SPARSE-LAGRANGIAN MULTIPLE MAPPING CONDITIONING SIMULATIONS OF LIFTED JET DIFFUSION FLAMES OF METHANE/AIR IN A VITIATED CO-FLOW

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Numerical simulations of a partially-premixed, turbulent jet diffusion flame stabilised in a hot vitiated co-flow are performed. For auto-igniting flames, an accurate prediction of flame stabilisation, which depends on a delicate balance between turbulent transport and chemical kinetics at the flame base, poses an enormous challenge to conventional turbulent combustion models. Multiple mapping conditioning/large eddy simulation (MMC-LES), a promising tool for modelling turbulence-chemistry interactions, has been successfully applied to simulate a variety of combustion applications involving gaseous, liquid, and solid fuels. MMC-LES is a full probability density function (PDF) method where MMC plays the role of the mixing model, emulating molecular mixing phenomenon. MMC attempts to produce accurate molecular mixing by localising mixing in an independent, composition-like reference space. Due to this enforced localised mixing, a sparse distribution of stochastic Lagrangian particles for may be used for the Monte-Carlo simulation of the sub-grid joint-composition PDF equation. In the present study, we employ MMC-LES to investigate the auto-igniting methane/air flames of UC Berkeley. A sparse resolution of 1 particle per 10 Eulerian finite-volume cells is used in this study, which offers much cheaper computing expenses in comparison to the conventional transported PDF approach. A skeletal chemical mechanism, based on GRI 3.0, containing 30 species and 184 reactions, represents the oxidation of methane.
The time-scale of molecular mixing is modelled using the recently published \textit{dyn-alSO} model to assess its performance in an auto-igniting configuration. The conditional and unconditional profiles of compositional scalars are compared with the data from experimental measurements. Moreover, the sensitivity of flame lift-off with different co-flow temperatures is investigated as well. MMC-LES is able to produce reasonably the location of the flame base as well as other flow and combustion characteristics.
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| Acronym | Definition                                      |
|---------|------------------------------------------------|
| gs      | grid scale                                     |
| sgs     | sub-grid scale                                 |
| slgs    | sub-Lagrangian-grid scales                     |
| a-ISO   | anisotropic mixing time-scale                  |
| BC      | boundary condition                             |
| CD      | Curl's coalescence and dispersion               |
| CEMA    | chemical explosive mode analysis               |
| CMC     | conditional moment closure                     |
| DNS     | direct numerical simulation                    |
| EMST    | Euclidean minimum spanning tree                |
| ESF     | Eulerian stochastic fields                     |
| FDF     | filtered density function                      |
| FMDF    | filtered mass-density function                 |
| FV      | finite-volume                                  |
| IEM     | interaction by exchange with mean              |
| LES     | large eddy simulation                          |
| LMSE    | linear mean-square estimation                  |
| M-Curl  | modified Curl's                                |
| MC      | mapping closure                                |
| MMC     | multiple mapping conditioning                  |
| PDF     | probability density function                   |
| r.m.s.  | root mean square                               |
| RANS    | Reynolds averaged Navier-Stokes                |
### List of Symbols

| Symbol | Unit | Description |
|--------|------|-------------|
| $C_p$  | J kg$^{-1}$ K$^{-1}$ | specific heat at constant pressure |
| $C_v$  | - | model coefficient for $sgs$ viscosity |
| $D$    | m s$^{-2}$ | molecular mass diffusivity |
| $D_a$  | - | Damköhler number |
| $\Delta$ | m | filter-width |
| $d_x$  | m | Lagrangian filter-width |
| $\mathcal{F}$ | - | filtered mass density function |
| $h_s$  | J kg$^{-1}$ | sensible enthalpy |
| $l_t$  | m | turbulent integral length-scale |
| $D$    | mm | diameter of the fuel-jet of the vitiated co-flow burner |
| $Y$    | - | mass fraction |
| $Z$    | s$^{-1}$ | mixture fraction |
| $X$    | - | molar fraction |
| $M_w$  | kg kmol$^{-1}$ | molar mass |
| $N_{eq}$ | - | number of equivalent species for density coupling |
| Symbol | Unit | Description |
|--------|------|-------------|
| $N_{pc}$ | - | number of stochastic particles per super-cell |
| $N_s$ | - | number of species |
| $\nu$ | m s$^{-2}$ | molecular viscosity |
| $\mathcal{P}$ | - | filtered-density function |
| $\phi$ | - | composition vector variable containing mass fraction and enthalpy (and mixture fraction) |
| $p$ | N m$^{-1}$ | thermodynamic pressure |
| $\Psi$ | - | sample space of composition |
| $\psi$ | - | extent of molecular mixing |
| $\widetilde{\mathcal{P}}$ | - | Favre filtered-density function |
| $Re$ | - | Reynolds Number |
| $\mathcal{W}$ | m$^3$ s$^{-1}$ | rate of reaction |
| $R_u$ | J mol$^{-1}$ K$^{-1}$ | universal gas constant |
| $\chi$ | - | scalar dissipation rate |
| $S_{ij}$ | s$^{-1}$ | strain rate tensor |
| $\tau_{ij}$ | N m$^{-1}$ | stress tensor |
| $T$ | K | gas phase temperature |
| $h$ | J kg$^{-1}$ | standardised enthalpy |
| $\varphi$ | - | fine-grained function |
| $u$ | m s$^{-1}$ | velocity |
INTRODUCTION

Power generation via combustion is pertinent in several industrial applications, such as furnaces, gas turbines, direct injection and rocket engines. Flames in such practical combustors must be ignited initially, and then the incoming reactants must be continuously mixed and should remain ignited by the hot burnt products present in the chamber for combustion to sustain. Such continuation of burning, called flame stabilisation, is a crucial design criterion for combustion chambers, especially for critical applications such as aircraft engines. Insufficient flame stabilisation may result in a combustor that cannot be operated safely or fluctuates dangerously. For low velocities of the fuel jet, flame stabilisation may happen at the rim of the burner. As practical combustion devices have high Reynolds number (Re) flows to enhance fuel-oxidiser mixing, flame stabilisation is necessary (Poinsot and Veynante, 2001 [68]) as rim-stabilisation is observed rarely in practice. Combustion products are often re-circulated to improve flame stability which may be provided using flow swirl (Cavaliere, Kariuki and Mastorakos, 2013 [5]), or a supporting pilot flame (Barlow and Frank, 1998 [1]) may be provided. If the fuel-jet Re is increased to a value much higher than the laminar burning velocity, the rim-stabilised flame elevates from the burner wall, and this configuration is called a ‘lifted’ flame.

Stabilisation of lifted jet diffusion flames is one of the fundamental research problem in combustion. Numerous studies exist in the literature on the dynamics and structure of lifted flames (Lyons (2007) [47], Lawn (2009) [43]). By increasing the fuel or surrounding coflowing air velocity, a rim-stabilised jet flame stabilises away from the burner lip without requiring a physical anchor. In many industrial applications, such as large industrial boilers, diesel engines, flames stabilise away from the burner rim, and thereby preventing damage of the hardware (Peters, 2000 [63]). Lifted flames exist over a range of jet velocities until it reaches a critical velocity at which flame extinguishes globally. Lifted flames are of interest since they are relatively simple, exhibiting important characteristics of finite-rate chemistry, turbulence-chemistry interaction, local extinction/re-ignition,
effects of heat release, and other effects. Hence, these flames have been a subject of joint modelling and experimental efforts in ongoing research to develop numerical models of turbulent combustion (Lyons, 2007 [47]).

Numerical prediction of lifted flames is also challenging for existing turbulent combustion models due to a delicate balance between chemical kinetics and turbulent transport at the base of the flame. Despite numerous studies (Vanquickenborne and Tiggelen (1966) [92], Pitts (1989) [67], Lyons (2007) [47], Lawn (2009) [43]), the stabilisation process is not entirely understood. The flame may be stabilised due to auto-ignition, partially premixed flame propagation, or other possible mechanisms. Numerical studies of these mechanisms in practical combustors are difficult to perform because of the detailed (and coupled) turbulent fluid mechanics and chemical kinetics. Therefore, to better understand such flame configuration, a simplified experimental setup is needed to decouple the influence of these complex phenomena from the flame dynamics. The International Workshop on Measurement and Computation of Turbulent Non-premixed Flames (TNF) is a platform that encourages strong coupling between experiments and calculations using burner geometries that are simple with well-defined boundary conditions to enable computational studies. Modellers can then use the data produced using such burners to validate their results. For studying lifted flames in a simplified setup, some popular experimental database are given by Cabra et al. (2002) [3] (Berkeley Burner), Markides and Mastorakos (2005) [49], Cabra et al. (2005) [2] and Markides, De Paola and Mastorakos (2007) [48]. The burner by Markides and Mastorakos [49] uses heated air to enable auto-ignition while enabling the composition of the co-flow to be devoid of combustion species. The disadvantage of using heated air as co-flow is that it makes it difficult to obtain very high temperatures. The design of Berkeley’s vitiated co-flow burner (VCB) utilises a lean premixed H$_2$/Air flame in the co-flow. Hence combustion products are mostly air and water, which should not greatly affect the auto-ignition process. Initially employed to study H$_2$/N$_2$ jet flames (Cabra et al., 2002 [3]), this burner was later extended to study CH$_4$/Air (Cabra et al., 2005 [2]) flames.
Modelling of turbulent flows may be divided into three approaches, i.e. direct numerical simulation (DNS), large eddy simulation (LES) and Reynolds averaged Navier-Stokes (RANS). Inherently time-averaged computational methods, e.g., RANS may struggle to capture the transient phenomena, such as temporal variation of flame lift-off height, occurring in real combustors. At the same time, DNS remains expensive for industrial applications due to the presence of a wide range of scales. With the increase in available computing resources, LES has emerged as a tool for predicting unsteady turbulent combustion involving complex turbulence–chemistry interaction, flame structure, and combustion dynamics. LES captures large energy-containing turbulent structures by solving governing equations for low-pass, spatially filtered quantities and modelling the contributions of sub-grid scale (sgs). Since chemical reactions occur at these small scales, accurate sgs models are needed to predict turbulence-chemistry interaction (TCI) correctly. Transient phenomena involving finite-rate chemistry, e.g., flame quenching and auto-ignition, require an appropriate sgs model for TCI. For both RANS and LES, in addition to the closure problem of the Reynolds stresses (Pope, 2000 [72]), this highly non-linear reaction rate also requires closure to model the TCI. A comprehensive review of various approaches used in literature to model turbulent reacting flows may be sought in Poinset and Veynante (2001) [68] and Echekki et al. (2011) [13].

Among the different approaches found in the literature, turbulent combustion models employing a statistical description of the unclosed reaction source term have gained significant attention. These methods use a one-point, one-time joint probability density function (PDF) of the composition (filtered density function (FDF) in LES context), or a subset of it, to obtain the filtered values of reactive scalars. The PDF/FDF methods may be broadly sub-classified into two categories. The first relies on evolving reactive scalars in a low-dimensional manifold comprised of mixture fraction and/or reaction progress variable whose joint PDF/FDF has a presumed form. The flamelet (Peters, 1984 [62]) and conditional moment closure (CMC) (Klimenko and Bilger, 1999 [40]) approaches fall into this category. Although these methods are attractive in terms of the computational cost, the confinement of the composition to the manifold means that these
models lack generality with different model variants required for non-premixed and premixed combustion regimes. They can struggle to accurately predict flames exhibiting strong extinction/re-ignition and auto-igniting flames. The alternative is the transported probability density function (TPDF) or transported filtered density function (TFDF) approach, which solves a transport equation of joint composition PDF/FDF or joint velocity-composition PDF/FDF without a priori assumption of the flame structure. Due to the multi-dimensionality of the PDF/FDF, its efficient solution is sought by solving stochastic differential equations over ensembles of Lagrangian stochastic particles (SPs) (Pope, 1985 [69]) or Eulerian stochastic fields (ESF) (Valiño, Bos and Dopazo, 1991 [91]).

The major advantage of the transported PDF/FDF method is that the non-linear filtered chemical source terms appear in closed form and require no special turbulence modelling (Pope, 1985 [69]). However, the effects of turbulent transport and conditional dissipation due to molecular diffusion (micro-mixing) are un-closed. The former is usually modelled based on the gradient diffusion hypothesis, whereas the latter is closed by a mixing model emulating the effects of molecular mixing in the composition space. Several mixing models have been developed, including interaction by exchange with mean (IEM) (Villermaux and Devillon, 1972 [94]), mapping closure (MC) (Pope, 1991 [71]), Curl’s coalescence and dispersion (CD) (Janicka, Kolbe and Kollmann, 1979 [33]), Euclidean minimum spanning tree (EMST) (Subramaniam and Pope, 1998 [87]), and their variants. Although these mixing models have been used extensively to simulate turbulent reactive flows, all of those listed above lack some of the properties required of a good mixing model, such as linearity, independence, and localness, as laid out by Subramaniam and Pope [87]. Molecular mixing is a local phenomenon driven by the small-scale gradients of scalar concentrations. Localness is particularly important as non-local mixing can lead to excessive diffusion of the composition across the thin reaction zone leading to non-physical outcomes such as exaggerated localised extinction events. Among the models mentioned above, EMST satisfies localness by explicitly confining the molecular mixing in the stochastic composition space; however, it violates the linearity and independence properties. For the other models listed above, mixing localness can be progressively
imposed by confining mixing to particles in the same finite-volume (FV) cell while using many stochastic particles per cell and reducing the cell size. For LES, where the number of FV cells is quite large to resolve smaller spatial scales, this refinement becomes prohibitive. Therefore, these intensive TPDF simulations are computationally expensive. Hence, besides satisfying the characteristics of a good mixing model, an ideal TPDF approach should also provide a cost-effective solution for practical combustion systems.

Klimenko and Pope (2003) [39] introduced the concept of multiple mapping conditioning (MMC) for modelling turbulent combustion, which is an amalgamation of the PDF, conditional moment closure (CMC), and MC approaches. In the evolution of the PDF, MMC plays the role of a mixing model by providing closure for the conditional scalar dissipation. A mathematically independent reference space mimicking important combustion quantities, such as the mixture fraction in non-premixed combustion (Cleary and Klimenko, 2011 [7]), and the progress variable (Straub et al., 2020 [85]) in premixed combustion, is used to ensure the conservation of the conditional means during molecular mixing. MMC satisfies the key requirements of a good mixing model, including linearity, independence, and localness. Due to the enforced localised mixing, sparse distribution of stochastic particles may be used in the MMC model within the LES framework (hereafter referred to as MMC-LES). Typically, fewer stochastic particles are used for the FDF of the reactive composition than the number of FV cells used for the solution of the filtered Navier-Stokes equation, making it a computationally attractive approach.

Numerous numerical studies of the Berkeley’s vitiated co-flow burner (VCB) with H₂ as fuel exists in both RANS and LES framework (Masri et al. (2004) [50], Cao, Pope and Masri (2005) [4], Gordon et al. (2007) [25], Patwardhan et al. (2009) [61], Navarro-Martinez and Kronenburg (2011) [58], Han, Raman and Chen (2016) [27], Sundaram et al. (2016) [88]). On the other hand, the computational studies of the methane fuelled VCB are relatively smaller in number, especially using the FDF approach. In their original paper on the methane VCB, Cabra et al. (2005) [2] applied the RANS-PDF approach and performed a comparative study of various mixing models (IEM, CD and EMST) with experimental predictions. A generous resolution of 400 SPs per FV cell was used, and
tuning of the mixing model constant (e.g. $C_{\phi} = 2$ for EMST) was needed to achieve the accurate predictions composition scalars (specie concentration and temperature). Gkagkas and Lindstedt (2007) [24] explored similar sensitivity of the model constant for the modified CD model, but the focus of the study was on the chemical kinetics of the species formed pre and during ignition. The authors concluded that the most important minor species during the pre-ignition playing a crucial role were $H_2$, $HO_2$ and $CH_2O$. Subsequently, Gordon et al. (2007) [25] used the EMST model with $C_{\phi} = 1.5$ and studied transport budgets of convection, diffusion, and reaction to conclude that auto-ignition is the most likely mechanism of flame stabilisation for the methane flame. The earliest study of the methane VCB using the presumed LES-FDF approach was performed by Domingo, Vervisch and Veynante (2008) [12] and Navarro-Martinez and Kronenburg (2009) [56], which used steady-flamelet and CMC model, respectively. Navarro-Martinez and Kronenburg [56] were able to capture the fluctuations of the flame base, which is not available from RANS predictions. Afterwards, Ihme and See (2010) [31] showed that using a steady flamelet model causes significantly faster ignition in this flame which is not in agreement with the measurements. It was concluded that the unsteady flamelet approach produced the correct lift-off behaviour. Jones and Navarro-Martinez (2009) [37] employed the LES-ESF approach to model these lifted flames and concluded that though the flame base is quite fluctuating, the model was able to capture it with reasonable expense. Other notable studies include using the LES-ESF with tabulation by Kulkarni, Zellhuber and Polifke (2013) [42], CMC with explicit extinction modelling by Roy, Kumar and Sreedhara (2014) [74], and LES Thickened Flame model by Schulz et al. (2017) [77].

In the past decade, MMC-LES has been successfully applied to a variety of turbulent flames (Galindo-López et al., 2018 [17]), but its application to lifted flames are scarcely any (Sundaram et al., 2016 [88]). In the RANS framework, some studies exist which employ intensive MMC method i.e. more SPs than FV cells (Wandel and Lindstedt (2019) [96], Ghai and De (2019) [23]). Therefore, the objective of the current study is to evaluate the performance of the sparse-Lagrangian MMC-LES to predict Berkeley lifted flame with the relatively complex methane fuel. The remainder of this thesis is structured as
follows:

Chapter 2 provides an articulate description of the mathematical formulation of modelling turbulent reacting flows in the LES framework with a focus on FDF based approaches.

Chapter 3 provides details of the experimental database and the corresponding numerical setup.

Comparisons with the experimental measurements are presented in Chapter 4.

Finally, conclusions from the current study are outlined in Chapter 5.
This chapter presents the gas-phase governing equations within the large eddy simulation (LES) framework for variable density, low-Mach number, turbulent reactive flows where acoustic interactions and compressibility effects are neglected. The modelling of the un-closed reaction term is discussed with a specific focus on probabilistic approaches. The chapter ends with details of the multiple mapping conditioning (MMC) method employed in the current study.

### 2.1 Filtered Governing Equations of Reacting Flows

In large eddy simulation (LES), the objective is to compute large scale energy-containing structures, greater than the grid size, while the small scale dissipative structures are modelled. Contrary to the Reynolds averaged Navier-Stokes (RANS) averaging procedure, where the governing equations are averaged in time, a spatial filtering operation is performed thereby preserving temporal information. Any instantaneous flow quantity, \( \Phi \), may be decomposed as

\[
\Phi = \bar{\Phi} + \Phi', \tag{1}
\]

\[
\Phi = \tilde{\Phi} + \Phi'', \tag{2}
\]

where the former is Reynolds decomposition for quantities per unit volume while the latter is density-weighted Favre filtering for per unit mass quantities. The \( .' \) and \( .'' \) denotes the un-resolved/sub-grid scale (sgs) terms. The following equations may be derived by decomposing the un-filtered conservation equations and performing spatial filtering operations. As the conservation equations contain non-linear terms, such as the convection term in the momentum equation, this decomposition and filtering procedure leads to un-closed terms. Solving transport equations for such terms leads to even higher-
order un-closed terms. This is known as the closure problem of turbulence [72], and hence modelling of these terms is needed.

The low-pass, spatial filtering operation may be defined as,

\[ \hat{\Phi} = \frac{\rho\Phi}{\bar{\rho}}, \]  

\[ \hat{\Phi}(x_j, t) = \int_{-\infty}^{\infty} \Phi(y_j, t)G(x_j - y_j, t) dy_j \]  

\[ = \int_V \Phi(y_j, t)G(x_j - y_j, t) dy_j, \]  

\[ \hat{\Phi}(x_j, t) = \frac{1}{\bar{\rho}} \int_V \rho(y_j, t)\Phi(y_j, t)G(x_j - y_j, t) dy_j, \]  

and

\[ \hat{\rho}(x_j, t) = \int_V \rho(y_j, t)G(x_j - y_j, t) dy_j. \]

Here the integral is over the entire computational domain \( V \) and the filter function, \( G \) of kernel width \( \Delta \), satisfies \( G(x) = G(-x) \), and \( \int_V G(y) dy = 1 \). Note that the subscript \( j \) denotes the index of spatial direction. Filtering removes the small-scale fluctuations, but the influence of these unresolved quantities, on the resolved scales is modelled in terms of the \( sgs \) stresses/fluxes. Thus, the filtered conservation equation of mass, momentum, energy and species conservation may be written as follows,

### 2.1.1 Conservation of mass

\[ \frac{\partial \hat{\rho}}{\partial t} + \frac{\partial \hat{\rho} u_i}{\partial x_i} = 0 \]  

(8)

where \( u_i \) is the bulk fluid velocity component in the \( x_i \)-direction.

### 2.1.2 Conservation of momentum

\[ \frac{\partial \hat{\rho} u_i}{\partial t} + \frac{\partial \hat{\rho} u_j u_i}{\partial x_j} = -\frac{\partial \hat{\rho}}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial \tau_{ij}^{sgs}}{\partial x_i} \]  

(9)
2.1 FILTERED GOVERNING EQUATIONS OF REACTING FLOWS

where \( \tau_{ij} = 2\mu \tilde{S}_{ij} \) is the stress tensor. The strain rate \( S_{ij} \),

\[
\tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij},
\]

is the deviatoric component, while the hydrostatic part of the stress is added to the pressure term although it is negligible for low mach flows. The term \( \tau_{ij}^{sgs} \) is the sub-grid stress, modelling of which is discussed in the next sub-section.

2.1.3 Conservation of species mass fractions

\[
\frac{\partial \rho \tilde{Y}_\beta}{\partial t} + \frac{\partial}{\partial x_j} (\rho \tilde{u}_j \tilde{Y}_\beta + \overline{V_{\beta,j}} \tilde{Y}_\beta) = -\frac{\partial q_{sgs,\beta,j}}{\partial x_j} + \rho \tilde{W}_\beta
\]

where \( Y_\beta \) is the mass fraction of the \( \beta \)th species \( (\beta = 1, 2, \ldots, N_s) \), \( \overline{V_{\beta,j}} \tilde{Y}_\beta \) is the filtered molecular diffusion flux modelled using Fick’s law [89],

\[
\overline{V_{\beta,j}} Y_\beta = -\rho \overline{\mathcal{D}}_\beta \frac{\partial \tilde{Y}_\beta}{\partial x_j}
\]

\( \overline{\mathcal{D}} \) is the molecular mass diffusion coefficient, and \( \tilde{W}_\beta \) is the rate of production of specie \( \beta \) per unit volume. Note that \( V_{\beta,j} \) is the \( j \)th component of diffusion velocity of specie \( \beta \).

2.1.4 Conservation of energy

\[
\frac{\partial \tilde{h}_s}{\partial t} + \frac{\partial \rho \tilde{u}_j \tilde{h}_s}{\partial x_j} = \frac{D \rho}{Dt} + \frac{\partial}{\partial x_j} \left( \rho \alpha \frac{\partial \tilde{h}_s}{\partial x_j} \right) - \frac{\partial q_{sgs,\beta,j}}{\partial x_j} + \tau_{ij} \frac{\partial \tilde{u}_i}{\partial x_j} + \rho \tilde{W}_h
\]

where \( h_s \) is the sensible enthalpy of the fluid, \( \alpha \) is the filtered thermal diffusion coefficient, and \( \tilde{W}_h \) is the heat release rate due to chemical reactions. For low mach number flows, the pressure contribution and the viscous dissipation term (second last term on right
hand side) are small and hence neglected. Note that some reacting flow codes solve the transport of the the standardised enthalpy, $h$

$$h = \sum_{\beta=1}^{N_s} h_{\beta}^c Y_{\beta} + h_s,$$

$$h_s = \sum_{\beta=1}^{N_s} \int_{T^0}^{T} C_{p,\beta}(T) dT,$$

where $h_{\beta}^c$ is the chemical enthalpy or enthalpy of formation at $T^0 = 298.15$ K and $p^o = 1$ atm, and $C_p$ is the specific heat at constant pressure. For the conservation of $h$, the chemical source term (last) in Equation (12) does not exist.

### 2.1.5 Equation of State

The density of the fluid may be evaluated from the equation of state assuming ideal gas,

$$\rho = \frac{p}{R_u \cdot \sum_{\beta} \frac{Y_{\beta}}{M_{w\beta}} \cdot T},$$

(13)

where $p$ is the thermodynamic pressure, $M_{w\beta}$ is the molecular weight, and $R_u$ is the universal gas constant.

In equations Equations (9), (11) and (12), there are un-closed sub-grid stresses/fluxes, representing the contribution of the un-resolved scales, which need to be modelled. As the chemical reactions are also a sub-grid phenomenon, approximation of $W$ is also needed to close the system of equations.

### 2.2 Sub-Grid Scale Model

The closure of the sub-grid terms described in Sections 2.1.2 to 2.1.4 is presented in this section. The modelling of the reaction rate is left for the next section. The model coefficients for the closed terms may be evaluated dynamically.
The sub-grid stress, \( \tau_{ij}^{sgs} = \rho(\tilde{u}_i \tilde{u}_j - \bar{u}_i \bar{u}_j) \), may be modelled using Boussinesq assumption [72],

\[
-\tau_{ij}^{sgs} = 2\rho \nu_{sgs} \tilde{S}_{ij} - \frac{2}{3} \rho k_{sgs} \delta_{ij}.
\] (14)

Here \( S_{ij} \) is the deviatoric strain rate (Eq. (10)) and \( k_{sgs} = \frac{1}{2} \tau_{kk} \) is the kinetic energy contained in the un-resolved scales.

The sub-grid viscosity, \( \nu_{sgs} \), may be modelled using the simple algebraic model proposed by Smagorinsky [83] from dimensional analysis as

\[
\nu_{sgs} = C_\nu \Delta^{4/3} l_t^{2/3} ||\tilde{S}_{ij}||,
\]

where the \( l_t \) is the turbulence integral length scale assumed equal to the filter width \( \Delta \). \( C_\nu \) is a model coefficient having default value of \( \sqrt{C_\nu} = 0.16 \), but may be varied between \( 0.1 - 0.2 \) [22]. Here \( ||\tilde{S}_{ij}|| = \sqrt{\tilde{S}_{ij} \tilde{S}_{ij}} \) is the Frobenius norm of \( S_{ij} \). Therefore,

\[
\nu_{sgs} = C_\nu \Delta^{2} ||\tilde{S}_{ij}||, \quad (15)
\]

\[
\nu_{sgs} = C_\nu \Delta^{2} \sqrt{\tilde{S}_{ij} \tilde{S}_{ij}}. \quad (16)
\]

### 2.2.1 Dynamic procedure

In the previous sub-section, the model coefficient for the \( sgs \) viscosity, \( C_\nu \), were presented which may be tuned to achieve the correct level of turbulent fluctuations. Another method is to evaluate this coefficient dynamically from the local flow properties as originally proposed by Germano et al. [22]. The basic idea behind the dynamic procedure is to use information at the grid scale (gs) to find the coefficient for the closure for the \( sgs \) terms. The method was suggested to rectify the problems with the excessive damping caused by the single, static value of coefficients of eddy-viscosity type closures for the \( sgs \) stress terms [15]. To find the closure coefficient, a coarser secondary filter compared to the LES filter, known as the “test” filter (\( \cdot \)), is employed to find a relationship between
the sgs term at the two filter widths. This subsection provides details of the procedure considering the sgs stress as the un-closed non-linear quantity, and more details may be sought in \[15, 22, 44, 64\].

Mass-weighted, secondary (test) spatial filtering of any quantity, $\Phi$, is defined as

$$\tilde{\Phi} = \frac{\hat{\rho} \Phi}{\hat{\rho}}, \quad (17)$$

analogous to Equation (3), with the size of this filtering window usually considered as $\hat{\Delta} = 2 \cdot \Delta$. With this idea the model constant for eddy viscosity is defined as,

$$C_\nu = \frac{1}{2} \frac{\left| L_{ij} \cdot M_{ij} \right|}{\left| M_{kl} \cdot M_{kl} \right|}. \quad (18)$$

Here $L$ and $M$ are Leonard and Model terms defined as,

$$L_{ij} = \hat{\rho} \hat{u}_i \hat{u}_j - \hat{\rho} \hat{u}_i \hat{u}_j, \quad (19)$$
$$M_{ij} = \hat{\rho} \hat{\Delta}^2 \left| \hat{S}_{ij} \right| \hat{S}_{ij} - \hat{\rho} \hat{\Delta}^2 \left| \hat{S}_{ij} \right| \hat{S}_{ij}. \quad (20)$$

The procedure outlined by Germano et al. [22] is known to produce unphysical values of constants as they contracted Equation (18) with the strain rate tensor (rather than $M$), and hence some global averaging procedure was needed to achieve a stable solution. To avoid this, Lilly’s modification [44] which uses the modelled tensor, $M_{ij}$, and least squares to calculate the coefficient $C_\nu$ is applied in the current work. With this, unphysically large values are avoided as Equation (18) approaches zero when the model term approaches zero. Operator $\| \|$ denotes local averaging over the finite volume cells to further damp isolated large values.

As first observed by Germano et al. [22] and Lilly [44], the numerator of Equation (18) may become negative, essentially representing an unrealistic backscatter of energy from small unresolved scaled to resolved scales. This causes the sgs model to amplify turbulent
fluctuations rather than damping it i.e. $\nu_{sgs} < 0$. A popular method used in literature [98] is to force a zero effective viscosity,

$$\nu_{eff} = \nu + \nu_{sgs} \geq 0 \text{ if } C_s < 0,$$

$$\nu_{sgs} \geq -\nu \text{ if } C_s < 0$$

and hence allowing some back-scatter, which may still provide stable solutions. Here, $\nu$ is the molecular momentum diffusivity. Alternatively, following the works of Verma and Mahesh [93] and Meneveau et al. [52], only positive (or zero) values can be enforced for the $sgs$ model coefficients, considering only the dissipative nature of the turbulence model.

2.2.1.1 SGS Kinetic Energy

The $sgs$ kinetic energy, Equation (14), may be evaluated following the procedure above as

$$k_{sgs} = \frac{1}{2} \tau_{k_k}^{sgs} = \frac{1}{2} C_k \Delta^2 ||\tilde{S}_{ij}||^2,$$

(21)

where

$$C_k = \frac{|L \cdot M|}{|M \cdot M|},$$

(22)

$$L = \hat{\rho} \bar{u}_i \bar{u}_j - \hat{\rho} \tilde{u}_i \tilde{u}_j,$$

(23)

$$M = \hat{\rho} \Delta^2 ||\tilde{S}_{ij}||^2 - \hat{\rho} \tilde{\Delta}^2 ||\tilde{S}_{ij}||^2.$$  

(24)
2.2.1.2 SGS Scalar Fluxes

The un-closed terms, $q_{\beta,j}^{sgs}$ and $q_{h,s,j}^{sgs}$, in the specie mass and energy conservation Equations (11) and (12) may be defined as,

$$q_{\beta,j}^{sgs} = \bar{\rho}(\tilde{u}_j \tilde{Y}_\beta - \tilde{u}_j \tilde{\phi}_\beta),$$

$$q_{h,s,j}^{sgs} = \bar{\rho}(\tilde{u}_j \tilde{h}_s - \tilde{u}_j \tilde{\phi}_s).$$ (25) (26)

These non-linear terms are usually modelled using the gradient diffusion hypothesis as,

$$q_{\beta,j}^{sgs} = -\bar{\rho} D_{\beta,sgs} \frac{\partial \tilde{Y}_\beta}{\partial x_j},$$

$$q_{h,s,j}^{sgs} = -\bar{\rho} \alpha_{sgs} \frac{\partial \tilde{h}_s}{\partial x_j},$$ (27) (28)

where $D_{\beta,sgs}$ and $D_{th,sgs}$ are the sgs mass and thermal diffusivity, respectively. These flow properties may be approximated similar to $\nu_{sgs},$

$$D_{sgs} = C_d \Delta^2 ||\tilde{S}_{ij}||,$$

$$D_{th,sgs} = C_a \Delta^2 ||\tilde{S}_{ij}||,$$ (29) (30)

where the coefficients may be evaluated dynamically similar to the process defined above for $\nu_{sgs},$

$$\mathcal{L}_j = \hat{\rho} \tilde{u}_j \tilde{\phi} - \hat{\rho} \tilde{u}_j \tilde{\phi}_s, \quad \mathcal{M}_j = \hat{\rho} \Delta^2 ||\tilde{S}_{jk}|| \frac{\partial \tilde{\phi}}{\partial x_j} - \hat{\rho} \Delta^2 ||\tilde{S}_{jk}|| \frac{\partial \tilde{\phi}_s}{\partial x_j}. $$ (31)

Here $\phi_\alpha = \{Y_\beta, h \text{ or } T, Z\}$ is the composition vector and assuming binary diffusion with equal mass diffusivity for all species ($D_\beta = D$; differential diffusion neglected), a single sgs mass diffusivity may be evaluated using the local mixture fraction, $Z$. The thermal diffusivity is obtained from temperature or a unity Lewis number ($Le = D_{th}/D$) assumption may be employed as in this current work.
2.3 FILTERED CHEMICAL SOURCE TERM

The current section focuses on the closure of the filtered reaction rate, $\rho W$, which should be valid for different combustion regimes such as pre-mixed, partially pre-mixed or non-premixed. Considering Arrhenius rate law \[89]\ based approximation of $W$, it is a non-linear function of the composition $\phi$. Decomposing and filtering the reaction rate via Equation (1) causes higher-order un-closed terms to appear due to this non-linearity. Closure of the filtered $W$ by considering only the filtered composition, $\tilde{\phi}$ i.e.

$$\tilde{W}(\phi, T) \neq W(\tilde{\phi}, \tilde{T}),$$

is an over-simplification and may be reasonably accurate for some stable flames. This approximation may fail in cases where the turbulence-chemistry interaction (TCI) is strong such as for flames with high local extinction as with this approximation, perfect mixing is assumed at the sgs, neglecting any fluctuations in composition $\phi". The interpretation of this assumption is that at the sub-grid scales, the composition is the same everywhere and equal to the filtered composition, $\tilde{\phi}$. Therefore, a better closure of the filtered $W$ is needed to be able to model highly turbulent flames.

2.3.1 Filtered Density Function (FDF)

Among the different approaches found in the literature, turbulent combustion models employing a statistical description of the un-closed reaction source term have gained significant attention [69]. The discussion in the current text is limit to these statistical models only. These methods use a one-point, one-time joint filtered density function (FDF) of the sgs composition, or a subset of it, to obtain the filtered values of reactive scalars. The
FDF, $\mathcal{F}$, may be defined for the sub-grid composition, $\phi = (Y_1, Y_2, \ldots, Y_\beta, \ldots, Y_{N_s}, h, Z)$, fluctuations as,

$$
\begin{align*}
\mathcal{F}(\Psi; x, t) &= \int_{-\infty}^{\infty} \rho(y, t) \varphi[\Psi, \phi(y, t)] G(x - y, t) dy, \\
&= \int \rho(y, t) \varphi[\Psi, \phi(y, t)] G(x - y, t) dy, \\
\varphi[\Psi, \phi(x, t)] &= \delta[\Psi - \phi] = \prod_{\alpha=1}^{N_s+2} \delta[\Psi_\alpha - \phi_\alpha].
\end{align*}
$$

where $\varphi$ is the fine-grained probability density function (PDF), and $\Psi$ is the sample space of composition. The fine-grained PDF, $\varphi[\Psi, \phi(x, t)] d\Psi$, represents the probability that at any $x$ and $t$, that composition lies between $\Psi_\alpha \leq \phi_\alpha \leq \Psi_\alpha + d\Psi_\alpha$, for all $\alpha$. The FDF is the density-weighted spatially filtered value of the fine-grained density $\varphi$, and hence it gives the density in the composition ($\Psi$) space of the fluid around $x$ weighted by the filter $G$. Interested readers may seek the more details on the FDF in Refs. [18, 32].

The FDF was initially introduced for constant density flows [11], and for variable density flows a filtered mass-density function (FMDF) ($\mathcal{F}$) definition was defined as mentioned earlier [32]. This distinction between FDF ($\mathcal{P}$) and FMDF is dropped and in the following only FDF notation in used. The relation between the two may be defined following Equation (3) as,

$$
\begin{align*}
\mathcal{P}(\Psi; x, t) &= \int_{-\infty}^{\infty} \varphi[\Psi, \phi(y, t)] G(x - y, t) dy, \\
\mathcal{F}(\Psi; x, t) &= \rho(x, t) \mathcal{P}(\Psi; x, t), \\
&= \rho(\Psi; x, t) \mathcal{P}(\Psi; x, t).
\end{align*}
$$

where one may define $\mathcal{P}$ and $\tilde{\mathcal{P}}$ as conventional- and Favre-filtered sub-grid FDF of sub-grid composition fluctuations, respectively [28].
The integral property of FDF states that integrating the joint composition FDF over the composition space recovers \([11, 32]\),

\[
\int_{-\infty}^{\infty} P(\Psi; x, t) d\Psi = \int_{-\infty}^{\infty} G(x - y, t) dy = 1, \tag{38}
\]

\[
\int_{-\infty}^{\infty} F(\Psi; x, t) d\Psi = \int_{-\infty}^{\infty} \rho(y, t) G(x - y, t) dy = \bar{\rho}. \tag{39}
\]

Also note that similar to the PDF, the filtered density functions also satisfy that \(F(\Psi; x, t) \geq 0\) and \(P(\Psi; x, t) \geq 0\). Important property of the FDF \([11]\) states that the filtered value of any scalar \(Q(x, t)\), which may be defined completely as the function of composition \(\phi(x, t)\), such as \(\rho(\phi(x, t))\) or \(W(\phi(x, t))\), may be obtained as,

\[
\bar{\rho}(x, t) \tilde{Q}(x, t) = \int_{-\infty}^{\infty} \rho(y, t) Q(y, t) G(x - y, t) dy, \tag{40}
\]

\[
= \int_{-\infty}^{\infty} \langle Q(x, t) | \Psi \rangle \mathcal{F}(\Psi; x, t) d\Psi, \tag{41}
\]

\[
= \int_{-\infty}^{\infty} Q(\Psi) \mathcal{F}(\Psi; x, t) d\Psi, \tag{42}
\]

\[
= \bar{\rho}(x, t) \int_{-\infty}^{\infty} Q(\Psi) \mathcal{P}(\Psi; x, t) d\Psi. \tag{43}
\]

Hence, the filtered value of any quantity, which is a function of scalar composition \((\phi = \{\phi_1, \phi_2, \ldots \})\), may be obtained by integration over the composition space. Here, \(\langle X|Y \rangle\) is the density weighted conditionally filtered value of \(X\) conditioned on \(Y\) and is defined as

\[
\langle Q(x, t) | \Psi \rangle = \frac{\int_{-\infty}^{\infty} \rho(y, t) Q(y, t) \phi(\Psi, y, t) G(x - y, t) dy}{\mathcal{F}}. \tag{44}
\]

The corresponding conventional (or Reynolds), conditionally filtered quantity may be defined as

\[
\overline{Q(x, t)|\Psi} = \frac{\int_{-\infty}^{\infty} \overline{\rho(y, t) Q(y, t) \phi(\Psi, y, t) G(x - y, t) dy}}{\mathcal{P}}. \tag{45}
\]
The relation between Equation (45) and Equation (44) may be defined similar to the Favre-filtering (Equation (35)) as,

\[ \langle Q(x,t) | \Psi \rangle = \rho(x,t) Q(x,t) = \rho(\bar{\Psi}) \tilde{Q}(\Psi), \]

where \( \tilde{Q}(\Psi) = \Omega(x,t) | \Psi \). Therefore, following the properties mentioned above we can evaluate the filtered reaction rate as,

\[ \rho(\bar{\Psi}) \tilde{W}(\phi(x,t)) = \int_{-\infty}^{\infty} W(\Psi) F(\Psi; x, t) d\Psi. \]

The FDF methods may be broadly sub-classified into two categories. The first relies on evolving reactive scalars in a low-dimensional manifold comprised of mixture fraction (Z) and/or reaction progress variable (C) whose joint FDF, \( F(\Psi = \{Z, C\}; x, t) \), has a presumed form. The alternative is the transported FDF approach, which solves a transport equation of full joint composition FDF or joint velocity-composition FDF, without a priori assumption of the flame structure. The following text briefly touches upon the popular FDF method mentioned in literature for modelling of turbulent non-premixed flames.

2.3.1.1 Flamelet Model

In non-premixed combustion, fuel and oxidiser are initially separated. Chemical reactions occur only because of mass diffusion or molecular mixing of these reactants. If the chemistry is considered fast enough, a reaction zone forms at about stoichiometric conditions. In this region, fuel and oxidiser diffuse from reactant sides and form reaction products. Combustion is typically controlled by the rate of molecular mixing if the chemical time-scales are smaller than the flow time scales (large Damköhler number, \( D_a \)). If the chemical time-scales are comparable to flow time-scales (low \( D_a \)), extinction can occur. This assumption of small chemical time-scale relative to the turbulent time-scale introduces an important simplification, since it eliminates many parameters such as those associated with chemical kinetics.

Introduced by Peters [62], the fundamental concept of flamelet modelling assumes the
structure of a turbulent diffusion flame as an ensemble of laminar diffusion flame element called \textit{flamelet}. The flamelet concept is assumed to be valid for high $D_a$, where $D_a = \frac{\tau_t}{\tau_c}$ i.e. the ratio of turbulent to chemical time-scales. The essential feature of the flamelet modelling is the representation of the laminar flame structure in terms of a \textit{conserved} scalar variable i.e. the mixture fraction ($Z$). The laminar flame may be represented by the Burke-Schumann [89] equilibrium solution ($\tau_c \rightarrow 0$ or infinitely fast chemistry), in terms of mixture fraction, which assumes a infinitely thin reaction zone and the reactants never co-exist. However, in real flames non-equilibrium (finite-rate chemistry) effects become important and need to be considered. The laminar counterpart of the specie (and enthalpy) Eq. (11) is transformed from spatial coordinates ($x$, $t$) to ($Z$, $t$) to obtain the steady flamelet equation,

$$
-\rho \chi \frac{\partial^2 \phi_\beta}{\partial Z^2} = \rho W_\beta, \tag{48}
$$

where $\chi = 2D \left( \frac{\partial Z}{\partial x_j} \right)^2$ is the scalar dissipation rate. The above equation is solved analytically for all species, $\beta$, to obtain the description of the flame structure in terms of mixture fraction $Z$. The values of the thermo-chemical chemical composition, as a function of $Z$, can be pre-computed for various values of $\chi_{st}$ (scalar dissipation rate at stoichiometry $Z_{st}$) and stored for the calculations of complex turbulent flame evaluations. More details may be found in Refs. [13, 62, 64].

To obtain the filtered quantities, $\tilde{Q}(x, t)$ (see Equation (40)), such as specie mass fraction or temperature, a low-dimensional (lower than the full composition $\phi = \{Y_\beta, h\}$) joint composition-FDF $\tilde{P}$ is presumed which is a function of $Z$ and $\chi$ i.e. $\Psi = \{Z = \zeta, \chi = \chi\}$,

$$
\tilde{Q}(x, t) = \int_{-\infty}^{\infty} Q(\Psi) \tilde{P}(\Psi; x, t) \, d\Psi, \tag{49}
$$

$$
= \int_{-\infty}^{\infty} \tilde{Q}(\zeta, \chi) \tilde{P}(\zeta, \chi; x, t) \, d\zeta \, d\chi, \tag{50}
$$
where $\zeta$ and $\chi$ are the sample space of $Z$ and $\chi$. Here, $\Omega(\Psi)$ is evaluated by solving Equation (48) to get any field variable $\Omega$ as a function of the composition $\Psi$. The filtered density may be obtained as

$$
\bar{\rho} = \left[ \int_{-\infty}^{\infty} \frac{\tilde{P}(\zeta, \chi; x, t)}{\rho(\zeta, \chi; x, t)} d\zeta \, d\chi \right]^{-1}.
$$

(51)

Assuming statistical independence between $Z$ and $\chi$, the joint-FDF may be written in terms of marginal PDF of $\tilde{P}$ as,

$$
\tilde{P}(Z = \zeta, \chi = \chi) = \tilde{P}(\zeta) \cdot \tilde{P}(\chi).
$$

(52)

In practice, a $\beta$-distribution is assumed for the mixture fraction while the scalar dissipation rate used is the stoichiometric dissipation rate, $\chi_{st}$, having a one-parameter log-normal PDF [35]. Other variants of the flamelet model such as with addition of the reaction progress variable ($C$), extension to the pre-mixed regime, etc. may be found in Refs. [28, 60, 62, 65].

2.3.1.2 Conditional Moment Closure (CMC)

The conditional moment closure (CMC) method was derived independently by Klimenko and Bilger [40]. Similar to the flamelet model, the CMC method uses the concept that there exists a correlation between the reactive scalars and the mixture fraction ($Z$), and hence the composition fluctuations may be linked to the fluctuations in $Z$-space ($\Psi = \{\zeta\}$). In non-premixed flows, where there is mixing between fuel and oxidiser streams, the reactive scalars within the mixing field depend strongly on the local and instantaneous value of mixture fraction $Z(x, t)$. Conditioning the reactive species ($\phi$) on $Z$, $\langle \phi(x, t)|Z = \zeta\rangle$, leads to relatively small fluctuations around the conditionally filtered quantities (see Equation (44)), and a simple first order closure for the filtered chemical source can be
found. Any instantaneous composition variable, such as mass fraction or enthalpy, may be decomposed in CMC as

\[ \phi_\alpha(x, t) = Q_\alpha(\zeta; x, t) + \phi_\alpha''(x, t), \] (53)

where \( Q_\alpha(\zeta; x, t) = \langle \phi_\alpha(x, t) | Z = \zeta \rangle \) denotes the conditionally filtered mean (see Equation (44)), while \( \phi_\alpha''(x, t) \) is the fluctuation around it. The transport equations for conditional scalars (temperature or enthalpy and species conservation), \( Q_\alpha(\zeta; x, t) \), can be derived using Equations (11), (44) and (46), complete details of which may be found in Refs. [40, 57]. This transport equation has an un-closed conditionally filtered reaction rate, \( \langle W_\alpha(\phi_\alpha) | \zeta \rangle \), which requires modelling. If this closure of the conditional scalars appearing in reaction rate term which needs to be modelled is achieved at the first moment level (Arrhenius law) by neglecting the conditional fluctuations \( \phi_\alpha'' \), the model is said to be ‘first-order CMC’ model i.e.

\[ \langle W_\alpha(\phi_\alpha) | \zeta \rangle = W_\alpha(Q_\alpha, \zeta). \] (54)

Finally, any un-conditionally filtered quantity may be evaluated from the filtered quantity using Equation (40) or Equation (49),

\[ \tilde{Q}_\alpha(x, t) = \int_{-\infty}^{\infty} Q_\alpha(\zeta) \tilde{P}(\zeta; x, t) \, d\zeta. \] (55)

The filtered density is evaluated similar to Equation (51). Here, similar to the flamelet model (Section 2.3.1.1), the sgs FDF can be presumed for the mixture fraction, \( \zeta \), and is usually assumed as a \( \beta \)-function [40].

The CMC model is able to predict complex reacting flows such as auto-igniting flames with reasonable accuracy [56], although flames with strong extinction require higher order closure of the conditionally filtered reaction rate [78].
2.3.1.3  Transported FDF

Till now the methods presented above used a presumed distribution of the sgs composition of scalars (see Sections 2.3.1.1 and 2.3.1.2) such as the $\beta$-distribution for the low-dimensional composition manifold ($\Psi = \{\zeta\}$). This assumption has been shown to be a reasonable approximation for various flames [56, 66, 78], but fails for cases such as having strong local extinction [20] or spray flames [21]. Moreover, these methods require different treatment for application to pre-mixed flames. An alternative, and more exact approach, is to solve a transport equation of the one-point, one-time, full joint-composition FDF, $\mathcal{F}(\Psi; x, t)$. Originally proposed by Pope [69] in the RANS context, the transport equation of the joint-composition PDF (or joint velocity-composition) was later extended to the sub-filter composition in the LES framework [11, 18]. As full composition ($\Psi$) is considered and no assumption is made about the correlation with flow quantities such as $Z$, the transported filtered density function (TFDF) methods are applicable to pre-mixed, non-premixed and partially-premixed reacting flows. More details on the historical developments of the TFDF methods may be found in Refs. [13, 14, 28]. The modelled transport equation of the FDF may be written as [32],

$$\frac{\partial \mathcal{F}}{\partial t} + \frac{\partial}{\partial x_j} (\bar{u}_j \mathcal{F}) = \frac{\partial}{\partial x_j} \left( \bar{\rho} (\mathcal{D} + \mathcal{L}) \frac{\partial (\mathcal{F}/\bar{\rho})}{\partial x_j} \right) - \frac{\partial^2}{\partial \Psi_\alpha \Psi_\beta} \left( \left\langle \frac{\partial \Phi_\alpha}{\partial x_j} \frac{\partial \Phi_\beta}{\partial x_j} | \Psi \right\rangle \mathcal{F}/\bar{\rho} \right) + \frac{\partial W_\alpha (\Psi) \mathcal{F}}{\partial \Psi_\alpha}.$$  \hspace{1cm} (56)

The FDF equation has a high dimension depending on the number of species representing the thermo-chemical composition $\Psi = \{\Psi_1, \Psi_2, \ldots, \Psi_{N_s}, \Psi_h, \zeta\}$, usually $N_s >> 1$. The salient feature of the transported PDF/FDF methods is that the chemical source term $W_\alpha$ appears as closed and requires no modelling. The second term on the right-hand side (RHS) is the sub-filter conditional scalar dissipation rate, representing the effect of molecular mixing (micro-mixing) at the sub-grid scales. This term requires the knowledge of the conditionally filtered scalar gradients and therefore requires modelling as the one-point, one-time FDF $\mathcal{F}$ does not contain such information. Numerous models for this sub-grid mixing, known as mixing models, have been suggested including interaction.
multiple mapping conditioning

The multiple mapping conditioning (MMC) approach is a rather new concept in the list of advanced modelling strategies for turbulent reacting flows. The following subsection presents the details of the MMC concept, mostly in the LES framework, which is used in the current work.

Introduced by Klimenko and Pope [39] in 2003, MMC is a combination of PDF/FDF [32, 69], CMC [40] and MC [71] concepts. Both deterministic and stochastic formulations of MMC exist. Deterministic MMC is the logical extension of CMC, while the stochastic MMC is a complete joint PDF method with MMC playing the role of a mixing model (see Equation (57)) which enforces localness within a defined manifold. MMC uses the concept of reference variables, which emulate physical quantities such as mixture fraction or enthalpy, in which space the sgs molecular mixing is localised. In the original model, the closure of the sgs scalar dissipation term, which dissipates the sgs fluctuations of composition scalars, with the IEM mixing model (also known as linear mean-square estimation (LMSE)) is given as,

$$\frac{\partial^2}{\partial \Psi^2} \left( \left\langle \rho \frac{\partial \phi_\alpha}{\partial x_j} \frac{\partial \phi_\beta}{\partial x_j} |\Psi| \right\rangle \frac{\mathcal{F}}{\rho} \right) = -\frac{\partial}{\partial \Psi} \left[ \frac{1}{\tau} (\Psi_\alpha - \tilde{\phi}_\alpha) \mathcal{F} \right], \tag{57}$$

where $\tau$ is the ‘time-scale of the sub-grid mixing’ and $\tilde{\phi}_\alpha$ is the resolved/filtered value of any composition variable, such as specie-mass fraction, for specie $\alpha$. The solution of transported FDF equation becomes infeasible using conventional numerical methods as the computational cost increases exponentially with an increase in the number of scalars ($N_s+1$) used to describe the joint FDF $\mathcal{F}$. Monte-Carlo method using Lagrangian particles [36, 69, 70] and Eulerian stochastic fields (ESF) method [53, 90] are often used to achieve a solution of the FDF Equation (56).
MMC (stochastic) [39], these reference variable (ξ) were derived to evolve as Markov processes [19] with standard Gaussian distributions. Recent developments [9] relaxed this restriction arguing that the evolution of the reference space may be better performed via Eulerian equations in LES or direct numerical simulation (DNS), referring it to as the generalised understanding of MMC. In the following, the details of only the stochastic MMC in the LES framework is provided. For more details see Refs. [8, 13].

2.4.0.1 Generalised MMC

As mentioned earlier, the solution of the FDF transport equation (viz. Equation (56)) becomes infeasible via finite-volume (FV) methods. Therefore, its solution is achieved by Monte-Carlo simulation using Lagrangian stochastic particles (SPs) as describe by Pope [69]. Equation (56) of the FDF $F(Ψ; x, t)$ is converted to equivalent set of stochastic differential equations (SDEs), by comparison to the Fokker-Plank equation [19], representing the evolution of SPs given as,

\[
\text{Transport in physical space: } dx_{jp}^sp = A_{jp}^sp \, dt + B_{jk}^sp \, d\omega_k,
\]

\[
\text{Transport in composition space: } d\phi_{sp}^α = [W_{sp}^α + S_{sp}^α] \, dt.
\]

Here, the drift and diffusion coefficients are given as,

\[
A_j = \tilde{u}_j + \frac{1}{\rho} \frac{\partial}{\partial x_j} \left( \rho[D + D_{sgs}] \right),
\]

\[
B_{jk} = \delta_{jk} [D + D_{sgs}],
\]

respectively. Here $\delta_{jk}$ is the Kronecker delta. The term $W_α$ represents the closed chemical/radiation source term for species and enthalpy, respectively, and $d\omega$ represents the increment of a Gaussian-Weiner process with zero mean and variance of $dt$. Note that $\tilde{u}_j$, $\bar{\rho}$, $D$ and $D_{sgs}$ are interpolated from the Eulerian fields to the SP locations, generally expressed as $\gamma^{sp} = \gamma^{eu}(x^{sp}, t)$. In the present work, tri-linear interpolation is used for these quantities.
The mixing operator is denoted by $\delta_\alpha$ which represents the effect of the sgs conditional scalar dissipation (cf. Equation (57)) on the evolution of particle composition. MMC imposes the aforementioned localness on the mixing operation through conservation of conditional mean scalar quantities in both physical ($x$) and reference ($\xi$) space, represented symbolically as,

$$\langle \delta_\alpha | X, \Xi \rangle = \langle \delta_\alpha | x = X, \xi = \Xi \rangle = 0,$$

where $X$ and $\Xi$ are the sample spaces for $x$ and $\xi$, respectively. In generalised MMC, referred hereafter as MMC-LES, the filtered evolution equation of the reference space, considered as mixture-fraction ($\xi = \tilde{f}$) in the current work, is written as,

$$\frac{\partial \tilde{f}}{\partial t} + \frac{\partial \tilde{u}_j \tilde{f}}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho \frac{\partial \tilde{f}}{\partial x_j} \right) - \frac{\partial q_{s, j}^{gs}}{\partial x_j}.$$

The sgs flux term is modelled using the gradient diffusion hypothesis, similar to Equation (27),

$$q_{s, j}^{gs} = -\rho \tilde{D}_{gs} \frac{\partial \tilde{f}}{\partial x_j}.$$

The reference space emulates important combustion quantities, such as the mixture fraction in non-premixed combustion [9], and the progress variable [85] or flame shadow position [81] in premixed combustion. It is mathematically independent of the real mixture fraction, $Z$, evolved on the stochastic particles (using Equations (58) and (59)). Hence, MMC satisfies the key requirement of independence of a good mixing model, laid out by Subramaniam and Pope [87]. Other requirements including linearity and localness, also satisfied by MMC, will be discussed mathematically in the following.

The composition increment of a stochastic particle due to micro-mixing (cf. Equations (57) and (59)) is expressed as,

$$d\phi_{sp} = -\frac{1}{\tau_L} [\phi_{sp} - \langle \phi_{sp} | X, \Xi \rangle]$$
where τ_L is the anisotropic mixing time-scale (a-ISO) model [95], at Lagrangian filter-width, d_x. It is defined as the ratio of reference mixture fraction variance and the scalar dissipation rate at the sub-Lagrangian-grid scales (slgs) i.e.,

$$\tau_L = \frac{\tilde{f}^2}{\chi_L} = C_L \frac{C_f d_x^2}{\mathcal{D} + \mathcal{D}_{sgs,L}},$$

where $C_L = 1$ is the natural value of the scaling constant. As the mixing model is linear function of composition, it satisfies a desirable property of a good mixing model. Using the procedure outlined in Section 2.2.1, this $\tau_L$ is evaluated dynamically due to $C_L$ and $\mathcal{D}_{sgs,L}$ calculated from local flow conditions. This dynamic time-scale model, referred to as dyn-aISO, has been successfully validated for a series of piloted flames [86]. With this approach the need to specify any mixing model constants is removed, decreasing the overall degrees of freedom of the model parameters.

In MMC-LES, there is an Eulerian filter scale, $\Delta_E$, associated with the LES grid and the filtering of the reference variable, and a Lagrangian filter scale associated with the distance between mixing particles, $d_x$. That is, the mixing phenomenon dissipates composition fluctuations, effectively imposing a Lagrangian filter over the stochastic particles. Hereon, to avoid confusion, one can refer to the sub-Lagrangian-grid scales using the abbreviation slgs, while sgs is now used specifically for the sub-Eulerian-grid-scales (see Equation (3)).

The mixing operation occurs in particle pairs, denoted $p$ and $q$, with the conditionally filtered means (see Equation (66)) estimated similar to modified-Curl's mixing model [6],

$$\langle \phi_\alpha | X, \Xi \rangle^{p,q} = \frac{m^p \phi_\alpha^p + m^q \phi_\alpha^q}{m^p + m^q},$$

where $m^p$ and $m^q$ are the particle weights. As the particle pairs to be mixed are localised in the reference mixture fraction space, it allows the MMC to use a sparse resolution of
Integrating Equation (66) over numerical time steps leads to,

\[
\phi_p^\alpha(t + \Delta t) = \phi_p^\alpha(t) + \psi(\langle \phi_\alpha | X, \Xi \rangle_t^{p,q}(t) - \phi_p^\alpha(t)), \quad (69)
\]

\[
\phi_q^\alpha(t + \Delta t) = \phi_q^\alpha(t) + \psi(\langle \phi_\alpha | X, \Xi \rangle_t^{p,q}(t) - \phi_q^\alpha(t)), \quad (70)
\]

where \(\psi = 1 - \exp(-\Delta t/\tau_L)\) is the extent of mixing. Particles \(p\) and \(q\) are selected by minimising the least square distance between particles in \((x, \tilde{f})\)-space,

\[
\bar{d}_{p,q}^2 = \sum_{i=1}^{3} \left( \frac{d_{p,q}^i}{r_m/\sqrt{3}} \right)^2 + \left( \frac{d_{p,q}^f}{f_m} \right)^2. \quad (71)
\]

Here, \(d_{\gamma}^{p,q} = |\gamma|^p - |\gamma|^q\) represents the distance between the particles \(p\) and \(q\) in \(\gamma\)-space with \(r_m\) and \(f_m\) being the characteristic normalisation distances in \((x, \tilde{f})\)-space, respectively. The smaller the characteristic distance, the greater is the weighting of the corresponding space. For non-premixed combustion of gaseous and multi-phase flames, \(f_m = 0.01\) has been found to produce accurate solutions \([29, 30, 76, 99]\). The parameter \(r_m\) is found from a fractal description of turbulent scalar topology \([9]\) and is defined as,

\[
r_m = 0.5 \left( \frac{d_{\tilde{f}}}{dn} \frac{\Delta_L^3}{\Delta_E^{2-D_f} f_m} \right)^{1/D_f}, \quad (72)
\]

where \(D_f = 2.36\) is the empirical fractal dimension \([84]\), \(\Delta_L\) is the nominal inter-particle distance calculated as the inverse of the cube root of particle number density, \(\Delta_E\) is inner cut-off scale given by the LES filter width, and \(d_{\tilde{f}}/dn\) represents the gradient normal to an iso-scalar sliver of reference mixture fraction \([10]\).

### 2.4.0.2 Eulerian-Lagrangian Equation Coupling

The Eulerian equations (viz. Equations (8), (9), (13) and (64)) governing the fluid flow dynamics, and the Lagrangian equations (viz. Equations (58) and (59)) evolving the chemical composition of the fluid, presented above are two-way coupled. Filtered and sgs quantities in SP evolution equation are interpolated from the Eulerian fields to stochastic particles.
particle locations, as discussed above. Stochastic particle density is coupled back to the Eulerian scheme to ensure mass consistency, achieved through a solution of additional Eulerian equations for equivalent composition fields $\tilde{\phi}^e_\alpha$. This approach is an adaptation of the equivalent enthalpy method of Muradoglu, Pope and Caughey [55], and produces a smooth Eulerian density field to prevent numerical oscillation. The Eulerian transport equation of the equivalent composition, $\tilde{\phi}^e_\alpha = (\tilde{\phi}^e_\beta, \tilde{h}^e)$, is written as:

$$\frac{\partial \tilde{\rho}^e_{\alpha}}{\partial t} + \frac{\partial \tilde{\rho}^e_{\alpha} \tilde{u}_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \tilde{\rho} (D + D_{sgs}) \frac{\partial \tilde{\phi}^e_{\alpha}}{\partial x_j} \right) + \tilde{\rho} \frac{\tilde{\phi}^e_{\alpha}|f - \tilde{\phi}^e_{\alpha}}{\tau_R}. \quad (73)$$

Note that $\tilde{\phi}^e_\beta$ represents the subset of the total chemical species, $N_{eq}$, which make up at least 99% of the mixture. The last term in Equation (73) is a source term conditioned on the reference mixture fraction, $\tilde{\phi}^e_{\alpha}|f$, which is calculated from the particles using the kernel estimation method [17]. This term provides the feedback from the Lagrangian particles to the Eulerian solver for calculating $\tilde{\phi}^e_{\alpha}$, which is ultimately used to evaluate the density from the equation of state (cf. Equation (13)),

$$\tilde{\rho} = \frac{\tilde{\rho}}{R_u \cdot \sum_{\beta=1}^{N_{eq}} \frac{\tilde{\phi}^e_{\beta}}{M_{w\beta}} \cdot \tilde{T}^e}, \quad (74)$$

where $\tilde{T}^e$ is obtained from $\tilde{h}^e$. The term $\tau_R$ in Equation (73) is a time scale used to relax the equivalent composition source by controlling the rate at which the equivalent composition is matched to the contribution from the particles. It is usually approximated as $N \cdot \Delta t$, where $N$ is the number of relaxation steps. It is taken as 10 in the current study and may be increased to prevent any numerical stability issues encountered.
This chapter provides details of the experimental configuration of the lifted methane flame series modelled in the current work. Subsequently, complete information of the corresponding numerical setup of large eddy simulation (LES) using the sparse-Lagrangian multiple mapping conditioning (MMC) model is provided.

3.1 EXPERIMENTAL CONFIGURATION

Lifted flames are quite challenging for numerical models, due to the complex chemical kinetics involved coupled with the fluctuations of the flame base. Prediction of such turbulent flames with complex flow re-circulation can pose a significant challenge for current combustion models [3]. Hence, to aid the understanding of such reacting flows, the vitiated co-flow burner of UC Berkeley, studied by Cabra et al. [3], provides a simplified setup consisting of a turbulent fuel jet issuing into a co-flow of hot combustion products generated from multiple, lean premixed flamelets. As the co-flow is large in diameter, it shrouds the flame from the laboratory air, rendering the problem a two-stream one. Hence, the vitiated co-flow burner allows for detailed experimental investigation of flame stabilisation and turbulent mixing of a fuel jet in hot combustion products, thereby avoiding the additional complexities of recirculating flow dynamics found in industrial combustors.
Initially introduced to study turbulent lifted H$_2$/N$_2$ jet flames [3], the Berkeley burner was later used to investigate the kinetically complex CH$_4$/Air flame [2]. The latter is the target flame series for the present work. The schematic of the burner is provided in Figure 1 along with a camera snapshot of the methane flame. As observed from the flame luminosity, the flame is not attached to the burner. The burner consists of a central pipe of diameter $D = 4.57$ mm from which a cold, partially pre-mixed methane air mixture exits at a velocity of $100 \text{ m s}^{-1}$. The Reynolds number of the jet is approximately 28,000. The wall of the jet has a thickness of 0.89 mm. The central jet is surrounded by a hot vitiated co-flow, from burnt products of multiple (2200 in number) lean-premixed H$_2$/Air flames having an equivalence ratio of $\approx 0.37$, spanning a diameter of 210 mm. Hence, the temperature obtained from the co-flow products is 1350 K. The stochiometric mixture fraction of the jet is $Z_{st} = 0.1769$. The summary of measured boundary conditions (BCs)
for the composition, based on Raman–Rayleigh–LIF technique [2], at one diameter from
the jet exit is provided in Table 2.

To understand the effect of the sensitivity of the flame lift-off height to co-flow temper-
ature, parametric variation is performed and the results compared with the experiments.
The three flames simulated are summarised in Table 3, where 1350 K is the base case for
which extensive validation is performed in Chapter 4.

3.2 Numerical Details

3.2.1 Solver Details

The MMC-LES model is implemented as a low-Mach, variable density solver known
as *mmcFoam* [17] within the open-source code OpenFOAM [97]. The spatially-filtered
transport equations, discussed in the previous chapter, employing a top-hat kernel [75]
are integrated in time using a second-order, fully implicit Crank-Nicolson method with
a maximum Courant number of 0.3. The convective term present in the momentum
equations (Equation (9)) are discretised using the second-order central-difference scheme,
while a normalised variable diagram (NVD) based differencing scheme [34] is employed to avoid unbounded values of scalars. The particle composition and position (Equations (58) and (59)) are solved by the fractional steps for advection, mixing and reaction [69]. The position of stochastic particles is integrated in time using the Euler-Maruyama method and the chemical source term is integrated using a semi-implicit Euler ODE solver SEULEX. The chemical kinetics of methane is represented by the skeletal mechanism of Lu and Law [46], derived from the GRI-3.0 scheme, and consists of 30 species and 184 reactions. To update the composition due to molecular mixing (viz. Equation (69)), particles are paired by minimising the least square distance between each particle in Equation (71) using a computationally efficient k-d tree algorithm [16]. The radiative heat transfer is not modelled in the course of the current work.

3.2.2 Domain Discretisation

A cylindrical computational domain extending to 14D x 80D in the radial and axial directions, respectively, is used for the computations. The MMC solver employs two grids: a LES-grid used for the finite-volume (FV) computation and a superMesh, solely for the stochastic Lagrangian particle number management. The cross-sectional view of both grids is shown in Figure 2. The LES-grid has a non-uniform distribution of 700 cells along the axial, 96 cells along the radial, and 48 cells in the azimuthal directions, with a refinement near the jet centreline and near the shear layers to resolve sharp gradients of velocity and scalars. The LES-grid is discretised into of a total of approximately 3,124,800 FV cells. The coarser superMesh contains 80 cells in the axial, 16 cells in the azimuthal, and 19 cells in the radial directions, for a total of 20,160 cells.

The particle number control allows $N_{pc}=15\pm5$ stochastic particles (SPs) per superMesh-cell, so that approximately 350,000 particles are introduced in the computational domain. This means that 1 stochastic particle is found for approximately 10 LES-mesh cells overall (1L/10E). As discussed in the Section 2.4 in the previous chapter, MMC allows a sparse resolution of SPs due to the enforced localness in the mathematically independent
reference space. Granted that higher order sub-grid scale (sgs) information may not be available due to this sparse nature, but first and second moments have shown to match reasonably well for numerous single and multi-phase flames [17, 79, 99]. Hence, this makes MMC method computationally desirable in comparison to conventional filtered density function (FDF) methods using intensive SP resolution of as high as 20 particles per FV cell (20L/1E) [73].

The value of the characteristic mixing distance in reference mixture fraction in Equation (71) is set to \( r_m = 0.01 \), while \( r_m \) is calculated according to Equation (72) using input parameters obtained in the high-gradient shear layer approximately 1/10 of a jet-diameter downstream of the exit-plane.

![Computational grids shown at one-jet diameter downstream of the jet-exit.](image)

**Figure 2:** Computational grids shown at one-jet diameter downstream of the jet-exit.

### 3.2.3 Boundary Conditions

Precursor pipe flow simulations were performed to provide fully-developed turbulent inlet BC for the main jet, commensurate with the measured velocity given in Table 2. The temporal statistics from the pipe-flow simulation are provided in Figure 3, with comparison to the empirical one/seventh power-law velocity profile, \( u/u_{max} = (1 - r/R)^{1/7} \). A time-varying inflow condition is prescribed for the co-flow based on the method of
turbulent spots [41] by imposing a top-hat velocity profile from the experiments. The integral length scale of the generated eddies is $1/10^{th}$ of the hydraulic diameter of the co-flow. Uniform values of the scalars, such as temperature, species mass fractions, and mixture fraction, have been provided using the measurements available near the burner exit plane (see Table 2). At the inlet plane, pressure is prescribed based on the Neumann BC, and a fixed total pressure is specified at the outflow and the side boundaries.

Figure 3: Mean and root mean square (r.m.s.) profiles of the boundary condition supplied at the fuel jet inlet in comparison to the $1/7^{th}$ power-law velocity profile.
RESULTS AND DISCUSSION

In this chapter, the results are presented for flames outlined in Tables 2 and 3. The presentation of the results is organised as follows. Section 4.1 presents a high-level picture of model performance through instantaneous snapshots of various scalar and vector fields, followed by conditional and unconditional flame characteristics in Sections 4.2 and 4.3, respectively. Finally, the effect of co-flow temperatures on the flame lift-off height are presented in Section 4.4. Note that unless otherwise specified, the results presented are for the base case having a co-flow temperature of 1350 K.

4.1 SNAPSHOTS OF PREDICTIONS

Figure 4 presents the instantaneous contours of the Favre-filtered velocity field magnitude and the corresponding velocity vectors. The turbulent jet (Re $\geq 28,000$) is clearly visible from this figure and the centreline velocity decays to less than half of its original value after approximately $x/D > 25$. The velocity vectors show that the co-flow gets entrained in the turbulent jet core region till $x/D < 35$, beyond which the velocity vectors point outwards towards the side boundaries hence decreasing the amount of fluid entrained. This transverse out-flow of fluid in the downstream region is due to thermal expansion because of ignition of the cold fuel-jet, which is corroborated by the temperature contours shown in Figure 5. As discussed by Muñiz and Mungal [54], heat release at the flame base decreases the entertainment of the surrounding fluid.
To explain the coupling between Eulerian and Lagrangian equations, discussed in Section 2.4.0.2, presented in Figure 5 are the contours of temperature on stochastic particles (SPs) and the corresponding Eulerian counterpart (see Equation (73)). It may be observed from these figures that the flame is lifted and its base is situated between $30 > x/D > 40$, before which only mixing between jet and hot co-flow occurs. As the conservation equation of the equivalent temperature contains the source term evaluated from the SPs using the kernel density estimation method [17], these figures closely resemble each other. These results show that the source term from the particles is accurately evaluated by the kernel density estimation method which uses a k-d tree algorithm. Therefore, a feedback from the SPs is provided to the Eulerian equations which are used for evaluation of the density field approximated by the ideal gas law.
Figure 5: Instantaneous contours of equivalent (left) and stochastic particle (right) temperature, respectively, sliced at the mid-plane.

In multiple mapping conditioning (MMC) for non-premixed combustion, there are two mixture fraction fields viz. reference mixture fraction ($f$) and the real mixture fraction ($Z$). The former, solved as an Eulerian quantity in large eddy simulation (LES) (Equation (64)), is used only to localise the molecular mixing in its space, while the latter is evolved on the stochastic particles (Equation (59)). Figure 6 presents the instantaneous contours of these aforementioned mixture fractions. Although these quantities evolve differently, it is observed from this figure that there exits a degree of correlation between them. This correlation is desirable as $\tilde{f}$ is just a mathematical quantity, while $Z$ is the quantity of interest and an imposed localness in $\tilde{f}$ also implies a mixing localness in $Z$. A quantitative plot of this correlation is provided in Section 4.2.
Figure 6: Instantaneous finite-volume contours of reference (left) and real (right) mixture fraction, respectively, sliced at the mid-plane.

4.2 CONDITIONAL STATISTICS

In the MMC method the turbulent composition-fluctuations are divided into major and minor. The major fluctuations are the fluctuations of the major scalar, i.e. reference mixture fraction for non-premixed combustion, modelled by the sub-grid scale (sgs) closure model (see Equation (65)). On the other hand, fluctuations around the mean conditioned on the reference variable, $\phi''' = \phi - \langle \phi | \Xi \rangle$, are called minor fluctuations, which are directly controlled by the mixing time-scale model (see Equation (67)). This behaviour is in contrast to conventional mixing models, such as interaction by exchange with mean (IEM), which do not make such distinctions between major and minor fluctuations and dissipate all fluctuations of reactive scalars. These minor fluctuations are generated due
to the molecular mixing phenomenon and are dissipated by the mixing operator (see Equation (66)). To introduce these fluctuations quantitatively, presented in Figure 7 are the scatter plots of the $Z$ vs. $\tilde{f}$. The positive correlation between these two mathematically independent quantities is clearly visible from the cigar-shaped scatter as well as the conditional mean, $\langle Z|\Xi \rangle$, aligned at $\approx 45^\circ$ from the abscissa and ordinate. Therefore, mixing in MMC preserves linearity and independence of mixing for all scalars as required of a good mixing model [86]. A control over the minor fluctuations, $Z''$, means essentially controlling the desired conditional composition fluctuations, $Z'' = Z - \langle Z|\zeta \rangle$ (note that these fluctuations are neglected in the conditional moment closure (CMC) method). It is worth mentioning that the minor fluctuations may be understood from Figure 7 as the departure of the scatter points from the conditional mean.

Figure 7: Scatter plots of particle mixture fraction ($Z$) vs reference mixture fraction ($\tilde{f}$) at four axial locations. Lines represent the conditional means.
To examine the structure of the flame, depicted in Figure 8, are the scatter plots of temperature versus mixture fraction from the simulations and the experiment at various axial locations. The equilibrium (fully burning) and the quenching (non-reacting or mixing) limits of a laminar diffusion flame are also presented for comparison. At $x/D = 30$, there is no burning with most points aligned with the mixing profile. The probability density function (PDF) of temperature and the scatter plot of OH mass fraction are also presented in Figures 9 and 10, respectively. The PDF at this location is uni-modal, while there is negligible production of the intermediate specie OH. Only a very few ignition events are observed at the lean side ($Z < Z_{st}$). As discussed by Mastorakos, Baritaud and Poinot [51], the mixture with the ‘most-reactive’ mixture fraction ignites first and this value was estimated to 0.04 for this flame [56]. Hence, prior to complete auto-ignition, the mixture starts igniting from the lean region and moves to the stochiometric mixture fraction as observed from Figure 8 at $x/D = 30, 40, 50$. This phenomenon is also corroborated by the predictions of Gkagkas and Lindstedt [24], which conclude that ignition occurs from lean to stochiometric mixtures. The flame reaches the fully burning state in a span of 40D from $x/D = 30$ to $x/D = 70$, clearly observed from Figure 8. Fluctuations at the flame base are observed till $x/D \leq 50$ as there are numerous samples lying on both mixing as well as the equilibrium lines. At $x/D = 50$ the number of experimental samples on the mixing line in the lean region are considerable, while the simulations do not predict the same. The PDF of temperature is multi-modal, and although all the peaks are predicted correctly, they are slightly shifted towards higher temperatures. At $x/D = 70$, the PDF becomes bi-modal in the simulations while experiments show only one peak. The scatter plots show rare events of cold central jet, which do not fully burn till this location, observed by existence of samples at larger values of mixture fraction values in comparison to the experimental measurement (see Figure 8). Nevertheless, the predictions from the MMC model are reasonable and similar predictions to the current work have been reported in the literature with different turbulence-chemistry interaction (TCI) models [2, 24, 82, 96]. The scatter plots of $Y_{OH}$ shown in Figure 10 are topologically similar from the experiments and the
simulation and the location of the peaks is reproduced quite well, but the mass fractions are somewhat higher in the experiments at $x/D \geq 40$. This may be attributed to the slightly higher temperature observed at these locations in Figure 8, although previous studies [24, 56] have produced similar over-predictions.

Figure 8: Scatter plots of particle mixture fraction ($Z$) vs temperature ($T$) at four axial locations from the experiment (left) and simulation (right). The dash-dotted and dashed lines represent the fully burning and quenched profiles of a laminar diffusion flame. The vertical solid line depicts the stoichiometric mixture fraction.
Figure 9: Probability distribution of the stochastic particle temperature from simulation compared with the experimental measurement.
Figure 10: Scatter plots of particle mixture fraction ($Z$) vs ($Y_{OH}$) at four axial locations from the experiment (left) and simulation (right). The dash-dotted and dashed lines represent the fully burning and quenched profiles of a laminar diffusion flame. The vertical solid line depicts the stochiometric mixture fraction.
The conditional mean and root mean square (r.m.s.) profiles of temperature, $Y_{O_2}$ and $Y_{CO}$ are presented in Figures 11 to 13. These figures complement the discussion presented above for the conditional scatter and provide a more quantitative comparison with the measurements. Considering the conditional mean peaks in these figures, it is observed that after auto-ignition at $x/D > 30$ the ignition proceeds from lean to stochiometric regions and to the rich region finally. The profiles of $\langle T|\zeta \rangle$, $\langle Y_{O_2}|\zeta \rangle$ and $\langle Y_{CO}|\zeta \rangle$ closely follow the equilibrium curve for lean mixtures at $x/D = 40 - 50$, and completely overlap with fully burning profile at $x/D = 70$. The rich region near stoichiometry is in good agreement with measurements for samples having $Z \leq 0.3$, although even richer samples remain somewhat cold at $x/D \leq 70$. Moreover, one may notice that the extent of the mixture fraction of the samples is broader from the simulations in comparison to the measurements. This broad width of the scatter samples is due to somewhat insufficient mixing in the simulations, especially from the jet central region, which causes some particles to remain fuel rich till $x/D \leq 70$. The un-conditional profiles of $Z$ shown in Figures 14 and 17 confirm this fact with slightly over-predicted $Z$ near the centre in the far-stream region. This trend has also been produced by previous simulations using other turbulent combustion models, including flamelet [31], CMC [59], modified Curl’s (M-Curl) [2], IEM [2], Euclidean minimum spanning tree (EMST) [2], etc.. Some over-predictions are noticed for $\langle T|\zeta \rangle$ at $x/D = 40, 50$, but the location and magnitude of peaks of the species $\langle Y_{O_2}|\zeta \rangle$ and $\langle Y_{CO}|\zeta \rangle$ are captured reasonably well.

The predictions of conditional r.m.s. values of reactive scalars in Figures 11 to 13 at $x/D = 30$ show non-zero values in lean mixtures ($Z < 0.1$), around the ‘most-reactive’ mixture in the pre-autoignition region [51]. This is due to the fact that the fuel/air mixture ignites from this region and subsequently mixes with surrounding fluid to stabilise the flame around $30 \leq x/D \leq 40$. As discussed above for the scatter plots in Figure 8, the $\sqrt{\langle T''^2|\zeta \rangle}$ values are somewhat lower than that measured during experiments for $Z < 0.2$ at $x/D = 50$. Also, the peak in conditional r.m.s. produced beyond $Z = 0.3$ at $x/D = 70$ is due to the few cold, essentially partially mixed, particles remaining in the jet central region discussed above in the previous paragraph. In general, the r.m.s. predictions for all...
4.2 CONDITIOINAL STATISTICS

Scalars are reproduced reasonably well for both major combustion species $\sqrt{\langle N^2_O | \zeta \rangle}$ and major radical $\sqrt{\langle N^2_C | \zeta \rangle}$ at $x/D = 40, 50$, by the MMC model. The large magnitude of the peaks in the r.m.s. values represent the bi-modal nature of the samples there, where they are mostly aligned at the extremes, i.e., either at equilibrium or mixing curve.
Figure 11: Means and r.m.s. of temperature conditioned on mixture fraction. The symbols represent the experimental measurements while the line are from the simulations. Note that the error bars are the experimental r.m.s. values. The dash-dotted and dashed lines represent the fully burning and quenched profiles of a laminar diffusion flame.
4.2 Conditional Statistics

Figure 12: Means and r.m.s. of $Y_{O_2}$ conditioned on mixture fraction. The symbols represent the experimental measurements while the line are from the simulations. Note that the error bars are the experimental r.m.s. values. The dash-dotted and dashed lines represent the fully burning and quenched profiles of a laminar diffusion flame.
Figure 13: Means and r.m.s. of $Y_{CO}$ conditioned on mixture fraction. The symbols represent the experimental measurements while the line are from the simulations. Note that the error bars are the experimental r.m.s. values. The dash-dotted and dashed lines represent the fully burning and quenched profiles of a laminar diffusion flame.
4.3 UN-CONDITIONAL STATISTICS

4.3.1 Axial Profiles

The centreline profiles provide information of the jet decay rate, which represents the accuracy of the sgs model employed herein. Figure 14 presents the centreline profiles of time-averaged quantities, namely mixture fraction, temperature, $Y_{\text{CH}_4}$ and $Y_{\text{CO}_2}$. Till $x/D \leq 35$, mixing between fuel jet (320 K) and the hot co-flow takes place, which is characterised by a gradual temperature rise and absence of product species. The decay rate of $Z$ and fuel mass fraction match reasonably well with experiments suggesting accurate modelling of mixing. Minor over-predictions in the downstream of the jet exit plane suggest that an even higher rate of molecular mixing is needed to exactly mimic the experiments. Subsequently, around $x/D \approx 40$, ignition is achieved and flame stabilises as evident by a sharp rise in temperature and $Y_{\text{CO}_2}$, followed by a constant equilibrium temperature (and no fuel remaining) for $x/D > 70$. 
4.3.2 Radial Statistics

The MMC-LES model allows use of a sparse resolution of stochastic particles, i.e. less particles in comparison to the number of finite-volume (FV) cells. For example, in the current work, a resolution of approximately 1 SP per 10 Eulerian FV cells (1L/10E) is employed, which is much less that the conventional models, such as IEM which require as high as 20 particle per FV cell (20L/1E). This sparse resolution can be employed due to the localisation of the molecular mixing in the f-space (in addition to x-space of course) which is controlled by the parameter \( f_m \) taken as 0.01 in the current study. According to Equation (71), localisation of mixing in f-space increases the distance between chosen pairs of the stochastic particles in the x-space. To check whether current setup resolves sgs fluctuations, presented in Figure 15 are the time-averaged profiles of mixing distance in physical \( d_x \) and reference space \( d_f \). At all locations, \( d_x \) is larger than 2.285 mm.
(jet radius), which is the upper limit of the integral length scale, suggesting that mixing model is able to resolve the energy bearing eddies. Also, the maximum distance in $\tilde{r}$ remains smaller than $f_m$, which shows the ability of the pair selection algorithm to maintain the chosen level of localness considering that $f_m$ is the only input parameter in the MMC model.

![Graphs showing average distance between mixing pairs of stochastic particles in physical (left) and reference space (right) at various axial locations.]

Figure 15: Average distance between mixing pairs of stochastic particles in physical (left) and reference space (right) at various axial locations.

Figures 16 and 17 present the radial statistics of mixture fraction and temperature from MMC-LES compared with the experimental measurements. It may be observed from Figure 16 that there is no reaction till $x/D \leq 30$ as the maximum temperature is 1350 K. These is rise in jet temperature due to mixing and entertainment of this hot co-flow. At $x/D = 40$, there is rise in temperature at the shear layer at $r/D \approx 4$, which supplements the discussion above that combustion progresses from lean co-flow region to rich jet-centre. This rise in temperature is also observed in the experiments, although it is slightly higher in the simulations. Visual observations of experimental images \[2\] conclude that the lift-off height is approximately near $x/D = 35$, this is also confirmed from Figure 16. The flame broadens with axial location as the peak temperature is observed at $r/D > 4$ at $x/D = 50$, where the jet central region also exceeds the co-flow temperature. Till $x/D = 70$ peak flame temperature of $> 2100$ K is reached signifying complete combustion. The profiles of $\sqrt{\langle T^2 \rangle}$ show a decrease in magnitude.
of fluctuations at \( x/D = 70 \) in comparison to \( x/D = 40, 50 \) signifying that a stable flame exists. The cold gas-phase particles observed in the temperature scatter in Figure 8 at \( x/D = 70 \) are also visible from \([T]\) at \( r/D < 1 \) upon close inspection. Near the jet exit till \( x/D < 30 \), the r.m.s. of temperature is over-predicted in comparison to the measurements. In the region \( x/D < 30 \), the mixing phenomenon tries to reduce the gradient between the two inlet streams and hence the r.m.s. of \( T \) and \( Z \) should become negligible for perfectly mixed fluid. From Figure 17, it is observed that the r.m.s. of mixture fraction is also slightly higher in this region. This may be attributed to insufficient mixing in this region as there is minor over-prediction in the mean profile of \( Z \), and hence the scatter plots in Figure 8 show a larger extent till \( x/D = 70 \). Nevertheless, the predictions in the flame region from \( x/D > 30 \) agree reasonably well with experiments for both mean and r.m.s. of \( Z \) and \( T \).
Figure 16: Radial profiles of the first and second temporal moments of temperature at various axial locations.
Figure 17: Radial profiles of the first and second temporal moments of mixture-fraction at various axial locations.
Radial profiles of temporal statistics of mass fractions of oxidiser $O_2$, product species $CO_2$, $H_2O$, and OH radical are presented in Figures 18 to 21. At $x/D = 30$, the mean profiles of oxidiser show mixing only between fuel jet and co-flow. Note that major product specie $Y_{H_2O}$ is not zero at the centre due to presence of water vapour in the fuel jet at the inlet. The fluctuations in product species $Y_{OH}$ and $Y_{CO_2}$ at this location show ignition of mixture, but a near zero mean of these quantities signify failed or rare events of auto-ignition. The means of major species and OH are in good agreement with the measurements at all axial locations, but the r.m.s. of $Y_{OH}$ is over-predicted. This observation is consistent with the scatter plots of $Y_{OH}$ shown above in Figure 10. This could be due to the uncertainty in measurements or the chemical kinetic mechanism considering the major species are predicted well, although a thorough analysis was not performed to conclude this statement. Nevertheless the topology of profiles of $\sqrt{\sqrt{Y_{OH}^2}}$ is similar to the measurements at all locations just shifted to higher values.

Figure 18: Radial profiles of temporal statistics of mass fraction of oxidiser at various axial locations.
Figure 19: Radial profiles of temporal statistics of mass fraction of H\textsubscript{2}O at various axial locations.

Figure 20: Radial profiles of temporal statistics of mass fraction of CO\textsubscript{2} at various axial locations.
4.4 EFFECT OF CO-FLOW TEMPERATURE

In this section, the sensitivity to the variation in co-flow temperature is examined by numerical experiments. A co-flow temperature of $T_{cf} - n \times 30$ K is chosen for the sensitivity study cases as outlined in Table 3, where $n = 0, 1, 2$. The resulting lift-off height predictions from the MMC-LES model are compared with results from popular studies in literature, within both Reynolds averaged Navier-Stokes (RANS) and LES frameworks, which provide a lift-off trend analysis. In addition to the experimental observation of Cabra et al. (2005) [2], the experimental correlation proposed by Kalghatgi (1981) [3], and the Well-mixed model assuming no $s_{gs}$ composition fluctuations are also plotted. Summary of these popular studies is given in Table 4.
Table 4: Popular numerical studies on the CH$_4$ fuelled vitiated co-flow burner (VCB) of Cabra et al. (2005) [2] and the proposed experimental correlation of Kalghatgi (1981) [38].

| STUDY                                      | TCI MODEL   |
|--------------------------------------------|-------------|
| Kalghatgi (1981) [38]                      | Experiments |
| Cabra et al. (2005) [2]                    | Well-mixed  |
| Cabra et al. (2005) [2]                    | M-Curl      |
| Navarro-Martinez and Kronenburg (2009) [56] | LES-CMC     |
| Roy, Kumar and Sreedhara (2014) [74]       | RANS-CMC    |
| Wandel and Lindstedt (2019) [96]           | RANS-MMC    |
| Ghai and De (2019) [23]                    | RANS-MMC    |

Figure 22: Time-averaged contours of temperature for three different co-flow temperatures.

To provide a global picture of the variation of co-flow temperature, provided in Figure 22 are the temporally averaged contours of the stochastic particle temperature for different T$_{cf}$. An increase in the flame lift-off height is clearly visible form these figures with decreasing co-flow temperature. This trend is expected considering that a higher temperature gradient between jet and co-flow is likely to diffuse to the cold-jet faster due to mixing phenomenon, thereby causing relatively early auto-ignition. Considering the
region of sharp temperature rise, it is seen from Figure 22 that a ≈ 4% change in co-flow temperature (60 K) causes more than 50% variation in the lift-off height.

For a quantitative analysis of the lift-off height variation, Figure 23 presents comparisons of the approximate location of the flame base with the values obtained in the literature as mentioned in Table 4. Cabra et al. [2] used flame luminosity from digital camera images to define the flame lift-off height from the experiments. These values are represented by black solid circles in this figure. A linear regression curve obtained from these experimental points is also provided. For a comparison of predictions to the experimental observation, Cabra et al. [2] considered concentration of intermediate species, namely C_2H_2 and C_2H_4, to determine the location of flame base for their PDF calculations. This criteria was chosen based on the finding, from auto-ignition calculations, that the time peak heat release is in unison with the time of culmination of C_2H_2 and C_2H_4.

The first axial location where the mole fraction of C_2H_2 and C_2H_4 reaches 2 ppm and 100 ppm, respectively, was noted and averaged to get the lift-off height. Employing this marker, Figure 24 provides the time-averaged contours of mole fraction of C_2H_2 and C_2H_4, for T_{cf} = 1350 K, with the location of the flame base highlighted. With this marker, the average value of lift-off height is ≈ 31 D. Apart from getting the location of flame base from averaged values of specie mole fractions, another method using instantaneous values of mole fraction of C_2H_2 and C_2H_4 from the stochastic particles was also considered. The axial location, from the domain inlet, of the first stochastic particle satisfying the marker criteria mentioned above is logged with time as shown in Figure 25. These values are labelled with the distinction ‘SP’ in Figure 23. An interesting observation from Figure 25 is that the flame base becomes less stable with a decrease in co-flow temperature, probably due to significant number of failed ignition events.

It is observed from Figure 23 that most studies produce a linear variation of the flame lift-off location with co-flow temperature, although the slope is quite different for each. This may be due to different chemical kinetic mechanisms used in these studies which cause a early/late onset of radical (C_2H_2, C_2H_4, etc.) pool build up, thus providing this variation. Moreover, different TCI models model the molecular mixing distinctly from
each other. The Well-mixed or no sgs TCI model predictions are much lower than all other models thereby depicting the importance of TCI modelling. The slope of the lift-off height from the experiments matches none of these studies, although a reasonable match of the un-conditional and conditional statistics was achieved with these different TCI models. The relation proposed by Kalghatgi [38] significantly under-predicts the lift-off. The height obtained from the MMC-LES produces as linear variation with change in $T_{cf}$ using both averaged contours and the SP method. The latter under-predicts the location of the flame base as these values obtained are from igniting particles which do not successfully burn, possibly due to subsequent mixing with colder fluid particle in its proximity. Asymmetric averaging of these instantaneous values may help improve the lift-off predictions from SPs. The slope of MMC-LES predictions is similar to that reported by Navarro-Martinez and Kronenburg [56], who used the CMC method. It is interesting to see that the slopes from the two studies employing RANS-MMC is quite different. Nevertheless, it is concluded from this figure that a better marker is needed to get a better match of the lift-off length with the measurements considering it was found from digital images, hence prone to errors.
Figure 23: Variation in lift-off heights with co-flow temperature from MMC-LES compared with experimental measurements and other studies mentioned in Table 4.
Figure 24: Time averaged contours of mole fraction of $\text{C}_2\text{H}_2$ (left) and $\text{C}_2\text{H}_4$ (right), respectively, sliced at the mid-plane for $T_{cf} = 1350$ K. The dash-dotted horizontal lines delineate the location of the flame base according to the criteria defined by Cabra et al. (2005) [2].
Figure 25: Normalised flame base location based on mole fraction of $C_2H_2$ and $C_2H_4$. The abscissa represents the number of computational time steps while the horizontal solid line denotes the mean location of the flame base.
CONCLUSIONS AND FUTURE WORK

The sparse-Lagrangian multiple mapping conditioning (MMC) approach is applied for the first time to successfully simulate a series of lifted methane flames stabilised above a hot vitiated co-flow. MMC in large eddy simulation (LES) framework is a full filtered density function (FDF) method, where MMC plays the role of a mixing model, localising the mixing in a reference space. Due to this localness of mixing, a sparse resolution of 1 stochastic particle (SP) per 10 finite-volume (FV) cells (1L/10E) was used, which is much lower than the conventional non-local mixing models such as interaction by exchange with mean (IEM). The performance of the recently proposed dynamically evaluated mixing time-scale, dyn-aISO, is also assessed for auto-igniting flames. Overall a reasonable agreement is achieved with the experiments by the MMC model for the conditional and un-conditional scalars, although some over-predictions in the temperature near the flame base were observed. The conditional predictions suggest that ignition starts from the lean side and moved towards the stoichiometric mixture. The mass faction of OH is slightly over-predicted in the flame region, while other species were produced well. The flame base shifts upwards with a decrease in co-flow temperature. It is observed that the flame base becomes quite unstable at lower co-flow temperatures. A linear variation of the flame lift-off height with co-flow temperature is observed, consistent with the previously published numerical results and the experimental measurements. However, the slope of this variation is different from the literature suggesting that a better marker for flame lift-off height is required for a proper comparison.

To gain more understanding into the flame stabilisation mechanism of these flames, chemical explosive mode analysis (CEMA) [45] may be performed. This analysis may be helpful in delineating whether the flame is stabilised due to auto-ignition or by propagation of premixed flame at the flame base. Species transport budget analysis [26] may also be performed to complement the current work in understanding of flame base stabilisation.
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