A comparison between direct numerical simulation and experiment of the turbulent burning velocity-related statistics in a turbulent methane-air premixed jet flame at high Karlovitz number

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Submitted to: Proceedings of the Combustion Institute

Total length: 6198 words

Main text: 4505

Tables: 60

Equations: 30

References: 716

Figures: 887, as follows: Fig. 1, 140; Fig. 2, 165; Fig. 3, 131; Fig. 4, 149; Fig. 5, 162; Fig. 6, 140.

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Abstract: A three-dimensional (3D) direct numerical simulation (DNS) of an experimental turbulent premixed jet flame at high Karlovitz number was studied. The DNS resolution adequately resolves both the flame and turbulence structures. A reduced chemical mechanism for premixed CH₄/air flames with NO_x based on GRI-Mech3.0 was used, including 268 elementary reactions, and 28 transported species. Consistent post-processing methods were applied to both the DNS and experimental data to evaluate turbulent burning velocity-related statistics, namely the flame surface density (FSD), and the flame curvature. Good agreement was achieved for the 2D comparisons. The DNS data were further analysed and provide 3D statistics unattainable from the experiment. The ratio of the 3D and 2D flame surface densities was estimated. The results are comparable with other values reported for various experimental flames. The 3D and 2D flame curvatures were also compared and their distributions are shown to be quite different owing to the round on-average geometry. Instantaneous images of the heat release surrogate, [CH₂O][OH], between the DNS and experiment agreed qualitatively. Various other experimentally obtainable surrogates for heat release rate including [CH₂O][H], [CH₂O][O], [HCO], and [CH] are also evaluated and compared using the DNS. The inner structure of the flame was compared between the DNS and experiment in terms of the joint PDFs of OH concentration and temperature. Generally good agreement was obtained; discrepancies may be due to the inconsistency of assumed equilibrium levels of OH concentration in the co-flow.

Keywords: Direct numerical simulation, high Karlovitz number, lean premixed combustion, turbulent burning velocity

1. Introduction

To minimise NO_x emissions, many modern gas turbines operate in a lean premixed mode. However, lean premixed combustion is susceptible to operability issues including combustion instability, blowout and flashback [1]. To enable improved designs, a better understanding of lean turbulent premixed combustion is required. In particular, one fundamental issue that underpins all these problems is the interaction of intense turbulence with flames that are relatively weak, due to high dilution with air.

In turbulent premixed combustion, a non-dimensional parameter, the Karlovitz number (Ka), has been introduced to classify different regimes of turbulence/flame interactions [2]. Ka is defined as the ratio of the flame to Kolmogorov time scales: $Ka = \tau_L / \tau_\eta$. For $Ka < 1$, turbulence is unable to penetrate the preheat or reaction zone, and the structure locally similar to laminar flames is observed. However, in high pressure lean premixed gas turbines, flames are expected to be located in the thin ($100 > Ka > 1$) or broken ($Ka > 100$) reaction zones regime, where Kolmogorov scales can disrupt the flame structure.

Relative to the situation at low Ka, understanding of flames in high Ka regimes is not particularly advanced. This has motivated a number of direct numerical simulation (DNS) studies of high Ka premixed combustion. Early work focused on flame-vortex interactions to understand stretching and quenching effects [3]. Later studies focused on isotropic turbulence, including two-dimensional (2D) detailed chemistry DNS [4-6], three-dimensional (3D) one-step chemistry DNS [7, 8], and 3D detailed chemistry DNS [9-12]. More recently, some cases have been reported including mean shear and non-trivial geometry in spatially developing slot jet methane flames [13] and temporally evolving, slot jet hydrogen flames [14]. Another notable trend in the literature is that DNS of real laboratory flames has recently become possible. Work in this direction includes DNS of rod-stabilised premixed flames [15], slot Bunsen flames [16], and swirl-stabilised flames [17]. However, these computations are at a relatively low Ka.

There has also been significant interest in achieving high Ka conditions in the laboratory, which have reported features such as a thickened reaction zone and local extinctions [18, 19]. Because of the large burner size and high Reynolds number (Re) of these experiments, DNS is currently not feasible; however recently a more accessible experiment with a small burner and moderate Re conditions was reported by the Lund University group [20, 21]. This study reported a series of co-flowing turbulent premixed jet flames in the thin and broken reaction zones regimes. Among the experimental conditions, of particular interest and feasibility for performing DNS is a methane-air premixed flame at high Ka and moderate Re (10,510), and at an equivalence ratio of 0.7. The present article reports the first DNS study of this flame. The present article is expected to be

the first to appear; however two other articles have been submitted based on the same DNS and are currently under review at the time of writing. In Ref. [22], quantitative comparisons of the DNS and experiment are reported, showing good agreement for the profiles of scalars and velocity; the DNS data further analyse the flame structure to understand the substantial flame broadening. In another paper [23], the statistics of the flame and flow and their interactions in the DNS are examined; the effects of heat release on the statistics are also discussed.

The particular objectives of this study are to examine key statistics in the DNS and experiment, including the flame surface density (FSD) Σ , flame curvatures, and experimental surrogates for heat release rate. The selection of these quantities is motivated by their availability in the experiments and their relevance to the turbulent burning velocity, S_T , which is outlined in the following. FSD influences S_T explicitly through the expression $S_T = S_L \cdot I_0 \cdot \int \Sigma d\zeta$ [24], where S_L is the laminar flame velocity, I_0 is the stretch factor, and ζ is the mean flame propagation direction. The turbulent burning velocity is also affected by stretch induced both by the tangential strain rate and propagation-curvature components. Stretch affects the burning velocity directly through the production/destruction of Σ and the effects on I_0 . Hence, flame curvature plays an important role in determining the overall burning rate. Finally, arguably the most direct measure of burning velocity would be determined by heat release rate; however, direct measurement of local heat release rate is impossible. Concentrations of HCO and CH have been proposed as surrogates of heat release rate [25]. It was also shown that, in laminar flame-vortex interaction simulations, the product imaging of OH and CH₂O is a good surrogate of heat release rate [26], as it measures directly the reaction rate of $\text{CH}_2\text{O} + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{HCO}$, and provides an estimate of the production rate of HCO. More recently, a H-atom based heat release rate surrogate, $[\text{CH}_2\text{O}][\text{H}]$, was also proposed for hydrocarbon flames [27]. In highly turbulent flames, turbulence may disturb the reaction zone and redistribute the heat and radicals, modifying the pathway of certain reactions and affecting the heat release. Hence, the performance of heat release surrogates has to be verified and quantified for these flames.

Direct comparisons of the above-mentioned statistics associated with turbulent burning velocity are performed between the DNS and experiment in the present study. The paper is organised as follows. Section 2 describes the computational approach and key parameters. Section 3 describes the data processing method used to extract FSD and curvature statistics. Statistical comparisons between the DNS and experiment, an evaluation of 3D/2D differences based on the DNS, and an evaluation the adequacy of heat release rate surrogates are presented in Section 4 before drawing conclusions in Section 5.

2. Numerical Methods

The experimental configuration is a round, piloted turbulent premixed methane-air burner operating at atmospheric pressure [20]. The jet bulk velocity is $U_b=110$ m/s, the jet equivalence ratio is $\phi=0.7$, and the jet temperature is $T_j=300$ K. The jet diameter is $D=1.5$ mm, and the jet Re based on U_b and D is $Re=10,510$. The small diameter and moderate Re render the DNS computationally feasible, while concurrently high Ka could be achieved. A wide laminar CH_4 /air co-flowing pilot flame having a velocity U_c of 1.8 m/s, measured temperature T_c of 1800K, and equivalence ratio ϕ of 0.9 is used to stabilise the flame. At these conditions, the laminar flame velocity is $S_L=0.19$ m/s, the flame thermal thickness is $\delta_L=0.66$ mm, and the flame time scale is $\tau_L=\delta_L/S_L=3.4$ ms. A photograph of the flame's natural luminosity is shown in Fig. 1a.

The DNS configuration corresponds to a premixed-fuel air jet issuing into an effectively infinite pilot flame. This is a reasonable approximation because the pilot is $40D$ wide, which is large enough to completely shield the flame from ambient air. Fig. 1b illustrates the DNS configuration, where the instantaneous flame front, denoted by the progress variable iso-surface (defined in Section 3), is delineated in red. The mean jet axial velocity profile at the inlet is specified using a power law velocity profile for an axisymmetric fully developed turbulent pipe flow. Superimposed on this mean profile is a turbulence field obtained by generating an auxiliary homogeneous isotropic turbulence field based on a prescribed Passot-Pouquet energy spectrum [28]. The turbulent velocity is 4 m/s and the integral length scale is 0.75 mm, consistent with the laser Doppler anemometry (LDA) measurement of the experiment [20]. The mean and root-mean-square axial velocity of the DNS has been compared with the LDA measurements in the near-field with good agreement [22], confirming the validity of the inlet velocity profile and inflow turbulence. Ka at the inlet is 253. The Damköhler number (Da) defined as the ratio of the integral time scale τ_f to the flame time scale τ_L is 0.054. For the large Ka and small Da in the present study, all turbulence time scales are smaller than the flame time scale, and the flame is in the broken reaction zones regime [2].

In the experiment the flame is attached to the rim of the burner, and the temperature and species profiles are somewhat ambiguous near the burner due to the absence of measurement at $x/D=0$. For simplicity the following profile is used to specify a scalar ψ (temperature or species mass fraction):

$$\psi = \psi_c + \frac{\psi_j - \psi_c}{2} \left(1 + \frac{\tanh \left(\frac{r}{\delta} \right)}{2} \right) \quad (1)$$

where ψ_j and ψ_c respectively denote the values of ψ in the jet and co-flow, r is the radial distance and δ is the thickness of the transition. ψ_c is determined from an equilibrium calculation of a CH_4 /air mixture with $\phi=0.9$ at

a defined temperature of 1800 K. ψ_j is computed based on a CH₄/air mixture with $\phi=0.7$ at 300 K. For $r<D/2$, δ is specified as $0.08D$; for $r>D/2$, δ is the half width of the burner surface to mimic the smooth transition between the co-flow and main jet. A similar inlet profile for scalars was used by Duwig and Dunn in their large-eddy simulation (LES) of highly turbulent piloted premixed flames [29]. This simple approach undoubtedly introduces some errors in the near burner region, but the main focus of this study is on the downstream region, which should be determined mainly by the jet and pilot conditions.

The physical domain is large 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, as illustrated in Fig. 1b. The resolution is chosen to adequately resolve both the flame and turbulence. A uniform grid spacing of $\Delta x = 30 \mu\text{m}$ is used in the streamwise direction x , while algebraic stretching is used in the lateral directions y and z outside of the shear zone. The grid in the y (z) direction is uniform with Δy (Δz) = $30 \mu\text{m}$ in the region between y/D (z/D) = -5 and 5, and gradually stretched outside of this region with a maximum relative stretching rate of 1.9%. 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 [14]. In the present high Ka case, the resolution of turbulence is more demanding. The Kolmogorov scale, defined as $\eta = (\nu^3/\epsilon)^{1/4}$, has a minimum of $10 \mu\text{m}$ in a narrow region near the potential core, where the flame does not overlap. The usual criterion for turbulence resolution, $\eta/\Delta x > 0.5$ [30], is satisfied elsewhere (see Supplement 1 for more details). Thus, the smallest scales of the turbulent flow are reasonably resolved in the flame region. The resultant grid is $N_x \times N_y \times N_z = 2400 \times 900 \times 900$. To flush out initialisation artefacts, the simulation was 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 were then mapped to the fine grid. The solution was advanced for another $10\tau_j$ to provide stationary statistics. It was found that statistical results of the half-resolution run and the production run are very similar, confirming the resolution is adequate.

The DNS code ‘S3D’ was employed to solve the compressible transport equations for continuity, momenta, species mass fractions and total energy [31]. The code uses a fourth-order Runge-Kutta method [32, 33] and a skew-symmetric, eighth-order explicit finite difference spatial scheme. A tenth-order filter was applied to damp high-wave number oscillations. A previously published reduced chemical mechanism for premixed CH₄/air flames with NO_x chemistry derived from GRI-Mech 3.0 was employed [34]. 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 [34]. Constant Lewis numbers, determined from a fit to mixture-averaged

transport properties in a premixed flame, were employed, and their values are provided in Supplement 2.

The simulation was performed on a Cray XC-40 located at the Pawsey Supercomputing Centre in Australia and required 10 million CPU-hours on 19,200 Intel Xeon Haswell processor cores for approximately 22 days.

3. Data Processing Methodology

In this section, methods for constructing the FSD and flame curvature from the experiment and DNS are described. Two different methods are utilised to extract the flame front. In many previous DNS studies [13, 14], flame fronts are typically located using the mass fraction of a major species. Major species are, however, not available in the experiment, while the temperature is not an optimal flame front marker due its limited signal-to-noise ratio (SNR). Information about the imaging quality and the SNR of measured scalars can be found in [21]. The SNR of OH is the highest among all scalars. Therefore, the flame front is extracted from OH images, being referred as the first method for the flame front identification. A 2×2 pixel filter was applied to reduce noise. The OH intensity is first normalised by its maximum value locally in each row (corresponding to a given axial location) of the image. Two iso-lines in the image are identified using a threshold level of 0.25. One corresponds to the location of maximum heat release rate. The other one is in the oxidation layer, which is not desirable. As CH_2O concentration in the oxidation layer is negligible, the second iso-line is excluded by multiplying the OH image with a binarised CH_2O image.

The motivation for introducing a second method is to extract and compare the statistics of 3D/2D flame front in the DNS. The iso-surface/iso-line of $c^* = 0.8$ is chosen to denote the 3D/2D flame front, corresponding to the location of maximum heat release rate, where c is the progress variable defined based on the O_2 mass fraction [12, 13], increasing monotonically from zero in the reactants to unity in the products.

To calculate FSD, the instantaneous flame front is binned into an interrogation box of size $0.375 \times 0.375 \text{ mm}^2$. The FSD values are found to be insensitive to the interrogation box size. The flame length in each box, L , is computed, and subsequently divided by the area of the interrogation box, A . This procedure is repeated for each image. The results are then averaged to obtain the spatial distribution of FSD, i.e. $\Sigma_2 = (\sum_{i=1}^{N_s} L_i) / (N_s A)$, where N_s is the number of images. In the DNS, a 2D OH concentration image of a typical x - r plane is exported for each snapshot; for consistency, the filtering from the experiment [20] was also applied to the DNS OH images. The same procedure described above is used to compute FSD from the DNS. Note that PLIF intensities are used in the experiment while species concentrations are used in the DNS. This difference can affect the

comparison. However, it was shown that the species PLIF image intensities may be interpreted qualitatively to be proportional to the species concentrations [20].

Most experimental measurements are performed in two or fewer spatial dimensions as is the case in the present study. Hence, it is necessary to develop a theoretical correction of the 2D measurements to estimate the corresponding 3D quantities [35, 36]. To this end, a comparison of the 3D and 2D FSD is performed in the DNS using the O₂-based flame front. The 3D FSD, Σ_3 , is calculated as the flame surface area per unit volume.

Due to preferential diffusion effects, the local burning rate correlates strongly with curvature even at high turbulence intensities [6]. Flame curvature statistics are compared between the DNS and experiment in 2D first. To calculate the 2D flame curvature, the instantaneous flame front is extracted from the OH images. The flame curvature at each discretised point along the flame front is determined. The flame curvature is positive (negative) when the centre of curvature is in the products (reactants).

The O₂-based flame front is then used to calculate the 3D/2D curvature in the DNS. The 3D curvature is calculated as $\nabla \cdot \mathbf{n}$, where $\mathbf{n}$ is the flame normal defined as $\mathbf{n} = -\nabla c / |\nabla c|$. Similarly, the 2D curvature is evaluated as $\nabla_2 \cdot \mathbf{n}_2$, where $\mathbf{n}_2 = -\nabla_2 c / |\nabla_2 c|$ is the 2D flame normal and ∇_2 denotes the vector-differential operator in x - r space.

4. Results and Discussions

4.1 Comparison of Flame Surface Density

Figure 2 shows a comparison of FSD contours from the DNS and experiment. The flame has two statistically symmetric branches in the x - r plane. In the upstream region, the FSD values are high and the distribution is narrow. As the flame develops, the FSD progressively becomes lower in magnitude and wider in spatial extent. Finally, the two branches merge due to complete consumption of the reactants and the corresponding flame annihilation. Overall, there is good agreement in the FSD between the DNS and experiment, both in terms of their spatial evolution and their magnitude. The main difference is that the DNS profile is slightly wider. This could be attributed to a number of factors; for example, the co-flow composition could be different from chemical equilibrium, and the difference in the FSD calculation between the DNS and experiment as described in Section 3. The comparison of the integral of the 2D FSD over the radial direction is displayed in Fig. 2c, and good agreement is obtained. The flame surface area approaches its maximum around $x/D=24$ and the flame length is approximately $38D$ in both profiles.

The profiles of FSD at two representative locations $x/D=10$ and 24 are shown in Figs. 3a and 3b, respectively. The left half of the figure shows the FSD results computed from the OH-based method, while the

right those computed from the O_2 -based method. It is seen that the FSD from the DNS and experiment quantitatively agree with a minor discrepancy in the position of the flame at $x/D = 10$ and the position and width at $x/D=24$. The simulated flame appears to be slightly shifted radially outwards compared to the experimental flame, consistent with the observation in Figs. 2a and 2b.

Figure 3 also shows that Σ_2 calculated with the O_2 -based method is slightly larger than that computed with the OH-based method at $x/D=10$, while they are comparable further downstream at $x/D=24$. This may be due to the greater degree of small-scale wrinkles at $x/D=10$, which might be smoothed by filtering the images in the OH-based method but not in the O_2 -based method. At $x/D=24$, the wrinkling scales are larger, and the effects of filtering on the FSD calculation are minimised. As a result, there is good agreement between the two methods of calculating FSD.

Because the experimental measurements are 2D, the FSD is underestimated. The extent of this underestimation can be assessed using the DNS. If we assume that the angle φ between the flame normal and the measurement plane has an isotropic distribution, it is expected that $\Sigma_3/\Sigma_2=4/\pi\approx 1.27$ [35, 36]. Close to the nozzle, Σ_3/Σ_2 approaches unity because the flame is not very wrinkled and φ is near-zero. Figs 3a and 3b show the profiles of Σ_3 and Σ_2 at $x/D=10$ and 24, respectively. It is observed that Σ_3 is generally larger than Σ_2 . The ratio, Σ_3/Σ_2 , at the location of peak FSD is 1.14 and 1.35 at $x/D=10$ and 24, respectively. Comparable values have been reported for various experimental flames [37, 38]. The results indicate that the flame is more wrinkled at $x/D=24$ than at $x/D=10$, and the distribution of the angle φ is different from isotropic. A detailed analysis of flame orientations is not within the present scope, but will be explored in the future.

4.2 Comparison of Flame Curvature

Figure 4 shows the PDFs of the flame curvature at $x/D=10$ and 24. The DNS results evaluated using the OH-based method are almost identical to the experimental results. Only a slight discrepancy is found at small curvature. This indicates that the DNS and experiment have very similar wrinkling scales. The PDFs of the 2D curvature using the O_2 -based method exhibit similar shapes. However, they are slightly shifted towards positive curvature, implying different wrinkling scales for the OH and O_2 fields; some differences should be expected due to their differing reactivity and diffusivities. It is worth noting that in the current high Ka condition, the flame wrinkling scales can be very small ($\sim 0.1\delta_L$), due to the interactions of the flame and small-scale turbulence, which is in contrast with those in low Ka flames [16].

The 2D curvature PDFs are symmetric and their means are near-zero. However, care should be taken when interpreting the 2D curvature results. The 3D curvature PDFs shown in Fig. 4 reveal that the curvature

distribution is positively skewed and the mean is negative. For a round jet flame, the mean flame front is nearly cylindrical and convex towards the product. As a result, the flame curvature has a negative mean, which can be roughly estimated as $-1/R(x)$, where $R(x)$ is the distance of the mean flame front to the centerline at the axial location x . The DNS results show that R increases with x until $x/D=24$, where it peaks. This explains why the mean curvature at $x/D=24$ is smaller than that at $x/D=10$.

4.3 Comparison of Flame Structure

The most direct measure of turbulent burning rate would be an evaluation of local heat release rate, however its direct measurement is not possible. Useful heat release rate surrogates have been studied in the literature [25-27], including $[\text{CH}_2\text{O}][\text{OH}]$, $[\text{HCO}]$, and $[\text{CH}_2\text{O}][\text{H}]$. By examining key elementary reactions and heat release rate distributions in CH_4/air laminar premixed flames and the turbulent flame, a new heat release rate surrogate, $[\text{CH}_2\text{O}][\text{O}]$, is proposed in the present work. Note that the three reactions, $\text{CH}_2\text{O} + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{HCO}$, $\text{CH}_2\text{O} + \text{H} \rightleftharpoons \text{H}_2 + \text{HCO}$ and $\text{CH}_2\text{O} + \text{O} \rightleftharpoons \text{OH} + \text{HCO}$, are the main contributors of HCO production in the present flame (not shown), and that the HCO pathway carries the largest share of the carbon flow [25]. It is also noted that, recently, improvement of H-atom and O-atom measurements using femtosecond two-photon PLIF has been explored [39]. Figs. 5a and 5b show a comparison of the instantaneous images of $[\text{CH}_2\text{O}][\text{OH}]$ between the experiment and DNS. While these are random realisations and not expected to agree one-to-one, the comparison indicates similar turbulence/chemistry interactions. The validity of heat release rate surrogates is examined using the DNS data. Figs. 5c-f show the heat release rate field, $[\text{CH}_2\text{O}][\text{H}]$, $[\text{CH}_2\text{O}][\text{O}]$ and $[\text{HCO}]$, respectively, in the DNS in a typical region. It is seen that the spatial distributions of all surrogates and heat release rate are similar. The good correlations between heat release rate and its surrogates are confirmed by the scatter plots shown in Figs. 5g and 5h. Downstream, some weak heat release rate is observed on the product side where $[\text{CH}_2\text{O}][\text{OH}]$, $[\text{CH}_2\text{O}][\text{H}]$, $[\text{CH}_2\text{O}][\text{O}]$ and $[\text{HCO}]$ are negligible. This is due to the oxidation reactions of CO and H_2 , i.e. $\text{CO} + \text{OH} \rightleftharpoons \text{CO}_2 + \text{H}$ and $\text{H}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{H}$, occurring downstream where CO , H_2 and OH are relatively abundant.

The correlations of heat release rate, $\dot{\omega}_T$, and its surrogate, ξ , are quantified. A correlation coefficient, $C_{\dot{\omega}_T-\xi}$, is proposed, i.e. $C_{\dot{\omega}_T-\xi} = (\langle \dot{\omega}_T \cdot \xi \rangle - \langle \dot{\omega}_T \rangle \langle \xi \rangle) / (\sqrt{\langle \dot{\omega}_T \cdot \dot{\omega}_T \rangle - \langle \dot{\omega}_T \rangle \langle \dot{\omega}_T \rangle} \cdot \sqrt{\langle \xi \cdot \xi \rangle - \langle \xi \rangle \langle \xi \rangle})$, which is a function of downstream distance. Three representative locations, $x/D = 8, 16$ and 24 , are selected for the analysis. In order to exclude regions where heat release is insignificant, the calculation is conditioned on $\dot{\omega}_T \geq 0.01\dot{\omega}_T^{\max}$. The correlation coefficients are shown in Table 1. Besides the above-mentioned surrogates, $[\text{CH}]$ as

an existing heat release rate surrogate is also evaluated. Two notable observations are made. First, the heat release rate surrogates perform well in the present flame, as evidenced by their high correlation coefficients. Comparatively, the performance of the proposed surrogate, $[\text{CH}_2\text{O}][\text{O}]$, is the best, while that of $[\text{CH}]$ is the worst. The relatively poor performance of $[\text{CH}]$ was also discussed in [25] and is related to its minor contribution to the carbon flow rate. At this stage, we stress that the surrogates may perform differently in different flame conditions [27]; it is necessary to assess them over a wide range of fuels, turbulent intensities, etc. Second, the correlations improve with downstream distance. This can be attributed to the increasing turbulent mixing, which includes the effects of unsteady strain rate and curvature [25] and the mixing of the jet and pilot, when the flame traverses downstream. Broadening of species layers, such as CH_2O and OH , was observed in both the experiment and DNS [20, 22], which can also modify the reaction pathways in different zones of the flame and affect the heat release.

Finally, the inner flame structure is compared between the DNS and experiment as shown in Fig. 6. The PLIF signals of OH were corrected to provide OH concentrations in the experiment [20]. It is seen that at $x/D=24$, the joint PDFs are in good agreement. At $x/D=10$, OH concentration from the DNS is lower than that of the experiment. One possible explanation for the discrepancy is that the assumed equilibrium OH concentration of the co-flow in the DNS is lower than the real concentration in the experiment. The wider scatter of data from the joint PDFs in the experiment can be attributed to noise in the measurements. The shot-to-shot based fluctuation of laser intensities is measured to be $\sim 1\%$ for OH PLIF, while the pixel-to-pixel fluctuation due to the read-out noise from the ICCD camera is $\sim 3\%$ at peak concentration.

5. Conclusions

DNS of a laboratory-scale turbulent premixed methane-air round jet flame, which features high Ka and moderate Re , was validated against the experiment comprehensively for various quantities related to the turbulent burning velocity. First, the FSD based on OH image was compared between the DNS and experiment, and good agreement was obtained. The 3D and 2D flame surface densities of the O_2 -based flame front were then compared in the DNS. The ratio, Σ_3/Σ_2 , at the location of peak FSD is 1.14 and 1.35 at $x/D=10$ and 24, respectively, comparable with values reported for other experimental flames.

Flame curvatures were also compared at various locations. The DNS results were almost identical to the experimental ones, indicating that the DNS and experiment have very similar wrinkling characteristics. Due to the interactions of the flame and small-scale turbulent structures under the high Ka condition, the wrinkling

scales of the flame surface can be very small ($\sim 0.1\delta_L$). The 3D and 2D flame curvatures evaluated with the O_2 -based method were compared in the DNS. The 3D curvature PDFs showed that the curvature distribution is positively skewed with a negative mean. The 2D curvature PDFs, however, were symmetric and their means were found to be near zero. The different behaviours between 3D and 2D curvatures were explained by analysing the flame geometry.

The validity of heat release rate surrogates is examined using the DNS data. A new surrogate, $[CH_2O][O]$, is proposed by examining key elementary reactions and heat release rate distributions. A correlation coefficient was also proposed to quantify the correlations of heat release rate and its surrogates. It was found that the performance of $[CH_2O][O]$ is the best, while that of $[CH]$ is the worst in the present flame; the correlation coefficient increases with downstream distance.

Acknowledgement

This work was supported by the Australian Research Council. This research used resources provided by the Pawsey Supercomputing Centre with funding from the Australian Government and the Government of Western Australia. The research was also supported by computational resources at Pawsey awarded through the National Computational Merit Allocation Scheme. The work at Sandia National Laboratories was supported by the Division of Chemical Sciences, Geosciences and Biosciences, the Office of Basic Energy Sciences, the US Department of Energy (DOE). Sandia National Laboratories is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the US Department of Energy under contract De-AC04-94-AL85000. The work at Lund University was supported by the Swedish Energy Agency and the ERC Advanced Grant, TUCLA.

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Figure Captions:

Figure 1. (a) Photograph of the turbulent flame from the experiment. (b) Schematic of the computational domain for DNS.

Figure 2. Comparison of the flame surface density Σ distribution: (a) DNS and (b) experiment. (c) Comparison of the integral of flame surface density in the radial direction $\int \Sigma(x, r) dr$.

Figure 3. Comparison of Σ along the radial direction at (a) $x/D=10$ and (b) $x/D=24$.

Figure 4. Comparison of flame curvature PDFs at (a) $x/D=10$ and (b) $x/D=24$.

Figure 5. Instantaneous images of (a) $[\text{CH}_2\text{O}][\text{OH}]$ from the experiment, and (b-f) $[\text{CH}_2\text{O}][\text{OH}]$, heat release rate, $[\text{CH}_2\text{O}][\text{H}]$, $[\text{CH}_2\text{O}][\text{O}]$ and $[\text{HCO}]$ from the DNS. (g) Scatter plots of $[\text{CH}_2\text{O}][\text{OH}]^+$ (red) and $[\text{CH}_2\text{O}][\text{H}]^+$ (blue) versus $\dot{\omega}_T^+$. (h) Scatter plots of $[\text{CH}_2\text{O}][\text{O}]^+$ (red) and $[\text{HCO}]^+$ (blue) versus $\dot{\omega}_T^+$. The superscript ‘+’ denotes a normalised value.

Figure 6. Comparison of joint PDFs of OH concentration and temperature from the (top) DNS and (bottom) measurements at $x/D=10$ and 24.

Table 1

The correlation coefficients of heat release rate and its surrogates.

x/D	$C_{\dot{\omega}_T-[\text{CH}_2\text{O}][\text{OH}]}$	$C_{\dot{\omega}_T-[\text{CH}_2\text{O}][\text{H}]}$	$C_{\dot{\omega}_T-[\text{CH}_2\text{O}][\text{O}]}$	$C_{\dot{\omega}_T-[\text{HCO}]}$	$C_{\dot{\omega}_T-[\text{CH}]}$
8	0.9150	0.9304	0.9579	0.9373	0.5866
16	0.9671	0.9511	0.9753	0.9708	0.7515
24	0.9747	0.9519	0.9791	0.9767	0.8279

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