Research Article

Conditional Moment Closure Modelling of a Lifted H_2/N_2 Turbulent Jet Flame Using the Presumed Mapping Function Approach

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A lifted hydrogen/nitrogen turbulent jet flame issuing into a vitiated coflow is investigated using the conditional moment closure (CMC) supplemented by the presumed mapping function (PMF) approach for the modelling of conditional mixing and velocity statistics. Using a prescribed reference field, the PMF approach yields a presumed probability density function (PDF) for the mixture fraction, which is then used in closing the conditional scalar dissipation rate (CSDR) and conditional velocity in a fully consistent manner. These closures are applied to a lifted flame and the findings are compared to previous results obtained using β -PDF-based closures over a range of coflow temperatures (T_c). The PMF results are in line with those of the β -PDF and compare well to measurements. The transport budgets in mixture fraction and physical spaces and the radical history ahead of the stabilisation height indicate that the stabilisation mechanism is susceptible to T_c . As in the previous β -PDF calculations, autoignition around the “most reactive” mixture fraction remains the controlling mechanism for sufficiently high T_c . Departure from the β -PDF predictions is observed when T_c is decreased as PMF predicts stabilisation by means of premixed flame propagation. This conclusion is based on the observation that lean mixtures are heated by downstream burning mixtures in a preheat zone developing ahead of the stabilization height. The spurious sources, which stem from inconsistent CSDR modelling, are further investigated. The findings reveal that their effect is small but nonnegligible, most notably within the flame zone.

1. Introduction

In a previous Conditional Moment Closure (CMC) study [1], the lifted H_2/N_2 turbulent jet flame of Cabra et al. [2] was thoroughly investigated using several CMC submodels and chemical kinetic mechanisms over a narrow range of coflow temperatures (T_c). For the most part, this work was aimed at the implementation of a fully consistent CMC realisation. Therefore, the consistency of the conditional CMC submodels with the mixture fraction Probability Density Function (PDF) transport equation was emphasised. The commonly used β -distribution was adopted throughout to presume the PDF. The Conditional Velocity (CV) fluctuations were modelled using the PDF gradient diffusion model of Pope [3].

One important feature of this model is its consistency with the first and second moments of the PDF [4] and with the modelling of the unconditional passive and reactive scalar fluxes [5, 6]. As for the closure of the Conditional Scalar Dissipation Rate (CSDR), the models of Girimaji [7] and Mortensen [8] were considered. Both models are derived by doubly integrating the PDF transport equations and using the same set of boundary conditions. The former is based on the homogeneous form of the equation, while, in the latter, the inhomogeneous terms are retained and PDF gradient modelling is applied to close the CV fluctuations. As such, Mortensen's model provides a fully consistent CSDR closure and degenerates exactly to Girimaji's when the inhomogeneous terms are discarded.

In both CMC realisations, it was found that autoignition is the controlling stabilisation mechanism over the considered T_c range. This conclusion is in full agreement with the findings of Stanković and Merci [9] and in partial agreement with those of Patwardhan et al. [10] and Navarro-Martinez and Kronenburg [11] who report stabilisation via premixed flame propagation as T_c is decreased. Another conclusion drawn in [1] is that Mortensen's fully consistent CSDR model results in delayed ignition and consequently yields larger liftoff heights. Hence, the occurrence of earlier ignition in the realisation employing Girimaji's model is attributed to the spurious (false) sources that arise from the inconsistency of this model with the CMC equations. Therefore, the consistent modelling of the CSDR is influential and ought to be investigated further.

The Mapping Closure (MC) devised by Chen et al. [12] has been frequently employed in the modelling of passive and reactive turbulent scalar mixing. O'Brian and Jiang [13] employ the MC to attain the Amplitude Mapping Closure (AMC) for passive scalar mixing. The closure is widely used in the CMC literature for the modelling of the CSDR [10, 14, 15]. It is the exact equivalent of the counterflow model employed in the framework of the Laminar Flamelet Model (LFM) [16]. Klimenko and Pope [17] employ a generalisation of the MC to formulate the Multiple Mapping Conditioning (MMC) for the modelling of turbulent reacting flows. MMC has close ties with the joint PDF approach [18] and CMC. When turbulent fluctuations are absent, MMC with the mixture fraction chosen as the only major conditioning scalar is equivalent to CMC. When all scalars in composition space are included, MMC is equivalent to the joint PDF approach [19].

In a recent work, Mortensen and Andersson [5] cast the solution of the MC for homogeneous turbulence into a Presumed Mapping Function (PMF) for inhomogeneous turbulent flows. Using a Gaussian reference field, the PMF yields a presumed PDF for the mixture fraction. The resulting PMF-PDF is employed to derive analytical closures for the CV and the CSDR. The CV closure is obtained by inserting the PMF-PDF into the PDF gradient diffusion model of Pope [3]. The CSDR closure is achieved by incorporating the PMF-PDF into the fully consistent, inhomogeneous CSDR expression previously devised by Mortensen [8]. To test the capabilities of the newly proposed approach, Mortensen and Andersson validate the PMF closures against the Direct Numerical Simulation (DNS) of a nonreacting Scalar Mixing Layer (SML). The PMF-PDF yields superior predictions compared to the β -PDF and the CV and CSDR closures yield a remarkable agreement with the DNS. It is shown that the CV closure is well-behaved at low probabilities compared to the β -PDF-based gradient diffusion model. The latter is known to result in instabilities in CMC as the CV diverges to infinity at small probabilities [20]. The authors further compare the homogeneous and inhomogeneous versions of the CSDR closure to DNS. They show that the influence of the inhomogeneous modification is small compared to the β -PDF approach [8]. The study concludes that the PMF approach is well suited for the modelling of mixing statistics in mixture fraction-based presumed PDF combustion models, such as CMC and the LFM.

The closures presented in [5] are concerned with binary mixing; nevertheless, PMF is extensible to the multistream mixing of multiple injections. The derivation and validation of PMF for trinary (three-stream) mixing are addressed in subsequent works. Cha et al. [21] validate the trinary PMF against the DNS of nonreacting Double Scalar Mixing Layers (DSML). The study reveals that trinary PMF is capable of capturing the fine-scale scalar mixing statistics manifesting in the DSML. Mortensen et al. [22] incorporate the trinary PMF into the CMC and stationary LFM of a reacting DSML. The investigated DSML is a representative problem for piloted nonpremixed flames where the fuel and oxidiser streams are separated by a pilot stream. Single-step reversible chemistry is employed in both the CMC and LFM computations. Given the negligible influence of the spurious sources, the CSDR is modelled using the homogeneous version of the trinary PMF closure. A remarkable agreement between both combustion models and DNS is achieved at low-to-moderate extinction levels. Deviations from DNS are reported for higher extinction levels. The discrepancies are attributed to issues specific to the considered combustion models (e.g., the first-order closure for the conditional chemical source in CMC, which is not suitable for the modelling of extinction). In a more recent work, El Sayed et al. [23] assess the trinary PMF in the context of a piloted methane/air flame. The study reveals that the pilot has significant influence on the structure of the flamelets in the near field where mixing is trinary. It is also shown that, compared to the classical flamelet approach that employs the counterflow solution for the modelling of the CSDR, flamelets generated using the trinary PMF can withstand higher strain rates before they extinguish and are more sensitive to transport by means of differential diffusion.

To date, a limited number of attempts have been made to implement PMF in the CMC of well documented laboratory-scale turbulent flames with detailed chemistry. Brizuela and Roudsari [24] use the *homogeneous* trinary PMF approach in the CMC calculations of Sandia flame D [25]. The reported results show that the PMF closures are more accurate than their classical counterparts (β -distribution for the PDF and the β -PDF-based AMC and gradient diffusion model for the CSDR and the CV, resp.) in the near field of the flame where the pilot influence is important. The current study is an extension to previous work [1] concerned with the CMC modelling of the lifted H_2/N_2 jet flame of Cabra et al. [2]. This flame has been thoroughly investigated using a number of turbulent combustion models such as CMC [9–11], PDF methods [2, 26–28], and the Eddy dissipation concept [2, 29]. To the authors' knowledge, the *inhomogeneous* PMF closures have never been applied to the CMC of laboratory-scale flames. In this paper, the lifted flame is revisited and investigated using CMC supplemented by the PMF approach. The PDF, the CV, and the CSDR are modelled using the *inhomogeneous binary* PMF closures since mixing occurs between two streams. The objectives of this study are to assess the applicability of the PMF-based submodels and to compare the obtained results to previous β -PDF results. As in [1], a range of coflow temperatures is considered and the stabilisation mechanism is determined by investigating the CMC budgets in mixture fraction and physical spaces

and through the analysis of the radical history ahead of the stabilisation height. In addition, the importance of the spurious sources, which are due to the inconsistent modelling of the CSDR, is thoroughly investigated.

2. Investigated Flame

The burner of Cabra et al. [2] consists of a central H_2/N_2 turbulent jet which issues into a hot coflow. The coflow consists of the combustion products of a lean premixed H_2 /air flame stabilised on a perforated disk. The disk is surrounded by an exit collar in order to delay the entrainment of ambient air into the coflow. The nozzle exit is placed above the surface of the disk so that the fuel stream exits into the coflow with a uniform composition. Table 1 shows the details of the experimental conditions. The experimental criterion for the determination of the liftoff height (H_{exp}) is taken as the first location where the mass fraction of OH reaches 600 ppm. The normalised measured height is $H_{exp}/d = 10$.

3. Mathematical Model

3.1. Conditional Moment Closure. As in the previous study [1], the turbulence-chemistry interactions are modelled by means of the first-order CMC [30]. For completeness, a brief overview of CMC theory is provided here. In CMC, a reactive scalar ϕ is conditionally averaged with respect to the mixture fraction, ξ , and its conditional transport equation is solved. The conditional average of ϕ is defined as $Q_\phi(\eta, x_i, t) = \langle \phi(x_i, t) \mid \xi(x_i, t) = \eta \rangle$, where η is a sample variable of ξ , such that $0 \leq \eta \leq 1$. Using the decomposition approach [30], ϕ is expressed as the sum of Q_ϕ and a fluctuation ϕ'' ($\phi = Q_\phi + \phi''$) such that $\langle \phi'' \mid \eta \rangle = 0$. The substitution of this sum into the transport equation of ϕ followed by the conditional averaging of the resulting expression leads to the equation of Q_ϕ . Applying this procedure to the mass fraction of a species κ (Y_κ) and the temperature (T) and invoking the primary closure hypothesis [30] yield

$$\frac{\partial Q_\kappa}{\partial t} = \underbrace{-\langle u_i \mid \eta \rangle \frac{\partial Q_\kappa}{\partial x_i}}_{\text{Convection}} - \underbrace{\frac{1}{\bar{\rho} \bar{P}(\eta)} \frac{\partial}{\partial x_i} [\bar{\rho} \langle u_i'' y_\kappa'' \mid \eta \rangle \bar{P}(\eta)]}_{\text{Diffusion in physical space}} + \underbrace{\frac{\langle \chi \mid \eta \rangle}{2} \frac{\partial^2 Q_\kappa}{\partial \eta^2}}_{\text{Diffusion in } \eta\text{-space (micro-mixing)}} + \underbrace{\frac{\langle \dot{\omega}_\kappa \mid \eta \rangle}{\langle \rho \mid \eta \rangle}}_{\text{Chemical source}}, \quad (1)$$

$$\begin{aligned} \frac{\partial Q_T}{\partial t} = & \underbrace{-\langle u_i \mid \eta \rangle \frac{\partial Q_T}{\partial x_i}}_{\text{Convection: } T_{C,x} \text{ and } T_{C,y}} \\ & - \underbrace{\frac{1}{\bar{\rho} \bar{P}(\eta)} \frac{\partial}{\partial x_i} [\bar{\rho} \langle u_i'' T'' \mid \eta \rangle \bar{P}(\eta)]}_{\text{Diffusion in physical space: } T_{D,x} \text{ and } T_{D,y}} + \underbrace{\frac{\langle \chi \mid \eta \rangle}{2} \left\{ \frac{\partial^2 Q_T}{\partial \eta^2} + \frac{1}{\langle c_p \mid \eta \rangle} \left[\frac{\partial \langle c_p \mid \eta \rangle}{\partial \eta} + \sum_{\kappa=1}^N \left(\langle c_{p,\kappa} \mid \eta \rangle \frac{\partial Q_\kappa}{\partial \eta} \right) \right] \frac{\partial Q_T}{\partial \eta} \right\}}_{\text{Diffusion in } \eta\text{-space (micro-mixing): } T_{MM}} \\ & - \underbrace{\frac{\sum_{\kappa=1}^N \langle h_\kappa \mid \eta \rangle \langle \dot{\omega}_\kappa \mid \eta \rangle}{\langle \rho \mid \eta \rangle \langle c_p \mid \eta \rangle}}_{\text{Chemical source: } T_{CS}} - \underbrace{\frac{\langle \dot{\omega}_r \mid \eta \rangle}{\langle \rho \mid \eta \rangle \langle c_p \mid \eta \rangle}}_{\text{Radiative Source: } T_{RS}}, \quad (2) \end{aligned}$$

where $Q_\kappa = \langle Y_\kappa \mid \eta \rangle$, $Q_T = \langle T \mid \eta \rangle$, $\langle u_i \mid \eta \rangle$ is the CV, $\langle \chi \mid \eta \rangle$ is the CSDR, $\langle u_i'' y_\kappa'' \mid \eta \rangle$ and $\langle u_i'' T'' \mid \eta \rangle$ are the conditional species and temperature turbulent fluxes, $\bar{P}(\eta)$ is the Favre mixture fraction PDF, $\langle \dot{\omega}_\kappa \mid \eta \rangle$ and $\langle h_\kappa \mid \eta \rangle$ are the conditional chemical source and enthalpy of species κ , N is the number of species, $\langle \dot{\omega}_r \mid \eta \rangle$ is the conditional radiative source, and $\langle \rho \mid \eta \rangle$ and $\langle c_p \mid \eta \rangle$ are the conditional density and specific heat. It is noted that in (1) and (2) the Lewis numbers are set to unity and all diffusivities are assumed to be equal.

The unconditional (Favre) averages of the reactive scalars are obtained by integrating their conditional counterparts weighted by the PDF over mixture fraction space via

$$\tilde{\phi} = \int_0^1 \langle \phi \mid \eta \rangle \bar{P}(\eta) d\eta, \quad \phi = Y_\kappa, T. \quad (3)$$

The quantities $\bar{P}(\eta)$, $\langle u_i'' y_\kappa'' \mid \eta \rangle$, $\langle u_i'' T'' \mid \eta \rangle$, $\langle u_i \mid \eta \rangle$, $\langle \chi \mid \eta \rangle$, $\langle \dot{\omega}_\kappa \mid \eta \rangle$, and $\langle \dot{\omega}_r \mid \eta \rangle$ appearing in (1)–(3) are unclosed

and require additional modelling. The submodels employed in this study are discussed in the following section.

3.2. The Presumed Mapping Function Approach. In CMC, an assumed distribution described by the moments of the mixture fraction is selected directly to presume the PDF. A commonly used distribution for the description of binary mixing statistics is the two-parameter β -PDF [30]. Although this choice is supported by DNS [7, 31], it lacks a sound physical basis. The recently proposed PMF approach of Mortensen and Andersson [5] employs the MC to offer a less *ad hoc*, naturally evolving alternative for the presumption of the PDF. In PMF, a known reference field is chosen and a mapping function between the true, unknown mixture fraction scalar field and the chosen reference field is established, ultimately leading to a presumed PDF. The PMF-PDF is subsequently utilised to derive fully consistent closures for the CV and CSDR. This section outlines the PMF approach and the resulting closures.

TABLE 1: Conditions of the lifted flame of Cabra et al. [2].

	Jet		Coflow
d (mm)	4.57	D (mm)	210
T_j (K)	305	T_c (K)	1045
U_j (m/s)	107	U_c (m/s)	3.5
X_{H_2}	0.2537	X_{H_2}	0.0005
X_{O_2}	0.0021	X_{O_2}	0.1474
X_{N_2}	0.7427	X_{N_2}	0.7534
X_{H_2O}	0.0015	X_{H_2O}	0.0989
ξ_{st}	0.474	ϕ	0.25

d = jet diameter; D = coflow diameter; T = temperature; U = velocity; X = mole fraction; ξ = mixture fraction; ϕ = equivalence ratio. Subscripts: j = jet; c = coflow; st = stoichiometric.

3.2.1. Probability Density Function. As in [5], the known reference field is denoted by ψ with sample space variable ϕ and consistent with conventional CMC notation and the unknown scalar field is denoted by ξ with sample space variable η . The reference field is mapped to the scalar field according to

$$\begin{aligned} X(\psi) &= \xi, \\ X(\phi) &= \eta, \end{aligned} \quad (4)$$

where X is a unique mapping function. The PDFs of ξ and ψ , $\tilde{P}(\eta)$, and $r(\phi)$ are related by

$$\tilde{P}(\eta) = \tilde{P}(X(\phi)) = r(\phi) \left(\frac{\partial X}{\partial \phi} \right)^{-1}. \quad (5)$$

A zero-mean Gaussian distribution is employed in [5] to prescribe the PDF of ψ . Accordingly,

$$r(\phi) = \frac{1}{\sqrt{2\pi}\sigma_r} \exp\left(-\frac{\phi^2}{2\sigma_r^2}\right), \quad (6)$$

where $\sigma_r^2 = 1 - 2\tau$ is the variance. The quantity τ is a scaled time parameter that is bounded by 0 (no mixing) and 0.5 (complete mixing). Using the cumulative distribution functions of $\tilde{P}(\eta)$ and $r(\phi)$, the mapping function is [5]

$$\begin{aligned} X(\phi) &= \frac{1}{2\sqrt{\pi\tau}} \int_{-\infty}^{+\infty} X(\phi', \tau=0) \exp\left[-\frac{(\phi' - \phi)^2}{4\tau}\right] d\phi', \end{aligned} \quad (7)$$

where $X(\phi', \tau=0)$ is the initial mapping. For binary mixing, the initial PDF of ξ evolves from the double-delta distribution

$$\tilde{P}(\eta, \tau=0) = (1 - \tilde{\xi}) \delta(\eta) + \tilde{\xi} \delta(\eta - 1), \quad (8)$$

where δ is the Dirac delta function and $\tilde{\xi}$ is the mixture fraction mean. The corresponding initial mapping is

$$X(\phi, \tau=0) = H(\phi - \alpha), \quad (9)$$

where H is the Heaviside step function. The parameter α in (9) is determined from

$$1 - \tilde{\xi} = \int_{-\infty}^{\alpha} r(\phi, \tau=0) d\phi. \quad (10)$$

Equation (10) has the analytical solution

$$\alpha = \sqrt{2\tau} \operatorname{erf}^{-1}(1 - 2\tilde{\xi}), \quad (11)$$

where erf^{-1} is the inverse error function. The substitution of (9) in (7) yields the mapping

$$X(\phi) = \frac{1}{2} \left[1 + \operatorname{erf}\left(\frac{\phi - \alpha}{2\sqrt{\tau}}\right) \right]. \quad (12)$$

Finally, the insertion (12) in (5) leads to the PMF-PDF

$$\tilde{P}(\eta) = \sqrt{\frac{2\tau}{\sigma_r^2}} \exp\left[E^2(\eta) - \frac{\phi^2}{2\sigma_r^2}\right], \quad (13)$$

where

$$\begin{aligned} \phi &= \alpha + 2\sqrt{\tau}E(\eta), \\ E(\eta) &= \operatorname{erf}^{-1}(2\eta - 1). \end{aligned} \quad (14)$$

The time parameter τ is obtained by finding the zero of

$$\tilde{\xi}^2 + \widetilde{\xi'^2} = \int_{-\infty}^{+\infty} X^2(\phi) r(\phi) d\phi, \quad (15)$$

where $\widetilde{\xi'^2}$ is the mixture fraction variance.

3.2.2. Conditional Velocity. The CV fluctuations are modelled using the PDF gradient diffusion model [3, 32, 33], which is the only known model that guarantees consistency with the modelling of the unconditional passive and reactive scalar fluxes. The CV expression takes the form

$$\begin{aligned} \langle u_i | \eta \rangle &= \tilde{u}_i - \frac{D_t}{\tilde{P}(\eta)} \frac{\partial \tilde{P}(\eta)}{\partial x_i} \\ &= \tilde{u}_i - D_t \left\{ \frac{\partial \ln[\tilde{P}(\eta)]}{\partial \tilde{\xi}} \frac{\partial \tilde{\xi}}{\partial x_i} + \frac{\partial \ln[\tilde{P}(\eta)]}{\partial \widetilde{\xi'^2}} \frac{\partial \widetilde{\xi'^2}}{\partial x_i} \right\}, \end{aligned} \quad (16)$$

where $\tilde{u}_i$ is the Favre-averaged velocity and $D_t = (C_\mu / Sc_t)(\bar{k}^2 / \bar{\epsilon})$ is the turbulent diffusivity, $\bar{k}$ is the turbulence kinetic energy, and $\bar{\epsilon}$ is the Eddy dissipation. The constant C_μ is equal to 0.09 and the turbulent Schmidt number Sc_t is set to 0.7 [34]. By inserting (13) in (16), it can be shown that [5]

$$\begin{aligned} \langle u_i | \eta \rangle &= \tilde{u}_i + \frac{D_t}{\sigma_r^2} \left\{ \frac{\partial \tilde{\xi}}{\partial x_i} \frac{d\alpha}{d\tilde{\xi}} \phi(\eta) \right. \\ &\quad - \frac{1}{2\tau} \left[\frac{\partial \tau}{\partial \tilde{\xi}} \frac{\partial \tilde{\xi}}{\partial x_i} + \frac{\partial \tau}{\partial \widetilde{\xi'^2}} \frac{\partial \widetilde{\xi'^2}}{\partial x_i} \right] \\ &\quad \left. \cdot \left[1 + \alpha \phi(\eta) - \frac{\phi^2(\eta)}{\sigma_r^2} \right] \right\}, \end{aligned} \quad (17)$$

where $d\alpha/d\tilde{\xi} = -\sqrt{2\pi}\exp(\alpha^2/2)$.

3.2.3. Conditional Scalar Dissipation Rate. Recently, Mortensen [8] derived a fully consistent closure for $\langle \chi \mid \eta \rangle$. The closure is obtained by the doubly integrating the inhomogeneous mixture fraction PDF transport equation subject to the boundary conditions $\langle \chi \mid \eta = 0 \rangle = 0$ and $\langle \chi \mid \eta = 1 \rangle = 0$. The CV fluctuations, which appear unclosed in this equation, are closed using the PDF gradient diffusion model. The CSDR closure is finally achieved by presuming the PDF with a distribution described by the vector of mixture fraction moments. When mixing is binary, the PDF is described by its first two moments, $\tilde{\xi}$ and $\tilde{\xi}''^2$, and the CSDR becomes (it is assumed in (18) that molecular diffusivity is negligible compared to D_t)

$$\begin{aligned} \langle \chi \mid \eta \rangle = & \frac{2}{\bar{P}(\eta)} \left\{ -\frac{\partial II(\eta)}{\partial \tilde{\xi}''^2} S_{\tilde{\xi}''^2} \right. \\ & + D_t \left[\frac{\partial^2 II(\eta)}{\partial \tilde{\xi}''^2 \partial \tilde{\xi}''^2} \frac{\partial \tilde{\xi}''^2}{\partial x_i} \frac{\partial \tilde{\xi}''^2}{\partial x_i} + \frac{\partial^2 II(\eta)}{\partial \tilde{\xi} \partial \tilde{\xi}} \frac{\partial \tilde{\xi}}{\partial x_i} \frac{\partial \tilde{\xi}}{\partial x_i} \right. \\ & \left. \left. + 2 \frac{\partial^2 II(\eta)}{\partial \tilde{\xi} \partial \tilde{\xi}''^2} \frac{\partial \tilde{\xi}}{\partial x_i} \frac{\partial \tilde{\xi}''^2}{\partial x_i} \right] \right\}, \end{aligned} \quad (18)$$

where

$$II(\eta) = \int_0^\eta \int_0^{\eta'} \bar{P}(\eta'') d\eta'' d\eta' \quad (19)$$

is the integral from 0 to η of the cumulative distribution function of η . The term $S_{\tilde{\xi}''^2}$ in (18) represents the source term of the mixture fraction variance transport equation. It is given by

$$S_{\tilde{\xi}''^2} = 2D_t \frac{\partial \tilde{\xi}}{\partial x_i} \frac{\partial \tilde{\xi}}{\partial x_i} - \tilde{\chi}, \quad (20)$$

where $\tilde{\chi}$ is the Favre-averaged scalar dissipation rate. Using (13) and (19) in (18), Mortensen and Andersson [5] show that CSDR can be expressed analytically as

$$\begin{aligned} \langle \chi \mid \eta \rangle = & \left\{ \tilde{\chi} - 2D_t \left[\left(\frac{\partial \tilde{\xi}}{\partial x_i} \right)^2 \left(2 + \frac{\tau_m^2 \tau_{vv}}{\tau_v^3} - \frac{\tau_{mm}}{\tau_v} \right) \right. \right. \\ & - 2 \frac{d\alpha}{d\tilde{\xi}} \frac{\partial \tilde{\xi}}{\partial x_i} \frac{\partial \tilde{\xi}''^2}{\partial x_i} A(\eta) - \left(\left(\frac{\partial \tilde{\xi}''^2}{\partial x_i} \right)^2 \tau_v \right. \\ & \left. \left. + 2 \frac{\partial \tilde{\xi}}{\partial x_i} \frac{\partial \tilde{\xi}''^2}{\partial x_i} \tau_m + \left(\frac{\partial \tilde{\xi}}{\partial x_i} \right)^2 \frac{\tau_m^2}{\tau_v} \right) B(\eta) \right] \right\} \frac{\langle \chi \mid \eta \rangle_H}{\tilde{\chi}} \\ & - 2D_t \left(\frac{\partial \tilde{\xi}}{\partial x_i} \right)^2 C(\eta), \end{aligned} \quad (21)$$

where

$$\begin{aligned} A(\eta) &= \frac{\alpha}{1-\tau} - \frac{\phi(\eta)}{\sigma_r^2}, \\ B(\eta) &= \frac{\alpha^2}{2(1-\tau)^2} \\ &\quad - \frac{1}{\sigma_r^2} \left(\frac{\phi(\eta)E(\eta)}{\sqrt{\tau}} + \frac{\phi^2(\eta)}{\sigma_r^2} - \frac{1}{1+\sigma_r^2} \right), \\ C(\eta) &= \sqrt{\frac{2}{\pi}} \left(\frac{d\alpha}{d\tilde{\xi}} + \frac{\tau_m}{\tau} \frac{\phi(\eta)}{\sigma_r^2} \right) \exp \left[-2E^2(\eta) + \frac{\alpha^2}{2} \right], \quad (22) \\ \tau_m &= \frac{\partial \tau}{\partial \tilde{\xi}}, \\ \tau_v &= \frac{\partial \tau}{\partial \tilde{\xi}''^2}, \\ \tau_{mm} &= \frac{\partial^2 \tau}{\partial \tilde{\xi}^2}, \\ \tau_{vv} &= \frac{\partial^2 \tau}{\partial \tilde{\xi}''^2}. \end{aligned}$$

The term $\langle \chi \mid \eta \rangle_H$ in (21) represents the homogeneous portion of (18); that is, $\langle \chi \mid \eta \rangle_H = 2\tilde{\chi}/\bar{P}(\eta) \partial II(\eta)/\partial \tilde{\xi}''^2$. Using (13) and (19), it can be shown that

$$\langle \chi \mid \eta \rangle_H = \tilde{\chi} \sqrt{\frac{1-\tau}{\tau}} \exp \left(-2E^2(\eta) + \frac{\alpha^2}{\sigma_r^2 + 1} \right). \quad (23)$$

Equation (23) is the exact equivalent of the AMC [13] and the counterflow model [16] as implied by the PMF-PDF.

3.3. Conditional Fluxes and Sources. The conditional turbulent fluxes are modelled using the gradient diffusion assumption given by

$$\langle \phi'' u_i'' \mid \eta \rangle = -D_t \frac{\partial \langle \phi \mid \eta \rangle}{\partial x_i}, \quad \phi = Y_\kappa, T. \quad (24)$$

This closure does not account for countergradient effects, which are mostly encountered in premixed flames. This approximation may not be suitable when lifted flames are stabilised by premixed flame propagation. A correction such as the one proposed by Richardson and Mastorakos [35] may be necessary. However, following previous CMC investigations of the same flame considered here [1, 9–11], (24) is adopted throughout this study.

The conditional chemical source, $\langle \dot{\omega}_\kappa \mid \eta \rangle$, is modelled using a first-order closure [30]. In this closure, the conditional fluctuations about the conditional averages of the reactive scalars are assumed to be small. Accordingly, $\langle \dot{\omega}_\kappa \mid \eta \rangle$

is modelled as a function of the conditional density, mass fractions, and temperature via

$$\begin{aligned} \langle \dot{\omega}_\kappa(\rho, T, \mathbf{Y}) | \eta \rangle \\ \approx \langle \dot{\omega}_\kappa(\langle \rho | \eta \rangle, \langle T | \eta \rangle, \langle \mathbf{Y} | \eta \rangle) | \eta \rangle \\ = \dot{\omega}_\kappa(\langle \rho | \eta \rangle, Q_T, \mathbf{Q}), \end{aligned} \quad (25)$$

where $\mathbf{Y} = \{Y_\kappa | \kappa = 1, 2, \dots, N\}$ and $\mathbf{Q} = \langle \mathbf{Y} | \eta \rangle$. This closure has been successfully applied in the CMC of lifted flames [1, 9–11, 14].

The conditional radiative source, $\langle \dot{\omega}_r | \eta \rangle$, is modelled using the optically thin assumption [36] with H_2O being the predominantly participating species. Previous modelling studies [1, 37] reveal that radiation has a negligible effect on the prediction of the stabilisation height in lifted flames. In the flame under investigation, this is due to the fact that H_2 in the fuel stream is highly diluted with N_2 . The radiative source is nevertheless retained here.

3.4. Other Considered Submodels. In addition to the PMF closures presented in Section 3.2, the β -PDF closures investigated in [1] are also considered in this work for the purpose of comparison with the PMF results. These closures are provided here for completeness. The β -PDF is given by

$$\bar{P}(\eta; \nu, w) = \frac{\eta^{\nu-1} (1-\eta)^{w-1}}{B(\nu, w)}, \quad (26)$$

where $\nu = \gamma\tilde{\xi}$ and $w = \gamma(1-\tilde{\xi})$ with $\gamma = \tilde{\xi}(1-\tilde{\xi})/\tilde{\xi}^{\prime\prime 2} - 1 \geq 0$ and $B(\nu, w) = \int_0^1 \eta^{\nu-1} (1-\eta)^{w-1} d\eta$ is the β -function.

Two β -PDF-based CSDR models are considered in [1]. The first is the homogeneous model of Girimaji [7]

$$\langle \chi | \eta \rangle = -2\tilde{\chi} \frac{\tilde{\xi}(1-\tilde{\xi})}{(\tilde{\xi}^{\prime\prime 2})^2} \frac{I(\eta)}{\bar{P}(\eta)}, \quad (27)$$

where

$$\begin{aligned} I(\eta) = \int_0^\eta \left\{ \tilde{\xi} \left[\ln \eta' - \int_0^1 \ln \eta'' \tilde{P}(\eta'') d\eta'' \right] + (1-\tilde{\xi}) \right. \\ \left. \cdot \left[\ln(1-\eta') - \int_0^1 \ln(1-\eta') \tilde{P}(\eta'') d\eta'' \right] \right\} \\ \times \tilde{P}(\eta') (\eta - \eta') d\eta'. \end{aligned} \quad (28)$$

The second is the inhomogeneous model of Mortensen given by (18) with $\bar{P}(\eta)$ presumed using the β -PDF. In this case, it can be shown that (19) simplifies to [8, 38]

$$\begin{aligned} II(\eta; \nu, w) = (\eta - \tilde{\xi}) I(\eta; \nu, w) \\ + \tilde{\xi}^{\prime\prime 2} \tilde{P}(\eta; \nu+1, w+1), \end{aligned} \quad (29)$$

where $I(\eta; \nu, w) = \int_0^\eta [\eta^{\nu-1} (1-\eta)^{w-1} / B(\nu, w)] d\eta$ is the incomplete β -function. When the inhomogeneous terms are

discarded, this version of Mortensen's model reduces exactly to (27). Hence, Girimaji's model is the exact equivalent of the homogeneous version of Mortensen's.

As for the closure of the CV, the PDF gradient diffusion model, (16), is employed with $\bar{P}(\eta)$ presumed using the β -PDF.

4. Implementation

The implementation details are available in [1]. Briefly, the calculations are performed on a two-dimensional axisymmetric computational domain. A quadratic unstructured mesh is used. The $k-\varepsilon$ model is employed to compute the mean flow quantities. Standard model constants are used except for $C_{\varepsilon 1}$ which is modified from 1.44 to 1.6 in order to improve the spreading rate predictions [39]. The mixing field is obtained by solving transport equations for $\tilde{\xi}$ and $\tilde{\xi}^{\prime\prime 2}$. It is important to emphasise that $\tilde{\chi}$ is not calculated algebraically. In practice, this quantity is computed by invoking the assumption of proportionality between the flow time ($\tilde{k}/\tilde{\varepsilon}$) and the time scale of scalar turbulence ($\tilde{\xi}^{\prime\prime 2}/\tilde{\chi}$) leading to $\tilde{\chi} = C_\chi \tilde{\varepsilon}/\tilde{k} \tilde{\xi}^{\prime\prime 2}$, where the time scale ratio C_χ is usually set to a constant value of 2. Alternatively, the transport equation of $\tilde{\chi}$ [40] is solved. This approach predicts correctly the asymptotic decay of the time scale ratio from high levels in the near field to a constant value in the neighbourhood of 2 at downstream locations (see Figure 3 in [1]). The SIMPLE algorithm is used for pressure-velocity coupling. Spatial discretisation is performed using the second-order upwind scheme. The inlet and coflow boundary conditions are set following the experimental conditions. Zero-gradient boundary conditions are applied elsewhere.

The CMC equations are discretised using the finite difference method. The first-order derivative of the convective term is discretised using the second-order upwind difference scheme with the kappa flux limiter [41]. The second-order derivatives appearing in the diffusive terms are discretised using the second-order central difference scheme. The mixture fraction grid consists of 80 evenly spaced points. Compared to the flow and mixing calculations, a relatively coarser mesh is used in physical space in order to achieve significant computational savings. This approach is valid due to the lower spatial dependence of the conditional averages compared to their unconditional counterparts. The ODE solver VODPK [42] is used to solve the system of equations. A three-step fractional method [43] is implemented in order to reduce stiffness of the system. The H_2 oxidation chemical kinetics mechanism of Mueller et al. [44] is employed throughout this study.

The details of the numerical implementation of the β -PDF-based submodels are available in [1] and are not repeated here for brevity. The PMF closures for the PDF (13), the CV (17), and the CSDR (21) are computed using the open-source code "PMFPack" [45]. The computation of the closures is straightforward. The major task is to determine τ and its partial derivatives. τ is determined by inserting (6) and (12) in (15) and finding the zero of the resulting equation in the interval $[0, 0.5]$. $\tilde{\xi}$ and $\tilde{\xi}^{\prime\prime 2}$ are available from the mixing

field. Bisection is used to accomplish this task and adaptive quadrature integration is employed to evaluate the integral. The partial derivatives of τ are determined by means of numerical differentiation.

5. Results and Discussion

5.1. Comparison of PMF and β -PDF Closures. In this section, the results of the PMF and β -PDF closures are presented. The coflow temperature is set to the experimentally reported value of 1045 K [2]. Three CMC realisations are compared. The first two correspond to the realisations investigated in [1]. In both, the PDF is presumed using the β -distribution, the CV is modelled using the β -PDF gradient model, and the CSDR is modelled using either Girimaji's mode (27) or Mortensen's model ((18) with $II(\eta)$ calculated using (29)). Hereafter, these realisations will be, respectively, referred to as CMC- β G and CMC- β M. The third realisation where the PMF closures are employed ((13) for the PDF, (17) for the CV and (21) for the CSDR) will be referred to as CMC-PMF.

5.1.1. Results in Physical Space. The contours of $\tilde{Y}_{OH}$ ($\times 10^{-3}$) are shown in Figure 1(a). As in the experiments of Cabra et al. [2], the criterion for the determination of the liftoff height is taken as the first location in the flow field where $\tilde{Y}_{OH}$ reaches 600 ppm. Given the experimental uncertainty of 10% in $\tilde{Y}_{OH}$ [2], the liftoff height uncertainty is roughly $\pm d$. The liftoff height normalised by d predicted by CMC-PMF is 9.80 compared to 10.50 for CMC- β G and 10.61 for CMC- β M. All heights fall within the experimental uncertainty. In comparison with the experimental value $H_{exp}/d = 10$, CMC-PMF results in the smallest relative error. The usage of the PMF closures does not affect the radial location of stabilisation (the distance from the stabilisation point to the centreline normalised by d) as CMC-PMF yields 1.47, which is exactly the same value predicted by CMC- β G and CMC- β M. The radial profiles of the Favre-averaged temperature and selected species mass fractions are shown in Figures 1(b)–1(f) at the axial locations $x/d = 8, 9, 10, 11, 14$ and 26. The profiles obtained using the three CMC realisations overlap at $x/d = 8$ and 9 and agree well with the experimental data of Cabra et al. [2]. Compared to the results of CMC-PMF, those of CMC- β G and CMC- β M are in better agreement with the experiments at $x/d = 10$. The temperature and product mass fractions are overpredicted while the reactant mass fractions are underpredicted in the range $1.1 \leq y/d \leq 1.8$ when the PMF closures are used. As indicated earlier, CMC-PMF predicts a liftoff height of 9.8 compared to 10.50 for CMC- β G and 10.61 for CMC- β M. Therefore, at $x/d = 10$, the mixture is not inert and a flame is present, which explains the higher levels of temperature and products and the lower levels of reactants. This effect propagates downstream. As shown at $x/d = 11$, the CMC-PMF results are overall in better agreement with the measurements. The differences between the three CMC realisations diminish at $x/d = 14$, with CMC- β G and CMC- β M being slightly closer to the experiments. Further downstream at $x/d = 26$ the results are almost identical.

5.1.2. Results in Mixture Fraction Space

Comparison of the Reactive Scalars. Figures 2(a) and 2(b) show the axial evolution of the conditional temperature, Q_T , and the conditional OH mass fraction, Q_{OH} , around the stabilisation locations indicated in Figure 1(a). In all three realisations, as x/d increases, the peaks of Q_T and Q_{OH} shift from lean mixtures towards stoichiometry and their amplitudes increase dramatically from the inert state. Compared to CMC- β G and CMC- β M, CMC-PMF yields relatively higher Q_T and Q_{OH} levels and therefore leads to the smallest liftoff height. The profiles of CMC- β G and CMC- β M are very similar, which explains why the liftoff heights resulting from these realisations are nearly identical (see Figure 1(a)). It is important to note that Q_T and Q_{OH} evolve differently in the CMC-PMF realisation. In CMC- β G and CMC- β M, Q_T and Q_{OH} start to increase around the “most reactive” mixture fraction ($\eta_{mr} = 0.0543$ [1]), as shown at $x/d = 8.86$, and their peaks remain around η_{mr} up to $x/d = 9.42$ before shifting slowly to less lean mixtures at $x/d = 9.69$ and eventually closer towards stoichiometry at $x/d = 11.09$. This behaviour indicates the occurrence of spontaneous ignition (autoignition) ahead of the stabilisation height. In CMC-PMF, although Q_T and Q_{OH} reach their maxima at η_{mr} at $x/d = 8.86$, it is obvious that their peaks shift more aggressively towards stoichiometry as x/d increases. This shows that the flame is stabilised by a different mechanism other than autoignition. As it will be shown in Section 5.3, a preheat zone exists ahead of the stabilisation height where lean mixtures are preheated by downstream burning mixtures as in premixed flame propagation.

Comparison of the Presumed PDFs. The evolution of the PDF is displayed in Figure 2(c). Both presumed PDFs peak at the same location in mixture fraction space. The PMF-PDF is slightly narrower than the β -PDF and presents a relatively higher peak. Although the differences between the two are small, the mildest changes in the shape of the PDF can have a nonnegligible impact on the CV and CSDR distributions and can affect the unconditional averages of the different reactive scalars (3).

Comparison of the CSDR Models. Figure 2(d) shows the evolution of the CSDR. Girimaji's homogeneous model results in almost symmetric profiles. The near-symmetric shape is due to the fact that $\tilde{\xi} \approx 0.474$ at the stoichiometric isoline. This value is very close to 0.5 at which the model is symmetric. The model can however yield skewed profiles when $\tilde{\xi} \neq 0.5$ [46]. On the other hand, Mortensen's inhomogeneous models (based on the β -PDF and the PMF-PDF) yield skewed profiles. The effect of inhomogeneity manifests away from the mean of the mixture fraction ($\eta \geq \tilde{\xi}$) as the PDF decays to zero (see Figure 2(c)). Mortensen's models are in general less dissipative as they produce substantially lower CSDR levels for $\eta \geq \tilde{\xi}$, most notably around stoichiometry and in rich mixtures. It is clear that the presumed form of the PDF in Mortensen's model affects the shape of the CSDR. Although the trends of the β -PDF and the PMF-PDF versions of the model are similar, significant difference can be clearly

FIGURE 1: Continued.

FIGURE 1: Results of the three CMC realisations for $T_c = 1045$: (a) contours of $\tilde{Y}_{OH}$ ($\times 10^3$) and radial profiles of (b) $\tilde{T}$, (c) $\tilde{Y}_{O_2}$, (d) $\tilde{Y}_{H_2}$ ($\times 10^2$), (e) $\tilde{Y}_{H_2O}$ ($\times 10^2$), and (f) $\tilde{Y}_{OH}$ ($\times 10^3$). In (a) the thick contours correspond to 600 ppm. The solid and dashed vertical lines correspond to the normalised numerical and experimental liftoff heights, respectively. In (b)–(f), dashed lines, CMC- βG ; thin solid lines, CMC- βM ; thick solid lines, CMC-PMF; symbols, experimental data [2].

seen around stoichiometry and in rich mixture, with the PMF-PDF version being less dissipative in these regions. This observation illustrates the strong influence of the presumed form of the PDF on the modelling of the CSDR.

Comparison of the CV Models. The axial and radial CV components, $\langle u | \eta \rangle$ and $\langle v | \eta \rangle$, are displayed in Figures 2(e) and 2(f), respectively. The β -PDF and PMF-PDF gradient diffusion models yield very similar results within two-to-three standard deviations of the mixture fraction mean. As in the CSDR profiles, the differences between the two closures become substantial away from the mean. The β -PDF gradient model tends to $\pm\infty$ as the PDF approaches zero. The PMF-PDF closure is generally better behaved over the whole mixture fraction space as it does not overshoot significantly at low probabilities. This behaviour demonstrates again the large influence of the presumed PDF. By inspecting Figure 2(e), although the trends of $\langle u | \eta \rangle$ are quite different, the results of the β -PDF and PMF-PDF closures are of the same order of magnitude and do not differ much from $\tilde{u}$. This is attributed to the fact that the axial velocity fluctuations are small, which is in turn due to the small magnitude of $\partial \ln[\tilde{P}(\eta)]/\partial x$ over the whole range of η . On the other hand, the magnitude of

$\partial \ln[\tilde{P}(\eta)]/\partial y$ can vary substantially, depending on the radial variations of the PDF at the point of interest. As shown in Figure 2(f), in the range where the PDF is finite ($0 < \eta \leq \tilde{\xi}_{st}$ in Figure 2(c)), the magnitude of $\partial \ln[\tilde{P}(\eta)]/\partial y$ is small regardless of whether the β -PDF or the PMF-PDF is used. However, at low probabilities ($\eta \geq \tilde{\xi}_{st}$), the two PDFs yield substantially different velocities. When the β -PDF is employed, $\partial \ln[\tilde{P}(\eta)]/\partial y$ is one order of magnitude larger than the PMF-PDF fluctuations. In the absence of experimental measurements, it is difficult to judge which closure is more accurate. Nevertheless, the fact that the PMF closure does not overshoot at low probabilities is desirable for numerical stability.

Comparison to Conditional Measurements. The conditional profiles of the temperature and species mass fractions obtained from the three CMC realisations are shown in Figure 3. The calculation of the conditional data from the experimental scatter is described in [1]. The numerical results are reported at the axial locations $x/d = 9, 10, 11, 14$ and 26 near the stoichiometric isocontour. As shown, the CMC-PMF results are generally in better agreement with the experimental data compared to CMC- βG and CMC- βM .

FIGURE 2: Continued.

FIGURE 2: Axial evolution of (a) Q_T (K), (b) Q_{OH} , (c) $\bar{P}(\eta)$, (d) $\langle \chi | \eta \rangle$ (1/s), (e) $\langle u | \eta \rangle$ (m/s), and (f) $\langle v | \eta \rangle$ (m/s) at $y/d = 1.47$ (the radial location of stabilisation). The thin vertical dash-dotted line indicates the location of the stoichiometric mixture fraction ($\eta = \xi_{st}$). The thick vertical dash-dotted line in (c)–(f) indicates the location of the mixture fraction mean ($\eta = \bar{\xi}$). The coflow temperature is 1045 K.

The improved predictions are mostly notable in lean mixture at $x/d = 10$ and 11 and in rich mixtures at $x/d = 14$. The results show that PMF is a reliable and accurate approach for the modelling of the unclosed terms in the CMC equations.

5.1.3. Effect of the PMF and β -PDF Closures. Having identified the differences between the β -PDF and the PMF-PDF closures, it becomes obvious why the results of CMC-PMF differ from those of CMC- β G and CMC- β M (Figures 2(a) and 2(b)). In [1], the differences between the results of CMC- β G and CMC- β M were solely attributed to the distinct CSDR levels at the “most reactive” mixture fraction, simply because the same presumed PDF (β -PDF) and CV model (the β -PDF gradient diffusion model) were employed in both realisations. It is obvious from Figure 2(d) that Mortensen’s model based on the PMF-PDF results in comparable CSDR levels at η_{mr} and produces profiles similar in shape and magnitude to those of the same model based on the β -PDF. Despite this, the predictions of the CMC-PMF realisation show departure from the CMC- β M results as shown in Figures 2(a) and 2(b). Thus, it becomes clear that the modelling of the CV also plays an important role in the modelling of this flame. Therefore, arguments based exclusively on the grounds of

intensity of micromixing at η_{mr} are not sufficient (though necessary) in order to explain the variability in the results. To illustrate this, the axial profiles of the CSDR models employed in the three realisations are plotted in Figure 4 at η_{mr} ($\langle \chi | \eta_{mr} \rangle$). Although the flame is stabilised by autoignition in CMC- β M [1] and by premixed flame propagation CMC-PMF (see Section 5.3), $\langle \chi | \eta_{mr} \rangle_{CMC-PMF}$ (thick solid lines) is lower than $\langle \chi | \eta_{mr} \rangle_{CMC-\beta M}$ (thin solid line). Hence, although the lower CSDR levels at η_{mr} favour the occurrence of autoignition, stabilisation is achieved by a different mechanism. For this reason, any analysis based exclusively on the CSDR is insufficient. Returning to Figure 2, the lower CSDR levels around stoichiometry in the CMC-PMF realisation lead to a decrease in the leakage of fuel and oxidiser from stoichiometric mixtures towards lean and rich mixtures. Therefore, the oxidation of the fuel becomes more intense in the vicinity of the stoichiometric mixture fraction. This behaviour, accompanied by the heating of lean mixtures in the preheat zone, promotes the early formation of a flame. Further, the smaller magnitude of $\langle v | \eta \rangle$ around stoichiometry and in rich mixtures results in a long residence time, which leads to increased chemical activity and hence higher Q_T and Q_{OH} levels.

FIGURE 3: Continued.

FIGURE 3: Conditional profiles near the stoichiometric isocontour: (a) Q_T (K), (b) Q_{O_2} , (c) Q_{H_2} ($\times 10^2$), (d) Q_{H_2O} ($\times 10^2$), and (e) Q_{OH} ($\times 10^3$). Dashed lines, CMC- β G; thin solid lines, CMC- β M; thick solid lines, CMC-PMF; symbols, experimental data [2]. The vertical grey dashed line indicates the location of the stoichiometric mixture fraction.

FIGURE 4: Axial profiles of $\langle \chi | \eta_{mr} \rangle$ at several radial locations for $T_c = 1045$ K: dashed lines, Girimaji's model ($\langle \chi | \eta_{mr} \rangle_{CMC-\beta G}$); thin solid lines, Mortensen's model based on the β -PDF ($\langle \chi | \eta_{mr} \rangle_{CMC-\beta M}$); thick solid lines, Mortensen's model based on the PMF-PDF ($\langle \chi | \eta_{mr} \rangle_{CMC-PMF}$). The vertical lines designate the ignition locations obtained with each CSDR model. The pattern of each vertical line follows that of the corresponding CSDR.

5.2. Sensitivity to the Coflow Temperature. Several CMC [1, 9–11] and PDF [27, 28] calculations show that the flame

under investigation is very sensitive to T_c . Cabra et al. [2] report an experimental uncertainty of 3% in the temperature measurements. As in [1], small perturbations ($\sim \pm 1.435\%$) are applied to T_c in order to assess flame response when the PMF closures are employed. Figure 5 shows the radial profiles of the Favre-averaged temperature and species mass fractions at the axial locations $x/d = 8, 9, 10, 11, 14$ and 26 for $T_c = 1030$ and 1060 K. The results of all three realisations are displayed. When T_c is decreased to 1030 K (black lines), the profiles of CMC-PMF are in close agreement with those of CMC- β G. This trend differs from the $T_c = 1045$ K case (Figure 1), where the profiles of CMC- β G and CMC- β M show closer agreement. In comparison to the experimental data, the predictions of CMC-PMF and CMC- β G are in general superior to those CMC- β M, particularly at $x/d = 11$ and 14 . Overall, the results of all three realisations remain in reasonable agreement with the experiments. When T_c is increased to 1060 K (grey lines), the profiles of CMC-PMF are in close agreement with those of CMC- β M. Again, this trend differs from those observed in the $T_c = 1030$ and 1045 K cases. The experimental measurements are grossly mispredicted at all axial locations as a result of the occurrence of early ignition (discussed in Section 5.3), which is in turn due to the higher coflow temperature.

FIGURE 5: Continued.

FIGURE 5: Radial profiles of (a) $\tilde{T}$, (b) $\tilde{Y}_{O_2}$, (c) $\tilde{Y}_{H_2}$ ($\times 10^2$), (d) $\tilde{Y}_{H_2O}$ ($\times 10^2$), and (e) $\tilde{Y}_{OH}$ ($\times 10^3$) obtained from the three CMC realisations for $T_c = 1030$ K (black lines) and 1060 K (grey lines). Lines: dashed, CMC- β G; thin solid, CMC- β M; thick solid, CMC-PMF; symbols, experimental data [2].

The normalised stabilisation coordinates obtained using the three realisations are displayed in Table 2. PMF-CMC yields the smallest liftoff height in the $T_c = 1030$ K case, followed by CMC- β G and then CMC- β M. Quantitatively, the CMC-PMF prediction is the closest to H_{exp}/d . The predicted radial stabilisation location is the same in all realisations (1.58) and is slightly larger than the one calculated at $T_c = 1045$ K (1.47). Therefore, the flame base becomes wider as T_c is decreased. When $T_c = 1060$ K, the liftoff height predicted in CMC-PMF falls between the heights calculated in CMC- β G and CMC- β M. The radial stabilisation locations obtained in CMC-PMF and CMC- β M are the same (1.26), while the predicted CMC- β G value is slightly smaller (1.16). As such, it can be seen that the flame base becomes narrower when T_c is increased.

5.3. Stabilisation Mechanism. Several stabilisation mechanisms have been proposed in the literature of lifted flames. Some are extinction due to excessive straining [47], premixed flame propagation [48, 49], and autoignition [50]. In the flame under investigation, the latter two theories are more plausible due to the presence of the vitiated coflow [50]. It was found in [1] to be autoignition-stabilised over a range of coflow temperatures (1030–1060 K) when the β -PDF closures

TABLE 2: Locations of the stabilisation points obtained using the three CMC realisations with the coflow temperatures 1030 K and 1060 K.

Realisation	$T_c = 1030$ K		$T_c = 1060$ K	
	x/d	y/d	x/d	y/d
CMC- β G	11.48	1.58	6.61	1.16
CMC- β M	11.91	1.58	7.39	1.26
CMC-PMF	11.22	1.58	6.97	1.26

are used (CMC- β G and CMC- β M). The distinction between stabilisation by autoignition and premixed flame propagation was achieved by means of the numerical indicators developed by Gordon et al. [28], which involve the analyses of the transport budgets and the history of radical build-up ahead of the stabilisation height. In this section, these indicators are invoked in order to determine whether the usage of the PMF approach changes the previous conclusions.

5.3.1. Budgets in Mixture Fraction Space. Figure 6 shows the transport budgets of the steady-state conditional temperature equation (the right-hand side terms of (2)) obtained using the CMC-PMF realisation for $T_c = 1030$, 1045 and

FIGURE 6: Transport budget of the steady-state Q_T equation (r.h.s. terms of (2)) obtained using the CMC-PMF realisation for different coflow temperatures: (a) $T_c = 1030$ K ($y/d = 1.58$), (b) $T_c = 1045$ K ($y/d = 1.47$), and (c) $T_c = 1060$ K ($y/d = 1.26$). T_{RS} : radiative source; T_{CS} : chemical source; T_{MM} : micromixing; $T_{C,x}$: axial convection; $T_{C,y}$: radial convection; $T_{D,x}$: axial diffusion; $T_{D,y}$: radial diffusion. The vertical dashed line corresponds to the location of the stoichiometric mixture fraction. All terms are scaled down by a factor of 10^5 and the units are K/s.

1060 K. For each T_c , the budgets are reported at three axial locations around the predicted stabilisation height covering the preflame, liftoff, and postflame regions. In the CMC- β G and CMC- β M realisations considered in [1], a balance in lean mixtures between the chemical source, T_{CS} , the axial convection term, $T_{C,x}$, and micromixing, T_{MM} , was found in the pre-flame region for all T_c . The axial and radial diffusion terms, $T_{D,x}$ and $T_{D,y}$, and the radial convection term, $T_{C,y}$, were found to have little contribution to the overall budget. This balance leads to the conclusion that the mixtures ignite spontaneously, and therefore the flame was deemed to be stabilised by autoignition. As shown in Figures 6(a) and 6(b), a different balance manifests in the preflame regions for $T_c = 1030$ and 1045 K (bottom panes) as $T_{C,x}$ is essentially counterbalanced by $T_{D,x}$. The contributions of the remaining terms are smaller in comparison, most notably that of T_{CS} . This balance suggests the presence of a preheat zone as in premixed flames. It is important to note that $T_{D,x}$ and $T_{C,x}$ do not peak at stoichiometry, but rather in lean mixtures. Therefore, as postulated by Patwardhan et al. [10], lean mixtures are preheated by downstream burning mixture. As such,

a premixed flame front propagates upstream and anchors the base of the lifted flame in lean mixtures. It is worth noting that when $T_c = 1045$ K, T_{CS} yields a larger contribution compared to the $T_c = 1030$ K case. This observation indicates that there is a weak competition from autoignition. However, T_{CS} is not sufficiently large to change the nature of the stabilisation mechanism. When T_c is increased to 1060 K, T_{CS} peaks at η_{mr} and the T_{CS} - $T_{C,x}$ - T_{MM} balance recurs in the preflame zone as displayed in Figure 6(c) (bottom pane), which indicates the occurrence of autoignition as in the CMC- β G and CMC- β M realisations [1]. At liftoff (middle panes in Figures 6(a)–6(c)), the peak of T_{CS} shifts to $\eta \approx 0.27$ and its amplitude increases dramatically. In the cases where $T_c = 1030$ and 1045 K, T_{CS} is balanced by $T_{C,x}$ and $T_{C,y}$. The terms T_{MM} and $T_{D,y}$ are more important than in upstream locations and $T_{D,x}$ is negligible. A similar balance is observed when $T_c = 1060$ K, except that T_{MM} is more prevalent. Compared to the CMC- β G and CMC- β M realisations [1], when $T_c = 1060$ K the roles of T_{MM} and $T_{C,y}$ vary significantly due to the different shapes of the CSDR and CV predicted by the PMF closures. T_{MM} has a weaker effect because of the smaller CSDR levels for $\eta \gtrsim \xi$

(not shown). Conversely, $T_{C,y}$ is more influential due to the larger residence time caused by the smaller magnitude of $\langle \nu | \eta \rangle$ over the same range of η (not shown). Further downstream in the postflame regions (top panes in Figures 6(a)–6(c)), T_{CS} peaks around the stoichiometric mixture fraction and it is essentially balanced by T_{MM} and $T_{C,y}$. $T_{C,x}$ remains important but its role diminishes from upstream locations, and $T_{D,x}$ is virtually zero. In comparison to the CMC- βG and CMC- βM in [1], for all T_c values, $T_{C,y}$ acts as the major heat sink around stoichiometry due to the larger residence time. Beyond the postflame locations indicated in Figure 6, $T_{C,x}$ and $T_{C,y}$ diminish gradually and the flame budgets approach the structure of a nonpremixed flame, which is largely characterised by a T_{CS} - T_{MM} balance.

5.3.2. Budgets in Physical Space. As in [1], the controlling stabilisation mechanism can be determined as well via the analysis the Integrated Transport (IT) budget of the conditional temperature in physical space. To compute the individual contributions, each term on the right-hand side of (2) is weighted by the appropriate presumed PDF and then integrated over the mixture fractions space. The axial profiles of the resulting contributions are shown in Figure 7 for all combinations of CMC realisations and coflow temperatures. The indicated y/d values correspond to the radial locations of stabilisation obtained in each realisation. As shown in the top and middle panes of Figures 7(a)–7(c), for all coflow temperatures in the CMC- βG and CMC- βM realisations IT_{CS} is balanced by $IT_{C,x}$ and IT_{MM} in the preflame regions. The remaining terms have little contribution to the overall balance. However, they become more important right ahead of the stabilisation height. The IT_{CS} - $IT_{C,x}$ - IT_{MM} balance indicates that the mixture ignites spontaneously, and therefore the flame is autoignition-stabilised for all T_c values. The nature of the controlling stabilisation mechanism in the CMC-PMF realisation depends on T_c . For $T_c = 1030$ (bottom pane in Figure 7(a)), there is a clear balance between $IT_{D,x}$ and $IT_{C,x}$ up to $x/d \approx 10.25$ and IT_{CS} is small. This structure indicates the presence of a preheat zone, which is indicative of stabilisation by means of premixed flame propagation. Beyond this location and prior to liftoff, IT_{CS} increases rapidly. The terms IT_{MM} , $IT_{C,y}$, and $IT_{D,y}$ become more important and $IT_{D,x}$ has the smallest contribution to the overall budget. Similar trends are observed for $T_c = 1045$ K (bottom pane in Figure 7(b)). However, in this case IT_{CS} is more significant in the preheat zone, which indicates that there is competition from the autoignition mechanism. Nevertheless, IT_{CS} is not sufficiently large in order for autoignition to happen. Increasing T_c further to 1060 K, the budgets in the preflame region (bottom pane in Figure 7(c)) are very similar to those of the CMC- βG and CMC- βM . IT_{CS} is primarily balanced by $IT_{C,x}$ and hence autoignition takes place. In the vicinity of the stabilisation height, the budgets of all realisations show similar structures as IT_{CS} is counterbalanced by $IT_{D,y}$, $IT_{C,x}$, $IT_{C,y}$, and IT_{MM} . However, the relative importance of $IT_{C,y}$ and IT_{MM} with respect to IT_{CS} and $IT_{C,x}$ varies significantly in the CMC-PMF realisations. Compared to CMC- βG and CMC- βM , $IT_{C,y}$ is larger in magnitude due to the lower radial CV component (longer residence time) whereas IT_{MM}

is smaller because of the lower CSDR levels. Beyond the stabilisation heights, the structure of a nonpremixed flame is gradually approached as IT_{CS} is primarily balanced IT_{MM} with smaller contributions from the remaining terms.

5.3.3. Radical History ahead of the Stabilisation Height. The analyses of the transport budgets of the temperature in mixture fraction and physical spaces reveal that the nature of the stabilisation mechanism becomes sensitive to the coflow temperature when the PMF approach is employed. Further analysis of the history of radical build-up ahead of the stabilisation height can provide more insight into this matter. Figure 8 shows the axial profiles of the normalised Favre-averaged temperature $((\tilde{T} - \tilde{T}_{\min})/(\tilde{T}_{\max} - \tilde{T}_{\min}))$ and mass fractions $(\tilde{Y}/\tilde{Y}_{\max})$ of H, O, OH, and HO_2 for all combinations of CMC realisations and coflow temperatures. The subscripts “min” and “max” denote the minimum and maximum values of the reactive scalars at the axial locations of stabilisation. For all coflow temperatures, the CMC- βG and CMC- βM realisations (top and middle panes in Figure 8) show that HO_2 builds up rapidly prior to the runaway of H, O and OH. Therefore, HO_2 acts as a precursor to the production of H, O, and OH as in autoignition scenarios [28]. The evolution of radicals in the CMC-PMF realisation (bottom panes in Figure 8) shows similar trends, which is at first glance indicative of the occurrence of autoignition. As shown by Gordon et al. [28], in premixed flame propagation radicals build up simultaneously in the preheat zone. It is obvious here that HO_2 builds up prior to the remaining radicals. However, for $T_c = 1030$ and 1045 K, there is a notable decrease in the axial distance between the runaway location of HO_2 and those of the remaining radicals (see the filled circles) and between the peak of HO_2 and the stabilisation height (distance between dash-dotted and dashed vertical lines). Hence, although radicals do not start building up at the same point, there is a clear tendency towards simultaneous radical production ahead of the stabilisation height. It is also important to note that when lifted flames are stabilised by means of premixed flame propagation, liftoff takes place at locations where the local mixture fraction mean, and $\tilde{\xi}$ is equal to the stoichiometric mixture fraction, ξ_{st} [51]. This is not the case here since the flame stabilises at $\tilde{\xi} = 0.183$ when $T_c = 1030$ K and $\tilde{\xi} = 0.139$ when $T_c = 1045$ K. These $\tilde{\xi}$ values are well below $\xi_{st} = 0.474$. Still, it is clear that $\tilde{\xi}$ approaches ξ_{st} as T_c is decreased. A further decrease in T_c is therefore expected to lead to a more simultaneous radical build-up.

5.4. Spurious Sources. Theoretically, if the closed CMC equations are multiplied by the PDF and then integrated over the mixture fraction space, the unconditional equations should be fully recovered [30]. When an inconsistent CSDR model (e.g., a homogeneous model or an inhomogeneous model employing an inconsistent CV closure), the process outline above would result in additional spurious (false) source terms. The analysis of the spurious sources is a valuable tool that enables the identification of the flaws of inconsistent

FIGURE 7: Axial profiles of the Integrated Transport (IT) budget of the steady-state Q_T equation (integrated r.h.s. terms of (2)) obtained using the three CMC realisations: (a) $T_c = 1030$ K, (b) $T_c = 1045$ K, and (c) $T_c = 1060$ K. The bottom, middle, and top panes correspond to CMC- β G, CMC- β M, and CMC-PMF, respectively. The indicated y/d values correspond to the radial locations of stabilisation. The vertical dash-dotted lines correspond to the stabilisation heights. IT_{RS} : radiative source; IT_{CS} : chemical source; IT_{MM} : micromixing; $IT_{C,x}$: axial convection; $IT_{C,y}$: radial convection; $IT_{D,x}$: axial diffusion; $IT_{D,y}$: radial diffusion. All terms are scaled down by a factor of 10^6 and the units are K/s.

FIGURE 8: Axial profiles of the normalised Favre-averaged temperature and mass fractions of H, O, OH, and HO₂ obtained using the three CMC realisations: (a) $T_c = 1030$ K, (b) $T_c = 1045$ K, and (c) $T_c = 1060$ K. The bottom, middle, and top panes correspond to CMC-βG, CMC-βM, and CMC-PMF, respectively. The indicated y/d values correspond to the radial locations of stabilisation. The vertical dash-dotted and dashed lines correspond to the axial locations of maximum HO₂ and liftoff height, respectively. The circles indicate the locations of the maximum slopes.

FIGURE 9: Axial profiles of the chemical and spurious sources at $y/d = 1.47$ (radial locations of stabilisation) for $T_c = 1045$ K: (a) HO_2 , (b) OH , and (c) H_2O . All spurious sources are multiplied by 10 and the units are s^{-1} . The vertical grey lines indicate the axial locations of the stabilisation heights: thin, β -PDF; thick, PMF-PDF.

CMC implementations. The spurious source associated with a species κ is calculated as [30, 52]

$$\tilde{S}_\kappa = \frac{1}{2} \int_0^1 [\langle \chi | \eta \rangle_i - \langle \chi | \eta \rangle_c] \frac{\partial^2 Q_{\kappa,i}}{\partial \eta^2} \tilde{P}(\eta) d\eta, \quad (30)$$

where $\langle \chi | \eta \rangle_i$ and $\langle \chi | \eta \rangle_c$ are, respectively, the inconsistent and consistent CSDR models (the same PDF is used in both) and $Q_{\kappa,i}$ is the conditional mass fraction of species κ obtained in the inconsistent realisation. The consistent inhomogeneous CSDR model of Mortensen [8], (18), is benchmarked against its inconsistent homogeneous version with $\tilde{P}(\eta)$ modelled using both the β - and PMF-PDFs. As such, the difference $[\langle \chi | \eta \rangle_i - \langle \chi | \eta \rangle_c]$ in (30) is exactly the negative of the inhomogeneous contribution of the model. The details of the two cases are as follows:

(i) β -PDF case is as follows:

- (a) $\langle \chi | \eta \rangle_i$: (27) (the equivalent of the homogeneous version of (18));
- (b) $\langle \chi | \eta \rangle_c$: (18) with $II(\eta)$ obtained from (29).

(ii) PMF-PDF case is as follows:

- (a) $\langle \chi | \eta \rangle_i$: (23);
- (b) $\langle \chi | \eta \rangle_c$: (21).

Figure 9 compares the axial evolution of the integrated conditional chemical sources (IT_{CS}) and spurious sources of HO_2 , OH , and H_2O for $T_c = 1045$ K. The profiles are plotted at the radial locations of stabilisation ($y/d = 1.47$ for the β -PDF case and $y/d = 1.37$ for the PMF-PDF case). As displayed in Figure 9(a), $\tilde{S}_{\text{HO}_2}$ is negligible in both cases before the runaway of HO_2 . Ahead of the stabilisation height, $\tilde{S}_{\text{HO}_2}$ acts as a source. It increases as the production of HO_2 proceeds and peaks in the vicinity of the maximum of $\text{IT}_{\text{CS},\text{HO}_2}$; then decreases as soon as the consumption of HO_2 begins, reaching a local minimum right ahead of the base of the flame. As the consumption of HO_2 continues, $\tilde{S}_{\text{HO}_2}$ increases again and peaks downstream of the stabilisation height before it decays gradually inside the flame zone. Overall, the magnitude of $\tilde{S}_{\text{HO}_2}$ is more important ahead of the stabilisation height. Figure 9(b) displays the axial

FIGURE 10: Radial profiles of the chemical and spurious sources obtained in the PMF-PDF case for $T_c = 1045$ K: (a) O_2 , (b) H_2 , (c) H_2O , and (d) OH . Thin lines, chemical sources; thick lines, spurious sources. The units are s^{-1} .

variation of $\tilde{S}_{OH}$. Similar to what is observed in Figure 9(a), $\tilde{S}_{OH}$ in Figure 9(b) acts as a source ahead of the stabilisation height. Its magnitude is negligible before the runaway of OH then increases as OH is produced and peaks in the vicinity of the maximum of $IT_{CS,OH}$. $\tilde{S}_{OH}$ decreases sharply at the base of the flame before increasing at a much slower rate in the flame zone (its magnitude decreases gradually with increasing x/d) and continues to act as a sink. As opposed to $\tilde{S}_{HO_2}$, $\tilde{S}_{OH}$ is more important in the flame zone compared to the region located ahead of the stabilisation height. The trends observed in the axial variation of $\tilde{S}_{H_2O}$ (Figure 9(c)) are similar to those of $\tilde{S}_{OH}$.

The comparison of the results of the β -PDF and PMF-PDF cases ahead of the stabilisation heights in Figures 9(a)–9(c) LOH reveals that the spurious sources in the PMF-PDF case yield higher maxima, however, prevailing over narrower axial bands. In the flame zone, the magnitude of the spurious sources obtained in the β -PDF case is smaller at all axial locations.

Overall, it can be concluded that the errors arising from the inconsistent modelling of the CSDR are small but nonnegligible. To ascertain this conclusion, the radial profiles of the chemical and spurious sources of O_2 , H_2 , H_2O , and OH are plotted in Figure 10. Only the PMF-PDF case is shown here. The results of the β -PDF case are very similar (see [1]). It is evident that the effect of the spurious sources is nonnegligible at all axial locations, particularly within the flame zone at $x/d = 14$ and 26. The ratios of spurious-to-chemical sources at the axial locations considered in Figure 10 (not shown) indicate that the spurious contribution increases with x/d , which is expected to take place as the scalar dissipation rate decays.

The findings presented in the current section show that inconsistent CMC implementations may influence the results as the additional spurious terms stemming from inconsistencies in the modelling of the CSDR can behave as significant sources or sinks.

6. Conclusions

A previously investigated lifted H_2/N_2 jet flame was revisited in order to assess the applicability of the PMF approach in the context of CMC. The findings were compared to previous results obtained using β -PDF-based closures over a range of coflow temperatures (T_c). In view of the current results, the following conclusions are drawn:

- (i) The PMF-PDF is in general narrower than the β -PDF and presents a higher peak. The shape of the PDF has a large influence on the modelling of the CSDR and the CV.
- (ii) Girimaji's CSDR model results in nearly symmetric profiles near the stoichiometric isoline whereas the Models of Mortensen (based on the PMF- and β -PDFs) yield skewed profiles. The latter models are less dissipative away from the mean of the mixture fraction.

- (iii) The gradient diffusion CV model is well-behaved over the whole mixture fraction space when the PMF-PDF is employed as it does not overshoot at low probabilities. The β -PDF-based model tends to infinity as the PDF approaches zero.
- (iv) The liftoff heights predicted in all realisations fall within experimental uncertainty. In comparison to the β -PDF-based calculations at $T_c = 1045$ K, the PMF approach yields improved results in physical and mixture fraction spaces and a more accurate liftoff height. The flame remains very sensitive to small perturbations in T_c .
- (v) As opposed to the β -PDF closures, the transport budgets in mixture fraction and physical spaces and the radical history ahead of the stabilisation height reveal that the nature of the stabilisation mechanism is sensitive to T_c when the PMF closures are used. For sufficiently high T_c (e.g., $T_c = 1060$ K), the mixture ignites spontaneously at the “most reactive” mixture fraction, and the flame is stabilised by autoignition. As T_c is decreased (e.g., to $T_c = 1045$ and 1030 K), lean mixtures are preheated by a premixed flame front propagating upstream, and, therefore, the flame is stabilised by means of premixed flame propagation.
- (vi) The effect of the spurious sources resulting from the inconsistent modelling of the CSDR is small in general but nonnegligible, in particular within the flame zone.

PMF is a consistent and reliable approach for the modelling of the conditional mixing and velocity statistics in CMC. Further application to other combustion phenomena is necessary to fully assess its applicability.

Disclosure

This work had been done at the University of Waterloo and the second address is the current address of the corresponding author Ahmad El Sayed.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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