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Effects of Fuel Molecular Weight on Emissions in a Jet Flame and a Model Gas Turbine Combustor

The objective of this study is to understand the effects of fuel volatility on soot emissions. This effect is investigated in two experimental configurations: a jet flame and a model gas turbine combustor. The jet flame provides information about the effects of fuel on the spatial development of aromatics and soot in an axisymmetric, co-flow, laminar flame. The data from the model gas turbine combustor illustrate the effect of fuel volatility on net soot production under conditions similar to an actual engine at cruise. Two fuels with different boiling points are investigated: n-heptane/n-dodecane mixture and n-hexadecane/n-dodecane mixture. The jet flames are nonpremixed and rich premixed flames in order to have fuel conditions similar to those in the primary zone of an aircraft engine combustor. The results from the jet flames indicate that the peak soot volume fraction produced in the n-hexadecane fuel is slightly higher as compared to the n-heptane fuel for both nonpremixed and premixed flames. Comparison of aromatics and soot volume fraction in nonpremixed and premixed flames shows significant differences in the spatial development of aromatics and soot along the downstream direction. The results from the model combustor indicate that, within experiment uncertainty, the net soot production is similar in both n-heptane and n-hexadecane fuel mixtures. Finally, we draw conclusions about important processes for soot formation in gas turbine combustor and what can be learned from laboratory-scale flames. [DOI: 10.1115/1.4037928]

Introduction

The increasing demand for aviation fuels, unstable fuel prices, stricter environmental rules, and need for energy security have led to an increased interest in alternative jet fuels. Extensive research in alternative jet fuels has led to approval of Fisher-Tropsch fuel (Annex 1 ASTM D7566) and hydrosprocessed renewable jet (Annex 2 ASTM D7566) to be used as blended fuels with current petroleum-derived jet fuels [1]. The components of the new alternative fuels may have very different molecular weights and structures than those of the currently approved fuels [2]. This variation in the fuel molecular-structure distribution generates new interest in understanding the effects of fuel composition on operability of current and future gas turbine engines.

The research efforts in the current project aim to aid in developing fundamental understanding of the effects of fuel molecular structure on emissions. To achieve this goal over a wide range of experimental conditions, a series of experiments and companion simulations were planned that progress in their level of complexity from simple laboratory flames to sector rigs [3]. The study at Penn State involves understanding the chemical effect of fuel molecular structure on aromatics and soot in jet flames, and testing the effect of fuel volatility on emissions in a model gas turbine combustor. The chemical effects of fuel molecular structure on soot have been discussed in Refs. [4] and [5].

The primary aim of the work presented here is to understand the effect of fuel volatility on emissions in an actual engine-like environment. The hypothesis of the study is that fuels with varying volatility will affect fuel droplet vaporization processes and hence, on fuel–air mixing and emissions. A fuel with a higher boiling point, i.e., a heavier hydrocarbon fuel, is expected to produce larger initial droplet sizes than a lighter hydrocarbon [6,7]: if the droplet vaporization time is longer than the convention time of the droplet from the injector exit to the flame front, the droplets will burn in a diffusion flame at a stoichiometric condition. As a result of this potentially incomplete vaporization, a heavier hydrocarbon fuel will likely have higher soot emissions as compared to a fuel with a lower boiling point.
In addition to testing the fuels in the model gas turbine combustor, the chemical effect of the two fuel mixtures on the aromatics and soot is investigated in a laminar, co-flow, axisymmetric burner under nonpremixed and rich premixed condition at atmospheric pressure. The aromatics are not only soot precursors, but are also classified as hazardous air pollutants themselves [8]. Nonpremixed flames play an important role in practical combustion systems; these flames display all major soot formation processes, which include soot nucleation, growth, and burnout processes, similar to those in real engines. The rich premixed conditions are selected in order to mimic conditions similar to those in the primary zone of an aircraft engine combustor. The n-alkane fuel mixtures studied here include n-heptane/n-dodecane (C7) and n-hexadecane/n-dodecane (C10) fuels. The fuel selection and experimental conditions are discussed in the Experimental Setup section. The C7 results are also discussed in more detail in Refs. [4] and [5]; we use them here as a means to understand fuel molecular weight and volatility effects, which are not discussed in Refs. [4] and [5].

Previous studies have investigated the soot development of higher-hydrocarbon fuels [9–11]. The n-hexadecane fuel, studied here, is representative of the molecular weight of components of jet fuel [12] and diesel fuel [13]. For example, Eddings et al. [14] studied a six component surrogate (Hex-11 and Hex-12) as a possible surrogate to match the volatility (the boiling point distribution) and sooting tendency of JP-8. The Hex-11 and Hex-12 had 5 mol % and 12 mol % of n-hexadecane as one of the surrogate components, respectively. The sooting limit and polycyclic aromatic hydrocarbons (PAH) formation of n-hexadecane has been studied in a microflow reactor at equivalence ratios of 1.5–4.5, and 4, respectively [15]. Pastor et al. [16] studied mixtures of n-decane and n-hexadecane fuels in a diesel engine. They found an increase in the n-hexadecane concentration resulted in an increase in the amount of soot formed in the flame. Douce et al. [16] studied soot formation from n-hexadecane in a shock tube. However, to the best of our knowledge, no study has reported aromatics and soot formation in both nonpremixed and rich-premixed jet flames involving n-hexadecane as a fuel. The results from the jet flame studies provide important validation-quality data for soot models.

The goal of this work is to understand the impact of fuel molecular weight on soot, and to compare laboratory flame results and the behavior of these fuels in actual gas turbines. The remainder of the paper presents the experimental configurations used in this study, as well as the measurement techniques. We provide details of the soot formation and oxidation processes in the laboratory flame, with quantitative measurements of soot volume fraction for the two fuels. Finally, we compare these soot measurements from jet flames to the model gas turbine combustor results. The results presented here on soot volume fraction in jet flames can be used to test chemical mechanisms and soot models for n-hexadecane in a well-characterized configuration. In addition, the results obtained from the model gas turbine combustor provide validation data for soot emissions in an environment similar to a gas turbine engine.

**Experimental Setup and Techniques**

**Laminar Flame Experiment.** The effect of fuel molecular weight on the spatial development of aromatics and soot is investigated in an axisymmetric, co-flow, laminar flame configuration at atmospheric pressure. The burner design is similar to the co-annular burner used by Santoro et al. [17]. The burner design is modified to operate it using prevaporized higher hydrocarbon fuels. The fuel tube is 4 mm above the exit plane of the burner. The vaporized fuel is carried by nitrogen gas from the vaporization unit to the burner exit. The energy for fuel vaporization is provided by several heating tapes wrapped around the outside surface of the tubing system. The air inlet, which is only used to study premixed flames, is situated after the two vaporization units. The temperature of the system is maintained at 300 ± 10 °C to prevent fuel condensation in the system. The gas chromatography analysis of the recondensed fuel from the tube exit indicates absence of fuel pyrolysis in the tubing system. The further details of the burner system are described in Ref. [4].

The co-flow air is set at a constant flow rate of 4 scfm. The flame is shielded from the surroundings using a brass chimney (400 mm long) with screens on the top. Four slots are machined at symmetrical locations on the chimney to provide access for the measurement techniques. A stepper motor (Velmex PK266) and a Velmex bislide, with step resolution of 6.5 μm and 5.00 μm, are used to move the burner in the horizontal and vertical directions, respectively.

The two-dimensional (2D) soot volume fraction in the jet flames is obtained using laser-induced incandescence (LII) [18]. The LII is calibrated using laser extinction (LE). The 2D aromatics profile is obtained using laser-induced fluorescence (LIF). The optical setup, data collection, and analysis of measurement techniques used in this study are identical to that described in Refs. [4] and [5]. A brief description of the technique is provided here. The LII is obtained using a Nd:YAG laser (Spectra Physics GCR 270-10, 10 Hz, 7 ns, 532 nm). The laser beam is expanded into a laser sheet and focused on the flame center using a combination of a plano-convex cylindrical lens and a convex lens. The laser fluence is maintained at 0.3 J/cm² to be in the “plateau” region of LII [18] for the LII experiment. In the LIF experiment, a 266 nm, 585 μJ laser pulse from the Nd:YAG laser is used for exciting the aromatic molecules.

The LII and LIF signal is recorded using a Princeton Instruments ICCD camera with a sensor size of 512 × 512 pixels using an f/2.8 105 mm UV lens. A spatial resolution of 0.1 mm/pixel of camera is achieved using the optical setup. The LII signal is collected using a narrow band interference filter centered at 430 nm with 10 nm FWHM [19]. The LII signal collection duration is 100 ns, after a delay of 20 ns following the laser pulse. For LIF signal collection, camera gate-width is 170 ns; the camera gate is opened 20 ns before the laser pulse. The study by Zizak et al. [20] found that the fluorescence wavelength shifts to longer wavelength as the aromatic molecule size increases. This property is implemented in the current study to identify two different classes of aromatics. The signal for the small (one and two ring) aromatics is obtained using two filters (WG5320 and UG11), which have transmission in the wavelength band 320–380 nm. The signal for large (three–five ring) aromatics is obtained using a filter (500FS20-50), which has transmission in the wavelength band of 380–500 nm.
488–514 nm. The small and large aromatics are further discussed in Ref. [4]. The LII and LIF signals are corrected for background noise, pixel-to-pixel responsivity of the detector, and variation in the laser intensity across the laser sheet.

A calibration factor of 3350 LII counts equals 1 ppm of soot is obtained using LE. A value of \( m = 1.57 - 0.56i \) is used as the refractive index of soot to be consistent with previous published work [19,21]. The estimated uncertainty in soot volume fraction measurement through laser extinction and calibration of LII data is ±15%. The measurement uncertainty are discussed in detail in Refs. [4] and [5]. The LIF measurements are presented as raw counts, because the fluorescence in each wavelength band is collected from a number of aromatic species; the fluorescence quantum yield and temperature dependency of absorption cross section of each aromatic species are not well characterized.

Model Gas Turbine Combustor. In practical devices like gas turbine engines, the physical properties of the fuel can have an important impact on the engine’s performance. Experiments in a model gas turbine combustor can help to understand the fuel volatility effect on emissions in a realistic combustion device. The schematic of the model gas turbine combustor is shown in Fig. 2. It consists of two sections: the inner section where the combustion occurs and the outer co-flow section for regenerative cooling.

The compressed air from the air delivery system enters the outer co-flow section of the combustor. The passage through this section preheats the air, thereby cooling the quartz window on the combustor chamber and removing heat from the exhaust stream. The preheated air then enters an electric heater, where it can be heated to a maximum temperature of 800 K. The heated air enters the combustion chamber after passing through a 7.39 mm inlet vent and a 45 deg flat vane swirler. The schematic of the air swirler is shown in Fig. 3. The geometric swirl number based on Ref. [22] is 0.77.

The liquid fuel injector used in this study is the same as used in Ref. [21], shown in Fig. 4. It consists of two concentric stainless steel tubes. The liquid fuel under pressure from the fuel delivery system enters the inner tube of the injector and is forced out through the 0.005 in diameter, 12 radial injector holes. The injection point is 36.8 mm upstream of the dump plane. A part of the primary air is diverted to flow through the annular region surrounding the inside tube of the injector to prevent the fuel from vaporizing inside the inner tube. The annulus is tapered at the end to create a shearing force to break the liquid fuel into small droplets. A stainless steel bluff body is attached at the end of the injector for flame anchoring.

The fuel–air mixture then flows into the 45 mm diameter, 307 mm long combustion chamber. The combustion products exit the combustor through a choked nozzle. The choked inlet and outlet help to isolate the impact of combustion instabilities on inlet air or fuel flow rate and inhibit pressure oscillations from the exit section to propagate to the combustion zone. The exit nozzle is maintained at a temperature of 480 K using air and water cooling. Two quartz windows of 12.5 mm in diameter are installed at the exit of the combustor to provide optical access for laser extinction technique. The quartz windows are purged with nitrogen gas to maintain the temperature of the windows and prevent soot deposition on them.

Line-of-sight soot volume fraction is measured at the exit of the combustor, 24.8 cm downstream of the dump plane. The LE
lent mixing, and spray as is present in a real combustor operating under the same experimental conditions. The experimental conditions for the model gas turbine combustor are outlined in Table 2. The experimental conditions for model combustor, respectively. The global equivalence ratio \( \Phi_{\text{global}} \) is varied from 0.9 to 1.8 by changing the fuel flow rate. An exit nozzle of 10.2 mm diameter is used to choke the flow to create a mean chamber pressure of 0.51 MPa. The combustor chamber pressure is held steady at 5 atm, within measurement uncertainty, for \( \Phi_{\text{global}} \) from 0.9 to 1.8. The flames are both statically and dynamically stable under these operating conditions. The fuels used had purity of >99% and 95% for the jet flame experiment and the model combustor, respectively.

### Fuel Selection and Experimental Matrix

The fuel matrix, shown in Table 1, is comprised of two binary mixtures: \( n \)-heptane/\( n \)-dodecane and \( n \)-hexadecane/\( n \)-dodecane, a high boiling point fuel; \( n \)-hexadecane has a boiling point of 287°C as compared to 216°C for \( n \)-dodecane and 98°C for \( n \)-heptane. The two binary mixtures are chosen such that the carbon fraction of \( n \)-dodecane and the added hydrocarbon is constant.

The flames investigated are nonpremixed (jet equivalence ratio \( \Phi_{\text{jet}} = \text{Inf} \)) and rich premixed (\( \Phi_{\text{jet}} = 24 \) and 6). The total carbon flow rate is held constant for all the flames at 0.011 mol/min. The carbon flow rate is defined as the summation of the product of each component flow rate and the corresponding number of carbon atoms. The carbon flow rate is fixed to match carbon flow from the base flame, a 75% \( n \)-dodecane and 25% \( n \)-xylene mixture [4]. The flow rate of nitrogen, 0.2 slpm, is used to carry the vaporized fuel to obtain a stable flame.

The effect of fuel volatility on soot emissions, for the fuels listed in Table 1, is investigated in a model gas turbine combustor. This experiment replicates the complexity of bulk mixing, turbulent mixing, and spray as is present in a real combustor operating on liquid fuels. The combustor has been used in previous studies on combustion instablility, soot, and emissions [21,23]. In addition to the two binary fuel mixtures, JP-8 (POSF 5699) fuel is tested to compare the results obtained in this study to previous published data [21], which involved testing of soot emission from JP-8 under the same experimental conditions. The experimental conditions for the model gas turbine combustor are outlined in Table 2. The air mass flow rate and inlet temperature are kept constant at 32 g/s and 560 ± 10 K for all the fuels tested. The inlet air temperature is measured at the location upstream of the critical venturi.

The soot production can be impacted by the fuel droplet size and droplet evaporation time. The initial droplet size depends on the type of injector used [6]. For a particular size droplet, the droplet evaporation time would depend on the initial temperature of the droplet and the adiabatic flame temperature. A higher inlet temperature would increase the adiabatic flame temperature, which would result in faster droplet evaporation. The faster evaporation results in less premixed combustion, leading to less soot production. The inlet air temperature is held constant for all the flames, C

### Table 1 Fuel matrix

<table>
<thead>
<tr>
<th>Name</th>
<th>Component</th>
<th>Volume fraction (%)</th>
<th>( H_2 ) content (%)</th>
<th>( H/C ) ratio</th>
</tr>
</thead>
</table>
| C

<table>
<thead>
<tr>
<th>Inf</th>
<th>( C_6 )-heptane</th>
<th>31.3</th>
<th>15.6</th>
<th>2.20</th>
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<tr>
<td>C16</td>
<td>( C_6 )-hexadecane</td>
<td>28.4</td>
<td>15.4</td>
<td>2.15</td>
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<tr>
<td>C16</td>
<td>( C_6 )-dodecane</td>
<td>71.6</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Table 2 Experimental conditions for model gas turbine combustor

<table>
<thead>
<tr>
<th>Condition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air mass flow rate</td>
<td>32 g/s</td>
</tr>
<tr>
<td>Inlet air temperature</td>
<td>560 ± 10 K</td>
</tr>
<tr>
<td>Injector</td>
<td>MP, 12 hole, 0.005 in diameter</td>
</tr>
<tr>
<td>Swirl angle</td>
<td>45 deg</td>
</tr>
<tr>
<td>Chamber pressure</td>
<td>0.51 MPa (5 atm)</td>
</tr>
<tr>
<td>Chamber length</td>
<td>307 mm</td>
</tr>
</tbody>
</table>

### Results and Discussion

**Laminar Flame: Visible Flame Heights.** Figure 5 shows the visible flame images for all the flames obtained using a Canon camera at some operating settings (ISO = 80, f-stop, and exposure time). From left to right, the flames are C

<table>
<thead>
<tr>
<th>Flame</th>
<th>Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_7 )-inf</td>
<td>(a) ( C_7 )-jet = Inf</td>
</tr>
<tr>
<td>( C_7 )-phi24</td>
<td>(b) ( C_7 )-jet = Inf, ( C_7 )-phi24 = 24</td>
</tr>
<tr>
<td>( C_7 )-phi6</td>
<td>(c) ( C_7 )-jet = 24, ( C_7 )-phi6 = 6</td>
</tr>
<tr>
<td>( C_16 )-phi24</td>
<td>(d) ( C_16 )-jet = 24, ( C_16 )-phi24 = 6</td>
</tr>
<tr>
<td>( C_16 )-phi6</td>
<td>(e) ( C_16 )-jet = 6</td>
</tr>
<tr>
<td>( C_16 )-phi6</td>
<td>(f) ( C_16 )-jet = 6</td>
</tr>
</tbody>
</table>

Fig. 5: Visible flame images obtained at same camera operating condition: (a) \( C_7 \)-jet = Inf, (b) \( C_7 \)-jet = Inf, (c) \( C_7 \)-jet = 24, (d) \( C_16 \)-jet = 24, (e) \( C_7 \)-jet = 6, and (f) \( C_16 \)-jet = 6.

In this work, the flame height is defined as the distance from the tube exit to the flame tip. The flame tip is obtained from the visible flame images, shown in Fig. 5. The flame tip has a fluctuation of ±2 mm over the duration of the experiment. At a particular \( \Phi_{\text{jet}} \) within measurement uncertainty, the flame heights are similar for both the fuels. As the level of premixing is increased, the flame height decreases. The flame heights decrease by approximately 18% for both the fuels from the \( \Phi_{\text{jet}} = \text{Inf} \) condition to \( \Phi_{\text{jet}} = 6 \) condition. In these six buoyancy-driven flames, the similar flame height, at a particular \( \Phi_{\text{jet}} \) indicates that the residence time in the flame for soot formation and oxidation is similar for the two fuels, if the soot nucleation is at similar height above burner (HAB).

**Laminar Flame: Development of Aromatics.** Figure 6 shows the 2D spatial development of small aromatics for the two fuels at three different \( \Phi_{\text{jet}} \). In all the 2D LIF and soot volume fraction figures comparing the six flames, Figs. 6(a)-6(f) show the 2D profiles for \( C_7 \)-jet = Inf flame, \( C_7 \)-jet = Inf flame, \( C_7 \)-phi6 = 24 flame, \( C_16 \)-jet = 24 flame, \( C_16 \)-jet = 6 flame, and \( C_16 \)-phi6 = 6 flame, respectively. The minimum and maximum value of the scale are shown on the top of each figure, for example, [0 27,000], [0 15,000], and [0 6] means the lowest value of the scale is 0; 27,000, 15,000, and 6 corresponds to the maximum value of the scale. At a particular \( \Phi_{\text{jet}} \), the 2D profiles are plotted...
on the same scale for the two fuels. However, the scale is different for the three $\Phi_{\text{jet}}$ to show the effect of premixing on the spatial development of small aromatics, large aromatics, and soot distinctly.

In Fig. 6, an iso-contour of approximately 15% of the peak LIF count is shown in white on the 2D plots for the three $\Phi_{\text{jet}}$ to distinguish the spatial extent of the small aromatics for the two fuels. Figures 6(a) and 6(b) show that the spatial distribution of the small aromatics is similar for both the fuels under nonpremixed condition; however, the peak small aromatics LIF count is approximately 35% higher in the C$_{16}$ fuel as compared to the C$_{7}$ fuel. The first location of the detection of small aromatic LIF signal is similar for both the fuels; the small aromatics LIF signal is visible in the flame annular region at approximately 3 mm HAB and at 6 mm HAB on the flame centerline. The LIF signal from small aromatics initially increases as the one and two ring aromatic species formation processes are dominant. Further downstream, the signal peaks and then decreases as the small aromatics consumption processes through oxidation or formation of larger aromatics are dominant.

Figures 6(c) and 6(d) shows that for the $\Phi_{\text{jet}} = 24$ condition, the spatial distribution of small aromatics is similar for the two fuels; the small aromatics LIF signal is first detected in the annular region at lower HAB at approximately 4 mm HAB as compared to 7 mm HAB on the flame centerline. Similar to the $\Phi_{\text{jet}} = \text{Inf}$ flame, the peak small aromatics LIF count is higher in the C$_{16}$ flame as compared to the C$_{7}$ flame by approximately 30%. The small aromatics spatial distribution for the two fuels at the $\Phi_{\text{jet}} = 24$ condition is similar to the $\Phi_{\text{jet}} = \text{Inf}$ condition. However, for the two fuels, the peak count of small aromatics decreases at $\Phi_{\text{jet}} = 24$ as compared to the corresponding $\Phi_{\text{jet}} = \text{Inf}$ flame.

With increased level of air addition to the fuel, at $\Phi_{\text{jet}} = 6$ shown in Figs. 6(e) and 6(f), the spatial distributions and the peak level of small aromatics are similar in both the fuels. It could be possible that the LIF technique is unable to resolve the differences in the level of small aromatics in the two fuels at the $\Phi_{\text{jet}} = 6$ condition because of low signal-to-noise ratio. In addition to the decrease in the peak LIF count of small aromatics in the $\Phi_{\text{jet}} = 6$ flame as compared to the $\Phi_{\text{jet}} = 24$ flame, substantial differences are visible in the spatial distribution of small aromatics in the $\Phi_{\text{jet}} = 6$ as compared to the $\Phi_{\text{jet}} = \text{Inf}$ and 24 flames. First, in the $\Phi_{\text{jet}} = \text{Inf}$ and 24 flames, the peak small aromatics LIF count is higher in the annular region than on the centerline. However, in the $\Phi_{\text{jet}} = 6$ flames, the peak LIF count of small aromatics is near the centerline at 20–25 mm HAB. Furthermore, with the increase in the premixing, the location where small aromatics LIF signal is first detected on the flame centerline shifts to higher HAB; this location is approximately 6 mm HAB for $\Phi_{\text{jet}} = \text{Inf}$ and 24 flames, and 10 mm HAB for $\Phi_{\text{jet}} = 6$ flame. This shift in the location and reduction in small aromatics with more premixing could be due to a combination of dilution, chemical, thermal, residence time of small aromatics, and LIF signal quenching due to oxygen, as discussed in detail in Ref. [5].

The differences evident in the peak level of small aromatics of the two fuels can be due to differences in temperature in the flame and/or chemical effects of the fuel. The comparison of radial temperature measurement at 5 mm HAB, shown in Figs. 7(a)–7(c), and the centerline temperature measurement until 20 mm HAB, shown in Figs. 7(d)–7(f), for the two fuels and three $\Phi_{\text{jet}}$ indicate that within measurement uncertainty, the temperature is similar for the two fuels at a given $\Phi_{\text{jet}}$. Therefore, in a similar
temperature field, the difference in the peak level of small aromatics of the two fuels at a particular \( \Phi_{\text{jet}} \) is likely due to the chemical effect of the fuel breakdown process and growth to the one and two ring aromatics. We used a detailed chemical mechanism developed as part of the program [3] to compare the pyrolysis of the pure \( n \)-dodecane and the \( n \)-heptane/\( n \)-dodecane fuel blend. In addition, we used the LLNL high temperature \( n \)-alkane mechanism [25] to compare the pyrolysis of the \( C_{16} \) and \( C_7 \) fuels. Figure 8 shows the consumption of \( n \)-heptane, \( n \)-dodecane, and \( n \)-hexadecane in a pyrolysis simulation under homogeneous reactor conditions at a constant temperature and pressure of 1600 K and 1 atm. These simulations show that \( n \)-dodecane and \( n \)-hexadecane decompose more quickly than \( n \)-heptane. The faster decomposition of \( n \)-hexadecane results in higher concentrations of reaction products, including the \( C_3/C_4 \) species that form the first aromatic ring. For example, Fig. 9 shows the comparison of the mole fraction of \( C_3H_3 \) and \( C_4H_6 \) species for the \( C_7 \) and \( C_{16} \) fuel mixtures in a pyrolysis (with no air in reactants) simulation under homogeneous reactor condition at constant temperature (1600 K) and pressure (1 atm) using \textsc{chemkin}. These simulations show that the peak mole fraction of \( C_3H_3 \) and \( C_4H_6 \) is higher in \( C_{16} \) fuel mixture as compared to the \( C_7 \) fuel mixture. The \( C_3H_3 \) radical can lead to benzene formation through a self-addition reaction [26]. The \( C_4H_6 \) can form \( i-C_3H_5 \) or \( n-C_3H_5 \), which can form benzene through pathways described in Ref. [26]. The homogeneous reactor simulation with addition of air to the fuel (\( \Phi_{\text{jet}} = 24 \) and 6) under the same temperature and pressure conditions shows that the \( n \)-hexadecane decomposes faster than \( n \)-heptane even under premixed conditions.

To complete the discussion of the LIF results, Fig. 10 shows the 2D spatial development of large aromatics for the two fuels at three \( \Phi_{\text{jet}} \). Figures 10(e) and 10(f) includes LII signal at 30–33 mm HAB, which is comparable to the LIF signal at 20–25 mm HAB. The LII signal appears because the laser beam intensity could not be lowered further than 585 \( \mu \)J, as doing so would reduce the LIF signal-to-noise ratio in other flame conditions. As a result of the low signal levels, no conclusions can be drawn about the large aromatics in the \( \Phi_{\text{jet}} = 6 \) flames.

Figures 10(a) and 10(b) show that the spatial distribution of large aromatics is similar for \( C_{16} \) and \( C_7 \) nonpremixed flames; the large aromatics LIF signal is first detected at approximately 6 mm

HAB and 11 mm HAB in the annular region and on the flame centerline, respectively. Similar to the small aromatics shown in Figs. 6(a) and 6(b), the peak LIF count of large aromatics is higher in the flame annular region as compared to the centerline. Quantitatively, the peak large aromatic LIF count is similar, within measurement uncertainty, for both the fuel mixtures. Figures 10(c) and 10(d) show that the spatial distribution of large aromatics for \( \Phi_{\text{jet}} = 24 \) flames is similar to the \( \Phi_{\text{jet}} = \infty \) flames, shown in Figs. 10(a) and 10(b). Within experimental uncertainty, the peak LIF count of large aromatics is similar for both the fuels. Similar to small aromatics discussed earlier, the peak LIF count of large aromatics decrease as compared to the nonpremixed flame with the increase in air addition to fuel jet for both \( C_{16} \) and \( C_7 \) fuels. As expected, for each flame condition, the HAB where large aromatics LIF signal is first detected is at higher HAB as compared to the location at which small aromatics LIF signal is first detected, because large aromatics form from the small aromatics. The spatial or temporal development of small aromatics to large aromatics is discussed in detail in Refs. [4] and [5].

Laminar Flame: Soot Volume Fraction. Figure 11 shows the 2D spatial development of soot volume fraction for the two fuels at three \( \Phi_{\text{jet}} \). An iso-contour of approximately 10% of peak soot

Fig. 10 Two-dimensional large aromatics (counts) obtained for: (a) \( C_7 \) \( \Phi_{\text{jet}} = \infty \), (b) \( C_{16} \) \( \Phi_{\text{jet}} = \infty \), (c) \( C_7 \) \( \Phi_{\text{jet}} = 24 \), (d) \( C_{16} \) \( \Phi_{\text{jet}} = 24 \), (e) \( C_7 \) \( \Phi_{\text{jet}} = 6 \), and (f) \( C_{16} \) \( \Phi_{\text{jet}} = 6 \).
Fig. 11 Two-dimensional soot volume fraction (ppm) obtained for: (a) C7 \( \phi_{\text{jet}} = \text{Inf} \), (b) C16 \( \phi_{\text{jet}} = \text{Inf} \), (c) C7 \( \phi_{\text{jet}} = 24 \), (d) C16 \( \phi_{\text{jet}} = 24 \), (e) C7 \( \phi_{\text{jet}} = 6 \), and (f) C16 \( \phi_{\text{jet}} = 6 \)

Soot volume fraction is shown to illustrate the spatial extent of LII signal and compare the results at three \( \phi_{\text{jet}} \). The horizontal stripes visible in the images are an artifact from variation in the local fluence of the laser sheet. Figure 11 shows that the LII is first detected in the flame annular region, and further downstream, the soot field develops toward the flame centerline for all six flames. The spatial development of soot in this co-flow flame is consistent with the previous published literature on nonpremixed and partially premixed flames [17].

With the increase in premixing level, the spatial extent of the LII signal reduces for both the fuels; the LII signal is first detected at approximately 12 mm, 15 mm, and 20 mm HAB in the flame annular region for the \( \phi_{\text{jet}} = \text{Inf} \), 24, and 6 flames, respectively. Furthermore, the location at which the LII signal is first detected in the annular region shifts further downstream with increased premixing for both the fuels; the LII signal is first detected at approximately 18% and 50% for the \( \phi_{\text{jet}} = 24 \) and 6 flames, respectively. For all the three \( \phi_{\text{jet}} \), the soot volume fraction increases initially due to dominant soot growth processes, reaches a peak, and then decreases at higher HAB as oxidation processes are dominant.

Figures 12(a)–12(c) show the comparison of the centerline soot volume fraction for the two fuels at \( \phi_{\text{jet}} = \text{Inf} \), 24, and 6 flames, respectively. For all the three \( \phi_{\text{jet}} \), the soot volume fraction increases initially due to dominant soot growth processes, reaches a peak, and then decreases at higher HAB as oxidation processes are dominant. Figures 12(d)–12(f) show the maximum soot volume fraction for the \( \phi_{\text{jet}} = \text{Inf} \), 24, and 6 flames, respectively, for the two fuels. At a particular HAB, higher value of maximum soot volume fraction as compared to the centerline soot volume fraction, indicates that the peak soot volume location is in the flame annular region. The C16 and C7 \( \phi_{\text{jet}} = \text{Inf} \) flames have a peak soot volume fraction of approximately 5 ppm, in both the flame annular region and on the centerline. Similar to the nonpremixed flames, the C16 and C7 \( \phi_{\text{jet}} = 24 \) flames have a peak soot volume fraction of approximately 4 ppm, in both the flame annular region and on the centerline. In contrast to the \( \phi_{\text{jet}} = \text{Inf} \) and 24 flames, Figs. 12(c) and 12(f) show that the \( \phi_{\text{jet}} = 6 \) flames have peak soot volume fraction of approximately 2.7 ppm on the flame centerline for both the fuels.

The LII measurements in the jet flames using prevaporized fuels shows that the C16 fuel result in slightly higher peak soot volume fraction. Even though the differences in the soot volume fraction among the two fuels at a particular \( \phi_{\text{jet}} \) is within the measurement uncertainty, the trend of slightly higher soot volume fraction in the C16 flames as compared to the corresponding C7 flames is repeatable. The trend of increase in soot volume fraction with increase in the carbon number in the n-alkane family is consistent with previous work [27,28]; the threshold sooting index, a global sooting parameter, showed a trend of increasing threshold sooting index with increase in the carbon number of the n-alkane fuels.

The peak soot volume fraction is lower for the two fuels at the \( \phi_{\text{jet}} = 24 \) and 6 conditions as compared to the nonpremixed flame. The percentage reduction in peak soot volume fraction is similar for both the fuels; the peak soot volume fraction reduces by approximately 18% and 50% for the \( \phi_{\text{jet}} = 24 \) and 6 flames, as compared to the nonpremixed flames.

In order to understand the spatial location of peak soot volume fraction, we plot the soot volume fraction on a streamline that passes through the flame center and maximum soot volume fraction along the downstream direction. Figures 12(a)–12(c) show the comparison of the centerline soot volume fraction for the two fuels at \( \phi_{\text{jet}} = \text{Inf} \), 24, and 6 flames, respectively. For all the three \( \phi_{\text{jet}} \), the soot volume fraction is slightly higher in the C16 flame as compared to the C7 flame for both nonpremixed and rich premixed flames.
volume fractions as compared to the C7 fuel under both nonpremixed and rich premixed conditions. With a nearly identical temperature field and soot residence time, the differences in the soot volume fraction between the two fuels are most likely due to the chemical effect of the fuel. In the laminar flame experiment, both fuels were prevaporized, whereas in a model combustor, both the differences in chemical structure and fuel volatility may impact the combustor soot emissions. In order to understand the effect of the fuel volatility of the two fuels: n-heptane and n-hexadecane, which varies by 189°C, on soot emission, the fuel mixtures are tested in a model combustor.

Soot Emissions From the Model Gas Turbine Combustor. Figure 13 shows the comparison of line-of-sight soot volume fraction results as a function of $\Phi_{\text{global}}$ for the two binary mixtures and JP-8 fuel. $\Phi_{\text{global}}$ is defined as the ratio of inlet fuel-to-air ratio. The plot shows result from two different experiments for each of the three fuels. Each experiment is comprised of three or four sweeps in $\Phi_{\text{global}}$, from 0.9 to 1.8 and then again from 1.8 to 0.9 in increments of 0.1. The uncertainty in the equivalence ratio is estimated to be ±2.6% [21]. The line-of-sight soot volume fraction at the exit of the combustor provides an estimate of the net soot produced in the combustor.

The soot emission increases with the increase in the $\Phi_{\text{global}}$ for all the three fuels; this result is reflected in the laminar flame studies, where higher $\Phi_{\text{jet}}$ results in higher peak soot volume fraction. Additionally, the increase in $\Phi_{\text{global}}$ would result in lower adiabatic flame temperature, thereby leading to slower droplet evaporation. The slower evaporation rate may result in relatively bigger size droplets, at $\Phi_{\text{global}} = 1.8$ as compared to at 1.0, to connect to the flame front, thereby increasing soot formation due to fuel rich regions. The comparison of soot volume fraction among the three fuels shows that the net soot produced by the two binary mixtures is substantially less as compared to the JP-8 fuel in the range of $\Phi_{\text{global}}$ from 1.0 to 1.8. At $\Phi_{\text{global}} = 1.8$, the soot emission from JP-8 is approximately 6 ppm, nearly a factor of six higher than the soot emission from the two fuel mixtures, which emit approximately 1 ppm of soot. Furthermore, for the two n-alkane fuels, the $\Phi_{\text{global}}$ at which measurable amount of soot using the LE technique is first detected is at a richer $\Phi_{\text{global}}$ of approximately 1.4 as compared to at approximately $\Phi_{\text{global}} = 1.2$ for the JP-8 fuel. Additionally, the factor by which the soot volume fraction is higher in JP-8 fuel as compared to the two fuel mixtures, increases with the increase in $\Phi_{\text{global}}$ from 1.4 to 1.8. Within experimental uncertainty, the C16 and C7 fuels have a similar amount of net soot production for $\Phi_{\text{global}}$ of 1.0–1.8.

The JP-8 fuel emits more soot as compared to the two binary fuel mixtures, because JP-8 contains a range of aromatic species, 20% by mass [29]; the aromatic components in a fuel can result in a higher soot production as compared to a fuel that has no aromatic content. The higher soot production in a fuel containing aromatic species is consistent with our recent study done in jet flames [4,5]. In the nonpremixed flames, replacing 25% volume fraction of n-dodecane with m-xylene, thereby maintaining constant mass fraction flow rate, resulted in an increase in the peak soot volume fraction by approximately three times the amount produced in the n-dodecane flame. Furthermore, the m-xylene/n-dodecane flame emits smoke since the soot produced is not completely oxidized. This increase in soot production is because the m-xylene reacts to form radicals such as m-xylol that react to form two-ring PAH, thereby accelerating the formation of larger aromatic species that are involved in the formation of incipient soot particles. The faster production of PAH also leads to higher concentrations of these species, which increases the amount of soot mass through condensation processes.

The hypothesis of this study was that fuels with different boiling points would affect the fuel droplet vaporization processes, and that a fuel with a higher boiling point would produce higher levels of soot. However, Fig. 13 shows that soot emission from both the C16 and C7 fuels is quite similar in the gas turbine combustor. It is possible that the current design of the injector and combustor results in the complete vaporization of the fuel droplets before the combustion zone. If the fuel droplets are vaporized before the combustion zone, the impact of fuel boiling point on soot emission may not be evident in the current experiment, just as it was not in the prevaporized laminar flame. In future, the fuel–air mixing and droplet size measurements need to be done to better interpret the results. The chemical effect of the fuel molecular weight on soot is expected to remain. However, the experiment in jet flames show that the chemistry has relatively small effect on the peak soot volume fraction, which cannot be resolved by the LE technique applied on the model gas turbine combustor.

Conclusions

The effect of fuel volatility on soot emissions is tested in a model gas turbine combustor. The change in the fuel volatility did not affect the soot emissions in the model combustor operating at $\Phi_{\text{global}} = 1.0–1.8$. The absence of the impact of fuel volatility on soot emission could be likely due to unique design of the injector and combustor, and hence, it is recommended to test the fuel matrix in other types of combustors. The JP-8 fuel has significantly higher soot emission as compared to the two fuel mixtures. In addition, the LE technique first detects soot emission approximately at richer $\Phi_{\text{global}} = 1.4$ for the n-alkane fuel mixtures as compared to at $\Phi_{\text{global}} = 1.2$ for the JP-8 fuel.

The two binary fuel mixtures are also tested in co-flow flame under nonpremixed and rich premixed conditions to simulate the fuel rich conditions present in the primary zone of the combustor. This experiment aids in understanding the chemical impact of the two fuel mixtures on aromatics and soot volume fraction. The LII measurement shows that the C16 fuel produces slightly higher peak soot volume fraction as compared to the C7 fuel at all three $\Phi_{\text{jet}}$; however, the difference in soot volume fraction between the two fuels is within the measurement uncertainty of ±15%. Additionally, the C16 produces approximately 35% higher peak level of small aromatics as compared to the C7 fuel at $\Phi_{\text{jet}} = \text{Inf}$ and 24. For both nonpremixed and premixed flames, the peak large aromatics level is similar for the two fuel mixtures, within the measurement uncertainty. The addition of air results in the decrease in the peak level of small aromatics, large aromatics, and soot volume fraction in $\Phi_{\text{jet}} = 24$ and 6, as compared to $\Phi_{\text{jet}} = \text{Inf}$, for both the fuels. The LII-LIF results presented here provide a unique dataset to test chemical mechanisms and soot models for the n-alkane fuels. Furthermore, the results from model combustor can be used to validate numerical models in an engine-like environment.
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Nomenclature

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\begin{align*}
C_7 & = \text{n-heptane/n-dodecane mixture} \\
C_{16} & = \text{n-hexadecane/n-dodecane mixture} \\
HAB & = \text{height above the burner} \\
Inf & = \text{nonpremixed flame} \\
LE & = \text{leather extinction} \\
LIF & = \text{laser induced fluorescence} \\
LII & = \text{laser induced incandescence} \\
PAH & = \text{polycyclic aromatic hydrocarbons} \\
2D & = \text{two-dimensional} \\
\Phi_{\text{jet}} & = \text{jet equivalence ratio in jet flames} \\
\Phi_{\text{global}} & = \text{global equivalence ratio in model gas turbine combustor}
\end{align*}
\]

References


