A direct numerical simulation study of flame structure and stabilisation of an experimental high Ka CH₄/air premixed jet flame

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Abstract: In the present work, a direct numerical simulation (DNS) of an experimental high Karlovitz number (Ka) CH₄/air piloted premixed flame was analysed to study the inner structure and the stabilisation mechanism of the turbulent flame. A reduced chemical mechanism for premixed CH₄/air combustion with NO_x based on GRI-Mech3.0 was used, including 268 elementary reactions and 28 transported species. The evolution of the stretch factor, I_0 , indicates that the burning rate per unit flame surface area is considerably reduced in the near field and exhibits a minimum at $x/D = 8$. Downstream, the burning rate gradually increases. The stretch factor is different between different species, suggesting the quenching of some reactions but not others. Comparison between the turbulent flame and strained laminar flames indicates that certain aspects of the mean flame structure can be represented surprisingly well by flamelets if changes in boundary conditions are accounted for and the strain rate of the mean flow is employed; however, the thickening of the flame due to turbulence is not captured. The spatial development of displacement speeds is studied at higher Ka than previous DNS. In contrast to almost all previous studies, the *mean* displacement speed conditioned on the flame front is *negative* in the near field, and the dominant contribution to the displacement speed is normal diffusion with the reaction contribution being secondary. Further downstream, reaction overtakes normal diffusion, contributing to a positive displacement speed. The *negative* displacement speed in the near field implies that the flame front situates itself in the pilot region where the inner structure of the turbulent flame is affected significantly, and the flame stabilises in balance with the inward flow. Notably, in the upstream region of the turbulent flame, the main reaction contributing to the production of OH, $H+O_2 \rightleftharpoons O+OH$ (R35), is weak. Moreover, oxidation reactions, $H_2+OH \rightleftharpoons H+H_2O$ (R79) and $CO+OH \rightleftharpoons CO_2+H$ (R94), are influenced by H₂O and CO₂ from the pilot and are completely quenched. Hence, the entire radical pool of OH, H and O is affected. However, the fuel consumption layer remains comparably active and generates heat, mainly via the reaction $CH_4+OH \rightleftharpoons CH_3+H_2O$ (R93).

Key words: Direct numerical simulation; turbulent flame; flame structure; displacement speed; reaction rate

1. Introduction

To achieve high thermal efficiencies and low NO_x emissions, lean premixed combustion is usually employed in modern stationary energy gas turbines. However, these combustors are susceptible to operability issues including combustion instability, blowout and flashback [1, 2]. Various methods are available to stabilise the flames, which generally operate by creating regions of low velocity and/or by enhancing mixing between cold reactants and hot combustion products, such as pilot flames [3, 4], swirl [5], rods [6] and bluff bodies [7]. Most of these configurations involve the flame being located in a region of strong shear. Also, due to high pressure, enhanced turbulence, and due to the flame being relatively weak, these devices operate at high Karlovitz numbers (Ka). For sufficiently high Ka (traditionally more than 100 [8]), small eddies can penetrate and disrupt reaction zones. Strong shear sustains the production of such eddies, but also may have a direct influence on the flame if strong enough. Improved understanding of the structure and stabilisation mechanisms of such highly sheared, high Ka flames is needed to enable improved combustor design.

The structure of freely propagating laminar methane-air flames is well known. Asymptotic analyses and numerical calculations with detailed chemistry [9-11] have revealed a multilayer structure comprising preheat, fuel consumption and oxidation zones. Reaction in the preheat zone is negligible, where species transport is balanced by convection and diffusion. In the fuel consumption zone, CH_4 is attacked by radicals, including OH , H and O , to produce CO , H_2 and other intermediates. Heat release is predominantly produced in the fuel consumption zone with secondary heat release produced in the CO oxidation layer. In the fuel consumption zone, reaction is primarily balanced by diffusion. In the oxidation zone, CO and H_2 are further oxidised to form CO_2 and H_2O . However, since at high Ka one or more of these zones may be perturbed, it is as yet unclear whether a similar structure exists in highly turbulent flows, and whether the same reaction pathways are active.

Turbulent premixed flames stabilised in shear layers are subjected to mean strain and turbulent motion. Both effects modify the inner flame structure through stretch, and influence the burning rate of the flame. In some cases, they may even lead to extinction of the flame. The response of the flame structure to stretch has been extensively studied [12-18]. Based on strained laminar flame calculations in a reactant-to-product counterflow configuration, it is known that in the limit of low strain rates, the flame structure is similar to that of an unstrained laminar flame. At large strain rates, the flame can shift to the product side of the stagnation plane, and exhibits a negative displacement speed [12]. Consequently, when subjected to large strain rates, the products of combustion may affect the flame structure. Depending on the composition of the products, the

flame can either be extinguished due to the enhanced diffusion of radicals to the product side of the flame [14] or be sustained if there is an excess of oxidising species in the lean products [15].

The displacement speed reflects the propagation of the flame relative to the flow and should be distinguished from the consumption speed based on the fuel consumption rate or heat release rate. The displacement speed is used directly in the G-equation modelling approach [19]. The concept of a locally negative displacement speed in laminar premixed flames has been well established. There is also evidence of its presence in DNS studies of turbulent premixed flames in canonical configurations [20-25]. Negative displacement velocities are observed in highly curved regions with the centre of curvature in the products [20] and at large tangential strain rates [24] when the diffusion flux exceeds the adverse convection flux. Despite the significance of the negative displacement speed in turbulent premixed combustion, it is infrequently reported in experimental measurements due to the difficulty of tracking the flame surface, flame normal vector, and flow field under turbulent reacting conditions and in three dimensions [26]. Coriton et al. [27, 28] studied turbulent premixed flames in a counter-flowing configuration of fresh reactants issuing against burnt products. They found that the flame extinguishes when it approaches the stagnation plane, where a negative displacement speed can be achieved. Quenching of the oxidation layer was found to be responsible for local or global extinction of the flame at high strain rates [27]. The flame was also affected by heat loss and dilution of the reaction zone [28].

As earlier mentioned, high Ka lean piloted premixed jet flames that stabilise in shear layers are relevant to industrial combustors. The pilot represents the entrainment of product gases in the recirculation zone of a practical combustor. It is of importance to examine the effects of the pilot, shear layer and strong turbulence on the flame structure and extinction behaviour. It has been previously shown that a turbulent flame can be quenched locally when it is subjected to intense stretch [3], and total quenching may occur as well [4, 29]. There have been several experimental investigations on the extinction behaviour of laboratory-scale turbulent premixed flames. Dunn et al. [4] explored finite-rate chemistry effects and reported an extinction region of a highly turbulent flame (PM1-150) in a high Ka piloted premixed jet burner. They found that further downstream the turbulence intensity relaxes and reignition occurs. The extinction and reignition regions were identified through chemiluminescence, $[CO][OH]$ and $[CH_2O][OH]$ measurements. The extinction of the upstream flame was attributed to the high levels of turbulence. However, the detailed mechanism of extinction and reignition remained to be explored.

In the present work, direct numerical simulation (DNS) is employed to study the structure of an

experimental high Ka lean piloted premixed jet flame. DNS plays an increasingly important role in revealing the structure of turbulent flames in that it resolves all of the relevant turbulence and chemistry scales involved [30]. A few DNS studies of high Ka flames have been carried out [31-34], and these have been limited to canonical isotropic turbulence freely propagating flame configurations, where the influence of mean shear is absent. Local extinction in these studies was found to be insignificant. Extinction is rarely observed in these flames because of enhanced turbulent mixing between cold reactants and hot products, and the small straining of the mean flow field. By comparison there have been relatively few multi-step chemistry DNS of premixed flames with mean shear. Sankaran et al. [35, 36] performed DNS of turbulent premixed flames in a spatially developing slot-jet configuration in the thin reaction zones regime, while Hawkes et al. [37, 38] studied a temporally evolving slot-jet configuration, where mean shear drives strong turbulent mixing in the flame. Again, extinction was not obvious in these flames.

Recently, Zhou et al. [39] carried out a series of experiments of high Ka CH₄/air premixed jet flames. In the experiments, the jet Reynolds number (Re) was varied between 6,000 and 40,000 and Ka was varied between 25 and 1470. A large pilot flame was used to prevent the entrainment of ambient cold air into the jet flame. Simultaneous planar laser-induced fluorescence (PLIF) measurements of OH and CH₂O and Rayleigh scattering measurements of temperature were carried out. Among the experimental conditions, of particular interest and feasibility for performing DNS is a methane-air premixed flame at high Ka and moderate Re at an equivalence ratio of 0.7. In recent previous work [40, 41], we reported a DNS of this flame. In Ref. [40] we reported a study of turbulent burning velocity related statistics and comparisons to experiment, including qualitative comparisons of key species involved in heat release reactions, and quantitative comparisons of flame surface density and flame curvatures, with good agreement. Another study [41] focused on more detailed comparisons to experiment, including quantitative mean temperatures, species, and velocity, and further analysed the flame structure to understand the substantial flame broadening that is observed in both the experiment and DNS.

The objective of the present study is to investigate the structure and stabilisation mechanism of the high Ka piloted premixed flame subjected to strong mean shear rate using the DNS. In particular, the instantaneous and statistical flame structure is shown; a comparison of the turbulent and laminar flame structure is performed; the displacement speed statistics are studied; the effect of the negative displacement speed on the inner flame structure is revealed and the mechanism for the upstream flame stabilisation is analysed. The paper is organised as follows. Section 2 describes the numerical methods and the DNS database. The

evolution of the burning rate, the displacement speed statistics and the reaction rates of some key species and elementary reactions are presented in Section 3. Finally, some conclusions are made in Section 4.

2. Numerical methods

The DNS are described in full in Wang et al. [40, 41], so only a brief description is provided here. A round jet burner employed in the experiment of Zhou et al. [39] is replicated in the DNS. The burner consists of a porous sintered-brass plate (61 mm in diameter) with a central jet diameter of $D = 1.5$ mm. The central jet operates at 1 atm and 300 K. The jet bulk velocity is $U_b = 110$ m/s and the equivalence ratio of the CH_4/air mixture is $\phi_j = 0.7$. At these conditions, the laminar flame speed $S_L = 0.193$ m/s, the flame thermal thickness $\delta_L = 0.663$ mm, and the flame time scale $\tau_L = \delta_L/S_L = 3.44$ ms. The jet Reynolds number based on U_b and D is $\text{Re}_j = 10,510$. A pilot flame of CH_4/air mixture at $\phi_c = 0.9$ was established surrounding the burner to provide a hot co-flow to assist with flame stabilisation. The temperature of the pilot flame is 1800 K and the velocity is 1.8 m/s.

The mean jet axial velocity and scalar profiles at the inlet are specified to match those of the experiment, to within the extent that these are known. A fluctuation velocity of about 4% of the bulk velocity is obtained by generating an auxiliary isotropic field, which is then superimposed on the mean inlet velocity using Taylor's hypothesis (Ref. [41] compared the DNS and experimental velocities at $x/D = 4$ with good agreement). The Karlovitz number is evaluated as $\text{Ka} = \tau_L/\tau_\eta$, where τ_η is the Kolmogorov time scale defined as $\tau_\eta = (\nu/\epsilon)^{1/2}$ (here, ν is the viscosity and ϵ is the kinetic energy dissipation rate). The Damköhler number (Da) is calculated as $\text{Da} = \tau_f/\tau_L$. The turbulence time scale, τ_f , is defined as $\tau_f = l_t/u'$, where u' is the turbulent velocity and l_t is the turbulence length scale calculated as $l_t = k^{3/2}/\epsilon$ (here, k is the turbulent kinetic energy). The values of Ka and Da evaluated at various axial locations along the mean flame front (defined in Section 3.2) are shown in Table 1. It is noted that both Ka and Da evolve in the axial direction as the jet turbulence develops. In such a flame with large Ka and small Da , all turbulence time scales are smaller than the chemical time scale. Therefore, the flame is expected to reside in the broken reaction zones regime [8], which is relevant for example, to ultra-lean, high pressure gas turbines for power generation. Further details of the boundary conditions are provided in Ref. [41].

The physical domain for the simulation is large by DNS standards owing to the long flame length: $L_x \times L_y \times L_z = 48D \times 36D \times 36D$ in the streamwise x and lateral directions y and z , respectively. The resolution of the DNS is chosen to adequately resolve both the flame and turbulence. A uniform grid spacing of $\Delta x = 30$ μm

is used in the streamwise direction x . The grid in the y (z) direction is uniform with Δy (Δz) = 30 μm in the region between y/D (z/D) = -5 and 5, and gradually stretched outside of this region. Approximately 22 grid points across δ_L are obtained with this spatial resolution, which in the present code is sufficient for accurate resolution of the flame structure [37]. In the present case, the spatial resolution is limited by turbulence. The Kolmogorov length scale defined as $\eta = (\nu^3 / \varepsilon)^{1/4}$ exhibits a minimum of 10 μm in a very narrow region near the potential core, where the flame does not overlap. The criterion, $h / D_x > 0.5$ [42], is satisfied elsewhere. Thus, the smallest scales of the turbulent flow are reasonably resolved. The resultant number of grid points is $N_x \times N_y \times N_z = 2400 \times 900 \times 900$.

To flush out initialisation artefacts, the simulation is first advanced for $10\tau_j$ on a half-resolved grid, where τ_j is the flow through time defined as $\tau_j = L_x / U_b$. The results are then mapped to the fine grid. The solution is advanced for another $10\tau_j$ to provide stationary statistics. It is found that statistical results of the half-resolution DNS and the production DNS are very similar (the maximum difference in mean temperature is less than 5%), confirming the resolution is adequate.

The DNS code ‘S3D’ [43] was employed to solve the compressible transport equations for continuity, momenta, species mass fractions and total energy. The code uses a fourth-order Runge-Kutta method for time integration [44, 45] and a skew-symmetric, eighth-order explicit finite difference spatial scheme. A tenth-order filter was applied every 10 time steps to damp high-wave number oscillations. A previously published reduced chemical mechanism for premixed CH_4/air flames with NO_x chemistry derived from GRI-Mech 3.0 was employed [46]. The mechanism contains 268 elementary reactions and 44 species, of which 16 species are identified as quasi-steady state species. The remaining 28 species are transported on the DNS grid. The mechanism has been validated against the detailed mechanism comprehensively [46]. Molecular diffusion should be properly modeled in order to predict the flame structure accurately [47]. In the present study, constant Lewis numbers, determined from a fit to mixture-averaged transport properties in a premixed flame, were employed. The Lewis numbers are given in Ref. [40].

3. Results and discussions

3.1 General flame structure

Firstly, the general characteristics of the turbulent flame are illustrated. Fig. 1 shows a photograph of the turbulent flame from the experiment and an instantaneous contour of the OH mass fraction revealing the basic flame structure from the DNS. As mentioned earlier, in the experiment the burner plate has an inner diameter

of 1.5 mm and an outer diameter of 61 mm. Due to the low flow velocity and long residence time above the plate, radicals like OH are able to accumulate in this region and to assist in flame stabilisation. Downstream of the nozzle a region with reduced OH concentration exists in the DNS, consistent with the reduced luminosity of the flame brush observed in the experiment. Further downstream, OH concentration increases and the flame burns more vigorously.

The instantaneous flame structure is examined to provide information regarding the flame response to turbulence. The progress variable, c , is defined to measure the progress of reaction based on the mass fraction of a major species as:

$$c = (Y - Y_u) / (Y_b - Y_u), \quad (1)$$

where Y_u is the species mass fraction in the reactants at the inlet and Y_b is the species mass fraction in the pilot flame. According to the definition, c increases monotonically from zero in the reactants to unity in the products. For most of this article, the O_2 mass fraction is used to define the progress variable, though different definitions based on CH_4 , CO_2 and H_2O will also be studied. In the following discussions, only the O_2 -based progress variable is used unless it is specifically stated otherwise.

The instantaneous distributions of the vorticity and species mass fractions of CO, H_2 and OH in the y - z plane at $x/D = 16$ is shown in Fig. 2. The progress variable isolines of $c^* = 0.5, 0.8$ and 0.9 are also superimposed. Note that in the unstrained laminar flame, the region where the heat release rate exceeds 35% of its maximum value spans approximately $c^* = 0.5$ to 0.9 . It is readily observed that due to the high turbulence intensity induced by the shear layer, the inner flame structure is significantly influenced. Consequently, the local flame thickness can be considerably larger compared with the laminar flame thickness. The mechanism for flame thickening was investigated in detail in Ref. [41].

It is also worth noting before proceeding that the present flame (in both the DNS and experiment) exhibits significant flame/flame interaction in the downstream region due to the merging of the preheat zone across the jet (and eventually the reaction zone in the flame tip). This is partly a consequence of the relatively small jet diameter in relation to the flame thickness, and partly as a consequence of the substantial flame thickening that occurs. To qualitatively gauge the extent of this effect and its possible influence on the results later discussed, Fig. 3 shows an instantaneous contour of formaldehyde mass fraction, which is a good marker for the preheat zone, in the x - r plane, where $10\delta_L$ is shown for comparison. It may be noted that the merging of the preheat zones across the jet begins around $x/D = 16$. As such, in the region downstream of $x/D = 16$, the

present DNS are not representative of a situation of a flame interacting with an infinite domain of unburned reactants, a fact which should be kept in mind when interpreting the present results. One could also anticipate that for larger jet diameters, the onset of flame/flame interaction across the jet would occur further downstream than in the present DNS. However, due to flame thickening at high Ka , this cannot be assessed simply by comparing the unperturbed flame thickness to the jet diameter; for instance, recent measurements [48] of a high Ka burner with a much larger jet diameter show extremely thickened preheat zones exceeding 20 mm (with a 0.36 mm unperturbed thickness) that also interact significantly across the jet well upstream of the flame tip (at least 60 mm – see Fig. 5 of [48]). Thus, while the present results are certainly affected by flame/flame interaction across the jet, this is not necessarily an atypical situation in larger burners at sufficiently high Ka .

3.2 Turbulent burning rate and stretch factors

The evolution of the burning rate of the flame along the streamwise direction is examined. A non-dimensional parameter, the stretch factor I_0 , is employed to quantify the local burning rate per unit flame surface area. I_0 influences the turbulent burning speed S_T directly through $S_T = S_L \cdot I_0 \cdot A'$ [49], where S_L is the unstrained laminar flame speed, and A' is the ratio of the wrinkled to unwrinkled flame surface area. From this expression, turbulence affects the flame by increasing the flame surface area through wrinkling (A') and by modifying the burning rate of the flame per unit surface area with respect to a laminar flame (I_0). A number of previous studies report values of I_0 for 2D isotropic pseudo-turbulence conditions [50-52]. However, very few studies report downstream development of I_0 , particularly in high Ka conditions where it can be significantly different from unity. Also, few if any studies report whether progress variables based on different species result in different I_0 values, which might be the case at high Ka due to non-flamelet behaviour.

The flame front is represented by an iso-surface given by a progress variable. In the case of the O_2 -based progress variable, the instantaneous flame front is defined as $c^* = 0.8$, which corresponds to the location of the maximum heat release rate in the unstrained laminar flame. The mean flame front is defined as $\bar{c} = 0.8$, where $\bar{c}$ is the mean progress variable computed by averaging the progress variable field in the azimuthal direction and in time. The mean flame front is outlined in red in Fig. 1b. The progress variable iso-surfaces representing the instantaneous flame front based on CH_4 , CO_2 and H_2O , corresponding to the location of the maximum heat release rate, are $c^* = 0.92$, 0.7 and 0.8, respectively.

To obtain an overall picture of the flame structure, Fig. 4a shows the instantaneous contours of progress

variable defined based on different species. The white line delineates the corresponding instantaneous flame front. One notable feature is that the progress variable along the centreline based on CH_4 approaches unity at a location that is further upstream compared with other species. This is because CH_4 is consumed completely in the fuel consumption zone and its reaction in the oxidation zone is negligible. The instantaneous flame fronts based on different species are almost identical as expected, as they are selected according to the locations of the maximum heat release rate. The instantaneous distributions of the progress variable reaction rate, $\dot{\omega}_c$, are shown in Fig. 4b. It is readily observed that $\dot{\omega}_c$ varies locally in space. The distribution of $\dot{\omega}_c$ also varies between different species. For example, CH_4 burns more intensively in a narrower region. This is due to the different chemical pathways of different species. Next, this variation is further quantified.

In the present study, a local analysis of the stretch factor, $I_0(x)$, is performed. By assuming a local balance between the consumption of reactants and turbulent flame propagation in each y - z plane, the turbulent burning speed $S_T(x)$ is defined as:

$$S_T(x) = \frac{\iint \dot{\omega}_c(x, y, z) dy dz \Delta x}{\rho_u A_L(x)}, \quad (2)$$

where $A_L(x)$ is the unwrinkled flame area at the axial location x , which is determined by $A_L(x) = 2\pi r(x)\sqrt{1 + r'^2}\Delta x$, where $r(x)$ is the distance of the mean flame front to the centreline and r' is dr/dx . Finally, the local stretch factor is written as:

$$I_0(x) = \frac{S_T(x)}{S_L} A'(x) = \frac{S_T(x)}{S_L} \frac{A_L(x)}{A_T(x)}, \quad (3)$$

where $A_T(x)$ is the wrinkled flame area at the axial location x computed through triangulation of the instantaneous flame front, computing the area of each triangle at this location, and summing all of the triangular areas. In the following analyses, time averaging is applied over all snapshots (~ 400) to provide converged statistics. The results for I_0 , A' and S_T/S_L with O_2 as the progress variable defining species are shown in Fig. 5a. It is seen that I_0 is below unity throughout the domain, indicating that the burning rate of the turbulent flame per unit area is always less than that of the unstrained laminar premixed flame. The evolution of I_0 suggests that the burning rate is considerably reduced in the near field and approaches its minimum value at $x/D = 8$. Downstream, the stretch factor gradually increases, consistent with the observations in Fig. 1. Near the inlet, the flame front is essentially flat and the turbulent flame area ratio, A' , is close to unity. As the flame develops, A' increases progressively until the flame tip. It should be noted although A' increases

monotonically with downstream distance, the turbulent flame area, A_T (not shown), exhibits its maximum value at $x/D = 24$, after which it decreases due to flame annihilation. Comparing the present results to those in the literature, stretch factors less than unity were inferred in DNS of high Ka premixed flames in isotropic turbulence by Lapointe et al. [33], but they are still higher than the current DNS results, due to the absence of mean shear. The stretch factor was also found to be higher in DNS of temporally evolving lean hydrogen-air slot-jet flames [37], in which the mean shear was comparable to the current DNS. However, the fuel was hydrogen, which has a different response to stretch than methane, and the Ka were lower for the flames there. The spatial variations of stretch factor were also studied in DNS of spatially developing lean methane-air slot-jet flames [36]. Consistent with the present work, the stretch factor was found to be smaller in the near field and became larger than unity in the far field. The stretch factor in Ref. [36] is still higher than the current result, which is probably because the mean shear was weaker than that in the present flame. Based on the above discussion, it can be inferred that both small scale turbulence and mean shear can affect the stretch factor. Their importance on the flame structure will be further investigated in the next section.

In low Ka conditions, it is expected that values of I_0 , A' , and S_T/S_L would be insensitive to the choice of the species defining the progress variable [52]; however this is not necessarily the case at high Ka . Differences in the evolution of the flame dynamics can be expected when the progress variable is defined based on different species due to differences in the turbulence/species interaction and species reactivity (and perhaps diffusivity). The evolution of I_0 , A' , and S_T/S_L for the progress variable definitions based on CH_4 , CO_2 and H_2O , respectively, is shown in Figs. 5b-d. It is seen that A' evolves similarly for all the cases. However, the evolution of I_0 is different. In particular, Fig. 5c indicates that I_0 based on CO_2 near $x/D = 8$ is close to zero, implying that the reaction rate of CO_2 is negligible. Note that CO_2 is predominantly produced in the oxidation layer through the reaction $CO + OH \rightleftharpoons CO_2 + H$ (R94). The near-zero stretch factor is consistent with the weakening/quenching of the oxidation layer in that region. In contrast, the stretch factors based on O_2 , CH_4 and H_2O are non-zero at $x/D = 8$, indicating the fuel consumption layer is more active compared with the oxidation layer. Comparatively, the CH_4 -based stretch factor is the largest; the stretch factor is slightly larger when it is calculated based on H_2O than O_2 . A more complete discussion of the reaction pathways is given in Section 3.5, but at this point it is worth noting that although the production of H_2O , through the reaction $H_2 + OH \rightleftharpoons H + H_2O$ (R79), in the oxidation layer is dramatically reduced, its production, through the reaction $CH_4 + OH \rightleftharpoons CH_3 + H_2O$ (R93), in the fuel consumption layer remains active.

3.3 Turbulent and laminar flame structures

There have been a number of past studies regarding the turbulent flame structure conditional both on progress variable [25] and on temperature [31-33]. In the present study, it is important to identify how local regions can be identified within the flame structure. Defining a local flame normal is ambiguous given the high degree of flame wrinkling and large flame curvatures encountered in the intense turbulence conditions. Hence, a distance function L_D is introduced, which represents the spatial distance with respect to the flame front [36]. L_D is defined such that at each point in the computational domain it signifies the shortest normal distance to the flame front, computed by solving the Eikonal equation in the 3D domain:

$$|\nabla L_D| = 1. \quad (4)$$

L_D is set to zero on the $c^* = 0.8$ iso-surface, negative in the reactants and positive in the products.

For flames in the flamelet regime, it is expected that iso-contours of the scalars and distance function are parallel to one another. However, in the present high Ka flame, the correlations between the distance function and the scalars are no longer obvious. Nevertheless, the averages of various quantities conditionally averaged on the distance function are still useful to understand the mean flame structure.

The profiles of temperature and equivalence ratio conditionally averaged on the distance function are shown in Fig. 6. The local equivalence ratio is defined as $\phi = (Y_H / 2W_H + 2Y_C / W_C) / (Y_O / W_O)$, where Y_k is the mass fraction of the element k and W_k is its atomic weight. The reactants are significantly preheated and diluted due to turbulent mixing. The temperature and equivalence ratio of the reactants downstream differ from those given at the inlet. For example, the mean temperature (equivalence ratio) along the centreline is 300 K (0.7) at the inlet and approaches 1102 K (0.78) at $x/D = 24$. As mentioned before, the pilot flame consists of hot products of CH_4/air at $\phi = 0.9$. Therefore, the local equivalence ratio across the flame increases progressively from 0.7 in the reactants to 0.9 in the products, resulting in a gradient of ϕ .

The results presented in Sections 3.1 and 3.2, and Fig. 6 suggest that, as anticipated for high Ka, a laminar-like flame structure may no longer exist in the present flame due to significant perturbations resulting from turbulence. In order to better quantify this effect, it is of interest to compare the mean turbulent flame structure with that of a strained laminar flame.

A reactant-to-product counterflow configuration, following previous recommendations [23], is chosen for the strained laminar flame calculations. To properly represent the local structure of the turbulent flame, the boundary conditions for the strained laminar flames need to be justified. Fig. 6 indicates that the streamwise

evolution of the temperature and composition of the reactants and products plays an important role in determining the local flame structure. Therefore, the temperature and composition in the reactants and products of the laminar flames are determined from Fig. 6. This is in contrast with typical flamelet models, which assume the flame is thin and determine the boundary conditions for tabulation based solely on the inlet free-stream conditions [53, 54]. Before discussing the results, it is important to note that this adjustment reflecting a change in boundary conditions also includes the effect of flame/flame interactions due to the merging of the flame in the centre, which is partly a consequence of the small jet diameter as earlier mentioned. For larger burners, this effect is likely to be less significant overall and the onset is likely to occur further downstream towards the flame tip; however even for much larger burners with sufficiently high Ka , experimental results show significant flame/flame interaction across the centre of the jet can still occur [48].

Figure 7 shows a comparison of the laminar flame structure with the mean turbulent flame structure conditionally averaged on the distance function. The profiles of the turbulent flame are in reasonable agreement with those from the strained laminar flames with selected strain rates, i.e. 3,400/s, 4,300/s and 4,500/s at $x/D = 8, 16$, and 24 , respectively. These strain rates were selected such that the peak heat release rate of the strained laminar flame matches that of the turbulent flame. It is also seen that the strained laminar flames reproduces the heat release rate and OH reaction rate in the DNS well. The main difference between the laminar and turbulent flames is that the turbulent flame is thicker than the laminar flame, characterising the effects of strong turbulence within the mean flame structure. Notably, the thickening of the CO layer is more evident compared with that of the H_2 and OH layers.

One important point to note from Fig. 7 is that despite the imposed strain rates being similar between the laminar flame profiles fitted at different downstream locations, the peak heat release, OH reaction rate, and species concentration levels are substantially different. Since the laminar flames do not consider effects of small scale turbulence, unsteadiness, curvature, etc., except indirectly through the boundary conditions, it can be speculated that the higher reaction rates downstream observed in the DNS are also principally due to the changes in reactant reactivity.

As earlier mentioned, the strain rates used to generate the profiles in Fig. 7 were determined such that the peak heat release of the laminar and turbulent flame matched. It is of interest to see whether this corresponds to the actual strain rate experienced by the flame, i.e. the tangential strain rate, a_t , defined as:

$$a_t = (\delta_{ij} - n_i n_j) S_{ij}, \quad (5)$$

where S_{ij} is the strain rate tensor and n_i is the i th component of the flame normal vector, $\mathbf{n}$, defined as:

$$\mathbf{n} = -\nabla c / |\nabla c|. \quad (6)$$

By definition, $\mathbf{n}$ points towards the reactants. The evolution of a_t conditionally averaged on the flame surface along the streamwise direction is shown in Fig. 8a. It is seen that the net of a_t is relatively small near the inlet. This seems to be counter-intuitive as the fluid dynamic strain rate is high in the near field due to the large jet velocity and small shear layer thickness. However, the fluid dynamic strain rate and a_t can differ significantly. In particular, it is known that a_t is sensitive to the alignment of the flame with respect to the flow [55, 56]. Near the inlet, the flame is aligned neither with the most extensive strain rate nor with the most compressive strain rate, resulting in a low value of a_t , as shown in a previous study of this flame [56]. The flame tends to align with the most extensive strain rate of the flow with increasing downstream distance, and a_t becomes larger. It is seen that a_t peaks at $x/D = 12$ and decreases further downstream due to the jet decay. Comparison of the total tangential strain rates experienced by the flame (order 20,000/s) and those needed to match the turbulent and laminar flame profiles (order 4,000/s) reveals that the latter are significantly smaller. Indeed, steady laminar flamelets experiencing the total tangential strain rate are in fact nearly completely quenched (not shown).

To understand this discrepancy, it is noted that the total tangential strain rate shown in Fig. 8a is likely to be highly fluctuating such that the flame may be unable to respond readily. Therefore, Fig. 8b shows the strain rates imposed by the mean shear, which are calculated as $(\delta_{ij} - \langle n_i n_j \rangle_s) \langle S_{ij} \rangle_s$ [50], where $\langle \cdot \rangle_s$ denotes a surface average. It is seen that the strain rates employed in the laminar flame calculations correspond well to the strain rates imposed by the mean shear (4,200/s at $x/D = 8$, 4,400/s at $x/D = 16$ and 3,400/s at $x/D = 24$) to leading order, suggesting that the mean flame responds primarily to the strain rate induced by the mean flow, which is persistent.

The present DNS results indicate that, even in the broken reaction zones (non-flamelet) regime, steady laminar flames can still represent certain aspects of the mean flame structure if the boundary conditions and strain rates for the laminar flame calculations are properly accounted for, e.g. the inlet free stream conditions should not be used. However, the laminar flame structure is unable to represent the thickening of the turbulent flame, resulting from strong turbulent eddy perturbations.

3.4 Statistics of the displacement speed

There have been many studies of displacement speed statistics [20-25]. However, very few report the spatial development of these statistics, and none to our knowledge report the spatial development at Ka as high as in the present work. In this section, the displacement speed statistics and the flame position with respect to the flow are examined. The transport equation for the progress variable is given as:

$$\rho \frac{Dc}{Dt} = \frac{\partial}{\partial x_i} \left(\rho D_c \frac{\partial c}{\partial x_i} \right) + \dot{\omega}_c, \quad (7)$$

where D_c is the diffusivity of the progress variable. The displacement speed, S_d , measures the flame front speed relative to the flow normal to the flame front and is defined as [24]:

$$S_d = \frac{1}{|\nabla c|} \frac{Dc}{Dt} = \frac{\dot{\omega}_c}{\rho |\nabla c|} + \frac{1}{\rho |\nabla c|} \frac{\partial}{\partial x_i} \left(\rho D_c \frac{\partial c}{\partial x_i} \right). \quad (8)$$

S_d can be further decomposed into its reaction ($S_{d,r}$), normal diffusion ($S_{d,n}$) and curvature ($S_{d,c}$) components as:

$$S_d = \underbrace{\frac{\dot{\omega}_c}{\rho |\nabla c|}}_{S_{d,r}} + \underbrace{\frac{1}{\rho |\nabla c|} \frac{\partial}{\partial n} \left(\rho D_c \frac{\partial c}{\partial n} \right)}_{S_{d,n}} - \underbrace{D_c \nabla \cdot \mathbf{n}}_{S_{d,c}}, \quad (9)$$

where n is the distance along the flame normal direction, and $\nabla \cdot \mathbf{n}$ is the flame curvature.

Figure 9a presents the displacement speed conditionally averaged on the flame front along the streamwise direction. To take into account the thermal expansion effects across the flame, the density weighted displacement speed, $S_d^* = \rho S_d / \rho_u$, is considered [21]. The streamwise evolution of its three components is also displayed. It is seen that the *mean* displacement speed is *negative* in the near field, where the dominant contribution to the displacement speed is normal diffusion. The negative displacement speed persists until $x/D = 18$. Downstream of this position, reaction overtakes normal diffusion, contributing to a positive displacement speed. Note that the downstream increase in the magnitude of the reaction component is due to the combined effect of the reduced $|\nabla c|$ and the enhanced reaction rate of the progress variable, as will be further discussed in Fig. 11. It is also noted that while locally negative displacement velocities have been reported in many previous studies [20-25], displacement velocities that are, on average, negative have only been reported by Sankaran et al. [36], and the spatial extent of the negative displacement speed region there was much more limited owing to the lower Ka conditions. While the present analysis framework is based on a flame-surface concept, it is worth pointing out that the observed negative displacement speed could also be interpreted from an auto-ignition standpoint; that is, as there is insufficient residence time in the near field to ignite the incoming fresh reactants, the reaction component of the displacement speed is significantly reduced.

The flame front speed in the laboratory frame, $\mathbf{w}$, can be written in terms of the flow velocity, $\mathbf{u}$, the flame normal vector, $\mathbf{n}$, and the displacement speed, S_d , as follows [57]:

$$\mathbf{w} = \mathbf{u} + S_d \mathbf{n}, \quad (10)$$

As the flame is statistically stationary, it is expected that the mean absolute velocity of the flame front, $\langle \mathbf{w} \cdot \mathbf{n} \rangle_s$, approaches zero:

$$\langle \mathbf{u} \cdot \mathbf{n} + S_d \rangle_s = 0, \quad (11)$$

The flow velocity in the flame normal direction is superimposed in Fig. 9a. Note that the velocity is weighted by its local density, consistent with the treatment of S_d^* . The figure shows that the evolutions of S_d and $-\mathbf{u} \cdot \mathbf{n}$ are almost identical. It is confirmed that $\mathbf{u} \cdot \mathbf{n}$ indeed balances the displacement speed on average. Note that, in the near field, the flame is typically aligned with its normal vector pointing radial inward, thus a positive $\mathbf{u} \cdot \mathbf{n}$ corresponds to a radially inward flow.

The sensitivity of the displacement speed statistics based on different species is also studied. The evolution of the displacement speed and its components, with the progress variable defined based on CH_4 , CO_2 and H_2O , respectively, are shown in Figs. 9b-d. It is observed that the evolution of the net displacement speed is similar in all cases. The minor discrepancy can be attributed to the slight differences in the flame front location for different definitions of the progress variable. Interestingly, however, the displacement speed components evolve differently. For example, the reaction term is the largest based on CH_4 and the smallest based on CO_2 . The reaction term based on H_2O is slightly larger than that based on O_2 . These trends are in line with those of the stretch factor based on different species as discussed earlier (Fig. 5). By definition, the reaction term is closely related to the species reaction rates. The reaction rate of CO_2 is attenuated to such a degree upstream that the normal diffusion term is nearly equal to the net displacement speed, i.e. CO_2 is mostly behaving as a passive scalar. It is interesting, however, that despite the significant differences in the reaction terms, the overall flame speeds are similar; it is deduced that there is a natural adjustment of the normal diffusion term which partly accounts for changes of reaction terms for the different species.

Figure 9 indicates that the mean displacement speed is mainly determined by reaction and normal diffusion, and the contribution of the curvature term to the mean displacement speed is negligible throughout the flame. This is consistent with other results for flames in 2D isotropic pseudo-turbulence [20, 21]; however here a small positive contribution is noted. The mean flame curvature has been calculated and its magnitude is found to be close to $-1/r(x)$ (recall that $r(x)$ is the radial distance of the mean flame location to the

centreline) [40]. Therefore the mean of the curvature term, $-\rho D_c \nabla \cdot \mathbf{n} / \rho_u$, is positive.

Despite its small contribution to the mean, the curvature term plays an important local role in the displacement speed in highly curved regions of the turbulent flame, affecting the local flame stretch. To evaluate this, Fig. 10 shows the local density weighted displacement speed and its components conditionally averaged on local curvature. The overall response of S_d^* with curvature evolves downstream, with the negative slope becoming larger with downstream distance for negative curvatures, but lower for positive curvatures. The component breakdown reveals that this change is principally a result of the reaction term. This term is nearly zero in the partially quenched near field region ($x/D = 8$), where normal diffusion and curvature components dominate, and increases in importance in the far field of the jet. The curvature term $-\rho D_c \nabla \cdot \mathbf{n} / \rho_u$ is linearly proportional with curvature $\nabla \cdot \mathbf{n}$, weighted by the molecular diffusivity D_c , which does not vary significantly along the flame front. In the near field ($x/D = 8$), it is confirmed that, in regions with large curvatures, the dominant contribution to the displacement speed is from the curvature term. However, in the far field ($x/D = 24$), the reaction term also plays a significant role. It is worth noting that although the curvature term is large in large curvature regions, the net contribution of the curvature term to the mean displacement speed depends on the probability density function of curvature. If the mean curvature is zero, the net contribution of the curvature term would be zero (because the curvature response of the curvature term is linear). In the current configuration, the mean flame curvature is slightly negative [40]. Therefore, there is a small positive contribution of the curvature term to the mean displacement speed.

To better understand the behaviour of the reaction term, the variables, $\dot{\omega}_c$ and $|\nabla c|$, which appear in the reaction term, are studied. Fig. 11a shows $\dot{\omega}_c$ conditionally averaged on local curvature at various locations. It is seen that $\dot{\omega}_c$ increases with downstream distance, which is consistent with the analysis of burning rate and stretch factor in Section 3.2. The enhanced reaction rates are also consistent with the earlier discussion of the reaction rate profiles in the strained laminar flame cases (Fig. 7), in which enhanced reactivity of the reactants (e.g. as measured by temperature, radical levels, etc.) caused increased peak reaction rates. Fig. 11b indicates that $|\nabla c|$ decreases with downstream distance, and is smaller in highly curved regions. The enhanced $\dot{\omega}_c$ and reduced $|\nabla c|$ are, therefore, responsible for the increasingly important role of the reaction term with increasing downstream distance.

As mentioned earlier, premixed flames may exhibit a negative displacement speed at large positive strain

rates. The displacement speed of the strained laminar flames as a function of strain rate is shown in Fig. 12a. Note that following Section 3.3, the laminar flame calculations employ local boundary conditions corresponding to a given axial position in the turbulent flame from the DNS. The local displacement speed of the DNS conditionally averaged on the local instantaneous strain rate is also shown. Considering first the laminar flame conditions, it is confirmed that the displacement speed decreases with strain rate and can be negative by crossing the stagnation plane. The displacement speed response to strain rate varies with axial location due to the different local boundary conditions. Note that as the normalisation always uses the unstrained laminar flame speed with inlet free-stream conditions, the normalised displacement speed in the low strain rate limit can be larger than unity downstream due to preheating of the reactants. The response of both the turbulent and laminar flames in Fig. 12a suggests a negative response of the flame to the tangential strain rate, although the response is weaker in the turbulent case potentially due to unsteadiness effects [58]. It is also found that the displacement speed at $x/D = 16$ and 24 decreases with increasing compressive strain rate due to curvature effects, consistent with previous DNS results by Sankaran et al. [36]. In particular, regions with highly compressive strain rate correspond with positive curvature as revealed in Fig. 12b, leading to smaller displacement speed due to the negative correlations of displacement speed and curvature (see Fig. 10).

The displacement speed response to the tangential strain rate is significantly different at various axial locations, which has not previously been reported. In Section 3.3, we showed that the mean flame structure mainly responds to the strain rate induced by the mean flow. However, it should be noted that local quantities on the flame front, such as the displacement speed, respond to the strain rate by the instantaneous flow, and this local response can be different from the overall effect. Fig. 12a shows the response becomes stronger and progressively more similar to the laminar flame response with increasing downstream distance, while the displacement speed is also shifted positively. The increasing strength of the response downstream is likely due to the increasing turbulence time scale with streamwise evolution of the jet; as a result, the flame has more time to respond to the applied strain rate. The increasing strength of a flame's response to lower frequency velocity perturbations has been demonstrated by theory [59], in laminar flame studies [16, 60], and in previous 2D isotropic pseudo-turbulence DNS cases at different turbulent intensities [58]. The positive shift of the mean flame speeds in the streamwise evolution is governed by two factors. Firstly, as already shown, the tangential strain rate due to the mean flow decreases downstream; unlike the fluctuating strain, this strain is persistent and therefore can have a net effect on the displacement speed. Secondly, given the positive offset of displacement speed between the DNS and the strained laminar flame calculations at all three axial locations,

the evolution of the local temperature and composition conditions due to turbulent stirring resulting in reactant preheating may be responsible.

In premixed round jet flames, the mean flame generally propagates in the radial direction. Therefore, the distributions of radial velocity of the flow and species radial flux are of interest. OH is an important radical in both of the fuel consumption and oxidation zones as will be discussed in the next section, so that it is selected to perform the flux analysis. Quantities conditionally averaged on the distance function are studied, consistent with the discussion of the mean flame structure. In particular, the radial flux is denoted as $\langle \widetilde{u_r Y_{OH}} | L_D \rangle$, where the tilde denotes a Favre average. The profiles of radial velocity, total OH radial flux¹ and OH mass fraction of at $x/D = 8, 16$ and 24 are shown in Fig. 13. It is seen that the radial velocity first increases and then decreases in the radial direction. At $x/D = 8$, the radial velocity is negative when the distance function is larger than zero, resulting in a negative radial flux of OH (i.e., radially inward transport). As OH concentration is higher in the oxidation zone, it is suggested that OH can be transported to the fuel consumption zone, the effect of which on chemical pathways will be explored in Section 3.5.

3.5 Flame stabilisation - chemical pathway analysis

In the literature, there is little knowledge of the effects of shear-generated turbulence and the pilot on high Ka flame stabilisation, due to the limitations of measurements [4, 29] and the scarcity of DNS of high Ka flames with strong shear. It is expected that the flame would be extinguished generally at the high strain rate as it is diluted by major species in the pilot, such as CO_2 and H_2O . However, the DNS results show that the present flame is nonetheless stabilised, although the flame is considerably weakened in the near field. To analyse the mechanism by which the flame stabilises, the reaction rates of key elementary reactions are examined.

Figure 14 shows the reaction rates of several key elementary reactions involved in OH production and consumption conditionally averaged on the distance function. The chosen reactions were selected from a complete reaction path analysis as the most important reactions for evolution of OH and other species. Their importance will be elaborated upon separately in the following.

The main reaction contributing to the production of OH is $\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$ (R35). Fig. 14 shows that, at $x/D = 8$, the reaction rate of $\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$ (R35) is reduced. Consequently, OH production is considerably

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¹ Note that the fluctuating part of the radial flux is small compared with the total radial flux with the conditional averaging method employed here, so that only the total is presented rather than breaking it into mean and fluctuating parts.

decreased in the near field. Note that another reaction, $\text{CH}_4 + \text{O} \rightleftharpoons \text{CH}_3 + \text{OH}$ (R11), also produces OH. However, its contribution is relatively small and not discussed in the paper.

A complete reaction path analysis indicated that, for unstrained and moderately strained premixed flames, H_2 and CO are mainly oxidised by OH to produce H_2O and CO_2 in the oxidation layer via the reactions $\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$ (R79) and $\text{CO} + \text{OH} \rightleftharpoons \text{CO}_2 + \text{H}$ (R94), respectively. However, Fig. 14 shows that these two reactions are essentially quenched at $x/D = 8$. Recall that, at $x/D = 8$, the flame front is in regions of negative mean radial velocity. Therefore, the reactions $\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$ (R79) and $\text{CO} + \text{OH} \rightleftharpoons \text{CO}_2 + \text{H}$ (R94) are affected by H_2O and CO_2 in the pilot, resulting in a significant reduction in the forward reactions. In regions of high H_2O and CO_2 , the reversal of these reactions consume H atoms and generate H_2 and CO. Fig. 15 shows scatter plots of the reaction rates of these two elementary reactions conditionally averaged on progress variable at various axial locations. It is readily observed that, at $x/D = 8$, small amounts of H_2 and CO are indeed produced via the reactions $\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$ (R79) and $\text{CO} + \text{OH} \rightleftharpoons \text{CO}_2 + \text{H}$ (R94), respectively. As a result, the production of H_2O and CO_2 in the oxidation layer largely vanishes. The results are consistent with computations of laminar premixed flames with high strain rates [15]. However, to the best of our knowledge, the quenching of the oxidation layer has not been reported in DNS studies before. Conversely, Fig. 14 shows that in the fuel consumption layer the reaction $\text{CH}_4 + \text{OH} \rightleftharpoons \text{CH}_3 + \text{H}_2\text{O}$ (R93), which is the dominant reaction attacking the fuel at high strain rate is comparably active at $x/D = 8$. Note that a complete set of chemical pathways for CH_4 has been extracted using the DNS data. In particular, the reaction, $\text{CH}_4 + \text{OH} \rightleftharpoons \text{CH}_3 + \text{H}_2\text{O}$ (R93), accounts for $\sim 70\%$ of the total consumption of CH_4 at the location $x/D = 8$. Another two reactions, $\text{CH}_4 + \text{H} \rightleftharpoons \text{CH}_3 + \text{H}_2$ (R50) and $\text{CH}_4 + \text{O} \rightleftharpoons \text{CH}_3 + \text{OH}$ (R11), have secondary contributions of $\sim 20\%$ and $\sim 10\%$, respectively. So that in the current study we mainly focus on the reaction $\text{CH}_4 + \text{OH} \rightleftharpoons \text{CH}_3 + \text{H}_2\text{O}$ (R93).

Next, the reaction rates of CO and OH in the turbulent flame are investigated. The particular emphasis here is placed on the examination of the species reaction rates in the fuel consumption and oxidation layers. It was previously shown in laminar premixed flame calculations that when the oxidation layer quenches at high strain rates, the entire radical pool of OH, H and O is affected and abrupt extinction of the flame may occur [15]. However, if the hot products were generated from a flame with an excess of oxidising species, which is analogous to the present DNS configuration, the flame structure would be more robust and resistant to extinction. It is of importance to check if these findings are still valid in highly turbulent flames.

Figure 16 shows the CO mass fraction and CO reaction rate conditionally averaged on the distance function at $x/D = 8, 16$ and 24 . It is seen that at $x/D = 8$ the CO mass fraction is low and the CO reaction rate

is reduced. Moreover, CO is produced in the fuel consumption layer, but no longer consumed in the oxidation layer, signifying the quenching of the oxidation layer. Consequently, the entire radical pool is also reduced. The results are consistent with those of laminar premixed flame calculations [15] and turbulent premixed flame experiments [27, 28]. In contrast, at $x/D = 24$, the CO production is high in the fuel consumption layer. The CO consumption is also active in the oxidation layer via the reaction $\text{CO} + \text{OH} \rightleftharpoons \text{CO}_2 + \text{H}$ (R94).

The OH reaction rate and OH mass fraction conditionally averaged on the distance function at various axial locations are shown in Fig. 17. OH is primary produced via the reaction $\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$ (R35), which spans both the fuel consumption and oxidation layers. At $x/D = 8$, the reaction $\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$ (R35) is weak as shown in Fig. 14. The net production of OH in the oxidation layer is negligible. Surprisingly, the consumption of OH remains comparably active, mainly via the reaction $\text{CH}_4 + \text{OH} \rightleftharpoons \text{CH}_3 + \text{H}_2\text{O}$ (R93). Although the production of OH significantly decreases, Fig. 17 shows that the OH concentration in the pilot is relatively abundant. As the flame is located in regions with negative mean radial velocity at $x/D = 8$ (see Fig. 13), OH is transported into the fuel consumption layer through advection, assisting the flame stabilisation.

4. Conclusions

A three-dimensional DNS of an experimental turbulent piloted premixed round jet flame was analysed with respect to the flame structure and stabilisation mechanism. The flame features high Ka and moderate Re , and resides in the broken reaction zones regime of the premixed combustion diagram. The resolution of the DNS is chosen to adequately resolve both the flame and turbulence structures. The resultant number of grid points required is approximately 2 billion. A reduced mechanism for premixed CH_4/air flames with NO_x chemistry derived from GRI-Mech 3.0 was used for the DNS.

The similarity of the DNS profiles with strained flamelet profiles was examined. It is found that although certain aspects of the mean flame can be captured more accurately than was expected by strained flamelet profiles, they are not able to capture the thickening of the turbulent flame due to strong turbulent eddy perturbations. Moreover, the boundary conditions in the strained laminar flame calculations require special treatment to account for turbulent mixing between the reactants and products, and flame/flame interactions due to the merging of the flame across the centre of the jet. The results also indicate that the mean flame mainly responds to the strain rate of the mean flow.

The evolution of the stretch factor, I_0 , suggests that the burning rate per unit surface area is considerably reduced upstream. A region of predominantly *negative* displacement speed region is identified in the near field,

which balances an inward flow. The negative mean displacement speed region arises from weak reactions leading to a low reaction-rate contribution, while normal diffusion remains negative. The curvature term plays an important role locally throughout the flame in the displacement speed in highly curved regions, but does not contribute significantly to the mean displacement speed, in line with previous studies without a net round geometry. The local curvature response of the displacement speed changes downstream in the jet, principally as a result of the changing reaction rate contribution. There is a general negative correlation between the displacement speed and the tangential strain rate, which does, in contrast to the curvature term, contribute to the mean displacement speed due to large mean strain rates. The response of the conditional mean of the displacement speed to strain changes significantly with downstream distance. The response becomes stronger and more similar (for positive strains) to a laminar flame response with downstream distance, which is consistent with downstream decreases of Karlovitz number. The displacement speeds are positively shifted with downstream distance, which is consistent with reactant preheating due to turbulent stirring, and a decreasing strength of the mean flow strain rate.

The sensitivity of stretch factor and displacement speed based on different species was also investigated. Qualitative trends for I_0 were similar for all major species; however I_0 based on CO_2 showed more upstream quenching as compared to I_0 based on CH_4 , O_2 and H_2O . As to displacement speed, the mean displacement speed was generally consistent between different species, but the breakdown into components differed significantly; with the normal diffusion term adjusting according to changes in the reaction term between different species, suggesting an underlying production-dissipation balance exists for species gradients.

It was shown that, in the near field, the mean flame front resides well within the pilot region with a negative mean radial velocity. The inner flame structure is considerably affected by the pilot. Both oxidation reactions, $\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$ (R79) and $\text{CO} + \text{OH} \rightleftharpoons \text{CO}_2 + \text{H}$ (R94), are influenced and even driven backwards to produce H_2 and CO in the oxidation layer. CO is produced in the fuel consumption layer, but no longer consumed in the oxidation layer, signifying quenching of the oxidation layer, consistent with the observed lower I_0 for CO_2 . OH production is considerably reduced due to the reduced reaction rate of $\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$ (R35). The consequence is that the entire radical pool of OH , H and O is affected. However, it is shown that the fuel consumption layer still remains comparably active, primarily via the reaction $\text{CH}_4 + \text{OH} \rightleftharpoons \text{CH}_3 + \text{H}_2\text{O}$ (R94).

Overall it is shown that, for the present high Ka jet flame, the strong shear layer and the pilot have significant impact on the flame structure and stabilisation. Mean shear causes significant near field flame

weakening, resulting in negative displacement speed and the flame residing on the product side of the stagnation plane. In the near field the oxidation layer is almost completely quenched, while fuel consumption remains active due to transport of radicals, principally OH, from the pilot region. Downstream the flame recovers as mean strain rates relax while at the same time the flame is progressively thickened, increasing the reactivity of reactants, which enhances the overall burning rate. Future work will examine aspects such as exploring validity of model assumptions for high Ka flames, and assessing existing modelling approaches.

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Table 1. The Karlovitz and Damköhler numbers evaluated at different axial locations.

x/D	8	16	24
Ka	488	337	232
Da	0.014	0.033	0.058

Figure Captions

Figure 1. (a) Photograph of the turbulent flame from the experiment. (b) Instantaneous contour of the OH mass fraction from the DNS. The red line delineates the mean flame front.

Figure 2. Instantaneous distributions of the (a) vorticity, $1/s$, (b) Y_{CO} , (c) Y_{H_2} , and (d) Y_{OH} in the y - z plane at $x/D = 16$. The isolines of the progress variable are delineated: (black) $c^* = 0.5$, (red) $c^* = 0.8$ and (white) $c^* = 0.9$. The nozzle diameter, D , and the distance between $c^* = 0.5$ and 0.9 in the unstrained laminar flame, l_c , are also added for reference.

Figure 3. Instantaneous contour of formaldehyde mass fraction. The length of $10\delta_L$ is shown for reference, where δ_L is the laminar flame thickness.

Figure 4. Instantaneous contours of (a) the progress variable and (b) its reaction rate based on different definitions. The maximum progress variable reaction rate in these plots is 560, 1290, 400, and 670 $kg/m^3 \cdot s$ for O_2 , CH_4 , CO_2 and H_2O , respectively.

Figure 5. Evolution of the stretch factor, I_0 , the turbulent flame area ratio, A' , and the turbulent burning rate ratio, S_T/S_L . The progress variable is defined based on (a) O_2 , (b) CH_4 , (c) CO_2 , and (d) H_2O .

Figure 6. Profiles of temperature and equivalence ratio of the turbulent flame at various axial locations conditionally averaged on the distance function.

Figure 7. Profiles of heat release rate, OH reaction rate, temperature, Y_{CO} , Y_{H_2} , and Y_{OH} of the turbulent flame at various axial locations conditionally averaged on the distance function. The strained laminar flames are also presented for comparison.

Figure 8. (a) The tangential strain rate, and (b) the strain rate on the flame front imposed by the mean velocity

gradients, $\left(\delta_{ij} - \langle n_i n_j \rangle_s \right) \langle S_{ij} \rangle_s$, along the streamwise direction.

Figure 9. Density weighted displacement speed and $-\mathbf{u} \cdot \mathbf{n}$ conditionally averaged on the flame front along the streamwise direction. The progress variable is defined based on (a) O_2 , (b) CH_4 , (c) CO_2 , and (d) H_2O .

Figure 10. Density weighted displacement speed and its components conditionally averaged on the flame curvature at (a) $x/D = 8$, (b) $x/D = 16$, and (c) $x/D = 24$.

Figure 11. (a) $\dot{\omega}_c$ and (b) $|\nabla c|$ conditionally averaged on the flame curvature at $x/D = 8$, $x/D = 16$ and $x/D = 24$.

Figure 12. (a) Density weighted displacement speed conditionally averaged on the flame tangential strain rate at $x/D = 8$, 16 and 24. Thin lines denote the results of the strained laminar flame calculations using local boundary conditions from the DNS. (b) Curvature conditionally averaged on the flame tangential strain rate at $x/D = 8$, 16 and 24.

Figure 13. Radial velocity, OH radial flux and OH mass fraction conditionally averaged on the distance function at $x/D = 8$, 16 and 24. The units for velocity and species flux are m/s.

Figure 14. Profiles of OH production rate in the reaction $\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$ (R35), H_2 consumption rate in the reaction $\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$ (R79), CO consumption rate in the reaction $\text{CO} + \text{OH} \rightleftharpoons \text{H} + \text{CO}_2$ (R94) and OH consumption rate in the reaction $\text{CH}_4 + \text{OH} \rightleftharpoons \text{CH}_3 + \text{H}_2\text{O}$ (R93) at $x/D = 8$, 16 and 24 conditionally averaged on the distance function. The units for reaction rate are $10^3 \text{ mole/m}^3 \cdot \text{s}$.

Figure 15. Scatter plots of (a) H_2 consumption rate in the reaction $\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$ (R79), and (b) CO consumption rate in the reaction $\text{CO} + \text{OH} \rightleftharpoons \text{H} + \text{CO}_2$ (R94) conditionally averaged on progress variable at $x/D = 8$, 16 and 24. The units for the consumption rate are $10^3 \text{ mole/m}^3 \cdot \text{s}$.

Figure 16. Profiles of CO reaction rate and CO mass fraction of the turbulent flame at $x/D = 8$, 16 and 24 conditionally averaged on the distance function.

Figure 17. Profiles of OH reaction rate and OH mass fraction of the turbulent flame at $x/D = 8$, 16 and 24 conditionally averaged on the distance function.

fig.3.eps

fig.4a.eps

fig.4b.eps

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