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Flame Self-Interactions in an Open Turbulent Jet Spray Flame

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ABSTRACT

A three-dimensional Direct Numerical Simulation database of an open turbulent jet spray flame representing a laboratory-scale burner configuration has been analysed to investigate flame self interactions (FSIs) in the presence of flow induced shear, to the best of the authors' knowledge, for the first time. The FSI occurrences (i.e. unburned gas mixture pockets (UBGPs), tunnel formations (TFs), tunnel closures (TCs) and burned gas mixture pockets (BGPs)) have been identified across the flame at different axial locations. It has been found that the interplays between turbulence, droplet evaporation and chemistry have a significant influence on the topological nature of the flame surface. Close to the jet exit, the FSI events are found to occur towards the burned gas side of the flame but moving further away from the jet exit there are significant occurrences of FSI events within the flame where increasingly fuel-rich, low Damköhler number conditions occur. In this study, the FSI events have been found to be predominantly TFs and TCs, which is consistent with previous analyses of turbulent premixed flames and combustion of droplet-laden mixtures. However, non-negligible occurrences of UBGPs and BGPs are also observed in this case. The results obtained from this analysis have important implications from a modelling perspective where flame topologies have a significant influence on the nature of the flame surface which will, in turn, affect the flame-surface based modelling approaches. Accordingly, the findings of the current analysis may need to be accounted for the development of flame surface-based closures in the context of turbulent spray flames.

KEYWORDS

Turbulent spray flames; Droplet-laden combustion; Flame self-interaction

1. INTRODUCTION

In turbulent combustion, the interaction of the flame and turbulent flow field gives rise to flame wrinkling and an increase in the flame surface area which, in turn, leads to an augmentation in the rate of burning. Under instances of high levels of wrinkling, the flame surface interacts with itself and the resulting local topologies due to these self-interactions can have a significant role in the burning characteristics of such flames. The use of scalar fields, such as reaction progress variable, is often necessary to characterise the local flame surface due to its relevance to flame surface area generation and burning rate. Previous studies have considered interaction between the gradient of the scalar fields and geometrical structures in turbulent flows¹, whilst other studies² outlined the topological structures associated with the scalar fields in 2D and 3D turbulence based upon the eigenvalues of the Hessian tensor of the scalar. Moreover, the tile-like and flat topologies discussed in these analyses have been found to be main topologies for non-reacting mixing³ as well as in turbulent premixed flames⁴⁻⁶. Furthermore, it has been documented that the local flame topology plays a central role in characterising flame-flame interactions in turbulent premixed combustion⁷⁻¹⁴. A number of approaches have been considered in the identification of flame-flame interactions including Minkowski functional techniques^{10,11}, automatic feature extraction techniques using complex wavelet transform methods^{7,8} and critical point theory^{9,12,13}. Whilst considerable analysis into flame-flame interactions in turbulent premixed combustion has been considered, the analysis of such phenomena in turbulent spray flames is limited¹⁵. Indeed, to the best of the author's knowledge, the topological nature of flame self-interactions (FSIs) in an open turbulent jet spray flame in the presence of a flow induced shear is yet to be analysed in the existing literature. The use of Direct Numerical Simulations (DNS) to glean fundamental insights of phenomena in both non-reacting and reacting turbulent flows has become an invaluable resource¹⁶⁻¹⁹. The analysis of the combustion of droplet-laden flows is one of on-going academic interest^{20,21}. Accordingly, to address the aforementioned gaps in the existing literature, a DNS database of an open turbulent jet spray^{22,23} corresponding to an experimental Ethanol spray flame²⁴ has been considered. As such, the main aims and objectives of the current study are:

- (a) To analyse an open turbulent jet spray flame for identifying the predominant topological structures associated with FSIs.

(b) To conduct a statistical analysis involving principal curvatures of the open turbulent jet spray flame to gain insight into the physical processes leading to the formation of the identified FSI topologies.

The remainder of the paper is organised as follows. In the next section, the mathematical background and numerical implementation pertaining to this analysis are presented. This is followed by the presentation of results and their discussion. In the final section of this paper, the main findings are summarised, and conclusions are drawn.

2. MATHEMATICAL BACKGROUND & NUMERICAL IMPLEMENTATION

In the current study, the DNS configuration corresponds to an experimental investigation of the Ethanol spray EtF3 flame²⁴. The spray and carrier gas are injected from a central jet nozzle ($D_j = 10.5\text{mm}$) with a bulk velocity $U_j = 24\text{m.s}^{-1}$ surrounded by a coaxial pilot annulus ($D_p = 25\text{mm}$; $U_p = 11.6\text{m.s}^{-1}$; $T_p = 2493\text{K}$) and an air coflow ($U_c = 4.5\text{m.s}^{-1}$). The pilot is composed of the fully burned products of a stoichiometric mixture of 5.08% Acetylene (C_2H_2), 10.17% Hydrogen (H_2) and 84.75% air by volume and provides the heat necessary for the evaporation of the fuel droplets. The flame is stabilised in the shear layer formed between the pilot and inner jet streams. The mass flow rate of liquid Ethanol in the jet is 45 g/min. Amongst the polydisperse droplets formed by the nebulizer, some droplets evaporate prior to reaching the nozzle exit, resulting in a partially gaseous fuel at the exit. The Ethanol mass flow rates at the nozzle exit are 14.3 g/min for the gaseous phase and 30.7 g/min for the liquid phase, resulting in a gaseous equivalence ratio of 0.85 at the jet exit.

The DNS database used in the current analysis has been generated by Pillai and Kurose^{22,23}. The simulation has been conducted using the FK³ code²⁵⁻³² employing a two-step chemical mechanism. This chemical mechanism accurately captures the equivalence ratio dependence of unstrained laminar burning velocity³³. Although simplified chemistry is used in this simulation, the configuration of the jet spray is relatively complex in terms of DNS and took more than 1.1 million CPU-hours. It has been shown in earlier investigations^{22,23} that the results obtained from the DNS database are consistent with the experimental findings of Gounder et al.²⁴. The standard conservation equations for mass, momentum, energy and species for reacting flows are solved for the Eulerian gaseous phase. The standard transport equations of position, diameter, momentum, and energy are solved for individual liquid fuel droplets in a

Lagrangian framework^{22,23,25-27,29,30}. Coupling between the Eulerian and Lagrangian phases is achieved by the Particle-Source-In-Cell approach^{22,23,25-27,29,30} where particles are modelled as spherical point masses. A polydisperse spray with a diameter distribution matching that of the experiment is injected based on a log-normal distribution with diameters ranging from $1\mu m$ to $80\mu m$ (the most likely diameter is $\sim 20\mu m$). Interested readers are directed to Pillai and Kurose¹⁶ for further information on the details of particle diameter distribution. The collisions and break-up have been neglected as this is a dilute flame with an inflow droplet volume fraction of $\sim 5 \times 10^{-4}$.

A DNS case with a domain of $94D_j \times 49D_j \times 49D_j$ is used for the current study which is discretised by a non-uniform $1160 \times 400 \times 400$ Cartesian grid. Large stretching is applied in all directions towards the boundaries to form absorbing zones that minimise reflection and contamination of the acoustic field near the jet^{22,23}. Due to the coupling strategy between the Eulerian and Lagrangian phases, the minimum cell size must be larger than the droplet size to accurately capture the evaporation process^{22,23}. To ensure an appropriate resolution of both the turbulence and the flame structure, the smallest cell size at the nozzle exit is taken to be $\Delta x = \Delta y = \Delta z = 150\mu m$. Further details on the boundary conditions and mesh can be found elsewhere^{22,23,25-27,29,30}. Due to the decay of turbulence downstream of the jet exit the turbulence intensity decreases and the integral length scale increases. Consequently, the Kolmogorov length-scale η_k increases continuously in the downstream direction from $\eta_k \approx 170\mu m$ (i.e. the largest value of the ratio $\Delta x/\eta_k$ is $\Delta x/\eta_k \approx 1.35$) at the nozzle lip, and the ratio of grid spacing to the Kolmogorov length scale throughout the domain remains consistent with the DNS grid requirement (i.e. $\Delta x/\eta_k \sim 2.0$) recommended by Pope³⁴. The turbulent Reynolds number Re_t is in the range of 50-100 in the high shear regions of the axial locations considered as discussed in detail in previous studies involving this simulation^{23,27,30}. A two-step global chemistry is used as the reaction model which requires significantly less spatial resolution in comparison to more detailed chemical mechanisms. The thermal flame thickness of the corresponding laminar premixed stoichiometric flame is $\delta_{L,th} = 536\mu m$ and, as such, the grid resolution is sufficient to resolve the flame thickness inside the jet flame region. Further information on the numerical implementation of this DNS database including the variations of the longitudinal integral length scale L_{11} and the Kolmogorov length scale η_k in the axial direction has been presented in detail elsewhere^{22,23,27,30} and thus are not repeated here. Interested readers are directed towards Refs. ^{22,23,27,30} for further information.

2.1 Relevant mathematical background

The evaporation of droplets leads to mixture inhomogeneities that can be characterised by the mixture fraction ξ , defined as³⁵:

$$\xi = \frac{(\beta - \beta_O)}{(\beta_f - \beta_O)} \quad (1)$$

where:

$$\beta_f = \frac{6.0}{W_{C_2H_6O}}; \beta_O = -\frac{Y_{O\infty}}{W_O} \quad \text{and} \quad \beta = \frac{2Y_C}{W_C} + 0.5 \frac{Y_H}{W_H} - \frac{Y_{O\infty}}{W_O} \quad (2)$$

where Y_α and W_α are mass fraction and the molar mass of element α , respectively^{27,29,30}. A reaction progress variable c based on the oxidiser mass fraction can be defined, as done so in several previous analyses^{19,29,30,36-44}, in the following manner:

$$c = \frac{[(1-\xi)Y_{O_2\infty} - Y_{O_2}]}{[(1-\xi)Y_{O_2\infty} - Y_{O_2}^{Eq}]} \quad (3)$$

where Y_{O_2} is the oxygen mass fraction, $Y_{O_2\infty}$ is the oxygen mass fraction in the pure oxidiser stream and $Y_{O_2}^{Eq}$ is the equilibrium oxidiser mass fraction (i.e. $Y_{O_2}^{Eq} = f(Y_{O_2}, \xi)$). Furthermore, the definition of c is consistent with a number of previous studies of turbulent stratified flames where variations in mixture fraction exist⁴⁵⁻⁵¹. For the analysis of the topology of turbulent flames, the behaviour of the critical points within the flame in relation to the reaction progress variable c is of central importance^{9,12,13}. Indeed, it should be noted that the gradient of the reaction progress variable c vanishes at critical points within the flame and, therefore, the Taylor series expansion around a critical point can be written in the following manner^{9,12,13}:

$$c(\mathbf{a} + \mathbf{x}) = c(\mathbf{a}) + (\mathbf{x}^T/2)\underline{\underline{H}}(c(\mathbf{a}))\mathbf{x} + \dots \quad (4)$$

The FSI topologies can be found using the eigenvalues of the Hessian $\underline{\underline{H}}(c)$. The shape factors θ and ϕ can be defined using the eigenvalues (i.e. $\lambda_1 > \lambda_2 > \lambda_3$) of the Hessian $\underline{\underline{H}}(c)$ in the following manner^{9,12,13}:

$$\theta = \frac{6}{\pi} \arctan \left(\frac{(\lambda_1 - 2\lambda_2 + \lambda_3)/6^{1/2}}{(\lambda_1 - \lambda_3)/2^{1/2}} \right) \quad (5i)$$

$$\phi = \frac{2}{\pi} \arctan \left(\frac{(\lambda_1 - 2\lambda_2 + \lambda_3)\cos(\theta\pi/6)/3^{1/2}}{(\lambda_1 - \lambda_3)/2^{1/2}} \right) \quad (5ii)$$

The Flame Self-Interaction topologies in the $\theta - \phi$ space can be represented graphically as shown in Fig. 1. In Fig. 1, moving from left to right, the signs of the eigenvalues of the Hessian $\underline{\underline{H}}(c)$ changes from $(- - -)$ to $(- - +)$ to $(- + +)$ to $(+ + +)$ where the black lines indicate the change in the sign of the eigenvalues. On the right-hand-side of Fig. 1, the eigenvalues with the signs of $(+ + +)$ correspond to Unburned Gas Mixture Pocket (UBGP) topologies whereas, on the left-hand-side of Fig. 1, the eigenvalues with the signs of $(- - -)$ correspond to Burned Gas Mixture Pocket (BGP) topologies. Furthermore, in Fig. 1, the eigenvalues with signs of $(- + +)$ correspond to Tunnel Closure (TC) topologies whereas the eigenvalues with signs of $(- - +)$ correspond to Tunnel Formation (TF) topologies. From a physical perspective, a Tunnel Closure (TC) topology is a cylindrical flame topology and propagates inwards whereas a Tunnel Formation (TF) topology grows outwards in a cylindrical manner.

Figure 1 Diagram of Flame Self-Interaction topologies characterised by shape factors θ and ϕ . The colouring of the quadrants is based upon the different types of FSI topologies (■ = BGP, ■ = TC, ■ = TF, ■ = UBGP). Examples of the topologies are shown in the quadrants.

In the current analysis, the FSI statistics are extracted at different axial locations (e.g. $x/D_j = 2, 4, 6, 8, 10, 12$) of the open turbulent spray flame. Moreover, the FSI statistics are conditioned on the reaction progress variable c across the range of $0.01 \leq c \leq 0.99$ which will ensure that the identification of the FSI topologies are limited to those locations where combustion occurs.

Figure 2 Instantaneous plots at normalised time $t_{sim} \cdot S_{L,st} / \delta_{L,th} = 22.54$ (where $S_{L,st}$ and $\delta_{L,th}$ are laminar burning speed and thermal flame thickness of the premixed stoichiometric mixture, respectively) of (a) $c = 0.75$ iso-surface coloured with ξ / ξ_{st} , (b) T at the central $x - y$ plane and (c) FSI topologies (■ = UBGP, ■ = TF, ■ = TC, ■ = BGP) at the central $x - y$ plane.

3. RESULTS & DISCUSSION

3.1 General flame behaviour and structure

Figure 2a shows the instantaneous iso-surface of reaction progress variable $c = 0.75$ coloured with normalised mixture fraction ξ / ξ_{st} where ξ_{st} stoichiometric mixture fraction ($\xi_{st} = 0.0914$). It is evident from Fig. 2a that significant wrinkling of the jet flame occurs due to flame-turbulence and flame-droplet interactions. Furthermore, Fig. 2a shows that moving away from the jet exit there is an increase in ξ / ξ_{st} as fuel droplets evaporate resulting in increasingly fuel-rich conditions with increasing axial distance. Figure 2b shows the instantaneous fields on the central $x - y$ plane of temperature T where the variations in temperature are indicative of the changes in burning rates due to the variations in equivalence ratio caused by droplet evaporation. Figure 2b shows that the injection of cold gaseous fuel in the inner jet whilst the temperature T increases as the inner jet mixes with the pilot stream and subsequently gives rise to droplet evaporation. The droplet evaporation occurs relatively quickly for smaller droplets, with small regions of gaseous fuel-rich mixture visible close to the jet exit (e.g. $x / D_j \approx 2$) but

large droplets also evaporate and give rise to larger hot regions of gaseous fuel-rich mixtures beyond approximately $x/D_j \approx 5$, as shown in Figs. 2a and 2b, while the largest droplets do not evaporate until far downstream of the jet exit. The variations in the burning characteristics of the flame will be associated with variations in the topographical nature of the flame. Figure 2c shows the instantaneous fields on the central $x - y$ plane of the FSI topologies (i.e. UBGP, TFs, TCs and BGPs). It is evident from Fig. 2c that all four FSI configurations are found across the flames at different axial locations suggesting that the TC and TF configurations are the predominant topologies.

Figure 3 PDFs of ξ/ξ_{st} for $0.01 \leq c \leq 0.99$ at $x/D_j = 2, 4, 6, 8, 10$ and 12 .

Figure 3 shows the PDFs of ξ/ξ_{st} within the flame (i.e. $0.01 \leq c \leq 0.99$) at the different axial locations considered in the current study (i.e. $x/D_j = 2, 4, 6, 8, 10$ and 12). It is evident from Fig. 3 that close to the jet exit (e.g. $x/D_j = 2$ and 4) there are both fuel-lean (due to the gaseous phase) and fuel-rich (due to droplet evaporation, typically smaller diameter fuel droplets) contributions with peaks for the PDFs typically close to the stoichiometric conditions. Moving further away from the jet exit, there is a greater level of droplet evaporation, particularly for larger fuel droplets, which leads to significant fuel-rich contributions. This is indicated by the shift in the peaks of the PDFs towards larger values of ξ/ξ_{st} as x/D_j increases. Accordingly, it is evident from Fig. 3 that combustion takes place under predominantly fuel-rich conditions at axial locations $x/D_j = 8, 10$ and 12 . These findings are consistent with the observations made in Figs. 2a. Furthermore, the fuel-rich conditions at axial locations $x/D_j = 8, 10$ and 12 are expected to lead to a reduction in the local temperature which is consistent with observations for Fig. 2b. Moreover, for such fuel-rich conditions, low Damköhler number

conditions are prevalent within the flame³⁰. It is anticipated that such conditions will influence the frequency of FSI within the flame with such behaviour offering important insights for the fundamental understanding of flame surface topology in turbulent spray flames.

Figure 4 Scatter plots of ϕ with θ for $0.01 \leq c \leq 0.99$ at (a) $x/D_j = 2$, (b) $x/D_j = 4$, (c) $x/D_j = 6$, (d) $x/D_j = 8$, (e) $x/D_j = 10$ and (f) $x/D_j = 12$. The scatter is coloured based upon the different types of FSI topologies (■ = UBGP, ■ = TF, ■ = TC, ■ = BGP).

x/D_j	BGP	TF	TC	UBGP
2	0.12	0.43	0.39	0.05
4	0.11	0.57	0.30	0.02
6	0.15	0.57	0.27	0.01
8	0.13	0.55	0.30	0.01
10	0.12	0.54	0.33	0.01
12	0.10	0.52	0.35	0.03

Table 1 Fractions of the FSI topologies (i.e. BGP, TF, TC and UBGP) at $x/D_j = 2, 4, 6, 8, 10$ and 12.

Figure 5 Histograms, with inserts at the lower frequencies, at $x/D_j =$ (a) 2, (b) 4, (c) 6, (d) 8, (e) 10 and (f) 12 of the four different FSI topologies BGP (■), TF (■), TC (■), UBG (■) across $0.01 \leq c \leq 0.99$.

3.2 Histograms of FSI topologies

Figure 4 shows the scatter plots of the shape factors ϕ with θ , coloured by FSI topology (i.e. UBGP, TF, TC and BGP) for $0.01 \leq c \leq 0.99$ at all axial locations considered in the current study (i.e. $x/D_j = 2, 4, 6, 8, 10$ and 12). It is evident from Fig. 4 that all four FSI topologies occur within the flame across all axial locations. However, it is evident from Fig. 4 that the frequency of the FSI topology occurrences varies from one axial location to another. This can more easily be explained by considering Fig. 5, where the histograms of the FSI topologies (i.e. UBGP, TF, TC and BGP) across c for all axial locations considered are shown (i.e. $x/D_j = 2, 4, 6, 8, 10$ and 12). It can be seen from Fig. 5 that the FSI events predominantly occur towards the burned gas side of the flame front (i.e. $0.95 \leq c \leq 0.99$) for axial locations. These observations are qualitatively similar to the findings for globally stoichiometric spherically expanding flames propagating into fuel droplet-mists for different turbulence intensities¹⁵. Indeed, closer to the jet exit (e.g. $x/D_j = 2, 4$ and 6) there are negligible FSI events in the unburned gas side of the flame, as shown in Figs. 5a-c, which is due to the higher shear experienced near the jet exit as a consequence of the high flow velocity. However, moving further away from the jet exit (i.e. $x/D_j = 10$ and 12), there are FSI events occurring towards the burned gas side of the flame front, as shown in Figs. 5e and 5f. It should also be noted that the observed behaviours are not consistent with turbulent premixed jet flames⁹ where there are significant FSI events found towards the unburned gas side of the flame. These differences are not unexpected considering the physical differences between premixed gaseous and spray flames, but it is worth noting that such behaviours must be taken into consideration particularly when formulating models for turbulent spray flames. It can further be seen from Fig. 5 that the greatest occurrences of FSI events are for TFs and TCs. Table 1 shows the fraction for each topology for the FSI events at each axial location indicating that TF accounts for around 50% of FSI events and TC accounts for around 30% of the FSI events for each axial location. Instances of UBGP and BGP at the axial locations considered are relatively limited. This observation is consistent with those made in previous analyses of FSI phenomena in turbulent premixed gaseous flames¹² where the rapid consumption of UBGP was provided as the reason for the low occurrence of UBGP. Previous analyses⁴⁴ have shown that droplet size can affect the distribution of flame curvature and can influence the characteristics of the flame topology. Therefore, presence of fuel droplets with varying diameters is expected to alter FSI topology distributions at different axial locations. Closer to the jet exit the smaller droplets are likely to be consumed but moving further away from the jet exit the larger droplets are more likely to

be evaporated and consumed. The effects of this on the flame curvature in the presence of the shear layer imposed by the flow conditions must be considered particularly in the development of models for turbulent spray flames based on the flame surface approaches.

3.3 Mean and Gaussian curvature behaviour

Following previous analyses¹⁵, the topologies of FSI can be characterised based on the local mean curvature $\kappa_m = 0.5\nabla \cdot (-\nabla c/|\nabla c|) = (\kappa_1 + \kappa_2)/2$ and the Gaussian curvature $\kappa_g = \kappa_1\kappa_2$ ^{3,4,15} where κ_1 and κ_2 are the two principal curvatures. Figure 6 shows the scatters of the four different topologies (i.e. UBG, TF, TC and BG) for $0.01 \leq c \leq 0.99$, $0.01 \leq c \leq 0.10$, $0.10 \leq c \leq 0.90$ and $0.90 \leq c \leq 0.99$ at $x/D_j = 2, 4, 6, 8, 10$ and 12 . It should be noted that a positive value of the local mean curvature κ_m corresponds to a flame surface which is concave to the unburned reactants whereas a negative value of the local mean curvature κ_m corresponds to a flame surface which is convex to the unburned reactants. A positive value of Gaussian curvature κ_g corresponds to elliptical “cup-like” topology whereas a negative value corresponds to a hyperbolic “saddle” topology. Those locations where κ_g disappears correspond to convex topologies when $\kappa_m > 0$ but correspond to concave topologies when $\kappa_m < 0$. Furthermore, the region of $\kappa_g > \kappa_1\kappa_2$ is not realisable due to complex principal curvatures. Examining Fig. 6, based upon the earlier discussion, the BGs (e.g. outward propagating topologies) are associated with convex “cup-like” topologies whereas the UBGs (e.g. inward propagating topologies) are associated with concave “cup-like” geometries which is shown at all axial locations considered in the current analysis. It can also be seen from Fig. 6 that the TF topologies are predominantly associated with hyperbolic “saddle” geometries but also convex “cup-like” topologies. The TC topologies are predominantly associated with hyperbolic “saddle” geometries but also concave “cup-like” topologies. Further examination of Fig. 6 reveals that close to the jet inlet (shown in Fig. 6a) the FSI topologies occur predominantly towards the burned gas side of the flame (i.e. $0.90 \leq c \leq 0.99$) with a relatively small number of occurrences in the rest of the flame. However, moving further away from the jet exit, a greater number of FSI occurrences towards the unburned gas side of the flame can be observed. These behaviours originate because the fuel droplets generally do not evaporate until closer to the burned gas side of the flame close to the jet inlet (i.e. $x/D_j = 2$). However, evaporation for large fuel droplets at the axial distances further away from the jet inlet increases the potential of FSI occurrences closer to the unburned gas side of the flame.

By considering Figs. 4-6 as well as Table 1, a comparison of the FSI events shows that there are a greater number of FSI events found closer to the jet exit (i.e. $x/D_j = 2$) than further away from the jet exit. This due to the availability of the smaller droplets to be evaporated and fuel consumed closer to the jet exit where relatively higher levels of shear and turbulence are present. However, moving further away from the jet exit, greater extent of droplet evaporation occurs, including larger droplets, resulting in fuel-rich combustion but still allowing for FSI occurrences and an increase in the frequency of FSI can be noticed at $x/D_j = 12$ relative to at $x/D_j = 8$ and $x/D_j = 10$. Moreover, whilst the predominant topologies found are TFs and TCs, there are still small but non-negligible occurrences of UBGP and BGPs. Examining Figs. 2c, 5a and Table 1, it is evident that close to the jet exit there are relatively larger occurrences of UBGP compared to further away from the jet exit. To explain this behaviour, it is worthwhile to consider the instantaneous reaction progress variable c iso-surfaces coloured with the local values of $\kappa_m \times \delta_{L,th}$. Figure 7 shows the $c = 0.9$ iso-surface at the normalised time $t_{sim} \cdot S_{L,st}/\delta_{L,th} = 22.54$ coloured with the local values of $\kappa_m \times \delta_{L,th}$ with a focus on close to the jet exit (i.e. close to $x/D_j = 2$). Figure 7 shows that there are dimples with relatively large negative values of $\kappa_m \times \delta_{L,th}$ occurring on the $c = 0.9$ iso-surface, and Fig. 6 suggests that UBGP surviving towards the burned gas side of the flame are associated with negative values of $\kappa_m \times \delta_{L,th}$. These dimples become less apparent further away from the jet exit suggesting that, further downstream, as droplets are more likely to be evaporated in the central jet and within the flame and thus are less likely to survive towards the burned gas side of the flame. Due to the abundance of fuel found at the downstream axial locations it reduces the likelihood of finding localised isolated pockets of reactants or, indeed, localised pocket of products as indicated by Fig. 5. However, further downstream the likelihood of FSIs increases closer to the unburned gas side of the flame. It has previously been shown for the presently considered flame in previous analyses³⁰ that the characteristic Damköhler number drops moving away from the jet exit and the increased likelihood of FSIs closer in the unburned gas side for smaller values of Damköhler number is consistent with previous analyses¹². Such observations for FSI topologies play a key role in the likely burning characteristics of the flame surface generation which must be accounted for from a modelling perspective and is discussed in the following section.

Figure 6 Scatter of $\kappa_g \times \delta_{L,th}^2$ with $\kappa_m \times \delta_{L,th}$ for the FSI events at (a) $x/D_j = 2$, (b) $x/D_j = 4$, (c) $x/D_j = 6$, (d) $x/D_j = 8$, (e) $x/D_j = 10$ and (f) $x/D_j = 12$ for (i) $0.01 \leq c \leq 0.99$, (ii) $0.01 \leq c \leq 0.10$, (iii) $0.10 \leq c \leq 0.90$ and (iv) $0.90 \leq c \leq 0.99$. The scatter is coloured based upon the different types of FSI topologies (■ = UBGp, ■ = TC, ■ = TF, ■ = BGP).

Figure 7 Instantaneous view of $c = 0.9$ iso-surface coloured with $\kappa_m \times \delta_{L,th}$ at normalised time $t_{sim} \cdot S_{L,st} / \delta_{L,th} = 22.54$.

3.4 Modelling Implications

It should be noted that the differences in the FSI events at different axial locations have several significant implications. The different frequencies and distributions of the FSI events indicate that the flame surface area annihilation because of FSI is expected to be different across a turbulent spray flame where the complexities of fuel droplet evaporation and variations in turbulence intensity are present. From a modelling perspective, further insight into the flame-flame interaction can be achieved by considering the statistical behaviours of the displacement speed of the reaction progress variable S_d and the surface density function σ (i.e. the magnitude of the gradient of the reaction progress variable $|\nabla c|$). The transport equation for the reaction progress variable c can be written as^{29,30,36,37}:

$$\rho \frac{\partial c}{\partial t} + \rho u_j \frac{\partial c}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial c}{\partial x_j} \right) + \dot{\omega}_c + \dot{S}_{ev} + \dot{S}_c \quad (6)$$

where ρ is the density, u_j is the j^{th} component of velocity, D is the diffusivity and $\dot{\omega}_c$ is the reaction rate of c . The first term on the right-hand-side of Eq. (6) arises due to molecular diffusion, the second term represents the reaction rate, the third term is the source/sink term due to droplet evaporation, and the final term is the cross-scalar dissipation term due to reactant inhomogeneity^{29,30,36,37}. The definitions of $\dot{\omega}_c$, $\dot{S}_{ev}$ and $\dot{S}_c$ depend on the local value of ξ . In Eq. (6), $\dot{\omega}_c$ is defined in the following manner^{29,30,36,37}:

$$\dot{\omega}_c = -\frac{[\xi_{st}\dot{\omega}_{O_2}]}{[\xi(1-\xi_{st})Y_{O_2\infty}]} \quad \text{for } \xi \leq \xi_{st} \quad (7i)$$

$$\dot{\omega}_c = -\frac{\dot{\omega}_{O_2}}{[(1-\xi)Y_{O_2\infty}]} \quad \text{for } \xi > \xi_{st} \quad (7ii)$$

where $\xi_{st} = (-\beta_o)/(\beta_f - \beta_o)$ is the stoichiometric mixture fraction. In Eq. (6), $\dot{S}_{ev}$ is defined as^{29,30,36,37}:

$$\dot{S}_{ev} = \left\{ -\frac{\xi_{st}}{[\xi^2(1-\xi_{st})Y_{O_2\infty}]} \right\} (\xi\dot{S}_O + (Y_{O_2\infty} - Y_{O_2})\dot{S}_\xi) \quad \text{for } \xi \leq \xi_{st} \quad (8i)$$

$$\dot{S}_{ev} = \left\{ -\frac{1}{[(1-\xi_{st})^2Y_{O_2\infty}]} \right\} ((1-\xi)\dot{S}_O + Y_{O_2}\dot{S}_\xi) \quad \text{for } \xi > \xi_{st} \quad (8ii)$$

where $\dot{S}_\xi = (\dot{S}_F - \dot{S}_O/s)/(Y_{F\infty} - Y_{O_2\infty}/s)$ is the droplet source/sink term in the ξ transport equation, $\dot{S}_F = (1 - Y_F)\Gamma_m$ and $\dot{S}_O = -Y_{O_2}\Gamma_m$ are the droplet source/sink terms in the fuel and oxygen transport equations, respectively, and Γ_m is the source term in the mass conservation equation due to evaporation. In Eq. (6), $\dot{S}_c$ is defined as^{29,30,36,37}:

$$\dot{S}_c = \left(\frac{2\rho D}{\xi} \right) \nabla c \cdot \nabla \xi \quad \text{for } \xi \leq \xi_{st} \quad (9i)$$

$$\dot{S}_c = \left\{ -\frac{2\rho D}{(1-\xi)} \right\} \nabla c \cdot \nabla \xi \quad \text{for } \xi > \xi_{st} \quad (9ii)$$

The transport equation of c , as provided in Eq. (6), can be rewritten in kinematic form as^{28,50,51}:

$$\frac{\partial c}{\partial t} + u_j \frac{\partial c}{\partial x_j} = S_d |\nabla c| \quad (10)$$

where S_d is the displacement speed, which is given by^{29,37,54,55}:

$$S_d = \underbrace{\frac{\vec{N} \cdot \nabla (\rho D \vec{N} \cdot \nabla c)}{\rho |\nabla c|}}_{S_n} + \underbrace{\frac{-2D\kappa_m}{S_t}}_{S_t} + \underbrace{\frac{\dot{\omega}_c}{\rho |\nabla c|}}_{S_r} + \underbrace{\frac{\dot{S}_{ev}}{\rho |\nabla c|}}_{S_{ev}} + \underbrace{\frac{\dot{S}_c}{\rho |\nabla c|}}_{S_c} \quad (11)$$

The transport equation of the surface density function $\sigma = |\nabla c|$ can be written as^{29,34,35,52,53}:

$$\frac{\partial |\nabla c|}{\partial t} + \frac{\partial (u_j |\nabla c|)}{\partial x_j} = a_T |\nabla c| + 2S_d \kappa_m |\nabla c| - \frac{\partial (S_d N_j |\nabla c|)}{\partial x_j} \quad (12)$$

where $a_T = (\delta_{ij} - N_i N_j) \partial u_i / \partial x_j$ is the tangential strain rate. Following Trivedi et al.¹³, the local topology can be considered and the four principal topologies (i.e. UBG, TF, TC and BGP) can be represented based on the scaled local coordinates x , y and z for small deviations from a critical point, in the following manner¹³:

$$c(x, y, z) = c_0 + \frac{1}{2}x^2 + \frac{1}{2}y^2 + \frac{1}{2}z^2 \quad \text{for UBG} \quad (13i)$$

$$c(x, y, z) = c_0 + \frac{1}{2}x^2 - \frac{1}{2}y^2 - \frac{1}{2}z^2 \quad \text{for TF} \quad (13ii)$$

$$c(x, y, z) = c_0 - \frac{1}{2}x^2 + \frac{1}{2}y^2 + \frac{1}{2}z^2 \quad \text{for TC} \quad (13iii)$$

$$c(x, y, z) = c_0 - \frac{1}{2}x^2 - \frac{1}{2}y^2 - \frac{1}{2}z^2 \quad \text{for BGP} \quad (13iv)$$

where c_0 is the reaction progress variable value at the critical point¹³. Based upon the expressions given by Eqs. 13i-13iv, it can be stated that an unburned gas pocket (UBG) will correspond to a local minimum (i.e. a central low value of the reaction progress variable with surrounding higher values) whereas a burned gas pocket (BGP) will correspond to a local maximum (i.e. a central high value of the reaction progress variable with surrounding lower values). For the unburned gas pocket (UBG) topology, the normal vector $\vec{N}$ can be given as $\vec{N} = (-x/r, -y/r, -z/r)^T$ (where the radius $r = (x^2 + y^2 + z^2)^{1/2}$) and twice the curvature of the flame surface κ can be given as $\kappa = -2/r$. For the burned gas pocket (BGP) topology, the normal vector $\vec{N}$ can be given as $\vec{N} = (x/r, y/r, z/r)^T$ and twice the curvature of the flame surface is given by $\kappa = 2/r$ ¹³. A tunnel formation (TF) topology, corresponds to a local saddle point with a minimum on the central axis of the tunnel (taken as the x direction) with a maximum in the two other directions where a tunnel formation (TF) topology, corresponds to a local saddle point with a maximum on the central axis of the tunnel (taken as the x direction) with a minimum in the two other directions. Accordingly, for the tunnel formation (TF) topology, $\vec{N} = (-x/r, y/r, z/r)^T$ and $\kappa = 2x^2/r^3$. For the tunnel closure (TC) topology, $\vec{N} = (x/r, -y/r, -z/r)^T$ and $\kappa = -2x^2/r^3$. Accordingly, it is possible to evaluate the terms in SDF transport equation using the expressions $\vec{N}$ and κ in the case of FSI events, which is beyond the scope of the current study and will form the basis of future analysis.

It should be noted that the behaviour of the displacement speed S_d (including its components) and the evolution of the surface density function $\sigma = |\nabla c|$ have been analysed for the currently considered flame in previous analyses^{29,30} and interested readers are directed to these studies. These analyses^{29,30} have demonstrated that the flame surface area is significantly affected by the interplay between the turbulence, droplet evaporation and chemistry. Accordingly, the qualitative behaviour in flame topology distributions for the FSI events found for turbulent spray flames imply that existing closures methodologies, including Flame Surface Density (FSD) approach^{56,57}, which depends on the flame surface topology, may need significant modifications to be valid for turbulent spray flames. Therefore, flame surface based modelling methodologies^{56,57} currently considered for premixed and stratified flames need to account for the aforementioned observations if they are to be extended for spray flames.

4. CONCLUSIONS

A three-dimensional Direct Numerical Simulation (DNS) database of an open turbulent jet spray flame representing a laboratory-scale burner configuration²⁴ has been analysed to investigate Flame Self Interactions (FSIs) in the presence of flow generated shear for the first time. The occurrences of FSIs (i.e. unburned mixture pockets (UBGPs), tunnel formations (TFs), tunnel closures (TCs) and burned gas mixture pockets (BGPs)) have been evaluated across the flame at different axial locations downstream of the jet exit. It has been found that the interplays between turbulence, droplet evaporation and chemistry have a significant influence on the topological nature of the flame. Close to the jet exit, the FSI events are found to occur towards the burned gas side of the flame but moving further away from the jet exit there are significant occurrences of FSI events within the flame where increasingly fuel-rich, and low Damköhler number conditions prevail. Consistent with previous analyses, the predominant FSI events have been found to be TFs and TCs, however, there are also non-negligible occurrences of UBGPs and BGPs. The results obtained from the current analysis have important implications from a modelling perspective where the flame topologies have a significant influence on the nature of the flame surface, which will, in turn, affect the flame-surface based modelling approaches. Accordingly, the findings of the current analysis might need to be accounted for when considering such flame surface based modelling in the context of turbulent spray flames, which will form the basis of future investigations.

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DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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