A Comparison of the Reactive OH Layer Structure between CH₄- and DME-Based Turbulent Non-premixed Jet Flames

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Dimethyl ether (DME) is a promising alternative to diesel fuel in compression-ignition engines and a possible substitute to natural gas in power-production applications. However, little is known about the fundamental combustion processes of DME-fueled systems under highly turbulent conditions. As a first step, laser-based imaging is used to examine the turbulent flame structure of turbulent DME flames and compare and contrast to well-characterized CH₄ flames under nearly identical conditions. Previously, we presented a series of canonical turbulent DME-fueled (Gabet et al., 2013) that were based off of the well-characterized DLR (.221 CH₄/.332 H₂/.447 N₂) jet flames that are used within TNF workshop. Using a fuel mixture of .221 DME/.332 H₂/.447 N₂ results in a jet flame with a stoichiometric mixture fraction (\(\varphi_s = 0.17\)), which is identical to the DLR flames. Thus the two flame systems can be compared directly with laser-based imaging to examine mixing, reaction zone structure, and reaction chemistry.

In this study we investigate the reactive layer structure of the two turbulent non-premixed jet flame systems at Reynolds number of 15,200 and 22,800 using OH planar laser-induced fluorescence (PLIF). The reaction layer, as represented by the OH radical distribution, provides information about flame structure and stability under various levels of turbulence regimes. By comparing OH PLIF data between "equivalent" CH₄- and DME-based flames, new insights into turbulent-chemistry interaction in the DME flames are gained. From the results, it is noted that although OH PLIF signal levels show negligible differences between the DLR and DME flames, notable differences in the structure of the OH field are observed. The OH PLIF layers within the DLR flames are much more wrinkled and display a significantly higher level of local extinction than the DME flames. At upstream axial locations near the nozzle, the OH field within the DME flames appears laminar-like, while the corresponding OH layers in the DLR flames are highly contorted and fragmented. Additional statistical analysis is presented for the flame curvature, OH layer thickness, and occurrence of local extinction as inferred from "holes" in the 2D OH layer. These results show that DME flames are affected much less by the local turbulence than the DLR flames at the same Reynolds numbers.

1. Introduction

Dimethyl ether (DME) is a promising substitute for diesel fuel in compression ignition engines. The use of DME can result in high thermal efficiencies and improved ignition properties as compared to diesel-fueled engines due to its high cetane number (Sorenson et al., 2001, Arcoumanis et al., 2008) and can be used as a "drop-in" replacement or supplement in existing CI engines. In addition, DME has shown a propensity for cleaner engine operation with decreases in particulate formation and nitrogen oxide emissions under certain conditions. Engine combustion is characterized by highly turbulent conditions, which results in complex relationships between unsteady fluid dynamics, species transport, finite-rate chemical kinetics, and non-equilibrium thermodynamics over a broad range of spatial and temporal scales. While each of these processes has received considerable attention over the last few decades, our knowledge of the effects of their complex coupling (even in laboratory-scale turbulent flames with simple fuels) remains incomplete. This combined with the potential operation of new fuels such as DME with variations in chemical and physical properties (as compared to conventional hydrocarbons) provides a formidable challenge for controlling combustion chamber processes and developing robust and predictive computational models.

DME also is an important fuel in the context of fundamental turbulent combustion research. Previously, there has been a substantial effort to obtain detailed measurements in various turbulent flames with "simple" fuels such as hydrogen and methane (Barlow, n.d.). Such measurements of velocity, temperature, and species concentrations have been used to study fundamental turbulent combustion processes and to assess and validate turbulent combustion models. In recent years, there has been a push to extend the benchmark data sets to include larger and more complex fuel
molecules. Experimentally, DME is promising due to its relatively low sooting levels, as compared to other gaseous fuels such as ethane or propane, which permits accurate non-intrusive laser-based diagnostics. In addition, DME has sufficient vapor pressures at elevated pressures such that elaborate pre-heating schemes are unnecessary (as in the case of larger, low-vapor pressure fuels), thus facilitating well-defined, canonical turbulent flames with repeatable boundary conditions and measurements with high precision (e.g. Fuest et al., 2012). Examples of recent measurements in turbulent DME flames include the 1D Raman/Rayleigh/LIF measurements of Fuest et al. (2012), planar laser-induced fluorescence (PLIF) imaging of CH\textsubscript{2}O by Gabet et al. (2013) and OH/CH\textsubscript{2}O PLIF and velocity imaging by Frank et al. (2010, 2012). Chemically, DME is the simplest ether and models describing its chemistry are manageable; that is detailed kinetic models involve less than 100 species and 500 reactions and accurate, reduced “skeletal” models involve 30 or fewer species (Zhao et al., 2008). Such reaction mechanisms are tractable for turbulent flame simulations. In this manner, DME represents one of the few “complex” or “alternative” fuels connecting chemical kinetic development, turbulent combustion modeling, and high-fidelity turbulent flame measurements. In a previous study by our research group, we reported laminar flame calculations, flame blow out conditions, CH\textsubscript{2}O PLIF and Mie scattering imaging in a set of “equivalent” methane- and DME-based flames to qualitatively compare and contrast compositional structure and turbulent flame behavior (Gabet et al., 2013). Starting with the well-known DLR jet flames (22.1%CH\textsubscript{4}/33.2%H\textsubscript{2}, 44.7% N\textsubscript{2}; Bergmann et al, 1998; Meier et al, 2000), the methane was directly replaced by DME, resulting in a second flame system with composition of 22.1% DME, 33.2% H\textsubscript{2}, and 44.7% N\textsubscript{2}. It is noted that this fuel composition results in the same stoichiometric mixture fraction (\(\xi_s = 0.17\)) as the DLR flames and when operated at the same Reynolds numbers, the two flame configurations represent a unique set of target flames for “direct” comparisons and turbulence-chemistry interaction investigations. The laminar flame calculations showed significant differences between the two flame systems in terms of fuel decomposition and consumption reactions including very rapid pyrolysis of DME which led to large levels of CH\textsubscript{2}O and H\textsubscript{2} under richer mixture fraction conditions. Flame blow out studies showed that the DME flames were more robust under high Reynolds number conditions and blew out at Reynolds numbers that were approximately 40% higher than the DLR flames. CH\textsubscript{2}O PLIF results showed that DME-based flames yielded CH\textsubscript{2}O signals that were approximately two orders of magnitude higher than the corresponding DLR flames. Furthermore, it was shown that CH\textsubscript{2}O was consumed more rapidly within the lower-temperature regions in the DME flames indicating more active low-temperature oxidation processes than the methane-based DLR flame.

In this paper, we present OH PLIF imaging results from the two flame configurations to examine differences in the turbulent flame structure with an emphasis on the high-temperature reaction layers in the upstream regions nearest the fuel nozzle. Although in general OH is characterized by rapid formation and slow three-body destruction reactions (which make it more suitable for marking high-temperature species transport), OH regions in the high-strain rate, near-field of non-premixed flames provide a suitable marker for the high-temperature reaction zone (Bergmann et al., 1998). In this manner, the instantaneous OH PLIF images provide a means for statistical analysis of the effects of turbulence on flame structure including flame (OH layer) curvature, OH layer thickness, and local flame (OH layer) extinction.

### 2. Experimental Methods

#### Flame Conditions:

The DLR and DME flames were operated at two Reynolds number conditions, Re = 15200 and Re = 22800, denoted flames “A” and “B”, respectively, following the convention previously established for the DLR flames (Bergmann et al, 1998; Meier et al, 2000). The composition of each flame is listed in Table 1. The “DLR” flames are operated with a composition of 22.1% CH\textsubscript{4}, 33.2% H\textsubscript{2}, and 44.7% N\textsubscript{2} to match the target cases that appear as part of the TNF workshop (Barlow et al., n.d.). For the DME flames, the methane was directly replaced by the DME, while keeping the mole fractions of the H\textsubscript{2} and N\textsubscript{2} the same as the DLR flames. This mixture resulted in a stoichiometric mixture fraction (\(\xi_s = 0.17\)) that is identical to that of the DLR flames. For all flames, the fuel mixture issued from a 0.8-cm-diameter tube into a 30 cm x 30 cm low-speed co-flowing stream of air at 0.3 m/s. The Reynolds numbers for A and B cases were calculated based on the diameter of the nozzle and all flames were operated within the same burner facility.

#### OH PLIF System:

A schematic of the OH PLIF system is shown in Fig. 1. The second harmonic-(532-nm-) output of an Nd: YAG laser (Continuum Surelite) with energy of 150 mJ/pulse was used to pump a dye laser (Lambda Physik) operating with Rhodamine 590 dye. The 566-nm dye-laser output was frequency-doubled with a BBO crystal to obtain 2.2 mJ/pulse at 283 nm. The dye laser was tuned such that the frequency-doubled UV output excited the Q(7) transition of the A'\Sigma^+ \rightarrow \Pi^+(1, 0) band of OH located at 283.31 nm. The 283.3 nm beam passed through a Galilean telescope and a set of sheet forming optics (cylindrical + spherical lenses) to produce a 50-mm tall laser sheet for OH PLIF imaging.
Table 1 Flame Configurations

<table>
<thead>
<tr>
<th>Flame</th>
<th>$X_{\text{CH}_4}$</th>
<th>$X_{\text{DME}}$</th>
<th>$X_{\text{H}_2}$</th>
<th>$X_{\text{N}_2}$</th>
<th>$Re_D$</th>
<th>$\xi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DLR A</td>
<td>0.221</td>
<td>-</td>
<td>0.332</td>
<td>0.447</td>
<td>15200</td>
<td>0.167</td>
</tr>
<tr>
<td>DLR B</td>
<td>0.221</td>
<td>-</td>
<td>0.332</td>
<td>0.447</td>
<td>22800</td>
<td>0.167</td>
</tr>
<tr>
<td>DME A</td>
<td>-</td>
<td>0.221</td>
<td>0.332</td>
<td>0.447</td>
<td>15200</td>
<td>0.169</td>
</tr>
<tr>
<td>DME B</td>
<td>-</td>
<td>0.221</td>
<td>0.332</td>
<td>0.447</td>
<td>22800</td>
<td>0.169</td>
</tr>
</tbody>
</table>

The OH emission from the A-X(1, 1), (0, 0) and B-X (0, 1) bands between 306 nm and 320 nm was detected by a lens-coupled ICCD camera system (PCO Sensicam CCD + LaVision IRO). The field-of-view for the ICCD camera system was 4.2 cm x 5.6 cm, resulting in a magnification of 0.08 or 82 mm/pixel. The combination of an f/1.8, 100-mm focal length UV camera lens (Cerco) and WG 305 longpass filter were mounted onto the ICCD to collect the OH PLIF emission and discriminate it from the background flame luminosity. Timing of all the devices was controlled by a function generator which synchronized the Nd:YAG laser to both the CCD camera and the lens-coupled intensifier. To further reduce the background signal, the image intensifier was gated for a short period of 100 ns with a camera shutter time of 500 μs.

Figure 1 - Schematic of the experiment setup for OH PLIF imaging.

Data Processing:

OH PLIF images were taken at axial positions of $x/d = 7, 10, 20, 30, 40, \text{ and } 60$ downstream of the fuel nozzle, where $d$ represents the diameter of nozzle. In this paper, statistical results are presented for $x/d = 7, 10, \text{ and } 20$. An average background image was first removed from the images, followed by a correction for spatial non-uniformities in intensity of the laser sheet. The average intensity distribution from a set of 200 laminar flame images was used as the intensity normalization within the turbulent flame images. Three hundred OH PLIF images were taken per axial position and were used to determine the mean and RMS fluctuations of the image sets. As noted above, several topographical flame characteristics were extracted from the data sets including OH layer curvature, OH layer thickness, and the probability of a “flame hole”, which was determined as a local discontinuity in the OH layer. Flame curvature is an important parameter which characterizes the effects of the local fluid strain on the reaction zone behavior, while flame thickness (inferred from OH layer thickness in this paper) is a notable parameter to study the coupling between the turbulent flow and flame chemical kinetics since flame stretching (due to large eddies) leads to thinner reaction zones and small eddies can enhance mixing to “thicken” the observed reaction zones.

First, the OH PLIF images were converted to a binary image (0 or 1) by defining a threshold as 10% of the peak signal intensity. In this manner, all pixels with counts less than 10% of the peak intensity were defined as zero and all other pixels were defined as one. Next, the edges of OH layer were extracted for calculating curvature and OH layer thickness. The local curvature of the OH layer was calculated by fitting a second order polynomial function to twenty sequential points. Negative curvature indicated the edge of the OH layer was turning toward the centerline of flame, while positive curvature indicated the edge was turning away from the centerline of flame.
calculated from the two outside contours that defined the local OH layer. A local normal vector was determined at each point along the OH layer, and the distance between the projection points along the normal vector to the opposite side of the OH layer contours were defined as the local OH layer thickness. In order to estimate local extinction effects in each flame, the number of two-dimensional OH layer holes were determined in each image and analyzed statistically. A “hole” was defined as a region where two continuous OH layers were completely disconnected from one another.

Results and Discussion

Figure 2 shows a comparison of typical instantaneous OH PLIF images in the DLR and DME flames at axial positions of x/d = 10, 20, 30, 40, and 60, and a Reynolds number of 22,800 (“B” flames). It is noted that none of the images were obtained simultaneously. The photographs in the middle of Fig. 2 are visible flame images from both the DLR B and DME B flames demonstrating the apparent similarity between the two flame configurations. However, from the OH PLIF images, it is noted that the DLR flames appear more wrinkled, with what appears to be significantly higher levels of local extinction (i.e., “holes” in the OH layer) than the DME-based flames. Simply put, it appears that the local turbulence is affecting the DME-based flames much less than the DLR flames. For example, at x/d = 10, the DME-based flame looks almost “laminar-like”, while the DLR flame is highly strained, wrinkled, and segmented. This agrees with the limited previous DME flame studies (Fuest et al., 2012, Frank and Coriton, 2012, Gabet et al, 2013) that show that DME appears to be more robust at high Reynolds numbers as compare to similar methane-based flames.

Figure 3 shows the mean and RMS OH PLIF intensity profiles for both DLR and DME flames A and B at x/d = 7. For the mean profiles, all results have been normalized by peak intensity of the mean profile for each respectively flame and the DLR flames have

![Figure 2](image_url)  
 Instantaneous OH PLIF images in Re = 22,800 CH4/N2/H2 and DME/N2/H2 flames. The photographs in the middle of the image show visible flame images of both the DLR B and DME B flames.

![Figure 3](image_url)  
 (Top) Mean OH PLIF profiles in the DLR and DME flames at x/d = 7. (Bottom) Normalized RMS fluctuation profiles in the DLR and DME flames at x/d = 7. The RMS profiles are normalized by the peak mean OH PLIF intensity.
been scaled to match the peak values of the mean DME profiles. The RMS intensities have been normalized by the peak of the mean profiles for each flame, respectively. First, it is noted that the peak mean intensity of OH is significantly higher in the DME flames as compared to the DLR flames. For example, the DLR profiles had to be scaled by 1.53 and 1.44 for flames A and B, respectively to match the peak mean values of the DME flames. While PLIF signals are a function of many parameters, it is expected that in these flames, the relative intensity between the two flames is proportional to a relative number density between the two flames. In this manner, the peak, spatially-averaged OH number density is much higher in the DME flames as compared to the DLR flames; however, it is noted that peak values in the instantaneous images were quite similar between the two flame configurations. This indicates that while instantaneous OH values may be similar between the DLR and DME flames, the DLR flames are more subject to spatial fluctuation due to more intense interactions with the local turbulent flow field. This is consistent with the “broader” mean OH profiles of the DLR flames as compared to the DLR flames and the higher relative RMS fluctuations of the DLR flames as compared to the DME flames at x/d = 7. For example, for DLR flame A, the peak RMS fluctuation of the OH signal is approximately 80% of the peak mean, while the RMS fluctuation is only 50% of the peak mean for DME flame A. Similar fluctuation levels are noted for DLR flame B and DME flame B as well.

At x/d = 10 (not shown), the OH profiles show the largest difference between the DLR and DME flames for the “A” flames, but the “B” flames are more similar to each other than at x/d = 7. For example, the peak OH intensity is approximately 60% lower in DLR flame A as compared to DME A and the relative RMS fluctuation is ~ 90% of the peak mean value for DLR A, while it is ~ 50% for DME A. The profiles of both the mean OH PLIF intensity and the RMS fluctuation are much broader than the DME cases. For the “B” flames, the peak mean OH intensity is ~ 30% lower in the DLR flame as compared to the DMR flame. While the relative RMS fluctuation still is ~ 90% of the peak mean for DLR flame B (as compared to DLR flame A), the relative RMS fluctuation for DME flame B has now increased to ~ 70% of the peak mean value. At x/d = 20, there is only 10% difference between the peak mean OH intensities and the relative RMS fluctuation between the DLR and DME “A” flames. For the “B” flames, the peak mean intensities and the relative RMS fluctuations are essentially identical. These results suggest that at the lowest axial positions, where strain rates are highest and the turbulence-chemistry interaction is most vigorous, the DME flames are more robust, but at downstream locations, where strain rates have presumably decreased, the DLR and DME exhibit similar characteristics in terms of mean and RMS fluctuations.

Figure 4 shows the probability density function (pdf) of the OH layer thicknesses at x/d = 7, 10, and 20 for the DLR A and DME A flames. For the Re = 15,200 cases, the median of the distribution is ~ 2 mm for the DLR flame and ~ 3 mm for the DME flame. In addition, the DLR flames exhibit a higher probability of smaller OH layer thicknesses (< 3 mm) and a longer tail exponential tail that decays slower than that of the DME flames. Both of these factors are quite indicative of the larger influence of the flow field turbulence on the OH layer structure in the DLR flames as compared to the DME flames. The higher probability of “thin” OH layer thicknesses in the DLR flames indicates the presence of larger eddies interacting with the OH layers, acting to “stretch” and thin the layers. This is consistent with the instantaneous images, which show higher levels of wrinkling in the DLR flames as compared to the DME flames. The higher probability of “thick” OH layers in the DLR flames (as compared to the DME flames) indicates the interaction of smaller eddies that act to enhance local mixing to “thicken” the observed OH layers (an indication of high-temperature regions) or may indicate some probability of small eddies penetrating the OH zone to directly thicken them. The “B” flame cases (not shown) are qualitatively similar, although the differences between the DLR and DME flames are much

Figure 4 – Probability density function (pdf) of OH layer thickness in the DLR A and DME A flames.
smaller. In any manner, the observed pdfs (especially in the “A” flame cases) indicate the stronger coupling between the turbulent flow field and the reaction chemistry/species transport in the DLR flames as compared to the DME flames.

Figure 5 shows the probability density functions (pdf) of the OH layer curvature at x/d = 7 and x/d =10 for the “A” flame cases. The top figures display the pdf in linear axes and the bottom figures are presented in a semi-log plot to highlight the tails of the pdf. Consistent with the previous results, DME flame A has a higher probability of small absolute curvatures (near zero) and a narrower distribution of curvature as compared to the DLR flame A results. It is noted that a curvature of near zero would be consistent with that of a laminar flame, with OH layers oriented parallel to the axial flow direction. Although not shown, the “B” cases exhibit the same qualitative trends as the “A” cases, although the differences between the DLR and DME flames are much less than those of the “A” cases. The overall conclusion from these topographical results is that the DME is more laminar-like and less wrinkled (or less affected by the local turbulent flow field) for the DME flames as compared to the DLR flames for an equivalent Reynolds number. The differences are the greatest at the lower Reynolds number operating case.

Finally, Figs. 6 and 7 display the probability distribution of OH layer “holes” existing within an image in flames A and B, respectively. As discussed in Sec. 2, the definition of OH layer holes is more intuitional/observational than theoretical as it characterizes the appearance of an OH disconnection which presumably is attributed to local flame extinction. Since the OH PLIF imaging results are two-dimensional, the disconnection of OH layer in the image does not necessarily imply that the flame is actually inconsistent, but could be connected in the out-of-plane dimension. For the Re = 15,200 cases, there is essentially no probability of finding a complete discontinuity or “hole” in the OH layer at x/d = 7 in the DME A flame, while the most probable number of OH layer holes is between 1 and 2 in the DLR A flame. Further downstream at axial positions of x/d = 10 and 20, the probable number of holes increases for both the DLR and DME flames, but at an increasing rate for the DLR flame. The average number of holes within the OH layers per image for the DLR flames is 1.2, 1.5, and 2.4 at x/d = 7, 10, and 20, respectively. For the DME A flame, the average number of OH layer holes per image is < 0.1, 0.1, and 0.5 at x/d = 7, 10, and 20, respectively. An interesting observation is that for the DLR B flame, the distribution of number of OH layer holes remains fairly constant as a function of axial position, with mean values of 3.8, 3.9, and 4.0 at x/d = 7, 10, and 20, respectively. In contrast, the DME flame B exhibits the same trends as the DLR and DME A flames; that is, there is an increasing probability of finding an OH layer hole with increasing axial position. The average number of OH layer holes per image for the DME B flame is 0.4, 0.5, and 1.4 at x/d = 7, 10, and 20, respectively.

3. Conclusions
This paper focused on the comparison of the reactive OH layer structure of the well-characterized DLR series of target jet flames with “equivalent” DME-based jet flames. The DME-based flames have been carefully matched to DLR flames in order to examine similarities and differences in turbulent flame structure. The observation of OH layer behavior was consistent with the previous CH2O imaging and blow out results (Gabet et al., 2013) in that the DME flames were more robust than DLR at the same Reynolds number. In this paper, statistical descriptions of the OH layer thickness, OH layer curvature, and OH layer “holes” (presumably local flame extinction sites) showed tangible
Figure 6 – Probability density function (pdf) of the existence of OH layer holes in an instantaneous OH PLIF image for DLR and DME flame A.

Figure 7 – Probability density function (pdf) of the existence of OH layer holes in an instantaneous OH PLIF image for DLR and DME flame B.
differences in the flame structure between the two flame systems, with significant differences occurring at the lowest Reynolds number (Re = 15,200) condition. The methane-based, DLR flames display higher probability of both thinner and thicker OH layer distribution, presumably due to higher levels of interaction with the local turbulent flow field. The DLR flames display higher probability of larger positive and negative curvature and number of OH layer holes per image. Future work includes simultaneous PIV and OH PLIF to directly examine the relationship between the local turbulent flow field (and its derivatives) and the OH layer structure.

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References