Statistics of Strain Rates and Surface Density Function in a Flame-Resolved High-Fidelity Simulation of a Turbulent Premixed Bluff Body Burner

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ABSTRACT

The statistical behaviour of the surface density function (SDF, the magnitude of the reaction progress variable gradient) and the strain rates, which govern the evolution of the SDF, have been analysed using a three-dimensional flame-resolved simulation database of a turbulent lean premixed methane-air flame in a bluff-body configuration. It has been found that the turbulence intensity increases with the distance from the burner, changing the flame curvature distribution and increasing the probability of negative curvature in downstream direction. The curvature dependences of dilatation rate $\nabla \cdot \vec{u}$ and displacement speed S_d give rise to variations of these quantities in the axial direction. These variations affect the nature of the alignment between the progress variable gradient and the local principal strain rates, which in turn affects the mean flame normal strain rate, which assumes positive values close to the burner but increasingly becomes negative as the effect of turbulence increases with axial distance from the burner exit. The axial distance dependences of curvature and displacement speed also induce a considerable variation in the mean value of the mean curvature stretch. The axial distance dependences of dilatation rate and flame normal strain rate govern the behaviour of the flame tangential strain rate, and its mean value increases in downstream direction. The current analysis indicates that the statistical behaviours of different strain rates and displacement speed and their curvature dependences need to be included in the modelling of Flame Surface Density and Scalar Dissipation Rate in order to accurately capture their local behaviours.

Keywords: Premixed flame, Surface Density Function, normal strain rate, tangential strain rate, curvature

1. INTRODUCTION

The statistical behaviour of the modulus of the reaction progress variable gradient $|\nabla c|$ (often referred to as the Surface Density Function, SDF¹) is of fundamental importance in turbulent premixed flame modelling because of its close relation with the generalised Flame Surface Density ($\Sigma_{gen} = \overline{|\nabla c|}$, where overbar indicates Reynolds averaging or LES filtering)² and Scalar Dissipation Rate ($SDR = D \nabla c \cdot \nabla c$, where D is the progress variable diffusivity).³ The evolution of SDF in premixed turbulent combustion using its transport equation has been analysed in detail from different viewpoints by several researchers^{1, 4-11}. Pope⁴ and Candel & Poinso⁵ derived the transport equation of the SDF and demonstrated the role of tangential strain rate and curvature in $|\nabla c|$ transport. Kollmann and Chen¹ focussed on the transport of $|\nabla c|$ and analysed pocket formation based on two-dimensional Direct Numerical Simulations (DNS). Chakraborty and co-workers^{6, 9-11} and Kim & Pitsch⁷ analysed strain rate and curvature dependence of the different terms of the SDF transport equation in different configurations for different turbulence intensities^{6,7}, fuels¹⁰, global Lewis numbers⁹ and mean flame radii.¹¹ The alignment of ∇c with the local principal strain rates has been analysed in detail in several previous studies^{7, 11-14}, which demonstrated that ∇c preferentially aligns with the most extensive principal strain rate when flame normal strain due to dilatation dominates over the straining induced by turbulent fluid motion. By contrast, a preferential alignment of ∇c with the most compressive principal strain rate is obtained when turbulent straining is stronger than the flame-induced strain. Recently, Dopazo and co-workers¹⁵⁻¹⁹ demonstrated the influences of normal and tangential strain rates arising from the non-material nature (i.e. flame normal motion) of the flame surface on the evolution of SDF. These strain rates induced by flame propagation have been termed as additional strain rates¹⁵⁻¹⁹ and the same terminology has been adopted in this paper. To date, most numerical investigations on the SDF transport and strain rate dependence of the SDF have been carried out on canonical configurations (i.e. flame in a box under decaying turbulence)^{1, 6, 7, 9-11, 14, 17-19}, but the analysis by Sankaran *et al.*⁸ and a recent paper by Wang *et al.*²⁰ considered a more realistic Bunsen flame and a high Karlovitz number jet, respectively. A recent investigation by Chaudhuri *et al.*²¹ analysed scalar gradient and scalar dissipation rate statistics for a temporally-evolving turbulent slot jet premixed flame. The investigation by Sankaran *et al.*⁸ suggested flame thickening in the mean sense, which contradicts findings²² from a canonical configuration. Similarly, the statistical behaviour of the

strain rates induced by flame propagation for high Karlovitz number jet flames²⁰ have been found to be in contradiction with the findings obtained for flames under decaying turbulence.¹⁷ Thus, further analysis is necessary to gain physical insights into the statistical behaviour of $|\nabla c|$ and strain rates, which affect the SDF transport, in a configuration that can be realised in laboratory-scale experiments. For the current analysis, a high-fidelity simulation dataset by Proch *et al.*^{23,24} for a turbulent lean methane-air (i.e. equivalence ratio $\phi = 0.75$) bluff-body burner configuration, which was developed and experimentally analysed at Cambridge University and Sandia National laboratories by Hochgreb, Barlow and their respective co-workers²⁵⁻³⁰, has been considered. It has been explained by Proch *et al.*^{23, 24} that the flame is well-resolved but some upstream regions in the unburned gas (at the feeding pipes) do not have sufficient resolution for a stringent definition of DNS. Thus, the simulation data can be considered to be a quasi-DNS for the flame. Chemical reactions are accounted for by the tabulation in accordance with the Premixed Flame Generated Manifolds (PFGM)^{23, 24, 32-37}, generated from one-dimensional freely propagating methane-air flames computed with the Cantera library³⁸ using the GRI-3.0³⁹ mechanism. The flamelets have been tabulated for the whole flammability range, within the equivalence ratio values of 0.45-1.8. The resulting manifold was mapped onto a two-dimensional look-up table in terms of the reaction progress variable c based on the combined mass fractions of CO, CO₂ and H₂O and the mixture fraction ξ . Interested readers can refer to Refs. 23, 32-37 for further information on the reaction rate modelling aspect of the simulation. The geometry of the bluff body flame allows for the analysis of the statistical behaviour of the SDF, its transport and its strain rate dependency at different spatial locations in a configuration which includes the effects of shear and can be realised in laboratory experiments (in contrast to numerical experimentation in canonical configurations). The main objectives of this analysis are:

- (a) To analyse and explain the effects of strain rates induced by fluid motion and flame propagation on the SDF transport at different axial locations of a lean methane-air flame.
- (b) To provide physical explanations for the strain rate dependence of the SDF.

2. MATHEMATICAL BACKGROUND

For the PFGM table the reaction progress variable is defined in terms of the combined mass fractions of CO₂, CO and H₂O (i.e. $Y_C = Y_{CO_2} + Y_{CO} + Y_{H_2O}$) in the following manner²³:

$$c = \frac{Y_C - Y_C^{min}(\xi)}{Y_C^{max}(\xi) - Y_C^{min}(\xi)} \quad (1)$$

In this equation, $Y_C^{max}(\xi)$ and $Y_C^{min}(\xi)$ are the maximum and minimum values of Y_C for a given mixture fraction value ξ , which is related to the equivalence ratio $\phi = (1 - \xi_{st})\xi / [(1 - \xi)\xi_{st}]$, where ξ_{st} is the stoichiometric mixture fraction (0.054 for methane-air mixture). The transport equation of c is given as:

$$\frac{\partial \rho c}{\partial t} + \frac{\partial (\rho u_j c)}{\partial x_j} = \dot{w} + \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial c}{\partial x_j} \right) \quad (2)$$

Here, u_j is the j^{th} component of the fluid velocity vector, $\dot{w}$ is the reaction rate of the progress variable, and D is the diffusivity of the progress variable. The molecular diffusion term $\nabla \cdot (\rho D \nabla c)$ can be split into its flame normal and tangential components in the following manner³⁹⁻⁴¹:

$$\frac{1}{\rho} \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial c}{\partial x_j} \right) = \frac{1}{\rho} \frac{\partial}{\partial x_N} \left(\rho D \frac{\partial c}{\partial x_N} \right) + 2\kappa_m D \frac{\partial c}{\partial x_N} \quad (3)$$

The flame normal co-ordinate is referred to as x_N , $\vec{N} = -\nabla c / |\nabla c|$ is the flame normal vector and $\kappa_m = 0.5 \nabla \cdot \vec{N}$ is the local mean of the principal curvatures of the flame surface. According to this convention, the flame normal points towards the reactants, and a flame surface which is convex to the reactants has a positive curvature. With the propagation velocity $v^c(\vec{x}, t)$ of a point $\vec{x}$ on the iso-surface at time t expressed as $v^c(\vec{x}, t) = u(\vec{x}, t) + S_d(x, t)\vec{N}(\vec{x}, t)$, equation 2 can be written in the kinematic form in the following manner:

$$\frac{\partial c}{\partial t} + u_j \frac{\partial c}{\partial x_j} = -S_d \frac{\partial c}{\partial x_N} \quad (4)$$

Here, S_d is the local displacement speed of the iso-surface relative to the flow velocity. It is possible to obtain an expression for the displacement speed based on equations 1 and 4 as⁴⁰⁻⁴²:

$$S_d = \underbrace{-\frac{1}{(\partial c / \partial x_N)} \left[\frac{1}{\rho} \frac{\partial}{\partial x_N} \left(\rho D \frac{\partial c}{\partial x_N} \right) \right]}_{S_n} \underbrace{- 2D\kappa_m}_{S_t} \underbrace{- \frac{\dot{w}}{\rho(\partial c / \partial x_N)}}_{S_r} \quad (5)$$

The three terms on the right-hand side of equation 5 signify the normal diffusion component S_n , tangential diffusion component S_t and the reaction component S_r of displacement speed.

For the further analysis, we will also consider the local rate of change in (a) magnitude of a non-material infinitesimal vector, $\vec{r} = (\Delta x_N) \vec{N}$ (between two points on adjacent iso-surfaces, $c(\vec{x}, t) = \Gamma$ and $c(\vec{x}, t) = \Gamma + \Delta\Gamma$), the local rate of change in (b) a surface area element A on the iso-surface $c(\vec{x}, t) = \Gamma$, and the local rate of change in (c) an infinitesimal volume $V = A(\Delta x_N)$, which have been obtained before¹⁷⁻¹⁹:

$$\frac{1}{\Delta x_N} \frac{d\Delta x_N}{dt} = a_N + \frac{\partial S_d}{\partial x_N} \quad (6)$$

$$\frac{1}{A} \frac{dA}{dt} = a_T + 2k_m S_d \quad (7)$$

$$\frac{1}{V} \frac{dV}{dt} = a_N + \frac{\partial S_d}{\partial x_N} + a_T + 2k_m S_d \quad (8)$$

Here, $a_N = N_i S_{ij} N_j$ and $a_T = (\delta_{ij} - N_i N_j) S_{ij}$ are the flow strain rates normal and tangential to the iso-surface and $S_{ij} = 0.5(\partial u_i / \partial x_j + \partial u_j / \partial x_i)$ is the flow strain rate tensor. The effective normal and tangential strain rates are defined here as¹⁷⁻¹⁹:

$$a_N^{eff} = a_N + \frac{\partial S_d}{\partial x_N} \quad \text{and} \quad a_T^{eff} = a_T + 2k_m S_d \quad (9)$$

The flow volumetric dilatation rate from heat release is $\nabla \cdot \vec{u} = a_N + a_T$. The quantities $\partial S_d / \partial x_N$ and $2k_m S_d$ originate from the nonmaterial nature of curved iso-surfaces, which propagate with a displacement speed S_d relative to the fluid.

While a_T^{eff} determines the effective flame stretch or area stretch factor, a_N^{eff} controls the production or destruction of scalar-gradients. Differentiating equation 4 with respect to x_i yields equation 10, where the gradient of c is denoted $c_{,i} = \partial c / \partial x_i$:

$$\frac{\partial c_{,i}}{\partial t} + u_j \frac{\partial c_{,i}}{\partial x_j} = -u_{j,i} c_{,j} - \frac{\partial S_d}{\partial x_i} \frac{\partial c}{\partial x_N} - S_d \frac{\partial c_{,i}}{\partial x_N} \quad (10)$$

Subsequent multiplication by $c_{,i}$ leads to:

$$\frac{1}{|\nabla c|} \left(\frac{\partial |\nabla c|}{\partial t} + v_j^c \frac{\partial |\nabla c|}{\partial x_j} \right) = -a_N^{eff} \quad (11)$$

Equation 11 provides the rate of change in time of $|\nabla c|$ following the nonmaterial iso-surface. A negative (positive) value of a_N^{eff} produces (destroys) scalar-gradients. Equation 11 can also be written as:

$$\frac{1}{|\nabla c|} \left(\frac{\partial |\nabla c|}{\partial t} + u_j \frac{\partial |\nabla c|}{\partial x_j} \right) = -a_N^{eff} - S_d \frac{N_j}{|\nabla c|} \frac{\partial |\nabla c|}{\partial x_j} \quad (12)$$

The statistical behaviour of a_N^{eff} and a_T^{eff} and their influences on $|\nabla c|$ and its transport in a bluff body burner configuration for a fuel-lean methane-air flame will be discussed in Section 4 of this paper.

3. NUMERICAL IMPLEMENTATION

The numerically methodology used for generating the dataset has been discussed by Proch *et al.*²³ and thus only a brief summary is given here. The Cambridge burner is a target flame of the Turbulent Non-premixed Flame (TNF) workshop and has been examined by various groups, using RANS/LES⁴³⁻⁴⁶ and the highly resolved simulation approach of the present case. Experimental validation data was provided by Hochgreb and Barlow²⁵⁻³⁰ with their respective co-workers, leading to the unique situation that “flame DNS” data could be validated against the statistical moments of a real flame experiment. Interested readers are referred to Refs. 25-30, 43-46 for further information on the experimental configuration and validation of previous experimental and computational analyses in this configuration. Further information on the comparison between experimental observation and the results from this dataset can be obtained from Ref. 23.

Figure 1: Schematic diagram of the investigated burner setup.

The burner geometry is illustrated in Fig. 1, which shows the bluff body and the two co-annular methane-air streams with an equivalence ratio of $\phi = 0.75$ at atmospheric conditions, which is

embedded in an air-coflow with a velocity of 0.4m/s. The burner was designed in such a manner that stratified flames can also be examined in this configuration by altering the mixture composition between the two annular channels^{24-30,46} but for premixed flame case the mixture composition remains same for outer and inner annuli. The case investigated here is the “base-line” case without stratification, where the mixture composition remains the same for the outer and inner annuli, but it should be stressed that there is shear between these two streams. The inlet flow velocities (i.e. U_i, U_o and U_{co}), root-mean-square turbulent velocity fluctuation u' , integral turbulent length scale l , equivalence ratio ϕ , unburned gas temperature T_u , Damköhler number $Da = lS_L/u'\delta_{th}$, Karlovitz number $Ka = (u'/S_L)^{1.5}(l/\delta_{th})^{-0.5}$ and, turbulent Reynolds number $Re_t = u'l/\nu$ are listed in Table 1 along with the values of the unstrained laminar burning velocity S_L and the thermal flame thickness $\delta_{th} = (T_{ad} - T_u)/\max|\nabla T|_L$ where ν is the kinematic viscosity, T_{ad}, T_u and T are the adiabatic flame temperature, unburned gas temperature and instantaneous temperature, respectively, and the subscript L refers to unstrained laminar flame values. As shown by Proch *et al.*²³, the flame burns in the corrugated flamelets regime near the burner, and further downstream in the thin reaction zones regime.⁴⁷

The simulation was performed using the in-house code ‘PsiPhi’^{23, 37, 46,48-51} that solves the governing equations in a low-Mach number finite-volume formulation. The inlet velocity fluctuations have been specified using a pseudo-turbulent field according to the filtering method proposed by Klein *et al.*⁵² in an efficient numerical implementation.⁵³ The spatial discretization of convection used a central-differencing scheme for momentum and a total variation diminishing (TVD) scheme for scalars relying on the non-linear CHARM limiter.⁵⁴ An explicit third order Runge-Kutta scheme is used for time-advancement and a CFL number of 0.5 is used for this simulation. An immersed boundary technique describes the last 12mm of the burner and the bluff body. Inside the immersed boundaries, a force resets momentum in such a manner that the velocities interpolated to the surface are zero, using averaged values at edges or corners. Diffusive scalar fluxes over the surface are set to zero, viscous momentum fluxes are evaluated from the velocity field. A zero gradient condition is applied for the pressure (correction) in surface-normal direction by copying the values from the flow-field into the immersed boundary. The computational domain consists of $1120 \times 1200 \times 1200$ equidistant cells with an edge-

length of $100\mu\text{m}$, which amounted to a total of 1.6 billion cells. The computation was carried out in parallel using MPI on the JUQUEEN BlueGene/Q at Jülich Supercomputing Centre, running on 64,000 cores to achieve a physical time of 0.34 seconds²³, which was shown to be sufficient for accurate statistical sampling in a previous LES study.⁴⁶

Stream	u' m/s	l mm	ϕ -	T_u K	Re -	S_L m/s	δ_{th} mm	Re_T -	Da -	Ka -
Inner	0.9	0.5	0.75	295	5,960	0.212	0.565	28.1	0.2	9.3
Outer	1.8	0.5	0.75	295	11,500	0.212	0.565	56.3	0.1	26.3
$U_i = 8.31\text{m/s}$, $U_o = 18.7\text{m/s}$ and $U_{co} = 0.4\text{m/s}$										

Table 1: Flame-turbulence interaction parameters for the inner and outer streams.

Figure 2: Contour plot of equivalence ratio in the mid-section of the burner, superimposed by an iso-surface of reaction progress variable at $= 0.5$. Reproduced with permission from Combust. Flame. Combust. Flame, 180, 321 (2017). Copyright 2017 Elsevier [23].

4. RESULTS & DISCUSSION

4.1 Flame-turbulence interaction

A three-dimensional visualization of the flame structure is shown in Fig. 2. The iso-surface of the reaction progress variable gets increasingly corrugated as the distance increases from the burner exit. Close to the burner, the flame develops a surface-wave pattern for which the iso-surfaces of c remain parallel to the mean flow direction. Further downstream, the iso-surfaces of c exhibit more wrinkles and less alignment with the flow, before getting highly corrugated. The same behaviour can be observed in the instantaneous distributions of the progress variable c and the absolute gradient $|\nabla c|$ in the midsection of the burner shown in Fig. 3. Islands of burned gases surrounded by reactants can be seen in the

instantaneous plots, in contrast no such instances can be seen in the three-dimensional plot. This suggests that the pockets seen in Fig. 3, may just be unburnt gas fingers pointing in the circumferential direction.

Figure 3: Distribution in the burner mid-section of the progress variable c and its normalised absolute gradient $|\nabla c| \times \delta_L$.

Downstream of $L_y = 35\text{mm}$, it can be seen from Fig. 3 that the contours of the reaction progress variable remain mostly parallel to each other on the burnt side, but they are rarely parallel to each other on the unburned side, exhibiting local flame thickening. This behaviour is indicative of the localised thin reaction zones regime⁴⁶ combustion, where turbulent eddies can enter into the preheat zone and perturb diffusive transport in this region, which is reflected in local flame thickening (or thinning).

The variations of averaged radial and axial velocity components, temperature and major species in the radial direction at different axial locations are shown in Figs. 7-11 of Ref. 23 and compared to

experimental data reported in Ref. 25 and thus these profiles are not shown here. Interested readers are referred to Ref. 23 for further information of the variations of mean and rms values of radial and axial velocity components, temperature and major species.

Figure 4: Variation of mean values of $|\nabla c| \times \delta_L$ conditional on c at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

Figure 5: Variation of mean values of $|\nabla c|/|\nabla c|_{max}$ conditional on c for both Laminar and Turbulent flames at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

4.2 Mean behaviour of SDF and flame thickness

Figure 4 shows the variation of the mean values of $|\nabla c| \times \delta_L$ conditioned on the respective progress variable at different axial locations, where δ_L is a flame thickness defined as $\delta_L = 1/\max |\nabla c|_L$ for an unstrained laminar flame. Here, the mean values conditioned on c means that the reaction progress variable space is divided into a number of bins and the quantities of interest are ensemble averaged for entries for these bins in order to obtain these plots. The same procedure was applied in several previous analyses.^{2,6,10,11} Figure 4 shows a peak conditional mean value of $|\nabla c| \times \delta_L = |\nabla c|/\max |\nabla c|_L$ assumes a value greater than unity, which indicates that the turbulent flame becomes thinner than the unstrained

laminar flame in a mean sense because, the peak value of $|\nabla c|$ can be taken to be a measure of flame thickness as $\delta \sim 1/\max|\nabla c|$ ⁸. In contrast, the flame would appear to be thickening if the peak mean value of $|\nabla c| \times \delta_L = |\nabla c|/\max|\nabla c|_L$ remains smaller than unity.

Figure 6: Variation of mean values of (a) the normalised displacement speed S_d/S_L , (b) its reaction component S_r/S_L , (c) its normal diffusion component S_n/S_L , (d) its tangential diffusion component S_t/S_L , and (e) combined reaction and normal diffusion component of displacement speed $(S_r + S_n)/S_L$ conditional on c at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

Contradictory evidences exist regarding the flame thickening/thinning under turbulence. Some numerical²² and experimental⁵⁵ analyses reported flame thinning in a mean sense under turbulence, whereas other experimental⁵⁶⁻⁵⁸ and numerical⁸ studies suggested otherwise. It is worth noting that all of these analyses have been done in different flow conditions (e.g. no mean shear for Hawkes and Chen²², and Chakraborty and Klein⁹ whereas a non-zero mean shear was present for Sankaran *et al.*⁸). Thus, it might be possible that these findings are not universal in nature and the flame thinning/thickening in a mean sense can be obtained depending on the flow condition. It can further be

seen from Fig. 4 that the flame thickness decreases with increasing axial distance. This also suggests that the flame surface area increases in the axial direction, which is consistent with the observations made from Fig. 3.

The profile of $|\nabla c|/|\nabla c|_{max}$ conditioned on respective progress variable for both laminar and turbulent flames is shown in Fig. 5, where $|\nabla c|_{max}$ represents the peak mean value of $|\nabla c|$ conditional upon c . The relative magnitudes of $|\nabla c|$ for laminar and turbulent flames provide a measure of the relative thickness of the reaction. It can be seen from the Fig. 5 that $|\nabla c|/|\nabla c|_{max}$ in the preheat zone under turbulent conditions remains smaller than the corresponding value obtained for an unstrained planar laminar flame, which suggests a thickening of the preheat zone relative to the overall flame thickness under turbulent conditions. By contrast, relative thinning of the turbulent flame happens towards the burned gas side of the reaction layer (see Fig. 5). In order to understand the observed behaviour of $|\nabla c|$ it is useful to examine the statistical behaviour of a_N , a_T , $\partial S_d/\partial x_N$ and $2S_d\kappa_m$ (see equations 7-9). Thus, it is necessary to understand the variation of S_d and its components S_r , S_n and S_t across the flame.

4.3 Mean behaviour of displacement speed and its components

The profiles of the mean values of the normalised displacement speed S_d/S_L , its reaction component S_r/S_L , its normal diffusion component S_n/S_L , tangential diffusion component S_t/S_L and the combined reaction and diffusion component of displacement speed $(S_r + S_n)/S_L$ conditional on c at different axial locations are shown in Fig. 6. The conditional mean of S_d/S_L remains mostly positive and shows that the mean value of S_d/S_L increases from the unburned to the burned gas side due to density variations. The mean values of S_d/S_L exhibits a considerable variation with the axial distance. It is also worthwhile to look into the behaviour of different components of displacement speed in order to explain the observed mean behaviour of S_d/S_L .

The mean value of S_r/S_L conditioned upon reaction progress variable assumes positive values throughout the flame, as can be seen from Fig. 6. Moreover, the mean behaviour of the normalised reaction component of displacement speed S_r/S_L remains unaffected by the axial distance. The location

of the peak mean values of S_r/S_L is determined by the relative location of peak values of $\dot{w}/\rho$ and SDF $|\nabla c|$. The mean values of $\dot{w}/\rho$ conditional on reaction progress variable are shown in Fig. 7a at different axial locations. One can also see from Fig. 7a that the variation of $\dot{w}/\rho$ is not affected by the axial location from the burner exit, which along with weak axial dependence of SDF leads to a weak axial distance dependence of the mean reaction component of displacement speed S_r/S_L . The mean normalised normal diffusion component of displacement speed S_n/S_L conditioned on reaction progress variable assumes small positive values in the unburnt region of the flame and large negative values on the burnt side of the flame (see Fig. 6). This behaviour originates from the positive (negative) values of the flame normal diffusion $\vec{N} \cdot \nabla(\rho D \vec{N} \cdot \nabla c)$ towards the unburned (burned) gas side of the flame. This can be substantiated from Fig. 7b where $\vec{N} \cdot \nabla(\rho D \vec{N} \cdot \nabla c)/\rho$ conditional on reaction progress variable are shown at different axial locations. Figure 7b also indicates a weak axial distance dependence of $\vec{N} \cdot \nabla(\rho D \vec{N} \cdot \nabla c)/\rho$ and of $|\nabla c|$, which results in a weak axial distance dependence of the mean normal diffusion component of displacement speed S_n .

It can be seen from equation 5 that the relative variations of $\vec{N} \cdot \nabla(\rho D \vec{N} \cdot \nabla c)/\rho$ and $|\nabla c|$ govern the mean variation of S_n/S_L . Figure 6 reveals that the mean values of S_t/S_L remain small in comparison to the other components of displacement speed, which suggests that S_r/S_L and S_n/S_L mainly affect the mean magnitude of S_d/S_L . This can be confirmed further by comparing the profiles of the mean values of S_d/S_L and $(S_r + S_n)/S_L$ from Figs. 6a and 6e, which reveal that the mean values of S_d/S_L and $(S_r + S_n)/S_L$ remain close to each other and large positive magnitude of S_r is partially nullified by the large negative value of S_n towards the burned gas side of the flame front. As S_t/S_L is proportional to the negative curvature (i.e., $S_t/S_L = -2D\kappa_m/S_L$), the mean value of S_t/S_L will assume higher values further downstream (at H3), because the flame is more wrinkled there than at H1 (as illustrated in Fig. 3). Moreover, Fig. 6 shows that the mean displacement speed depends on axial distance, mainly due to the mean variation of S_t/S_L .

Figure 7: Variation of mean values of (a) the normalised reaction source term $\dot{w}/\rho \times \delta_{th}/S_L$ and (b) the normalized flame normal diffusive flux $\vec{N} \cdot \nabla(\rho D \vec{N} \cdot \nabla c)/\rho \times \delta_{th}/S_L$ conditional on c at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

Figure 8: Variation of mean values of (a) $\nabla \cdot \vec{u} \times \delta_{th}/S_L$, (b) $a_N \times \delta_{th}/S_L$ and (c) $a_T \times \delta_{th}/S_L$ conditional on c at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

4.4 Mean behaviour of dilatation and fluid-dynamic strain rates

The mean values of the normalised flow dilatation rate $\nabla \cdot \vec{u}$ conditioned on c are shown in Fig. 8a at different axial locations. The mean value of the flow dilatation rate remains positive because of the thermal expansion due to chemical heat release. The curvature dependency of dilatation rate (i.e.

negative correlation between dilatation rate and curvature due to focussing of heat at negatively curved locations) gives rise to the axial distance dependency of the mean dilatation rate variation, as the magnitude of curvature increases with axial distance from the burner exit. Figure 8b shows the mean normal strain rate a_N conditioned on c , it exhibits mostly positive values near the burner (at H1) and negative values further downstream (at H2, H3) throughout the flame. The statistical behaviour of a_N is principally determined by the fluid-dynamics which can be explained in the following manner. The normal strain rate can be expressed as: $a_N = (e_\alpha \cos^2 \alpha + e_\beta \cos^2 \beta + e_\gamma \cos^2 \gamma)$ where e_α , e_β and e_γ are the most extensive (i.e. most positive), intermediate and the most compressive (i.e. most negative) principle strain rates with α , β and γ being the angles associated the eigenvectors with ∇c . It has been shown in several previous analyses^{7, 12-14} that ∇c preferentially aligns with the eigenvector associated with e_α (i.e., high probability of finding $|\cos \alpha| \approx 1.0$) and yields a positive value of a_N when the strain rate induced by flame normal acceleration (due to dilatation) overcomes turbulent straining. By contrast, ∇c preferentially aligns with the eigenvector associated with e_γ (i.e., high probability of finding $|\cos \gamma| \approx 1.0$) and gives rise to a negative value of a_N when the strain rate induced by flame normal acceleration is overcome by turbulent straining. The flame is quasi-laminar close to the burner exit and as a result ∇c preferentially aligns with the eigenvector associated with e_α for the major part of the flame except in the unburned gas where the effects of heat release are weak, so that a preferential alignment between ∇c and the eigenvector associated with e_γ is observed (see Fig. 19 in Ref.23). This alignment behaviour gives rise to positive mean normal strain rate for the major part of the flame at H1. The flame becomes more wrinkled downstream because of Kelvin-Helmholtz instability and combustion occurs in the highly turbulent shear layer between the inner and outer flows. Thus, the influence of turbulent straining increases with the distance from the burner exit. At H2, turbulent straining effects are stronger than at H1 and the mean normal strain rate at H2 assumes negative values towards the unburned gas side. Within the reaction layer, the mean normal strain rate at H2 remains largely positive, but with local negative values, whereas these values of a_N were always positive at H1. Moreover, the (still positive) mean value of a_N at H2 is smaller than at H1 because of the reduced extent of ∇c alignment with the eigenvector associated with e_α . Finally, at H3, turbulent straining becomes so strong that it overcomes the straining due to flame normal acceleration, resulting in a preferential

alignment between ∇c and the eigenvector associated with e_γ . This leads to negative mean values of a_N in almost the entire reaction layer at H3.

Figure 9: Variation of mean values of (a) $(S_{d,N})^+ = \partial S_d / \partial x_N \times \delta_{th} / S_L$, (b) $(S_{r,N})^+ = \partial S_r / \partial x_N \times \delta_{th} / S_L$, (c) $(S_{n,N})^+ = \partial S_n / \partial x_N \times \delta_{th} / S_L$, (d) $(S_{t,N})^+ = \partial S_t / \partial x_N \times \delta_{th} / S_L$, and (e) $(S_{r,N} + S_{n,N})^+ = (\partial S_r / \partial x_N + \partial S_n / \partial x_N) \times \delta_{th} / S_L$ conditional on c at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

The relative magnitudes and mean behaviour of $\nabla \cdot \vec{u}$ and a_N determine the mean behaviour of the tangential strain rate $a_T = \nabla \cdot \vec{u} - a_N$, which is shown in Fig. 8c, conditioned on c . The mean tangential strain rate a_T assumes mostly positive values for all values of c . At H1, where the flame is little affected by turbulence, the mean value of a_T decreases towards the burned side of the flame. The magnitude of a_T increases with increasing axial distance from the burner exit. The variation of the magnitude of the mean $\nabla \cdot \vec{u}$ remains small in comparison to that of a_N . It is therefore the increasingly negative a_N that causes the growth of $a_T = \nabla \cdot \vec{u} - a_N$ in downstream direction.

4.5 Mean behaviour of the strain rates due to flame propagation

The mean values of the normal strain rate component due to flame propagation $\partial S_d/\partial x_N$ conditional on c along with its components ($\partial S_r/\partial x_N, \partial S_n/\partial x_N, \partial S_t/\partial x_N$ and $\partial(S_r + S_n)/\partial x_N$) are shown in Figs. 9a-e. As the flame normal vector points towards the reactants, any increase of S_α (here $\alpha = d, r, n, t$) with c will produce a negative value of $\partial S_\alpha/\partial x_N$. Thus, the mean profiles of S_α shown in Fig. 6 provide an indication of the expected mean behaviour of $\partial S_\alpha/\partial x_N$. It can be seen that the mean value of $\partial S_d/\partial x_N$ remains positive in the unburnt and burnt region of the flame brush. A negative value of $\partial S_d/\partial x_N$ (and of $\partial S_\alpha/\partial x_N$) tends to bring c -iso-surfaces closer to each other and acts to increase $|\nabla c|$ and *vice versa*.

The mean conditional values of $\partial S_r/\partial x_N$ remain negative (see Fig. 9b) in accordance with the mean conditional values of S_r/S_L , which increase from the unburned side to the burned side of the flame brush (see Fig. 6b). The mean contribution of $\partial S_n/\partial x_N$ assumes small negative values on the unburnt side of the flame and increases towards a positive value on the burnt side of the flame. This can be expected from the behaviour of S_n/S_L in Fig. 6c, which decreases sharply towards a negative value on the burned side of the flame. The mean contribution of $\partial S_t/\partial x_N$ is small near the burner and increases with the height above the burner. A comparison between Figs. 6 and 9 reveals that S_r and S_n do not show a strong dependency on axial distance and accordingly $S_r/\partial x_N$, $\partial S_n/\partial x_N$ and $\partial(S_r + S_n)/\partial x_N$ do not exhibit any significant dependence on the axial distance. A comparison between Figs. 9a and 9e reveals that the variation of $\partial S_t/\partial x_N$ induces significant axial distance dependence of $\partial S_d/\partial x_N$. The considerable axial distance dependence of S_t gives rise to the similar dependency for $\partial S_t/\partial x_N$ with the height above the burner.

Figure 10: Variation of mean values of (a) $(2S_d\kappa_m)^+ = 2S_d\kappa_m \times \delta_{th}/S_L$, (b) $(2(S_r + S_n)\kappa_m)^+ = 2(S_r + S_n)\kappa_m \times \delta_{th}/S_L$, (c) $(-4D\kappa_m^2)^+ = -4D\kappa_m^2 \times \delta_{th}/S_L$ and (d) $\kappa_m^* = \kappa_m \times \delta_{th}$ conditional on c at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

The normalised mean profiles of $2S_d\kappa_m$ conditioned on c are shown in Fig. 10a. The mean values of $2S_d\kappa_m$ remain negative throughout the flame. To understand this behaviour, $2S_d\kappa_m$ can be split into components arising from the components of displacement speed:

$$2S_d\kappa_m = 2\kappa_m(S_r + S_n + S_t) = 2(S_r + S_n)\kappa_m - 4D\kappa_m^2 \quad (13)$$

The profiles of normalised mean values of $2(S_r + S_n)\kappa_m$ and $-4D\kappa_m^2$ conditioned on c are shown in Figs. 10b and 10c respectively, at different axial locations. A comparison between Figs. 10b and 10c reveals that the mean contributions of $(-4D\kappa_m^2)$ and $2(S_r + S_n)\kappa_m$ remain comparable and both remain negative throughout the flame at all distances from the burner exit. The term $(-4D\kappa_m^2)$ is always negative and its magnitude increases with the height above the burner exit due to the increased flame wrinkling. Moreover, the magnitude of $(-4D\kappa_m^2)$ increases from the unburned to the burned side of the flame due to the higher diffusivity D on the burned side.

The mean values of κ_m conditioned on c for all the species considered here are shown in Fig. 10d at different axial locations, which reveals that the mean value of κ_m remains predominantly negative in

this configuration. The correlation coefficient between $(S_r + S_n)$ and κ_m at different c values are shown in Table 2 at different axial locations. Table 2 indicates that the correlation coefficient between $(S_r + S_n)$ and κ_m remains weak throughout the flame. The combination of predominantly positive values of $(S_r + S_n)$ and negative values of κ_m along with weak correlation between these quantities leads to negative mean values of $2(S_r + S_n)\kappa_m$. The magnitude of the (negative) mean of $2(S_r + S_n)\kappa_m$ increases with the distance from the burner exit because of the increased magnitudes of curvature κ_m .

<i>Correlation coefficient between $(S_r + S_n) - \kappa_m$</i>				
<i>Axial location</i>	<i>unburnt</i>	<i>preheat</i>	<i>reaction</i>	<i>burnt</i>
H1	0.61	0.04	-0.15	-0.22
H2	0.42	0.35	-0.18	-0.34
H3	0.18	0.22	0.04	-0.10

Table 2: Correlation coefficients between $(S_r + S_n) - \kappa_m$ at different c -values corresponding to unburnt ($c = 0.1 - 0.3$), preheat ($c = 0.3 - 0.6$), reaction ($c = 0.6 - 0.8$), burnt ($c = 0.8 - 0.89$) at different heights above the burner corresponding to H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

4.6 Mean behaviour of effective normal and tangential strain rates

The mean profiles of a_N^{eff} conditioned on c are shown in Fig. 11a. A comparison between Figs. 8 and 9 reveals that the mean behaviour of a_N^{eff} is determined mainly by the normal strain rate component $\partial S_d / \partial x_N$ due to flame propagation. This behaviour is consistent with previous findings by Dopazo *et al.*¹⁷. As mean values of $\partial S_d / \partial x_N$ show axial dependence, the mean effective normal strain rate a_N^{eff} is also dependent on the axial location.

The negative (positive) values of a_N^{eff} are associated with flame thinning (flame thickening) and thus the negative mean value of a_N^{eff} in the region of the flame where the SDF attains its maximum value is consistent with the flame thinning observed in Fig. 4, which showed that the peak in the mean of $|\nabla c| \times \delta_L$ exceeds unity.

The mean value of $(u_j + N_j S_d)(\partial |\nabla c| / \partial x_j) |\nabla c|^{-1}$ conditioned upon the progress variable c is shown in Fig. 11b. The conditional mean of $(u_j + N_j S_d)(\partial |\nabla c| / \partial x_j) |\nabla c|^{-1}$ assumes negative values for the major part of the flame except towards the burned side, where the quantity shows high positive mean values. Similar to a_N^{eff} , the mean variation of $(u_j + N_j S_d)(\partial |\nabla c| / \partial x_j) |\nabla c|^{-1}$ also does not show a

significant dependence on the axial location above the burner exit. The mean values of $(u_j + N_j S_d)(\partial|\nabla c|/\partial x_j)|\nabla c|^{-1}$ and a_N^{eff} determine the mean behaviour of $(\partial|\nabla c|/\partial t)|\nabla c|^{-1}$. One can see from Fig. 11b that the negative mean contributions of $(u_j + N_j S_d)(\partial|\nabla c|/\partial x_j)|\nabla c|^{-1}$ almost nullify the positive mean values of a_N^{eff} to yield high negative values of $(\partial|\nabla c|/\partial t)|\nabla c|^{-1}$ towards the burned gas side of the flame. Thus, the mean value of $(\partial|\nabla c|/\partial t)|\nabla c|^{-1}$ remains negligible in Fig. 11c, which is consistent with the fact that the mean value of $|\nabla c|$ under turbulent conditions does not show much change in comparison to the corresponding laminar value (see Fig. 5). Moreover, the mean value of $(\partial|\nabla c|/\partial t)|\nabla c|^{-1}$ assumes small positive values for c at which the peak mean value of $|\nabla c|$ is obtained, which explains why the peak mean value of $|\nabla c| \times \delta_L = |\nabla c|/\max|\nabla c|_L$ is found to be greater than unity in this turbulent case. However, this is not a universal situation, and an overall flamelet thickening can be obtained under a different flow condition for a different turbulent premixed flame.

Figure 11: Variation of mean values of (a) $a_N^{eff+} = a_N^{eff} \times \delta_{th}/S_L$, of (b) $((u_j + N_j S_d)(\partial|\nabla c|/\partial x_j)|\nabla c|^{-1})^+ = (u_j + N_j S_d)(\partial|\nabla c|/\partial x_j)|\nabla c|^{-1} \times \delta_{th}/S_L$, of (c) $((\partial|\nabla c|/\partial t)|\nabla c|^{-1})^+ = (\partial|\nabla c|/\partial t)|\nabla c|^{-1} \times \delta_{th}/S_L$ and of (d) $a_T^{eff+} = a_T^{eff} \times \delta_{th}/S_L$ conditional on c at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

The profiles of the mean effective tangential strain rate a_T^{eff} conditioned on c are shown in Fig. 11d at different axial locations. The negative mean contribution of $2S_d\kappa_m$ dominates over the positive mean fluid-dynamic tangential strain rate a_T to yield negative mean values of a_T^{eff} , and this trend strengthens with increasing distance from the burner exit. The negative mean values of a_T^{eff} are indicative of the stabilisation mechanism associated with Huygens propagation, which suggests that a smooth perturbed flame surface will eventually form cusps and become flatter with time.

4.7 Local behaviour of strain rates and SDF

In order to understand the local behaviour of the strain rates, the joint probability density functions (PDFs) between various strain rate components and curvature κ_m have been utilised in this sub-section. The joint PDFs between normal strain rate a_N and curvature κ_m are shown in Fig. 12a for different locations within the flame. It can be seen from Fig. 12a that a_N and κ_m are negatively correlated for the major part of the flame before the correlation becomes positive towards the burned gas side.

The effects of thermal expansion are strong at negatively curved regions because of focussing of heat and thus the strain rate induced by thermal expansion overcomes turbulent straining to induce a preferential alignment of ∇c with e_α ^{7, 12-14}, which in turn leads to high values of $a_N = (e_\alpha \cos^2 \alpha + e_\beta \cos^2 \beta + e_\gamma \cos^2 \gamma)$. The effects of dilatation rate $\nabla \cdot \vec{u}$ are weak towards the burned gas side of the flame, and thus the curvature dependence of normal strain rate $a_N = \nabla \cdot \vec{u} - a_T$ is principally governed by the curvature dependence of tangential strain rate a_T . The joint PDFs between tangential strain rate a_T and curvature κ_m are shown in Fig. 12b for different locations within the flame. Figure 12b indicates a negative correlation between a_T and κ_m with the correlation strength weakening both on unburned and burned gas sides of the flame. This behaviour is consistent with several previous DNS^{6, 9, 39, 60, 61} and experimental⁶² analyses. This negative correlation between a_T and κ_m is a combined effect of thermal expansion and flame-eddy interaction, which was previously^{60, 61} discussed in detail and is not repeated here. The negative correlation between a_T and κ_m leads to the positive correlation between $a_N = \nabla \cdot \vec{u} - a_T$ and κ_m on the burned gas side where the effects of $\nabla \cdot \vec{u}$ are weak. It can

further be seen from Figs. 12a and 12b that the correlation strength weakens with increasing distance from the burner exit. The turbulent velocity fluctuation increases in downstream direction and the strength of the correlation between fluid-dynamic strain rates and curvature decreases with increasing turbulent fluctuation, which is consistent with previous findings^{6, 61, 63, 64}.

The joint PDFs between the additional normal (tangential) strain rate component $\partial S_d / \partial x_N$ ($2S_d \kappa_m$) and curvature κ_m are shown in Fig. 13a (Fig. 13b) for different locations within the flame. Figure 13a exhibits a weak correlation between $\partial S_d / \partial x_N$ and κ_m throughout the flame. It can be seen from Fig. 13b that the dependence between $2S_d \kappa_m = 2(S_r + S_n) - 4D\kappa_m^2$ and κ_m is non-linear and the net correlation remains negative. It has already been shown in Table 2 that $(S_r + S_n)$ and κ_m are weakly correlated but the additional tangential strain rate (or curvature stretch) component arising from tangential diffusion component $-4D\kappa_m^2$ induces the non-linear curvature dependence of $2S_d \kappa_m$. Moreover, $-4D\kappa_m^2$ is responsible for the net negative correlation between $2S_d \kappa_m$ and κ_m , which is consistent with the findings based on DNS in canonical configurations⁶⁴⁻⁶⁷. As observed earlier for fluid-dynamic strain rates, the correlations between additional strain rates and curvature weaken with the increasing distance from the burner exit due to increased turbulent velocity fluctuations.

(a)

(b)

Figure 12: Contours of joint PDFs of normalised (a) normal strain rate $a_N^+ = a_N \times \delta_{th}/S_L$ and (b) tangential strain rate $a_T^+ = a_T \times \delta_{th}/S_L$ with normalised curvature $\kappa_m^* = \kappa_m \times \delta_{th}$ at locations H1 (7–13mm), H2 (30–37mm) and H3 (60–68mm) for different c -values corresponding to unburnt ($c = 0.1 - 0.3$), preheat ($c = 0.3 - 0.6$), reaction ($c = 0.6 - 0.8$), burnt ($c = 0.8 - 0.89$) gases.

(a)

(b)

Figure 13: Contours of joint PDFs of normalised additional (a) normal strain rate $(S_{d,N})^+ = \partial S_d / \partial x_N \times \delta_{th} / S_L$ and (b) tangential strain rate $(2S_d \kappa_m)^+ = 2S_d \kappa_m \times \delta_{th} / S_L$ with normalised curvature $\kappa_m^* = \kappa_m \times \delta_{th}$ at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm) for different c-values corresponding to unburnt ($c = 0.1 - 0.3$), preheat ($c = 0.3 - 0.6$), reaction ($c = 0.6 - 0.8$), burnt ($c = 0.8 - 0.89$) gases.

(a)

(b)

Figure 14: Contours of joint PDFs of normalised effective (a) normal strain rate $a_N^{eff+} = a_N^{eff} \times \delta_{th}/S_L$ and (b) tangential strain rate $a_T^{eff+} = a_T^{eff} \times \delta_{th}/S_L$ with normalised curvature $\kappa_m^* = \kappa_m \times \delta_{th}$ at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm) for different c -values corresponding to unburnt ($c = 0.1 - 0.3$), preheat ($c = 0.3 - 0.6$), reaction ($c = 0.6 - 0.8$), burnt ($c = 0.8 - 0.89$) gases.

The joint PDFs between the effective normal (tangential) strain rate a_N^{eff} (a_T^{eff}) and curvature κ_m are shown in Fig. 14a (Fig. 14b). Figure 14a shows a weak correlation between a_N^{eff} and curvature κ_m throughout the flame front. This suggests that the curvature dependence of $\partial S_d / \partial x_N$ dominates over that of a_N . This is also consistent with the observations made from Fig. 11, which indicates that the mean behaviour of a_N^{eff} is determined principally by the additional normal strain rate $\partial S_d / \partial x_N$. Furthermore, Fig. 14a suggests that the distance from the burner exit does not seem to have any major influence on the correlation between a_N^{eff} and κ_m . It can be seen from Table 3 that $(u_j + N_j S_d)(\partial |\nabla c| / \partial x_j) |\nabla c|^{-1}$ remains weakly correlated with curvature. The combination of weak correlations of a_N^{eff} and $(u_j + N_j S_d)(\partial |\nabla c| / \partial x_j) |\nabla c|^{-1}$ with curvature κ_m leads to a weak correlation between $|\nabla c|$ and curvature κ_m , which can be substantiated from Table 4. Figure 14b shows that the net correlation between a_T^{eff} and curvature κ_m remains negative and this correlation remains weak towards the unburned gas side and the correlation strength decreases with increasing distance from the burner. The combination of negative correlations between a_T and curvature κ_m , and between $2S_d \kappa_m$ and curvature κ_m gives rise to a net negative correlation between a_T^{eff} and κ_m .

<i>Correlation coefficient between $(u_j + N_j S_d)(\partial \nabla c / \partial x_j) \nabla c ^{-1}$ and κ_m</i>				
<i>Axial location</i>	<i>unburnt</i>	<i>preheat</i>	<i>reaction</i>	<i>burnt</i>
H1	0.08	0.12	0.0	-0.02
H2	0.03	0.02	0.02	-0.03
H3	0.03	0.03	-0.05	-0.01

Table 3: Correlation coefficients between $(u_j + N_j S_d)(\partial |\nabla c| / \partial x_j) |\nabla c|^{-1} - \kappa_m$ at different c -values corresponding to unburnt ($c = 0.1 - 0.3$), preheat ($c = 0.3 - 0.6$), reaction ($c = 0.6 - 0.8$), burnt ($c = 0.8 - 0.89$) at different heights above the burner corresponding to H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

<i>Correlation coefficient between ∇c and κ_m</i>				
<i>Axial location</i>	<i>unburnt</i>	<i>preheat</i>	<i>reaction</i>	<i>burnt</i>
H1	0.41	0.47	0.25	0.02
H2	0.26	0.44	0.40	0.08
H3	0.02	0.06	0.10	0.02

Table 4: Correlation coefficients between $|\nabla c| - \kappa_m$ at different c -values corresponding to unburnt ($c = 0.1 - 0.3$), preheat ($c = 0.3 - 0.6$), reaction ($c = 0.6 - 0.8$), burnt ($c = 0.8 - 0.89$) at different heights above the burner corresponding to H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

4.8 Modelling implications

The foregoing discussion indicates that the statistics of the SDF and its evolution are determined by a combination of fluid-dynamic straining, chemical heat release and flame propagation. Along with fluid-dynamic straining, the flame normal gradients of displacement speed play a pivotal role in the SDF evolution. It is possible to obtain the transport equation of the generalised Flame Surface Density (FSD) (i.e. $\Sigma_{gen} = |\nabla c|$)² from equation 12:

$$\frac{\partial \Sigma_{gen}}{\partial t} + \frac{\partial (\overline{u_j})_s \Sigma_{gen}}{\partial x_j} = \overline{(a_T^{eff})}_s \Sigma_{gen} - \frac{\partial (\overline{S_d N_j})_s \Sigma_{gen}}{\partial x_j} \quad (14)$$

where $(\overline{Q})_s = \overline{Q|\nabla c|}/\Sigma_{gen}$ is the surface-averaging operation and the overbar denotes either Reynolds averaging or LES filtering as appropriate. Similarly, equation 12 can be manipulated to yield:

$$\frac{\partial |\nabla c|^2}{\partial t} + u_j \frac{\partial |\nabla c|^2}{\partial x_j} = -2a_N |\nabla c|^2 - 2N_j \frac{\partial S_d}{\partial x_j} |\nabla c|^2 - S_d N_j \frac{\partial |\nabla c|^2}{\partial x_j} \quad (15)$$

Algebraic manipulation of equation 15 provides the transport equation of scalar dissipation rate (SDR)

$$N_c = D_c |\nabla c|^2:$$

$$\frac{\partial (\rho N_c)}{\partial t} + \frac{\partial (\rho u_j N_c)}{\partial x_j} = -2\rho a_N N_c - 2\rho N_j \frac{\partial S_d}{\partial x_j} N_c - \rho S_d N_j \frac{\partial N_c}{\partial x_j} + \rho S_d N_j N_c \frac{1}{D_c} \frac{\partial D_c}{\partial x_j} + \frac{\rho N_c}{D_c} \left(\frac{\partial D_c}{\partial t} + u_j \frac{\partial D_c}{\partial x_j} \right) \quad (16i)$$

$$\frac{\partial (\rho N_c)}{\partial t} + \frac{\partial (\rho u_j N_c)}{\partial x_j} = -2\rho a_N^{eff} N_c - \rho S_d N_j \frac{\partial N_c}{\partial x_j} + \rho S_d N_j N_c \frac{1}{D_c} \frac{\partial D_c}{\partial x_j} + \frac{\rho N_c}{D_c} \left(\frac{\partial D_c}{\partial t} + u_j \frac{\partial D_c}{\partial x_j} \right) \quad (16ii)$$

By Reynolds averaging or LES filtering of equations 16i and 16ii, one can obtain the transport equation of the Favre-averaged or filtered SDR $\tilde{N}_c = \overline{\rho N_c}/\bar{\rho}$. It is evident from equations 14 and 16 that a_N , a_T , $N_j \partial S_d / \partial x_j$, $2S_d \kappa_m$, a_N^{eff} and a_T^{eff} play key roles in both the FSD and SDR transport, and that the local correlations between different strain rates and curvature discussed in this paper are expected to survive to a certain extent at the resolved scale for the LES. Thus, the physical processes which govern the aforementioned correlations and the observed mean behaviours of that a_N , a_T , $N_j \partial S_d / \partial x_j$, $2S_d \kappa_m$, a_N^{eff} and a_T^{eff} need to be modelled to enable accurate RANS and LES predictions based on either the FSD or SDR modelling methodologies.

5. CONCLUSIONS

The statistics of the ‘effective’ strain rates, and its implication on the evolution of the surface density function (SDF) $|\nabla c|$ have been analysed using a database from a three-dimensional, high-fidelity simulation of a turbulent lean ($\phi = 0.75$) methane-air bluff-body burner configuration, which was designed and examined at Cambridge University and Sandia National laboratories by Hochgreb, Barlow and their co-workers [25-30]. The peak value of the mean value of SDF conditioned on the reaction progress variable for the turbulent condition is found to be greater than the maximum value of the SDF in the corresponding unstrained laminar flame, which is indicative of the thinning of the reaction layer under turbulent conditions in comparison to the corresponding laminar flame in a mean sense. The statistics of dilatation rate, fluid-dynamic normal and tangential strain rates, and the additional normal and tangential strain rates arising from flame propagation have been analysed in detail and the influence of these statistics on the SDF magnitude and its evolution has been discussed. The mean value of dilatation rate $\nabla \cdot \vec{u}$ remains positive and exhibits a considerable dependence on the axial location above the burner exit. The mean fluid-dynamic normal strain rate a_N assumes positive values close to the burner exit but increasingly becomes negative as the effect of turbulence increases with axial distance from the burner exit. The mean contribution of additional normal strain rate due to flame propagation $\partial S_d / \partial x_N$ remains negative for the major part of the flame. The mean fluid-dynamic tangential strain rate a_T remains positive but this positive value is dominated by negative mean values of tangential strain rate due to flame propagation (or curvature stretch) $2S_d \kappa_m$ and this behaviour becomes more prominent further downstream as the effects of turbulence increase with axial distance. The mean curvature stretch $2S_d \kappa_m$ assumes mostly negative values throughout the flame brush due to the tangential diffusion component of the flame displacement speed $S_t = -2D\kappa_m$ and the correlation between $(S_r + S_n)$ and κ_m remains weak throughout the flame. The relative magnitudes of mean values of a_N and $\partial S_d / \partial x_N$ determine the mean behaviour of the effective normal strain rate a_N^{eff} and similarly the mean behaviour of a_T^{eff} is determined by the mean contributions of a_T and $2S_d \kappa_m$. The mean value of a_T^{eff} remains positive close to the burner exit and increasingly becomes negative as one moves away from the burner exit, suggesting that the curvature stretch component dominates over the fluid-dynamic tangential strain

rate as the axial distance increases. It has also been demonstrated that both $(u_j + N_j S_d)(\partial|\nabla c|/\partial x_j)|\nabla c|^{-1}$ and a_N^{eff} determine whether the flame thickens or becomes thin under the flame-turbulence interaction. The joint PDFs for the fluid-dynamic strain rates, and the ‘effective’ strain rates with curvature have been utilised to explain the local flame thickening/flame thinning. Detailed physical explanations have been provided for local curvature dependences of strain rates and SDF obtained from the aforementioned joint PDFs. It is expected that the local strain rate and curvature dependencies of the SDF transport will be evident also in the resolved scale in the context of generalised FSD (i.e. $\Sigma_{gen} = \overline{|\nabla c|}$) and Favre-filtered SDR $\tilde{N}_c$ transport. Thus, FSD and SDR transport models should be able to predict these local behaviours at the resolved scale to ensure a high-fidelity of LES predictions.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge the compute time granted on JUQUEEN at Jülich Supercomputing Centre (JSC), through the John von Neumann Institute for Computing (NIC). NC is grateful to the Engineering and Physical Sciences Research Council (EPSRC), UK and ARCHER for financial and computational support.

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Table 1: Flame-turbulence interaction parameters for the inner and outer streams.

Table 2: Correlation coefficients between $(S_r + S_n) - \kappa_m$ at different c -values corresponding to unburnt ($c = 0.1 - 0.3$), preheat ($c = 0.3 - 0.6$), reaction ($c = 0.6 - 0.8$), burnt ($c = 0.8 - 0.89$) at different heights above the burner corresponding to H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

Table 3: Correlation coefficients between $(u_j + N_j S_d)(\partial|\nabla c|/\partial x_j)|\nabla c|^{-1} - \kappa_m$ at different c -values corresponding to unburnt ($c = 0.1 - 0.3$), preheat ($c = 0.3 - 0.6$), reaction ($c = 0.6 - 0.8$), burnt ($c = 0.8 - 0.89$) at different heights above the burner corresponding to H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

Table 4: Correlation coefficients between $|\nabla c| - \kappa_m$ at different c -values corresponding to unburnt ($c = 0.1 - 0.3$), preheat ($c = 0.3 - 0.6$), reaction ($c = 0.6 - 0.8$), burnt ($c = 0.8 - 0.89$) at different heights above the burner corresponding to H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

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Figure 1: Schematic diagram of the investigated burner setup.

Figure 2: Contour plot of equivalence ratio in the mid-section of the burner, superimposed by an iso-surface of reaction progress variable at $c = 0.5$. Reproduced with permission from Combust. Flame. Combust. Flame, 180, 321 (2017). Copyright 2017 Elsevier [23].

Figure 3: Distribution in the burner mid-section of the progress variable c and its normalised absolute gradient $|\nabla c| \times \delta_L$.

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Figure 7: Variation of mean values of (a) the normalised reaction source term $\dot{w}/\rho \times \delta_{th}/S_L$ and (b) the normalized flame normal diffusive flux $\vec{N} \cdot \nabla(\rho D \vec{N} \cdot \nabla c)/\rho \times \delta_{th}/S_L$ conditional on c at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

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Figure 9: Variation of mean values of (a) $(S_{d,N})^+ = \partial S_d / \partial x_N \times \delta_{th}/S_L$, (b) $(S_{r,N})^+ = \partial S_r / \partial x_N \times \delta_{th}/S_L$, (c) $(S_{n,N})^+ = \partial S_n / \partial x_N \times \delta_{th}/S_L$, (d) $(S_{t,N})^+ = \partial S_t / \partial x_N \times \delta_{th}/S_L$ and (e) $(S_{r,N} + S_{n,N})^+ = (\partial S_r / \partial x_N + \partial S_n / \partial x_N) \times \delta_{th}/S_L$ conditional on c at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

Figure 10: Variation of mean values of (a) $(2S_d \kappa_m)^+ = 2S_d \kappa_m \times \delta_{th}/S_L$, (b) $(2(S_r + S_n) \kappa_m)^+ = 2(S_r + S_n) \kappa_m \times \delta_{th}/S_L$, (c) $(-4D \kappa_m^2)^+ = -4D \kappa_m^2 \times \delta_{th}/S_L$ and (d) $\kappa_m^* = \kappa_m \times \delta_{th}$ conditional on c at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

Figure 11: Variation of mean values of (a) $a_N^{eff+} = a_N^{eff} \times \delta_{th}/S_L$, (b) $\left((u_j + N_j S_d)(\partial|\nabla c|/\partial x_j)|\nabla c|^{-1}\right)^+ = (u_j + N_j S_d)(\partial|\nabla c|/\partial x_j)|\nabla c|^{-1} \times \delta_{th}/S_L$, (c) $\left((\partial|\nabla c|/\partial t)|\nabla c|^{-1}\right)^+ = (\partial|\nabla c|/\partial t)|\nabla c|^{-1} \times \delta_{th}/S_L$ and (d) $a_T^{eff+} = a_T^{eff} \times \delta_{th}/S_L$ conditional on c at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm).

Figure 12: Contours of joint PDFs of normalised (a) normal strain rate $a_N^+ = a_N \times \delta_{th}/S_L$ and (b) tangential strain rate $a_T^+ = a_T \times \delta_{th}/S_L$ with normalised curvature $\kappa_m^* = \kappa_m \times \delta_{th}$ at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm) for different c -values corresponding to unburnt ($c = 0.1 - 0.3$), preheat ($c = 0.3 - 0.6$), reaction ($c = 0.6 - 0.8$), burnt ($c = 0.8 - 0.89$) gases.

Figure 13: Contours of joint PDFs of normalised additional (a) normal strain rate $(\partial S_d/\partial x_N)^+ = \partial S_d/\partial x_N \times \delta_{th}/S_L$ and (b) tangential strain rate $(2S_d \kappa_m)^+ = 2S_d \kappa_m \times \delta_{th}/S_L$ with normalised curvature $\kappa_m^* = \kappa_m \times \delta_{th}$ at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm) for different c -values corresponding to unburnt ($c = 0.1 - 0.3$), preheat ($c = 0.3 - 0.6$), reaction ($c = 0.6 - 0.8$), burnt ($c = 0.8 - 0.89$) gases.

Figure 14: Contours of joint PDFs of normalised effective (a) normal strain rate $a_N^{eff+} = a_N^{eff} \times \delta_{th}/S_L$ and (b) tangential strain rate $a_T^{eff+} = a_T^{eff} \times \delta_{th}/S_L$ with normalised curvature $\kappa_m^* = \kappa_m \times \delta_{th}$ at locations H1 (7-13mm), H2 (30-37mm) and H3 (60-68mm) for different c -values corresponding to unburnt ($c = 0.1 - 0.3$), preheat ($c = 0.3 - 0.6$), reaction ($c = 0.6 - 0.8$), burnt ($c = 0.8 - 0.89$) gases.