams with different mixture composition and enthalpy are mixing in the experimental flame considered in this study, one must solve the total enthalpy equation. This also allows us to have sub-adiabatic conditions for the pilot and coflow streams.

Transport equations for the Favre-averaged progress variable and its variance are written as

\[
\frac{\partial \rho \tilde{c}}{\partial t} + \frac{\partial (\rho u_i \tilde{c})}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D_c \frac{\partial c}{\partial x_i} - \rho u_i'' c'' \right) + \tilde{\omega}_c, \quad (14)
\]

and

\[
\frac{\partial \rho c''^2}{\partial t} + \frac{\partial (\rho u_i c''^2)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D_c \frac{\partial c''^2}{\partial x_i} - \rho u_i'' c''^2 \right) - 2 \rho u_i'' c'' \frac{\partial \tilde{c}}{\partial x_i} - 2 \rho \tilde{c}^2 + 2 c'' \tilde{\omega}_c. \quad (15)
\]
The dissipation rate of $c^{\prime\prime}$ is modelled using Equation (12). The source terms $\bar{\omega}_c$ and $c^{\prime\prime}\bar{\omega}_c$ are modelled in a manner consistent with the CMC as

$$\bar{\omega}_c = \int_0^1 \langle \dot{\omega}_c | \zeta \rangle p(\zeta; x) \, d\zeta$$  \hspace{1cm} (16)$$

and

$$c^{\prime\prime}\bar{\omega}_c = \int \zeta \langle \dot{\omega}_c | \zeta \rangle p(\zeta) \, d\zeta - \bar{\omega}_c \int \langle \dot{\omega}_c | \zeta \rangle p(\zeta) \, d\zeta.$$  \hspace{1cm} (17)$$

The Reynolds PDF, $p$, is related to the Favre PDF through $\overline{p \tilde{p}} = \langle \rho | \zeta \rangle p$.

A schematic of the computational domain for the test flame used in this study is shown in Figure 3 along with the boundary conditions for various scalars. The progress variable variance is specified to be zero at all the boundaries. It must be noted that the three streams not only have different enthalpies but also have different composition and equivalence ratio as given in Table 1, and thus three passive scalars (fluid markers) are required to account for the mixing of these streams. Thus, transport equations for $\tilde{Z}_1$, $\tilde{Z}_2$ and $\tilde{Z}_3$, are included in the simulation and this equation for scalar $\tilde{Z}_k$ is written as

$$\frac{\partial (\overline{p \tilde{Z}_k})}{\partial t} + \frac{\partial (\overline{p \tilde{u}_i \tilde{Z}_k})}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D_{Z_k} \frac{\partial \tilde{Z}_k}{\partial x_i} - \rho u_i^{\prime\prime} \overline{Z_k^{\prime\prime}} \right).$$  \hspace{1cm} (18)$$
This helps us to track the fluids emerging from the jet, pilot and hot co-flow streams and to account for the effects of mixing of these streams with entrained air. Thus, each stream has its own designated markers, $\tilde{Z}_1$, $\tilde{Z}_2$ and $\tilde{Z}_3$ and their values are set to be unity at the inlet of the appropriate streams as shown in Figure 3. Furthermore, these markers obey the condition $\tilde{Z}_1 + \tilde{Z}_2 + \tilde{Z}_3 + \tilde{Z}_4 = 1$, which is used to obtain $\tilde{Z}_4$.

These markers are used in the following manner to obtain the average temperature $\tilde{T}$.

The total enthalpy computed using its transport equation at a given grid point in the physical space is written as

$$
\tilde{h} = h^s + \Delta h^o_{f, \text{mix}},
$$

where $\tilde{Y}_\alpha$ is the Favre-averaged mass fraction of species $\alpha$ at the grid point, which is computed using Equation (13). The symbols $\tilde{Y}_\alpha,2$ and $\tilde{Y}_\alpha,3$ denote the mass fractions of species $\alpha$ in streams 2 and 3 at the respective inlets. The enthalpy of formation for species $\alpha$ is $\Delta h^o_{f,\alpha}$ and the enthalpy of formation for air is taken to be zero. From the above equation, one can easily verify that the temperature of the incoming streams, given in Table 1, are recovered by using the boundary values for $\tilde{Z}_1$, $\tilde{Z}_2$ and $\tilde{Z}_3$ marked in Figure 3.

The progress variable is defined using the fuel mass fraction as noted in Section 2. This choice is guided by the expected physical behaviour of the flame brush in the chosen test cases and it gives a unique and unambiguous region for the flame brush which is expected between the jet and pilot streams. If one defines $c$ using the mass fraction of (CO+CO$_2$) then $\tilde{c}$ would be one for the stoichiometric pilot and zero for the jet co-flow containing products of H$_2$–air combustion and ambient air (see Figure 3). If the mass fraction of H$_2$O is used then $\tilde{c}$ would be zero for the jet, 1.51 for the pilot, 1.25 for the hot co-flow and zero for the ambient air. Values larger than one result from H$_2$O mass fractions in the pilot and hot co-flow streams being larger than the burnt mixture value for the CH$_4$–air jet reactant mixture at $\phi = 0.5$. If the temperature is used to define $c$ then $\tilde{c} = 0$ for the jet, one for the pilot, 0.606 for the hot co-flow and zero for the ambient air. From these boundary values, one sees that there will be more than one region (mixing layers) with non-zero gradient of $\tilde{c}$. The spatial variation of $\tilde{c}$ implies a flame brush since $c$ signifies changes due to chemical reaction in premixed combustion. Thus, one would see multiple flame brushes when $c$ is defined using the choices, except the fuel mass fraction, noted above. This behaviour is unphysical and not observed in the experiments of Dunn et al. Thus, $c$ based on the fuel mass fraction is used in this study and its boundary conditions are given in Figure 3.

The inlet velocity profile is specified using the bulk mean value, $U_0$, as $u(r)/U_0 = (1 - r/R)^{1/7}$, where $R$ is the radius of the main jet port. Uniform velocities of 0.8 and 0.7 m/s are specified at the inlets of the pilot and hot co-flow streams, respectively. A small uniform velocity of 0.2 m/s is specified for the surrounding air. A uniform value for the mean turbulent kinetic energy, $k_o$, at the centreline of the fuel nozzle exit, is obtained from $I = u'/U_0 = \sqrt{2k_o/3}/U_0$. The axial rms velocity, $u'$, for the cold and reacting conditions of both flames selected for this investigation is reported in the experimental study [30]. The
initial value for the turbulent kinetic energy dissipation rate, $\tilde{\varepsilon}_o$, at the centreline of the fuel nozzle exit is obtained using $\tilde{\varepsilon}_o = C_\mu \bar{\tilde{\varepsilon}}^3 / \Lambda$, with $C_\mu = 0.7$. The turbulence is modelled using a standard $k-\varepsilon$ model with changes to $C_\varepsilon$ (from 1.44 to 1.6) to account for the round jet anomaly [47].

A SIMPLER approach [48] is used to couple the velocity and pressure fields inside the computational domain. The CMC equations are then solved using the models described in Section 2 along with the mean fluid dynamic and turbulence quantities. Contributions from $e_{Q\alpha}$ are neglected based on an earlier investigation [27]. This simply implies that $e_{Q\alpha}$ contributions are relatively weak compared with contributions from other terms of Equation (2). The non-unity Lewis number effect is felt through the diffusion of the conditional average in the sample space (see the third term of Equation (2)) as noted in Section 2. The mean density obtained using the conditional density is fed back to the fluid dynamics solver part. These processes are iterated in a serial code until convergence criteria are met for all quantities of interest as shown in Figure 4. A single simulation on an Intel(R) Xeon(R) CPU X5450 3.00 GHz processor took about 700 hours on the wall clock to yield a fully converged solution. Nearly 85% of this time was spent on the CMC part, the loop marked ‘CMC solver’ in Figure 4. The computational time can be reduced by using parallel programming, which has yet to be implemented in this code.

The combustion kinetics is modelled using the GRI-mechanism [49]. An unstrained laminar flame computed using this mechanism as noted in Section 3 is used to specify the initial and boundary conditions for the CMC equations after mapping the laminar solution from the physical space to $\zeta$ space.

The computational domain spans 600 mm in the axial direction, $x$, and 300 mm in the radial direction, $r$. The CFD computational domain has 150 cells in the axial direction and

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**Figure 4.** Computational sequences in the CMC program.
100 × 100 cells in the other two directions. The computational grid is non-uniform near the jet, pilot and hot co-flow streams with the smallest cell size being 1 × 1.6 (in millimetres). As in the earlier study [27], the CMC grid has 500 non-uniform cells in ζ space, which were required to resolve the strong gradients in ζ space. Two cells in each direction of the physical space grid for the RANS equations are combined to create the physical space grid for the CMC equations since the conditional averages are expected to vary slowly in the physical space. The sensitivity of the computed solution to the grid size is tested by doubling the size of the smallest cell, while retaining the growth rate for the cell size. The solution shows negligible sensitivity, and thus the grid resolution noted above is used for the results reported in this paper. The solutions computed in this way by the RANS-CMC approach are compared with the experimental data reported in [29, 31] in the following discussion.

5. Results and discussion
The turbulence models and boundary conditions used in this calculation are assessed first by comparing the non-reacting flow results for both the PM1-200 and PM1-50 flames selected for this study. Figures 5 and 6 compare the calculated mean and rms values of the axial velocity. These values are normalised using the bulk mean velocity, $U_0$, at the jet exit. The non-reacting and reacting flows are denoted by the letter ‘N’ and ‘R’, respectively, in these figures. The normalised mean axial velocities agree well with the measurements for the non-reacting cases as shown in Figures 5(a) and 6(a). A similar level of agreement is also seen for $u'/U_0$ in Figures 5(b) and 6(b) for the non-reacting cases. These comparisons suggest that the boundary conditions used in the simulations mimic the experimental conditions well and the standard $k$-$\varepsilon$ turbulence model is adequate for the mixing of three streams. Also, the turbulence production due to shear is captured satisfactorily by the turbulence modelling used in this study.

It is to be noted that $u'$ shown in Figures 5(b) and 6(b) is obtained from the calculated $\tilde{k}$ using $u' = \sqrt{2\tilde{k}/3}$, whereas in the experiments it is a period weighted mean calculated using $u' = \sqrt{\sum_{i=1}^{n} [u(t_i) - \bar{U}]^2 \Delta t_i / \sum_{i=1}^{n} \Delta t_i}$, where $n$ is the number of realisations and $\Delta t_i$ is the gate period in the measurements for the $i$th realisation of the velocity [29].
The agreement in $\tilde{U}/U_0$ is very good for the PM1-50 flame as shown in Figures 5(a) and is satisfactory for the PM1-200 flame with some over-prediction as depicted in Figure 6(a). There are some differences in $u'/U_0$ as in Figures 5(b) and 6(b). However, the trend in the axial variation of the centreline quantities is captured satisfactorily in the calculation. The agreement between the measured and calculated $u'/U_0$ is acceptable for $x/D \leq 25$ in the PM1-50 flame and for $x/D \leq 10$ and $x/D \geq 35$ in the PM1-200 flame. The reason for this is as follows. Dunn et al. [30] showed that the flame brush in PM1-50 is conical extending up to $x/D \approx 40$ using a time-averaged luminosity image (see their figure 3) suggesting that the chemical (flame) effects on the fluid dynamics are strong in this region. The variation of $\tilde{U}/U_0$ shown in Figure 5(a) suggests that $\tilde{U}/U_0$ is nearly constant for $x/D \leq 25$ and thus the shear induced turbulence inside the flame brush is very small leading to small $u'/U_0$ as in Figure 5(b) for $x/D \leq 25$ and this variation is captured satisfactorily in the computation. As Figure 5(a) suggests, the shear effects on the turbulence start to increase for $x/D \geq 25$ and these effects are compounded by flame induced effects. Thus, the $u'/U_0$ value starts to increase for $x/D \geq 25$ and this compounded effect is not fully captured by the standard $k-\varepsilon$ turbulence modelling leading to substantial under-prediction in $u'/U_0$ for $x/D > 25$ as in Figure 5(b).

The flame luminosity image of Dunn et al. [30] for the PM1-200 case showed that the flame luminosity decreases beyond $x/D \approx 13$ and becomes very small for $x/D \geq 35$. This suggests that the flame induced effects on turbulence become negligible for $x/D \geq 35$. The variation of $\tilde{U}/U_0$ shown in Figure 6(a) suggests that the shear induced effects will increase for $x/D \geq 13$. Thus, the compounded effects of shear-turbulence and flame are strong in the region $10 \leq x/D \leq 35$ where the standard $k-\varepsilon$ model is unable to predict the variation of $u'/U_0$ as in Figure 6(b). Since turbulence effects dominate in the region $x/D \geq 35$, the standard turbulence modelling used in this study does a very good job in that region. Similar behaviour is also expected at large axial distances for the PM1-50 flame, but unfortunately no experimental data are available beyond $x/D = 40$ to confirm this.

5.1. Conditional mean mass fractions

The conditional mean mass fraction, $Q_\alpha$, is obtained by solving the CMC equation, Equation (2) without $e_{Q_\alpha}$. However, this does not imply that the Lewis number for different species is taken to be the same as noted in Sections 2 and 4. The typical variation of conditional mean mass fractions for some selected representative major and minor species is shown.
Figure 7. Variation of the conditional mean mass fraction with $\zeta$ for major (respectively, minor) species for the PM1-200 flame at $\tilde{c} = 0.45$ and (a) (respectively, (b)) $x/D = 4.5$, (c) (respectively, (d)) $x/D = 6.5$, and (e) (respectively, (f)) $x/D = 8.5$.

in Figure 7 for the PM1-200 flame. The results are shown for $\tilde{c} = 0.45$ for three axial locations, $x/D = 4.5, 6.5$ and 8.5. Note that the values of H$_2$ and OH are multiplied by 40 and 20, respectively, for plotting purposes. The unstrained laminar CH$_4$–air premixed flame with $\phi = 0.5$ shown in this figure is computed using the PREMIX code and the GRI-mechanism as noted earlier in Section 4 and flame parameters such as the flame speed and gradient based thickness computed in this study are close to those reported in [31].
Figure 8. Typical variation of the normalised conditional scalar dissipation rate, $(N_c|\zeta) = \langle N_c \rangle (\delta_o^s / S_o^s)$, obtained in the CMC calculations of PM1-50 and PM1-200 flames for $\tilde{c} = 0.45$ at $x/D = 4.5$ (a) and $x/D = 10.5$ (b).

Figure 9. Variation of the Favre PDF, $\tilde{p}(\zeta)$, at selected locations across the flame brush of the PM1-50 flame (a) and the PM1-200 flame (b).

The variation of conditional averages of major species in the sample space is very close to those found in the unstrained laminar flame. However, the representative minor species variation with $\zeta$ in the CMC calculation is similar to those observed in the laminar flame, except for molecular hydrogen. In the laminar flame, the hydrogen mass fraction varies

| $\tilde{c}$ | $\tilde{c}^{\nu^n}$ | $\tilde{Z}_1$ | $\tilde{Z}_2$ | $\tilde{Z}_3$ | $r/D$ |
|------------|----------------|------------|------------|------------|--------|
| 0.1        | 0.027          | 0.971      | 0.026      | 0.0025     | 0.17625 |
| 0.2        | 0.063          | 0.931      | 0.061      | 0.006      | 0.3152  |
| 0.3        | 0.097          | 0.894      | 0.094      | 0.011      | 0.3575  |
| 0.4        | 0.129          | 0.857      | 0.126      | 0.015      | 0.3875  |
| 0.5        | 0.161          | 0.821      | 0.158      | 0.020      | 0.4425  |
| 0.6        | 0.193          | 0.784      | 0.190      | 0.024      | 0.4725  |
| 0.8        | 0.145          | 0.635      | 0.308      | 0.055      | 0.6275  |
Table 3. Values of $\bar{c}$, $\bar{c}'$, $\bar{Z}_1$, $\bar{Z}_2$, $\bar{Z}_3$ and $\bar{Z}_4$ in the PM1-200 flame for the PDFs shown in Figure 9.

| $r/D$ | $\bar{c}$  | $\bar{c}'$ | $\bar{Z}_1$ | $\bar{Z}_2$ | $\bar{Z}_3$ | $\bar{Z}_4$ |
|-------|------------|------------|-------------|-------------|-------------|-------------|
| 0.1   | 0.030      | 0.964      | 0.0181      | 0.017       | 0.3102      |
| 0.2   | 0.051      | 0.925      | 0.035       | 0.039       | 0.3375      |
| 0.3   | 0.094      | 0.883      | 0.054       | 0.062       | 0.3975      |
| 0.4   | 0.143      | 0.848      | 0.069       | 0.081       | 0.42512     |
| 0.5   | 0.141      | 0.809      | 0.087       | 0.103       | 0.4875      |
| 0.6   | 0.205      | 0.761      | 0.101       | 0.136       | 0.5125      |
| 0.8   | 0.155      | 0.620      | 0.126       | 0.252       | 0.6601      |

Figure 10. Normalised mean velocities from the CMC calculation are compared with the experimental data [29] and transported PDF calculations in [29, 31] for the PM1-200 flame.
Figure 11. Normalised mean velocities from the CMC calculation are compared with the experimental data [29] and transported PDF calculations in [29, 31] for the PM1-50 flame.

little with a sharp drop near $\zeta = 0$ and $\zeta = 1$, but the conditional mean value for hydrogen shows a peak near $\zeta \approx 0.84$. The conditional averages of major and minor species does not seem to vary with axial distance as shown in Figure 7 and the radial variation is also observed to be negligible. A strong variation is seen only across the conditioning variable, $\zeta$. The variations of conditional means for the PM1-50 flame are similar to those shown here. These results suggest that the spatial variation in the unconditional means must come about through the changes in the PDF of $\zeta$ as per Equation (13).

5.2. Behaviour of $\langle N_c|\zeta \rangle$ and $\bar{\rho}(\zeta)$

The typical variations of the conditional dissipation rate, $\langle N_c|\zeta \rangle$, normalised using $S_{i,n}$ and $\delta_{i,n}$ are shown in Figure 8 for the PM1-50 and PM1-200 flames. The results are shown for $\bar{c} = 0.45$ at two axial locations; $x/D = 4.5$ and 10.5. The turbulence level in the PM1-200 flame is larger than in the PM1-50 flame, and thus the conditional mean dissipation rates are substantially larger in the PM1-200 flame. The variation of $\langle N_c|\zeta \rangle^+$ with $\zeta$ shown in Figure 8 is similar to that observed for the stoichiometric premixed methane–air flames in [27], but the $\langle N_c|\zeta \rangle^+$ magnitudes are different. This is because of the difference in the thermo-chemical and turbulence conditions of the lean flames considered here. The chemical reactions are expected to be strong around $\zeta \approx 0.8$ for hydrocarbon flames because of the large activation energy and thus $\langle N_c^+|\zeta \rangle$ peaks around this $\zeta$ value as shown in Figure 8. This behaviour remains the same as in Figure 8(b) for a downstream location as one would expect. However, the peak value of $\langle N_c|\zeta \rangle^+$ increases by about 20% between the two locations shown in Figure 8. This is because of the increase in turbulence level due to the shear production mechanism. The influence of turbulence on the conditional dissipation
Normalised rms velocities from the CMC calculation are compared with the experimental data [29] and transported PDF calculations in [29] for the PM1-200 flame.

rate can be seen in Equations (11) and (12). Thus, it seems that the conditional dissipation rate model used in this study captures the behaviour of $\langle N_c|\xi \rangle$ in the flamelets, turbulence effects and their interactions.

The Favre PDF of the progress variable, obtained using the presumed Beta function for the given Favre mean and variance is shown in Figure 9 for the PM1-50 and PM1-200 flames. The Favre mean, $\tilde{c}$, and variance, $\tilde{c}'^2$, are obtained from their respective transport equations, Equations (14) and (15). Their values along with the values of $\tilde{Z}_1$, $\tilde{Z}_2$ and $\tilde{Z}_3$ for the locations shown in Figure 9 are given in Table 2 and 3, respectively, for the PM1-50 and PM1-200 flames. These PDFs are shown for seven different radial positions, denoted by $\tilde{c}$, at a given axial location of $x/D = 4.5$. The corresponding radial positions are given in Table 2 and 3. Unlike for the stoichiometric premixed flames, F1 to F3 in Figure 2, computed by Amzin et al. [27], these PDFs are not bimodal across the flame brush. The bimodal PDF limit given by $c'c'' = \tilde{c}(1 - \tilde{c})$ is observed only for high values of $\tilde{c}$ as one observes in
Figure 13. Normalised rms velocities from the CMC calculation are compared with the experimental data [29] and transported PDF calculations in [29] for the PM1-50 flame.

Table 2 and 3 – at locations very close to the burnt side of the flame brush, i.e. $\tilde{c} \geq 0.85$, bimodal PDFs are observed for both the PM1-50 and PM1-200 flames. The mono-modal behaviour of this marginal PDF is typical of the distributed combustion regime.

5.3. **Comparison to measurements**

Variations of the centreline mean and rms values of the axial velocity are shown in Figures 5 and 6, which are discussed earlier in this section. The agreement between the measured and computed mean velocities is good although some over-prediction is observed for the PM1-200 flame. When the shear-turbulence effects are compounded by the flame effects, the turbulence models used in this study under-predict the rms velocity, otherwise the agreement between the measured and computed rms values is good. However, the general trend is captured quite well in this study.

The radial variation of the computed and measured mean velocity, normalised using $U_0$, in the streamwise direction is shown in Figures 10 and 11, respectively, for the PM1-200 and PM1-50 flames. The results are shown for six axial locations for the PM1-200 flame and four axial locations for the PM1-50 flame. The results for $u'/U_0$ are shown in Figures 12 and 13, respectively, for the PM1-200 and PM1-50 flames for the streamwise locations shown in the figures for the mean velocities. The trends and variations seen in these figures are typical for turbulent flames established in a piloted jet with co-flows. Also, results from earlier studies [29, 31] using the transported joint scalar PDF modelling approach with two turbulence models are shown in these two figures for comparison. These studies with the transported PDF methodology use $C_{\epsilon_1} = 1.6$ and the Euclidean Minimum Spanning Tree (EMST) mixing model to represent conditional diffusion, which is closely related to the
Figure 14. Mean temperatures computed in the CMC calculation are compared with the experimental data [29], the transported PDF calculations in [29] and the VFJPDF calculations in [32] for the PM1-200 flame.

conditional dissipation rate appearing in the CMC equation, Equation (2). The agreement between the measured and computed values using CMC is good for $x/D = 5$ and the CMC values are larger than the measurements for other locations in Figure 10. This is because of the compounded effects of flame, turbulence from the shear-production mechanism and their interactions noted earlier in this section. These effects are not fully represented in the standard $k-\varepsilon$ turbulence model. The results from the transported PDF calculations [29] seem to confirm this observation. Furthermore, a reasonably good comparison between the measurements and computational results, specifically for CMC, seen in Figures 11 and 13 offers further confirmation of this observation. Overall, the mean and rms values of axial velocity computed using the CMC methods are closer to the experimental values for the
Figure 15. Mean temperatures computed in the CMC calculation are compared with the experimental data [29], the transported PDF calculations in [29] and the VFJPDF calculations in [32] for the PM1-50 flame.

Figure 16. Radial variation of $Y_{CO} \times 10^3$ computed in the CMC calculation is compared with the experimental data [29], the transported PDF calculations in [29] and the VFJPDF calculations in [32] for the PM1-200 flame.
The small scale mixing was modelled using EMST and the reaction was modelled through the In Situ Adaptive Tabulation (ISAT) approach as in the transported PDF calculations reported in [29]. The VFJPDF results are shown only for \( x/D = 30 \) and 45 for the PM1-200 flame, and \( x/D = 15 \) and 25 for the PM1-50 flame, and the results for other axial locations are not reported in [32].

The adiabatic flame temperature for the jet mixture is 1480 K and thus the high temperature of about 2200 K seen at \( r/D \approx 1 \) for \( x/D = 2.5 \) is due to the stoichiometric CH\(_4\)-air pilot, which is located in the region \( 0.5 < r/D < 2.94 \) at \( x/D = 0 \). A temperature of about 1500 K seen for \( r/D \geq 3 \) is the product temperature for a \( \phi = 0.43 \) H\(_2\)-air mixture. The drop in the mean temperature to a value of about 1300 K near \( r/D = 3 \) for \( x/D = 2.5 \) in the measurement is due the heat transfer to the unignited stoichiometric pilot stream through the walls between the hot co-flow and pilot stream, as shown by Rowinski and Pope [32]. These heat transfer effects are not included in the CMC calculations reported in this study and thus the computed temperature is larger than the measured value for this location. If one wishes to include these effects then the computational boundaries shown in Figure 3 are expanded.
must include the wall and its thickness, and a conjugate heat transfer model should be used. They are excluded from this study for simplicity and also the sensitivity of the computed results to the heat loss is small for locations beyond \( x/D = 2.5 \), which is demonstrated by Rowinski and Pope [32].

The experimental data in Figure 15 suggest that the shrouding effect of the stoichiometric pilot persists (mean temperature larger than 1500 K) even at \( x/D = 15 \) for the PM1-50 flame, whereas it is seen only at \( x/D = 2.5 \) for the PM1-200 flame. The luminosity images shown in [31, figure 2] and [30, figure 3] suggest that the shrouding effect of the pilot persists for the full length \( (x/D \sim 40) \) of the PM1-50 flame and it prevails only up to \( x/D \sim 5 \) in the PM1-200 flame. There is a reasonable representation of these effects in the CMC calculations as one observes in Figures 14 and 15. The measured centreline \( (r/D = 0) \) values in the PM1-200 flame are captured quite well by all the computational models up to \( x/D = 15 \) as
Figure 19. Radial variation of $Y_{\text{OH}} \times 10^6$ computed in the CMC calculation is compared with the experimental data [29] and the transported PDF calculations in [29] for the PM1-50 flame.

one sees in Figure 14. Beyond this axial location, the computed mean temperature at $r/D = 0$ is substantially larger than the measured values. Rowinski and Pope [32] showed that just the mixing of the hot co-flow and products of the jet mixture occur beyond $x/D \sim 30$ by setting the reaction rate to zero in their calculation. It is also to be noted that the radiative heat loss is not included in the CMC and PDF calculations compared here. So this heat loss effect may be required for the downstream locations, while the upstream locations may be insensitive to this effect due to the shrouding of the hot pilot. Furthermore, as noted earlier in this section, the turbulence-chemistry interaction may be stronger beyond $x/D \sim 15$ and thus the first order CMC closure may be inadequate to capture the local extinction observed for this flame in the experiments. These observations need to be verified in a future study.

Since the shrouding effects extend far downstream in the PM1-50 flame, the agreement in the centreline values of the mean temperature is improved for the PM1-50 flame, although some over-prediction is observed for the $x/D = 25$ location. The radial variation at $x/D = 25$ computed in the CMC calculation is close to that from the VFJPDF calculation. In general, the temperature variations computed using CMC and different flavours of the transported PDF approach are not too far from one another.

The radial variation of the mean mass fractions of CO computed in this study using CMC are compared with the experimental measurements and results from PDF computations [29, 31] in Figures 16 and 17 for the PM1-200 and PM1-50 flames, respectively. Note that the mass fraction value is multiplied by $10^3$. Generally, the CMC results are closer to the measured CO mass fraction values in the PM1-50 flame as shown in Figure 17. For the PM1-200 flame, the peak value of the CO mass fraction inside the lean flame brush at $x/D = 2.5$ is under-predicted by the CMC and PDF methods. There is something of an
over-prediction for other locations, but the trend is captured quite well by the CMC and PDF models. The comparison of computed and measured mean mass fractions of OH is shown in Figures 18 and 19 for the PM1-200 and PM1-50 flames, respectively. At \( x/D = 2.5 \), the CMC gives good prediction compared with the PDF models for both the PM1-200 and PM1-50 flames, and for other locations there is a general over-prediction of OH mass fraction for both the CMC and PDF models. This over-prediction is too high for the PM1-200 flame and similar for both the CMC and PDF models. It is interesting to note a similar behaviour for the reactive scalar mean mass fractions and temperature, despite a vast difference in the modelling methods used. Rowinski and Pope [32] showed that the over-prediction for the PM1-200 flame is because the reaction rates in this flame are small and the reactions have to be slowed down by a factor of five in their PDF calculation to obtain a good match with measured mean mass fraction values and temperature. The CMC results shown here suggest that this observation also applies to the CMC calculation. Further calculations are, however, required to verify this, which forms a basis for future investigation.

6. Summary and conclusion

The conditional moment closure method has been well developed for non-premixed combustion in many past studies, but and its application to premixed combustion is rare. The CMC method has been applied to premixed combustion in a dump combustor in the past, showing good agreement with experimental results [26]. However, the closure for the conditional scalar dissipation rate used in that study was not fully satisfactory. The close coupling among turbulence, chemical reaction and molecular diffusion in premixed combustion and their influences on the conditional dissipation rate must be represented in the conditional dissipation rate model. Such a model developed in [43] was used by Amzin et al. [27] in conjunction with the CMC method to simulate turbulent piloted stoichiometric CH\(_4\)–air premixed combustion showing encouraging results. These flames of Chen et al. [28] are in the thin reaction zones regime of turbulent premixed combustion. Amzin et al. [27] also argued that the CMC method can be applied across the turbulent combustion regime. However, the validity is governed by the assumptions used to derive the sub-models for the CMC method. In this study, CMC is applied to piloted turbulent lean CH\(_4\)–air premixed combustion investigated experimentally by Dunn [29] and Dunn et al. [30, 31]. These lean flames, called PPJB flames, are in the distributed combustion regime and are thus considerably challenging for combustion modelling.

In this paper, the conditional dissipation rate required for the CMC method is closed using an algebraic model used in [27]. The reaction rate is closed using first order CMC closure and the combustion kinetics is mimicked using the GRI-3.0 chemical kinetics mechanism for methane–air combustion. The conditional scalar fluxes are modelled using the gradient flux approximation as in [27]. The PDF of the progress variable, the conditioning scalar \( \xi \), is obtained using an assumed Beta function shape. The turbulence is modelled using a standard \( k–\varepsilon \) closure. The computer code used by Amzin et al. [27] is also used in this study to simulate PM1-200 and PM1-50 flames of the PPJB set. These two flames have the extreme conditions in the experimental set shown in Figure 2. The boundary conditions and model setup are validated first by simulating the non-reacting cases in the PPJB set.

The conditionally averaged scalar mass fractions are observed to vary by a very small amount in the axial direction for both the PM1-200 and PM1-50 flames. The marginal PDF of \( \xi \) is found to be mono-modal, which is different from the commonly observed bi-modal shape (seen in [27] for the piloted stoichiometric flames) in premixed combustion.
However, the mono-modal shape is expected for combustion occurring in the distributed combustion regime. The computed values of mean and rms of the axial velocity agree quite well with the measured values in regions without the compounded effects of shear turbulence, combustion, and their interaction. A consistent behaviour for the temperature, scalar mass fraction, and velocity is seen in the CMC, calculation supporting the above observation. Generally, the computed values for the PM1-50 flame are in reasonably good agreement with the measured values, compared with the PM1-200 flame. This is because the finite rate chemistry effects, shear-turbulence, and their interactions are large in this flame, offering a considerable challenge for turbulent combustion modelling. Rowinski and Pope [32] systematically varied the local reaction rate using a scaling factor and showed that considerably low (five times smaller) reaction rates are required to observe good agreement with measured temperature and scalar mass fractions in the PM1-200 flame. This suggests a considerable level of local extinction (a large reaction intermittency) implying that a second order CMC closure may be required for the PM1-200 flame. The radiative heat loss may also have to be included to have the reduced reaction rate through reduced temperature. These factors will be addressed in a future study. It is also worth noting that the CMC results are comparable to the results from different flavours of the transported PDF method.

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References
[1] R.A. Houghton, The contemporary carbon cycle, in Treatise on Geochemistry, D.H. Holland and K.K. Turekian, eds., Pergamon, Oxford, UK, 2003, pp. 473–513.
[2] M. Maslin, Global Warming: Causes, Effects and the Future, LLC and Voyageur Press, Minneapolis, MN, 2007.
[3] C.N. Lane, Acid rain: Overview and Abstracts, Nova Science, New York, 2003.
[4] B.S. Brewster, S.M. Cannon, J.R. Farmer, and F. Meng, Modeling of lean premixed combustion in stationary gas turbines, Prog. Energy Combust. Sci. 25 (1999), pp. 353–385.
[5] S.M. Correa, A review of NOx formation under gas turbine combustion conditions, Combust. Sci. Technol. 87 (1993), pp. 329–362.
[6] J.B. Heywood, Pollutant formation and control in spark-ignition engines, Prog. Energy Combust. Sci. 1 (1976), pp. 135–164.
[7] J.F. Driscoll, Turbulent premixed combustion: Flamelet structure and its effect on turbulent burning velocities, Prog. Energy Combust. Sci. 34 (2008), pp. 91–134.
[8] Y. Huang and V. Yang, Dynamics and stability of lean-premixed swirl-stabilized combustion, Prog. Energy Combust. Sci. 35 (2009), pp. 293–364.
[9] T. Echekki and E. Mastorakos, Turbulent Combustion Modeling: Advances, New Trends and Perspectives, Springer, Heidelberg, 2011.
[10] N. Swaminathan and K.N.C. Bray, Turbulent Premixed Flames, Cambridge University Press, Cambridge, UK, 2011.
[11] D. Veynante and L. Vervisch, Turbulent combustion modelling, Prog. Energy Combust. Sci. 28 (2002), pp. 193–266.
[12] T. Lieuwen, H. Torres, C. Johnson, and B.T. Zinn, A mechanism of combustion instability in lean premixed gas turbine combustors, J. Eng. Gas Turb. Power 123 (2001), pp. 182–189.
[13] K.N.C. Bray, Laminar flamelets and the Bray, Moss, and Libby model, in Turbulent Premixed Flames, 1st ed., N. Swaminathan and K.N.C. Bray, eds., Cambridge University Press, Cambridge, UK, 2011, pp. 41–60.
[14] R.W. Bilger, Future progress in turbulent combustion research, Prog. Energy Combust. Sci. 26 (2000), pp. 367–380.
[15] R.W. Bilger, S.B. Pope, K.N.C. Bray, and J.F. Driscoll, Paradigms in turbulent combustion research, Proc. Combust. Inst. 30 (2005), pp. 21–42.
[16] A.Y. Klimenko, Multi-component diffusion of various admixtures in turbulent flow, Fluid Dynam. 25 (1990), pp. 327–334.

[17] R.W. Bilger, Conditional moment closure for turbulent reacting flow, Phys. Fluids A 5 (1993), pp. 436–444.

[18] A.Y. Klimenko and R.W. Bilger, Conditional moment closure for turbulent combustion, Prog. Energy Combust. Sci. 25 (1999), pp. 595–687.

[19] S.B. Pope, PDF methods for turbulent reactive flows, Prog. Energy Combust. Sci. 11 (1985), pp. 119–192.

[20] S.B. Pope and M.S. Anand, Flamelet and distributed combustion in premixed turbulent flame, Proc. Combust. Inst. 20 (1984), pp. 403–410.

[21] M.S. Anand and S.B. Pope, Calculations of premixed turbulent flames by PDF methods, Combust. Flame 67 (1987), pp. 127–142.

[22] A. Mura, F. Galzin, and R. Borghi, A unified PDF–flamelet model for turbulent premixed combustion, Combust. Sci. Technol. 175 (2003), pp. 1573–1609.

[23] R.P. Lindstedt and E.M. Vaos, Transported PDF modeling of high-Reynolds number premixed turbulent flames, Combust. Sci. Technol. 145 (2006), pp. 495–511.

[24] R.P. Lindstedt, Transported probability density function method for premixed turbulent flames, in Turbulent Premixed Flames, 1st ed., N. Swaminathan and K.N.C. Bray, eds., Cambridge University Press, Cambridge, UK, 2011, pp. 102–135.

[25] A. Kronenburg and E. Mastorakos, The conditional moment closure model, in Turbulent Combustion Modeling: Advances, New Trends and Perspectives, T. Echekki and E. Mastorakos, eds., Springer, New York, 2011, pp. 91–114.

[26] S.M. Martin, J.C. Kramlich, G. Kosály, and J.J. Riley, The premixed conditional moment closure method applied to idealized lean premixed gas turbine combustors, J. Eng. Gas Turb. Power 125 (2003), pp. 895–900.

[27] S. Amzin, N. Swaminathan, J.W. Rogerson, and J.H. Kent, Conditional moment closure for turbulent premixed flames, Combust. Sci. Technol. 184 (2012), pp. 1–25.

[28] M.J. Dunn, A.R. Masri, and R.W. Bilger, A new piloted premixed jet burner to study strong finite-rate chemistry effects, Combust. Flame 151 (2007), pp. 46–60.

[29] M.J. Dunn, A.R. Masri, R.W. Bilger, and R.S. Barlow, Finite rate chemistry effects in highly sheared turbulent premixed flames, Flow Turb. Combust. 85 (2010), pp. 621–648.

[30] D.H. Rowinski and S.B. Pope, PDF calculations of piloted premixed jet flames, Combust. Theory Model. 15 (2011), pp. 245–266.

[31] C. Duwig, K.-J. Nogenmyr, C. Chan, and M.J. Dunn, Large Eddy Simulations of a piloted lean premix jet flame using finite-rate chemistry, Combust. Theory Model. 15 (2011), pp. 537–568.

[32] N. Swaminathan and R.W. Bilger, Analysis of conditional moment closure for turbulent premixed flames, Combust. Theory Model. 5 (2001), pp. 241–260.

[33] M.D. Smooke and V. Giovangigli, Formulation of the premixed and nonpremixed test problems, in Reduced Kinetic Mechanisms and Asymptotic Approximations for Methane–Air Flames, M.D. Smooke, ed., Springer Verlag, New York, 1991, pp. 1–28.

[34] K. Bray, P.A. Libby, and J. Moss, Unified modeling approach for premixed turbulent combustion – Part I: General formulation, Combust. Flame 61 (1985), pp. 87–102.

[35] K.N.C. Bray, P.A. Libby, G. Masuya, and J.B. Moss, Turbulence production in premixed turbulent flames, Combust. Sci. Technol. 25 (1981), pp. 127–140.

[36] I.G. Shepherd, J.B. Moss, and K.N.C. Bray, Turbulent transport in a confined premixed flame, Symp. (Int.) Combust. 19 (1982), pp. 423–431. Available at http://dx.doi.org/10.1016/S0082-0784(82)80214-2.

[37] D. Veynante, A. Trouve, K.N.C. Bray, and T. Mantel, Gradient and counter-gradient scalar transport in turbulent premixed flames, J. Fluid Mech. 332 (1997), pp. 263–293.

[38] N. Swaminathan, R. Bilger, and B. Cuenot, Relationship between turbulent scalar flux and conditional dilatation in premixed flames with complex chemistry, Combust. Flame 126 (2001), pp. 1764–1779.
[41] E.S. Richardson, N. Chakraborty, and E. Mastorakos, Analysis of direct numerical simulations of ignition fronts in turbulent non-premixed flames in the context of conditional moment closure, Proc. Combust. Inst. 31 (2007), pp. 1683–1690.

[42] H. Kolla and N. Swaminathan, Strained flamelets for turbulent premixed flames – Part I: Formulation and planar flame results, Combust. Flame 157 (2010), pp. 943–954.

[43] H. Kolla, J.W. Rogerson, N. Chakraborty, and N. Swaminathan, Scalar dissipation rate modelling and its validation, Combust. Sci. Technol. 181 (2009), pp. 518–535.

[44] M.J. Dunn, A.R. Masri, R.W. Bilger, R.S. Barlow, and G.-H. Wang, The compositional structure of highly turbulent piloted premixed flames issuing into a hot co-flow, Proc. Combust. Inst. 32 (2009), pp. 1779–1786.

[45] R.J. Kee, J.F. Grcar, M.D. Smooke, J.A. Miller, and E. Meeks, A Fortran program for modeling steady laminar one-dimensional premixed flames, Report SAND85-8240, Sandia National Laboratories, Livermore, CA, 1985.

[46] J.W. Rogerson, J.H. Kent, and R.W. Bilger, Conditional moment closure in bagasse-fired boiler, Proc. Combust. Inst. 31 (2007), pp. 2805–2811.

[47] S.B. Pope, An explanation of the turbulent round-jet/plane-jet anomaly, AIAA J. 16 (1978), pp. 279–281.

[48] S.V. Patankar, Numerical Heat Transfer and Fluid Flow, Hemisphere, Washington, DC, 1980.

[49] G.P. Smith, D.M. Golden, M. Frenklach, N.W. Moriarty, B. Eiteneer, M. Goldenberg, C. Thomas Bowman, R.K. Hanson, S. Song, W.C. Gardiner, Jr., V.V. Lissianski, and Z. Qin, GRI-Mech 3.0, The Gas Research Institute, Des Plaines, IL, 2011. Available at http://www.me.berkeley.edu/grimech.