Flow Field and Scalar Measurements in a Series of Turbulent Partially-Premixed Dimethyl Ether/Air Jet Flames

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We present a series of benchmark flames consisting of six partially-premixed piloted dimethyl ether (DME)/air jet flames. These flames provide an opportunity to understand turbulence-flame interactions for oxygenated fuels and to develop predictive models for these interactions using a canonical burner geometry. The development of accurate models for DME/air flames would establish a foundation for studies of more complex oxygenated fuels. The flames are stabilized on a piloted jet burner similar to that of the partially-premixed methane/air jet flames that have been studied extensively within the context of the TNF Workshop. This series of six jet flames spans jet exit Reynolds numbers, Re_D , from 29,300 to 73,300 and stoichiometric mixture fractions, ξ_{st} , from 0.35 to 0.60. Flame conditions range from very low probability of localized extinction to a high probability of localized extinction and subsequent re-ignition. Measurements in the flames are compared at downstream locations from 5 to 25 diameters above the nozzle exit. Mean and fluctuating velocity components are measured using stereo particle image velocimetry (SPIV). Simultaneous laser-induced fluorescence (LIF) imaging of OH and CH₂O provides insights into the distribution of these intermediate species in partially-premixed DME/air flames. OH LIF imaging is also combined with SPIV to investigate the strain rate field across the reaction zone.

Keywords: DME, Turbulent Jet Flames, PIV, OH LIF, CH₂O LIF, TNF workshop.

1. Introduction

Dimethyl ether (DME) is a promising clean alternative fuel for use in ground transportation compression ignition (CI) engines [1-3]. DME's high cetane number and easy vaporization also make it a potential fuel candidate for homogeneous charge compression ignition (HCCI) engines [2]. DME-fueled engines have the potential of significantly reduced CO and soot emission levels because of the presence of oxygen and the absence of a carbon-carbon bond in the DME molecule ($\text{CH}_3\text{-O-CH}_3$) [4, 5]. DME can be produced from conversion of biomass, natural gas and coal [1]. Despite the potential of DME as a clean fuel, appropriate combustion technologies must be developed and a fundamental understanding of the interplay between DME chemistry and turbulence is required.

Turbulent jet flames provide a canonical geometry in which to study turbulence-flame interactions and have been used in the development and testing of turbulent combustion models. Within the context of the International Workshop on Measurements and Computation of Turbulent Flames (TNF) [6], the series of piloted methane/air jet flames (Sandia flames *C-to-F*) spanning Reynolds number of approximately 13,400 to 44,800 have been used extensively for experimental studies [7-10] and model development [11-15]. DME flames represent a step forward in chemical complexity and are a good starting point for studying turbulent combustion of oxygenated fuels since DME is the simplest ether [16-19]. The progression of turbulent combustion studies from methane to DME combustion not only provides insights into turbulence-chemistry interactions for an oxygenated fuel but also may reveal enhanced effects of turbulent transport for intermediate species relative to methane flames.

Detailed chemical-kinetic reaction mechanisms for DME/air combustion are available: Fischer/Kaiser *et al.*, 2000 [20, 21] consisting of 78 species and 351 reactions, Zhao *et al.*, 2008 [22] employing 55 species and 290 reactions. These mechanisms have been tested over a range of conditions using experimental data on ignition delay times, flame speeds, and flame species [21, 23-30]. However, there remain significant discrepancies in predictions of combustion intermediates such as formaldehyde, which plays a central role in the decomposition of DME [31, 32]. In turbulent flames, combustion intermediates can be subject to significant transport by turbulent mixing.

In the present paper, we establish a series of piloted partially-premixed DME/air jet flames that are analogous to the well-studied Sandia CH_4 /air jet flame series. The DME/air jet flames have increasing levels of localized extinction and Reynolds numbers from 29,300 to 73,300. The maximum Reynolds number of the DME/air jet flame series is approximately 60% larger than the CH_4 /air jet flames. The main DME/air jet flame series has an air-to-fuel ratio of 4:1 (by vol.), which results in the same stoichiometric mixture fraction of 0.35 as the 3:1 air-to-fuel ratio of the CH_4 /air flames. In addition, we

consider DME/air jet flames with larger air-to-fuel ratios of 6:1 and 8:1 that represent a progression toward premixed combustion. The mean location of the reaction zone in these flames is positioned in a different region of the jet shear layer closer to the jet axis as a result of the larger stoichiometric mixture fraction.

2. Experimental Methods

2.1. Piloted Jet Burner and Experimental Conditions

Experiments were performed on a series of six piloted partially-premixed DME/air jet flames (photographs displayed in Fig. 1) with jet exit Reynolds numbers, Re_D , and stoichiometric mixture fractions, ξ_{st} , as listed in Table 1. For the series of flames labelled D_{41} , E_{41} , F_{41} and G_{41} , characterized by a constant air-to-DME volume ratio of 4-to-1 corresponding to $\xi_{st} = 0.35$, the jet flow rate progressively increased from 120 LPM to 300 LPM, resulting in Re_D of approximately 29,300, 44,000, 58,600, and 73,300. The total volumetric flow rates of the jet flows in Flames D to F are the same for the DME/air and CH₄/air jet flame series [8]. The flames labelled F_{41} , F_{61} and F_{81} had a constant jet flow rate of 240 LPM and a varying air-to-DME volume ratio of 4-to-1, 6-to-1 and 8-to-1, respectively, resulting in increasing ξ_{st} values of 0.35, 0.48 and 0.60. The jet exit Reynolds numbers of the three F -flames were comparable with an approximately 10% decrease in Re_D between flames F_{41} and F_{81} as a result of the change in composition (Table 1).

The piloted jet burner was a slightly revised version of the well-established Sydney burner configuration from the Sandia series of partially-premixed CH₄/air jet flames [8]. Specific dimensions were: a central jet diameter of 7.45 mm (as opposed to 7.2 mm in the Sandia CH₄/air Flame series), inner and outer diameters of the pilot annulus of 8.0 mm and 18.2 mm, respectively, and a coflow diameter of 254 mm. The pilot reactant mixture had an equivalence ratio of 0.6 and was composed of C₂H₂, H₂, CO₂, N₂ and O₂ with the mole fractions listed in Table 2. The pilot and mean jet flow rates were scaled proportionally such that the energy release of the pilot is approximately 2% of the main jet for flames D_{41} , E_{41} , F_{41} and G_{41} , 2.9% for F_{61} and 3.7% for F_{81} . These values were smaller than for the Sandia CH₄/air flames where the pilot energy release was approximately 6% of the main jet. The burner was surrounded by an air coflow with an initial velocity of 0.9 m/s that was monitored using a hot-film anemometer.

The gas flows to the jet and pilot were regulated using mass flow controllers, which were calibrated using piston-displacement calibration units (Sierra CalTrak) with an accuracy of $\pm 0.25\%$. DME was supplied in pressurized liquid tanks preheated to 330K to ensure a steady supply of gas. At ambient temperature and atmospheric pressure, DME is stable in the gas phase. Preheating of the DME tank did not affect the jet inlet temperature of 294K. Accurate positioning of the burner was controlled using a three-way motorized translation stage with a resolution of $< 7 \mu\text{m}$.

2.2. OH LIF and CH₂O LIF Imaging

In one set of experiments, laser-induced fluorescence (LIF) imaging measurements of OH and CH₂O were combined using the experimental configuration depicted in Fig. 2a. For OH-LIF excitation, the frequency doubled output of a Nd:YAG-pumped dye laser was tuned to the Q₁(6) transition ($\lambda = 283.01 \text{ nm}$, 1.2 mJ/pulse) of the $A^2\Sigma^+ \leftarrow X^2\Pi^+$ ($v' = 1, v'' = 0$) band of OH. A passive, single-cavity pulse stretcher was employed to lengthen the effective duration of the UV laser pulse. The longer laser pulse enabled the use of greater laser energy while operating in the linear LIF regime. The OH fluorescence emission from the A-X(0,0) and (1,1) bands were imaged onto an intensified CCD camera using a UV-camera lens (f.l. = 45 mm, f/1.8) with color glass filters (UG11 and WG305) to block interferences, resulting in a projected pixel size of approximately $53 \mu\text{m}$ and a field of view of $3.5D \times 3.5D$. The OH-LIF measurements were corrected for spatial variations in the average beam profile and the throughput of the imaging system. Shot-to-shot fluctuations were negligible for the subsection of the dye-laser beam that was used for LIF imaging. The OH-LIF signals were not corrected for local variations in quenching rates or the Boltzmann population fraction of the OH ground state.

As in Refs. [31-33], laser-induced fluorescence of formaldehyde was excited by the third harmonic of an injection seeded Nd:YAG laser (42 mJ/pulse) with a pulse stretcher similar to that of the OH-LIF system. The diode seed laser was temperature tuned to $\lambda = 354.83 \text{ nm}$ ($\Delta\lambda \sim 0.003 \text{ cm}^{-1}$) to excite overlapping transitions in the 4_0^1 band of the $\tilde{A}^1A_2 \leftarrow \tilde{X}^1A_1$ system. In comparison to broadband excitation using the third harmonic output of an unseeded Nd:YAG laser [16, 34], narrowband excitation of formaldehyde resulted in higher fluorescence signal by a factor two [31] and reduced interferences from intermediate species [33]. The CH₂O fluorescence emission was imaged onto an intensified CCD camera using a medium-format camera lens, an AR-coated singlet (f.l. = -400 mm), and a 35-mm format lens, resulting in a projected pixel size of approximately $19 \mu\text{m}$ and a field of view of $2.5D \times 2.5D$. A color glass filter (GG375) in the imaging system blocked elastic scattering from the laser and transmitted the CH₂O-LIF signal. The laser beam was horizontally polarized to eliminate interference

from Rayleigh or Raman scattering. The CH₂O-LIF measurements were corrected for the average variation in the laser beam profile and the throughput of the imaging system. For these corrections, response images were obtained by filling the field of view with a uniform stream of methane and recording the average C-H stretch Raman scattering signal from the UV laser beam. A half-wave plate at 355 nm was used to rotate the polarization of the laser beam to vertical in order to maximize the Raman scattering signal without affecting the laser beam profile.

2.3. Stereo Particle Image Velocimetry Measurements

In a second set of experiments, OH LIF imaging was combined with velocity field measurements using the experimental configuration in Fig. 2b. Three-component velocity field measurements were performed using stereo particle image velocimetry (SPIV). The jet and coflow were seeded with 0.3 μm aluminum oxide particles, which were illuminated by the second harmonic output ($\lambda = 532 \text{ nm}$) of a dual-head pulsed Nd:YAG laser. The laser beam was expanded by a factor of 2.5 in the vertical direction using a cylindrical telescope and formed into an approximately 1 mm thick sheet. A pair of CCD cameras (Cooke PCO, 1280 x 1024 px²) equipped with Nikon 105-mm macro lenses were used to capture the particle scattering images. The cameras were mounted at 23 degrees with respect to the normal to the laser sheet. Imaging of particles in the laser-sheet plane was improved by the use of Scheimpflug mounts to compensate for tilting and shifting of the lenses with respect to the camera bodies. A narrow-bandwidth interference filter centered at 532 nm was placed in front of each camera lens to reduce interference from flame luminosity. The resulting field of view of the cameras was approximately 19 x 14 mm². The stereoscopic projections were calibrated using recordings of a dot-array target that was translated stepwise along the z-axis. This calibration was further improved using a self-calibration procedure based on a pinhole model [35], which resulted in a residual error of less than 0.2 px.

Velocity vector calculations for SPIV were performed using an iterative cross-correlation processing algorithm with dynamic windowing. After each processing pass, the size of the interrogation window was halved and offset by the displacement distance of the previous processing pass, which reduced the risk of correlation loss and provided finer spatial resolution. The aspect ratio of the interrogation windows was also iteratively elongated in regions of shear to improve the accuracy of the measurements [36]. The interrogation window size, Δ_w , was reduced to a final nominal area of 32 x 32 px² (474 x 474 μm^2) in flames D_{41} , E_{41} and the F -flame series and an area of 48 x 48 px² (711 x 711 μm^2) in flame G_{41} with 50% overlap between neighboring windows, which resulted in a

vector spacing of 355 μm in flame G_{41} and 237 μm in the other flames. The laser produced a pair of pulses at a repetition rate of 5 Hz with an inter-pulse time delay that varied from 3.0 μs to 8.1 μs . The pulse delay was adjusted for each flow condition to provide a maximum inter-frame particle displacement, Δx_p , between 8 and 24 px depending on the measurement location. For the ensemble velocity statistics of Section 3.1, a universal outlier detection algorithm [37] was used to eliminate spurious vectors that were not replaced and therefore not included in the statistics. For the calculation of the conditional mean velocity gradients in Section 3.4, the spurious vectors were detected and replaced using the post-processing method of Garcia [38]. The -3 dB cut-off frequency of the spatial filter was comparable to that of a two-pass top-hat filter with a kernel size of Δ_w . The velocity fields were then interpolated onto the OH LIF images using 2D spline fitting.

2.4. Accuracy of the Velocimetry Measurements

The dominant sources of error and bias in the velocity measurements arose from the dynamic range and spatial resolution of the PIV imaging system. For standard two-component PIV measurements, the average error in the determination of particle displacements using dynamic windowing cross-correlation algorithms has been estimated to be as small as 0.04 px by Westerweel *et al.* [39], but this estimation could be degraded by a factor of 2 to 3 in the presence of imaging noise and fluctuations in the particle image diameter and signal level [40-42]. In comparison, a stereoscopic imaging configuration with cameras angled at 46 degrees with respect to each other was estimated to reduce the error of the in-plane velocity components by 30% but yielded errors in the out-of-plane velocity that were approximately 2.3 times larger [43]. For SPIV measurements in the turbulent flames, the estimated uncertainties in determining particle displacements were $\Delta x_p \sim 0.08$ px for the in-plane velocity components and $\Delta x_p \sim 0.24$ px for the out-of-plane velocity component, which corresponded to velocities on the order of $0.003U_{bulk}$ and $0.01U_{bulk}$, respectively. In shear flows, velocity statistics could be biased in regions with small particle displacements [36, 44, 45]. The sensitivity of the ensemble velocity statistics to particle displacement was investigated by repeating the velocity measurements in flame D_{41} at $x/D = 5$ with a factor of two increase in the inter-pulse time, thereby doubling the maximum particle displacement from 12 px to 24 px. The results showed no noticeable effect on the velocity statistics.

The spatial resolution of the SPIV measurements was limited by the size of the interrogation window, Δ_w . Small-scale particle motions within an interrogation window introduced an additional source of measurement error [45, 46], and the presence of under-resolved turbulence lengthscales

resulted in underestimates of velocity fluctuations [47, 48]. The extent to which the SPIV measurements resolved the velocity field can be estimated by comparing the turbulence lengthscales with Δ_w . For the turbulent flame conditions, the outer lengthscale, δ , which is defined as the full width at half maximum (FWHM) of the radial profile of the mean axial velocity, varies from $\delta = 7.5$ mm for $x/D = 5$ to $\delta = 22.0$ mm for $x/D = 25$ (Section 3.1). Estimates of the Batchelor lengthscale, λ_B , using conventional scaling laws for non-reacting turbulent jets are in the range of 20 μm to 50 μm near the nozzle exit for the Reynolds numbers shown in Table 1 [49]. Although these values are relevant for the non-reacting air jets, the dissipative lengthscales in jet flames are larger than those of the corresponding non-reacting jets because of dilatation and increases in viscosity that result from the heat release. Using Rayleigh scattering imaging, Frank and Kaiser [50] found that the Batchelor lengthscales in the *near-field* of turbulent non-premixed jet flames were a factor of 2 to 3 larger than those in non-reacting jets of equivalent Reynolds numbers. Additionally, the dissipative lengthscales measured by Wang *et al.* [51] in the Sandia CH_4 -air flames *D* ($Re_D = 22,400$) and *E* ($Re_D = 33,600$) ranged between 65 μm and 106 μm for $x/D = 7.5$ -to-30. Using these results, we estimated that the Kolmogorov lengthscale, $\eta \approx \lambda_B$ for $Sc \approx 1$, in the reaction zone of the DME-air jet flames considered here ranged between 50 μm and 100 μm , which was approximately 5-to-10 times smaller than Δ_w for flames *D*₄₁, *E*₄₁ and *F* and 7-to-14 times smaller for flame *G*₄₁. Measurements of the finest scale turbulent velocity gradients with a bias of less than 10% would require a window size of less than 3η [47, 48, 51]. Given the resolution of the SPIV measurements, dissipative lengthscales could not be analyzed without significant bias. However, we were able to evaluate variations in the mean axial velocity across the reaction zone in Section 3.4. For all the flames, the shear layer thickness was between 3.5 mm and 5 mm at $x/D = 5$ and increased with downstream location. Therefore, the lengthscales associated with the mean shear were significantly larger than Δ_w , and these velocity gradient measurements were not significantly impaired by the SPIV spatial resolution.

3. Results and Discussion

Photographs of the chemiluminescence from the series of piloted jet flames are presented in Fig. 1. Burning conditions range from stable burning with small amounts of localized extinction in flame *D*₄₁ to less stable combustion with increased probabilities of extinction and intermittent flame ignition by the pilot gases in flames *F*₈₁ and *G*₄₁. The flames with constant stoichiometric mixture fraction, *D*₄₁, *E*₄₁, *F*₄₁ and *G*₄₁, have an average length of approximately 60 diameters, whereas the lengths of the flames

F_{6I} and F_{8I} decrease to approximately $50D$ and $40D$, respectively. Flow field and scalar measurements are performed in the developing region of these jet flames for $x/D \leq 25$.

3.1. Velocity Field Statistics

The turbulent jet is a canonical configuration that has been studied extensively in non-reacting [52-54] and reacting [7-17, 55-64] flows. The heat release in a jet flame introduces a decrease in gas density and an increase in viscosity that significantly reduce the entrainment rate of the coflow stream [55, 60]. The rates of entrainment and mixing are important for modeling of turbulent jet flames and ultimately determine the flame height [59]. Velocity statistics are required to understand the effects of heat release on turbulent mixing as well as to validate numerical simulations and to determine boundary conditions. Conventional scaling laws typically apply in the *far-field* region of turbulent jets, but the effects of combustion in the *near-field* can have significant consequences on the downstream turbulence properties [58]. In this work, the flow fields are measured in the *near-field* for $x/D \leq 25$, which is a transitional region of turbulent jets where turbulence grows in the shear layer. Measurements in jet flames are compared to those in turbulent air jets with the same volumetric flow rates. In order to discern the effects of combustion of the DME/air jet mixture on the flow field, the air jet measurements are performed while using the corresponding pilot flames from the jet flames.

Radial profiles of the velocity fields in flame D_{4I} and the turbulent air jet D_{air} are compared at axial locations of $x/D = 5, 10, 15, 20$ and 25 in Fig. 3. Although the flame and air jet have the same bulk exit velocity, U_{bulk} , the mean axial velocity, U , exhibits a faster decay as a function of downstream location in the air jet than in the flame (Fig. 3a) because of the reduced entrainment rate in the flame. Between $x/D = 5$ and 25 , the mean centerline velocity, U_o , decreases by 66% in the air jet and by only 22% in the flame.

The RMS of the axial velocity fluctuations, u' , normalized by the bulk velocity is plotted for D_{air} and D_{4I} in Fig. 3b. Turbulence initially develops inside the 7.45-mm diameter tube, resulting in a jet exit RMS velocity that is approximately 3.5% of the bulk velocity. Downstream of the nozzle, turbulence intensifies in the shear layer between the jet and coflow stream, as indicated by the off-axis peak in the profiles of u'/U_{bulk} at $x/D = 5$ and 10 for both D_{air} and D_{4I} . Further downstream, for $x/D \geq 15$, the magnitude of the turbulent fluctuations in the non-reacting jet decays, indicating that the turbulent kinetic energy dissipates. The RMS axial velocity fluctuations along the jet centerline, u'_0 , initially increase more rapidly in the turbulent air jet than in the turbulent flame because of the larger entrainment rate of the coflowing air into the core of the non-reacting jet. For $x/D \geq 20$, the RMS axial

velocity in D_{air} peaks near the centerline and decreases monotonically with increasing radial position, suggesting that coflowing air is fully entrained into the core of the jet at these downstream locations. In the flame, the radial profiles of u'/U_{bulk} for $x/D \leq 25$ maintain an off-axis peak as a result of the lower entrainment rate, dilatation in the reaction zone, and fluctuations in the burning rate. In contrast to the air jet, the RMS axial velocity along the centerline of flame D_{41} continues to increase as a function of downstream location attaining a value of 10% at $x/D = 25$. The off-axis maximum value of u' is approximately 18% of U_{bulk} for $x/D \geq 15$ at a radial position of $1.0 \leq r/D \leq 1.3$.

Profiles of the mean radial velocity component, V_r , normalized by the bulk velocity are plotted for D_{air} and D_{41} in Fig. 3c. The mean radial velocities are zero on the jet centerline and have peak positive values in the region of $r/D = 0.5-1.5$ and negative values in the outer regions of the jet where coflowing air is entrained. In the flame, the peak positive value of the mean radial velocity increases with increasing downstream location, whereas it progressively decreases in the air jet. As a result, the difference between the peak radial velocities in the reacting and non-reacting flows becomes increasingly larger. On the other hand, the minimum values of the mean radial velocity are systematically lower in the air jet than in the flame, indicating a stronger entrainment of the coflowing air into the jet for the non-reacting case. The velocity zero crossings indicate the locations in the mixing layer where the mean outward flow of jet gases merges with the inward flow of entrained air. The radial coordinate of the zero-crossing point diverges from the jet axis as the turbulent jet expands with increasing downstream location, and the rate of divergence is greater in the flame.

The downstream evolution of the velocity fields in the turbulent flames D_{41} - G_{41} and their non-reacting counterparts are summarized in Fig. 4. The entrainment rate and the effects of heat release on the flow field are characterized by outer variables such as the mean and RMS axial velocities along the jet centerline and the jet half-width. In the flames, the mean axial velocity on the jet centerline, U_o , decreases at a constant rate of approximately $-0.01U_{bulk}/D$ between $x/D = 0$ and 25, as shown in Fig. 4a. For $x/D \leq 10$, U_o/U_{bulk} is identical in the flames and air jets, which is partially attributable to the influence of the pilot gases near the nozzle. For $x/D \geq 15$, U_o decays more rapidly in the turbulent air jets than in the flames.

Axial profiles of the jet centerline turbulence intensity, u'_o/U_o , are shown in Fig. 4b. Note that the normalization factor used here is the mean centerline axial velocity at the corresponding downstream locations. The centerline turbulence intensity is lower in the turbulent flames than in the turbulent air jets, especially for $x/D \geq 10$. In the air jets, u'_o/U_o rises rapidly between the axial locations of $x/D = 5$ and 15, as result of the shear layer expansion onto the centerline. In the turbulent flames, the centerline

turbulence intensity increases slowly as a function of downstream location up to nearly 10% at $x/D = 25$. The reaction zone moderates the development of turbulence in the core of the jet. As reported by Pope [53], the centerline turbulence intensity in non-piloted, non-reacting turbulent free jets increases to a plateau value of 25% in the *far-field* region. According to the measurements in the piloted air jet, such a turbulence intensity is approximately reached at $x/D = 25$.

The streamwise expansion of the turbulent jets is quantified by the full width at half maximum of the radial profile of the mean axial velocity, δ , in Fig. 4c. For $x/D < 25$, the turbulent jet flames remain wider than the piloted air jets. At $x/D = 25$, the widths of the flames and air jets are approximately equal to $\delta \sim 2.8D$, and it is expected that the turbulent air jets become wider than the flames further downstream. All four jet flames have approximately the same spread rate of $\partial\delta/\partial x = 0.08$, in good agreement with the data reported in Refs. [59, 62]. This *near-field* spread rate of the flames is significantly smaller than the established *far-field* spread rate for non-reacting turbulent jets of $\partial\delta/\partial x = 0.2$ [53].

The overlap of the respective curves for the flames and air jets in Fig. 4 indicates that the downstream evolution of the normalized centerline velocity statistics from $x/D=5$ to 25 is relatively insensitive to the jet exit Reynolds number. The largest deviations occur for the turbulence intensity of the non-reacting jets at $x/D=10$. Though not shown, the statistics for flames F_{6I} and F_{8I} are consistent with those of flames D_{4I} - G_{4I} , indicating that there are no substantial variations in the streamwise evolution of the flow field for the range of Reynolds numbers and stoichiometric mixture fractions investigated.

3.2. Computations of laminar flame structure and LIF signals

In order to analyze the scalar measurements in the following sections, we use laminar flame calculations to investigate the chemical structure of the flames and to demonstrate the simulation of CH_2O and OH LIF signals. The chemical structures of the partially-premixed DME/air flames are computed using a one-dimensional, steady-state counterflow configuration (Chemkin Oppdif [65]) and two chemical-kinetic mechanisms, namely Kaiser et al., 2000 [21] and Zhao et al., 2008 [22], and their associated transport data. The results of the calculations for a strain rate $a = 300 \text{ s}^{-1}$ are plotted in Fig. 5.

The species profiles calculated for the 4:1 air:DME mixture ($\xi_{st} = 0.35$) using different chemical mechanisms are compared in Fig. 5a. Minor differences between the two mechanisms are evident for the major species, CH_3OCH_3 (DME), O_2 , H_2O , CO_2 , CO and H_2 (Fig. 5a top), as well as for some of the

intermediate species, CH_3 , H , OH and O (Fig. 5a bottom). However, the reaction mechanisms have a larger disparity in the mole fractions of CH_2O and CH_4 . For the Zhao mechanism, the peak mole fractions of CH_2O and CH_4 are 27% and 32% larger, respectively, than those of the Kaiser mechanism. Both CH_2O and CH_4 are formed in the decomposition of DME, which occurs by both unimolecular decomposition and abstraction of a hydrogen atom in reactions between DME and radicals such as H , OH , O , and CH_3 . For both chemical-kinetic mechanisms, CH_2O is predominantly produced by decomposition of the methoxy-methyl radical in the reaction $\text{CH}_3\text{OCH}_2 = \text{CH}_2\text{O} + \text{CH}_3$. The methoxy-methyl radical is formed by the dominant H-atom abstraction reaction of $\text{DME} + \text{H} = \text{CH}_3\text{OCH}_2 + \text{H}_2$. In the Zhao mechanism, the methoxy-methyl radical is also produced by the second most important DME decomposition reaction, $\text{CH}_3\text{OCH}_3 + \text{CH}_3 = \text{CH}_3\text{OCH}_2 + \text{CH}_4$. In contrast, the second most important decomposition reaction in the Kaiser mechanism is $\text{CH}_3\text{OCH}_3 = \text{CH}_3 + \text{CH}_3\text{O}$. The excess production of CH_3OCH_2 and CH_4 in the Zhao mechanism may explain the difference in the formaldehyde and methane mole fraction profiles for the two mechanisms.

The mole fractions of CH_2O and OH in partially-premixed DME/air flames with air:DME ratios of 4:1, 6:1, and 8:1 ($\xi_{st} = 0.35, 0.48$ and 0.60) are compared in Fig. 5b. The Kaiser mechanism was used for these calculations. As the amount of premixing increases, the reaction zone broadens in the direction of the fuel stream. Although the peak OH mole fraction is approximately unchanged as ξ_{st} increases from 0.35 to 0.60, the distribution of OH extends further toward the fuel stream. Greater premixing also shifts the distribution of CH_2O mole fraction toward the fuel stream, and its peak value decreases since the fuel stream contains less DME. Additional laminar flame calculations show that the extension of the OH distribution and shift in the CH_2O peak become less pronounced as the strain rate increases above 300 s^{-1} .

The two mechanisms differ somewhat in predictions of flame extinction. The extinction limits of strained laminar flames computed for $\xi_{st} = 0.35, 0.48$ and 0.60 are compared for the Kaiser and Zhao reaction mechanisms in Fig. 6. At low strain rates, both reaction mechanisms predict a similar increase in the maximum flame temperature as ξ_{st} increases. As the strain rate increases, the maximum temperature for the Zhao mechanism decreases faster than for the Kaiser mechanism. The Zhao mechanism predicts an extinction strain rate limit of approximately 800 s^{-1} for all three mixtures, which is approximately 15% lower than that of the Kaiser mechanism. Both mechanisms indicate that the extinction strain rate is relatively insensitive to variations in the amount of partial premixing, suggesting that same amount of localized extinction should be observed in the three turbulent flames F_{41} , F_{61} and F_{81} .

The analysis of CH₂O and OH LIF measurements in the following sections uses the LIF signals themselves without conversion to concentrations. This conversion would require additional simultaneous measurements of the major species and temperature to account for variations in Boltzmann population distributions and collisional quenching rates. In order to effectively compare experimental and numerical data, the LIF signals can be computed from the species and temperatures obtained from the simulations and directly compared to the measured LIF signals [31, 32]. Briefly, the simulated OH-LIF signal is proportional to the product of the OH concentration, the Boltzmann population fraction, and the fluorescence quantum yield, which is determined using collisional quenching cross-sections from Tamura *et al.* [66]. The simulation of CH₂O-LIF signals is more complicated and involves greater uncertainty due to the excitation of overlapping transitions and the lack of relevant temperature- and species-dependent quenching data. As described in Refs. 31 and 32, the Boltzmann population distributions of the lower states of the relevant formaldehyde transitions were computed using spectral simulation software [67], and the temperature dependence of the collisional quenching cross-sections were modeled as a power law of $T^{-0.5}$.

Profiles of computed CH₂O and OH LIF signals are included in Fig. 5b to demonstrate this approach using the strained laminar flame calculations. The LIF signals are scaled such that the peak LIF signals match the corresponding peaks in the OH and CH₂O mole fraction profiles for the flame with $\xi_{st} = 0.35$. The same scaling factors are applied to all three flames. The relative peak heights of the LIF signal profiles correspond very closely to those of the peak mole fractions. The profiles of the OH LIF signals are shifted slightly toward the oxidizer side relative to the OH mole fraction profiles, and the CH₂O LIF signal profiles show an even larger shift relative to the CH₂O mole fraction profiles. Profiles of the formaldehyde number density (not shown) are shifted closer to the CH₂O LIF profiles since the temperatures are lower and number densities are larger on the fuel-stream side of the CH₂O distribution.

3.3. Scalar Field Statistics

The scalar fields are first characterized in terms of ensemble statistics of the OH and CH₂O LIF imaging measurements performed at locations of $x/D = 5, 10, 15, 20$, and 25 . For all comparisons of the scalar measurements, the OH and CH₂O LIF signals are normalized by the respective peak values of the mean LIF signals in flame D_{41} at $x/D = 5$. Single-shot composite images of simultaneous OH LIF and CH₂O LIF measurements at all downstream locations are displayed in Fig. 7. Iso-contours of the OH LIF signal are overlaid on the CH₂O LIF images. The CH₂O LIF images show that an annular layer of

CH_2O forms near the nozzle exit and merges into the core of the jet at approximately $x/D = 15$. The CH_2O LIF images also reveal the presence of highly convoluted small scale structures in the core of the jet, which is indicative of significant turbulent mixing. In contrast, the OH layers are less corrugated since OH forms in the less-turbulent, high-temperature region of the reaction zone. The degree of corrugation and fragmentation of the OH layers increase as the Reynolds number increases. Isolated pockets of OH that are observed in some images, such as at $x/D = 20$ in flame F_{6I} , can result from flame dynamics subsequent to localized extinction or three-dimensional corrugations of the flame with respect to the imaging plane. Discontinuities in the OH layers, as observed at $x/D = 5$ in flame G_{4I} , correspond to regions of localized extinction, which occur with greater probability as the Reynolds number increases. The space between fragmented regions of OH radicals can contain significant CH_2O LIF signal. The fragmentation of the OH layers and the separation distance between the OH and CH_2O layers are further analyzed in Section 3.4. Overall, the snapshots in Fig. 7 reveal a stark contrast between the structure of the reaction zone in the turbulent flames and that of the laminar counterflow flames presented in Section 3.2. These qualitative discrepancies in the structure may have implications for the applicability of flamelet-based models for turbulent combustion [68].

Radial profiles of the mean and RMS OH LIF and CH_2O LIF signals, computed using 700-to-1000 LIF snapshots at each downstream location, are plotted for Flame D_{4I} in Fig. 8. As the jet flame evolves downstream, the mean OH LIF profile becomes broader and the peak value decreases (Fig. 8a). At the same time, the CH_2O LIF signal increases along the centerline. In Fig. 8b, the double-peaked profiles of the RMS fluctuations of the OH LIF signal are produced by the corrugations and fluctuations in the position of the OH LIF layers relative to the burner. The largest fluctuations in the CH_2O LIF signal occur at the interface with the OH layers between $r/D = 0.5$ and 1.0, and the magnitude of the fluctuations increases as a function of downstream location.

A comparison of the streamwise evolution of the mean scalar fields in the turbulent flames is plotted in Fig. 9, including variations of the peak mean OH LIF signal, the mean centerline CH_2O LIF signal, and the radial location of the peak mean OH and CH_2O LIF signals. Figure 9a shows that the maximum value of the mean OH LIF signal at $x/D = 5$ decreases with increasing jet exit velocity, by a factor 2 from D_{4I} to G_{4I} , as a result of the increased probability of localized extinction or incomplete ignition by the pilot flame. For $x/D \geq 10$, this peak value is comparable in the four flames with $\xi_{st} = 0.35$. Figure 9b shows that the mean centerline CH_2O LIF signal in all six flames reaches a maximum at $x/D = 20$ and decreases further downstream. For the four flames with $\xi_{st} = 0.35$, the centerline CH_2O LIF signal profiles are identical. For these flames, the axial profiles of both the peak

mean OH LIF signal at $x/D \geq 10$ and the mean centerline CH₂O LIF signal are independent of the Reynolds number.

Larger variations in the streamwise evolution of the LIF signals are observed for the flames with different stoichiometric mixture fractions. For each case in the *F*-flame series, Fig. 9a shows that the peak mean OH LIF signal varies relatively little as a function of downstream location but increases slightly as ξ_{st} increases. In contrast, Fig. 9b shows that the centerline mean CH₂O LIF signal decreases with increasing ξ_{st} for axial locations of $x/D \geq 15$, indicating that the increased premixing leads to more rapid fuel consumption at these downstream locations.

Figure 9c shows the difference in the evolution of the OH and CH₂O layers as the jet flame expands downstream. The peak mean OH LIF signal is displaced radially in all the flames, but the spreading rate is largest in the *D*₄₁-*G*₄₁ flames and decreases as the amount of premixing increases for flames *F*₆₁ and *F*₈₁. In contrast, the peak mean CH₂O LIF signal converges to the centerline at approximately $x/D = 20$. The rate of convergence increases slightly as the amount of premixing increases.

3.4. Turbulent Flame Structure

The structures of the turbulent premixed flames are analyzed in more detail using simultaneous SPIV and OH LIF measurements as well as simultaneous CH₂O LIF and OH LIF imaging. The combined PIV/OH LIF measurements provide conditional statistics on the flow field in the vicinity of the reaction zone. Radial profiles of the mean shear, $\langle \partial u / \partial r \rangle$, conditional on the distance from the interior of the OH layer are plotted in Fig. 10. The interior boundary of the OH layer is defined by the iso-contours of normalized OH LIF signal that are equal to 0.24 and located on the side of the OH layer closest to the jet axis. The abscissa in Fig. 10 corresponds to the radial distance from this boundary, with positive and negative values oriented toward the coflow and jet axis, respectively. The magnitude of $\langle \partial u / \partial r \rangle$ in Fig. 10 is normalized by the ratio U_{bulk}/R for each flame. For all the flames, the profiles of conditional mean shear reach a maximum near the boundary of the OH layer at $r = 0$ mm. The maximum shear decays rapidly from $x/D = 5$ to 10 and decreases more gradually further downstream. The decrease in the mean shear is associated with the expansion of the shear layer and the decrease in the axial velocity with increasing downstream location. The comparison of flames *D*₄₁, *E*₄₁, *F*₄₁ and *G*₄₁ in Fig. 10 shows that $\langle \partial u / \partial r \rangle$ decreases relative to the ratio U_{bulk}/R with increasing Reynolds number, even though the absolute value of $\langle \partial u / \partial r \rangle$ is larger in the more turbulent flames. The thickness of the conditional mean shear region across the reaction zone, defined as the FWHM of the radial profiles of

$\langle \partial u / \partial r \rangle$, increases as a function of downstream location. This shear region thickness varies from 3.5 mm at $x/D = 5$ to 8.5 mm at $x/D = 15$ in flame D_{4I} and from 5.0 mm at $x/D = 5$ to 9.8 mm at $x/D = 15$ in flame G_{4I} . For $x/D \geq 20$, the thickness becomes larger than 11 mm and could not be determined due to limitations in the field of view of the SPIV/OH LIF measurements. In flames F_{4I} , F_{6I} and F_{8I} , however, the profiles of $\langle \partial u / \partial r \rangle$ are quite similar to each other despite the variations in ξ_{st} . Although the increase in premixing for the F -flame series shifts the mean location of the reaction zone closer to the jet axis and deeper into the turbulent mixing layer, the local shear at the reaction zone remains essentially unchanged. As a result, the impact of flow shear on the flame chemistry is expected to be comparable for these three flames.

The interplay between combustion chemistry and turbulence in the jet mixing layer can hamper the ignition of reactants by the pilot gases and also cause the formation of burning pockets and extinguished regions, as is evident in the single-shot images of Fig. 7. The effects of the flow field on the flame structure are evaluated by analyzing the number of “holes” in the high-temperature reaction zone, as indicated by discontinuities in the OH layer. The hole counting procedure is described in detail in Ref. [69], including the limitations of this analysis. In brief, each normalized OH LIF image of dimensions $3.5D \times 3.5D$ is smoothed, binarized, and thresholded at a relative signal level of 0.24. Contiguous regions containing OH are labeled, and reaction zone holes are identified as the shortest connection between neighboring OH-containing regions with the boundaries of the imaging region treated according to Ref. [69]. The results are used for a comparison of the relative trends in reaction zone morphology for the different turbulent flames since the exact number of holes depends to some extent on the choice of signal threshold and is subject to inherent uncertainties. When the reaction zone is not strongly affected by the flow field, as exemplified in the snapshot in Fig. 7 for flame D_{4I} centered at $x/D = 5$, the OH LIF layer is singly-connected and zero holes are counted for that snapshot. However, more intense turbulence-chemistry interactions fragment the OH layer and the number of holes per snapshot increases. For instance, the snapshot for flame G_{4I} at $x/D = 5$ in Fig. 7 has two holes with three regions containing OH.

Probability density functions (PDFs) of the number of holes per OH LIF image and their variation with flow conditions and downstream position are shown in Fig. 11. The PDFs for flames D_{4I} to G_{4I} show a progression of increasing probability of hole formation as the turbulence and flow shear increase. The probability of finding zero reaction zone holes at $x/D = 5$ decreases from approximately 99% in flame D_{4I} to 3% in flame G_{4I} , and the most probable number of holes per snapshot shifts from 0 to 2.

The increased probability of hole formation at the higher Reynolds numbers can result from a combination of localized extinction and incomplete ignition of the reactants by the pilot gases.

The downstream evolution of the PDFs varies somewhat amongst the different flames. In flames D_{41} and E_{41} , the probability of finding zero holes is greatest at $x/D = 5$, where localized extinction and isolated pockets of OH radicals are relatively rare. Further downstream, the probability of detecting one or more holes per image increases because of a combination of increased localized extinction, flame pockets, and three-dimensional flame convolution. This result may appear to contradict the expectation that regions of the reaction zone that are closer to the nozzle would be disrupted by the higher shear at $x/D = 5$ (Fig. 10); however, combustion in the near field is actively supported by the pilot gases. However, this support becomes less robust at the larger flow rates in flames F_{41} and G_{41} . In these flames, the largest probability of detecting discontinuities in the reaction zone occurs at $x/D = 5$, and it decreases further downstream as the strain rate and shear decrease (Fig. 10).

The PDFs for flames F_{41} , F_{61} , and F_{81} show relatively small variations in the probability of fragmentation of the OH layers, although the probability decreases slightly with increased premixing. These variations are most pronounced at $x/D = 5$ -10. The difference in extinction probability within the F -flame series is not the result of the flow shear since the data in Fig. 10 show that the shear at the reaction zone is comparable in these flames. The increased premixing represents a progression from partially-premixed combustion to fully-premixed combustion, although even the largest amount of premixing with air:DME = 8:1 results in an equivalence ratio of 1.8 and a relatively small flame speed on the order of 10 cm/s [23, 28].

The effect of turbulent transport on distributions of combustion intermediate species is a key aspect of turbulence-chemistry interactions. The single-shot images in Fig. 7 show that the spatial overlap between formaldehyde and OH can fluctuate significantly within the series of turbulent flames. In some instances, the two species are located in close proximity, whereas in other instances, there are large gaps between the two species (e.g. snapshots of flames E_{41} , F_{41} , F_{61} at $x/D = 25$). The degree of overlap can affect the local reaction rates of these species, and the proximity of formaldehyde to the extinguished regions may affect the delay times for re-ignition. Extinguished regions can contain significant amounts of formaldehyde, as seen in the single-shot $\text{CH}_2\text{O}/\text{OH}$ LIF image at $x/D = 5$ for flame G_{41} .

The average separation distance between regions containing CH_2O and OH increases as a function of downstream position, as shown in Fig. 9c. The fluctuating separation distance between the CH_2O and OH distributions is quantified in each simultaneous $\text{CH}_2\text{O}/\text{OH}$ LIF snapshot following the approach described in Ref. [31]. The resulting PDFs of CH_2O -OH separation distances for the entire dataset are

plotted in Fig. 12. The PDFs are computed using a bin size of $18.9\ \mu\text{m}$, which equals the projected pixel size for the CH_2O LIF imaging measurements. For this analysis, the outer boundary of the CH_2O distribution and inner boundary of the OH layer are defined using the iso-contours of normalized LIF signals equal to 0.24. Although the PDFs depend to some extent on the iso-contour value that is used to determine the boundaries, the trends observed in Fig. 12 remain consistent with different values. For all the flames, the peaks of the PDFs are centered approximately at 0 mm. Except for flame F_{8I} , the PDFs are noticeably skewed toward positive values, indicating that the CH_2O and OH layers are preferentially separated. The PDF distributions broaden and extend toward larger positive values with increasing downstream location. Therefore, the separation between the two intermediate species increases with downstream location in concert with the decrease in mean shear (Fig. 10). The largest separation distances are measured in flame D_{4I} , and the PDF distribution tends to narrow with increasing bulk jet flow rate, which corresponds to increasing mean shear. These results are consistent with previous calculations of laminar partially premixed flames that show a reduction in separation distance with increases in strain rate [32]. The separation distance also decreases with increasing stoichiometric mixture fraction in flames F_{4I} to F_{8I} , which is consistent with the laminar flame calculations in Fig. 5b and the mean separation distance measurements in Fig. 9c.

4. Conclusions

Measurements in a series of piloted, turbulent partially-premixed DME/air jet flames were presented for varying Reynolds numbers and stoichiometric mixture fractions. These flames provide a framework for the development and validation of turbulent combustion models and simulation schemes. The flow field was determined using stereo-PIV, and the turbulent flame structure was measured using CH_2O and OH LIF imaging. Measurements were performed in the *near-field* region of the jets for $x/D \leq 25$, where strong variability of the velocity and LIF signal statistics were observed with downstream locations.

Ensemble mean and RMS statistics of the velocity components and the CH_2O and OH LIF signals were self-consistent across the range of Reynolds numbers, but the distribution of the mean LIF signals varied as a function of the stoichiometric mixture fraction. Simultaneous PIV and OH LIF measurements were used to evaluate conditional velocity gradients, enabling an analysis of the local shear at the reaction zone in each of the turbulent jet flames. The reaction zones in the jet flames that

had stoichiometric mixture fractions ranging from $\xi_{st} = 0.35$ to 0.60 experienced essentially the same amount of shear despite differences in the mean location of the flame within the jet mixing layer. The relationship between the topology of CH₂O and OH was investigated using simultaneous imaging of CH₂O and OH LIF. The combined measurements revealed that the regions occupied by these intermediate species are subject to maximum shear and that the flame structure can be highly disrupted by the flow field with formation of locally extinction regions and isolated pockets of OH radicals. In addition, there are large intermittent fluctuations in the separation distances between these species.

The scalar and velocity data will be made available for model development by contacting the authors.

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Tables

Table 1 – Turbulent flame conditions.

<i>Flame</i>	φ_{jet}	ξ_{st}	Re_D	U_{bulk} (m/s)
<i>D_{4I}</i>	3.6	0.35	29,300	45.9
<i>E_{4I}</i>	3.6	0.35	44,000	68.8
<i>F_{4I}</i>	3.6	0.35	58,600	91.8
<i>F_{6I}</i>	2.4	0.48	54,600	91.8
<i>F_{8I}</i>	1.8	0.60	52,500	91.8
<i>G_{4I}</i>	3.6	0.35	73,300	115.

Table 2 – Pilot mixture composition.

$X(CO_2)$	$X(N_2)$	$X(C_2H_2)$	$X(H_2)$	$X(O_2)$	φ_{pilot}
0.030	0.688	0.022	0.088	0.172	0.6

List of Figures

Figure 1 – Flame photographs (exposure time: 1.0 ms).	26
Figure 2 – Experimental configurations for (a) simultaneous CH ₂ O/OH LIF and (b) simultaneous PIV/OH LIF measurements.	27
Figure 3 – Radial profiles of mean and RMS axial velocities and mean radial velocity in piloted air jet D _{air} and flame D ₄₁	28
Figure 4 – Comparison of centerline velocity measurements in flames D ₄₁ , E ₄₁ , F ₄₁ and G ₄₁ . Profiles of a) U_o/U_{bulk} , b) u_o'/U_o and c) δ (FWHM of U radial profiles). Note that the normalization factor in Fig. 4b is the mean centerline velocity at each downstream location, U_o . ..	29
Figure 5 – Flame structure calculated for $a = 300/s$ using Chemkin Oppdif [65]. a) Comparison of species mole fractions computed using the Zhao (solid) [22] and Kaiser (dashed) [21] reaction mechanisms. b) Profiles of OH and CH ₂ O mole fractions for $\xi_{st} = 0.35$ (solid), 0.48 (dashed) and 0.60 (dotted) computed using the Kaiser mechanism. Profiles of simulated OH and CH ₂ O LIF signals.	30
Figure 6 – Strained laminar flame extinction limits computed using Chemkin Oppdif [65] and compared for the Zhao (solid) [22] and Kaiser (dashed) [21] reaction mechanisms. Calculated maximum laminar flame temperatures plotted as a function strain rate for $\xi_{st} = 0.35$ (blue), 0.48 (black) and 0.60 (red).	31
Figure 7 – Examples of single-shot OH LIF and CH ₂ O LIF measurements at locations of $x/D = 5, 10, 15, 20$ and 25 in all six turbulent flames. Images of the CH ₂ O LIF signal are overlapped with OH LIF signal iso-contours for $OHLIF = 0.24$ to 1.92 in steps of 0.24 . Dashed vertical lines indicate the jet centerline.	32
Figure 8 – Radial profiles of mean and RMS OH LIF (solid) and CH ₂ O LIF (dashed) signals in flame D ₄₁	33
Figure 9 – Comparison of a) peak mean OH LIF signal, b) centerline mean CH ₂ O LIF signal and c) radial position of peak mean LIF signals in all the turbulent flames.	34
Figure 10 – Mean radial gradient of the axial velocity conditional on OH LIF iso-contours of 0.24 . Velocity gradients are normalized by U_{bulk}/R for each flame.	35
Figure 11 – Number of reaction zone holes per OH LIF snapshot in the turbulent flames.	36
Figure 12 – PDFs of the spacing between the CH ₂ O and OH LIF layers in the turbulent flames. Negative values indicate that the layers are overlapping.	37

Figure 1 – Flame photographs (exposure time: 1.0 ms).

Figure 2 – Experimental configurations for (a) simultaneous CH_2O /OH LIF and (b) simultaneous PIV/OH LIF measurements.

Figure 3 – Radial profiles of mean and RMS axial velocities and mean radial velocity in piloted air jet D_{air} and flame D_{41} .

Figure 4 – Comparison of centerline velocity measurements in flames D_{41} , E_{41} , F_{41} and G_{41} . Profiles of a) U_o/U_{bulk} , b) u_o'/U_o and c) δ (FWHM of U radial profiles). Note that the normalization factor in Fig. 4b is the mean centerline velocity at each downstream location, U_o .

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Figure 8 – Radial profiles of mean and RMS OH LIF (solid) and CH₂O LIF (dashed) signals in flame D_{41} .

Figure 9 – Comparison of a) peak mean OH LIF signal, b) centerline mean CH_2O LIF signal and c) radial position of peak mean LIF signals in all the turbulent flames.

Figure 10 – Mean radial gradient of the axial velocity conditional on OH LIF iso-contours of 0.24. Velocity gradients are normalized by U_{bulk}/R for each flame.

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Figure 12 – PDFs of the spacing between the CH₂O and OH LIF layers in the turbulent flames. Negative values indicate that the layers are overlapping.