**Table 1.** Physical properties of n-heptane and 1-heptene at 20°C and 1atm.

<table>
<thead>
<tr>
<th></th>
<th>n-heptane</th>
<th>1-heptene</th>
</tr>
</thead>
<tbody>
<tr>
<td>Critical temperature, °C</td>
<td>540</td>
<td>537</td>
</tr>
<tr>
<td>Boiling point, °C</td>
<td>98.4</td>
<td>93.6</td>
</tr>
<tr>
<td>Density, kg/m³</td>
<td>690</td>
<td>697</td>
</tr>
<tr>
<td>Vapor pressure, kPa</td>
<td>4.7</td>
<td>7.9</td>
</tr>
<tr>
<td>Liquid viscosity, mPa.s</td>
<td>0.376</td>
<td>0.349</td>
</tr>
</tbody>
</table>

**Table 2.** Experimental conditions for non-reacting and reacting n-heptane sprays.

<table>
<thead>
<tr>
<th>Temperature, K</th>
<th>800 – 1300 (reacting)</th>
<th>1000 (non-reacting &amp; base case)</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₂ volume fraction, %</td>
<td>8 – 21 (reacting)</td>
<td>21 (base case)</td>
</tr>
<tr>
<td>Density, kg/m³</td>
<td></td>
<td>14.8</td>
</tr>
<tr>
<td>Injection pressure, MPa</td>
<td></td>
<td>150</td>
</tr>
<tr>
<td>Injection duration, ms</td>
<td></td>
<td>6.8</td>
</tr>
<tr>
<td>Injection mass, mg</td>
<td></td>
<td>17.8</td>
</tr>
<tr>
<td>Nozzle diameter, mm</td>
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<td>0.1</td>
</tr>
<tr>
<td>Discharge coefficient (Cₜ)</td>
<td></td>
<td>0.8</td>
</tr>
<tr>
<td>Area contraction coefficient (Cₜ)</td>
<td></td>
<td>0.86</td>
</tr>
</tbody>
</table>
Fig 1: Predicted and measured ignition delays for n-heptane/air at $p = 55$ atm and $\phi = 1$ (a), and for 1-heptene/air mixtures (b) at $p = 10$ atm, and three equivalence ratios, $\phi = 1.5$, $[\text{C}_7\text{H}_{14}] = 1248$ ppm, $\phi = 1$, $[\text{C}_7\text{H}_{14}] = 873.3$ ppm, and $\phi = 0.5$, $[\text{C}_7\text{H}_{14}] = 447.6$ ppm. Ignition delay is defined as the time for OH mole fraction to attain 50% of the peak value. Solid and dashed lines in Fig. 1b indicate simulation results with the reduced and detailed CRECK mechanisms, respectively.

Fig 2: Measured and predicted liquid penetration (a) and vapor penetration (b) distances for n-heptane non-reacting spray. Predictions are shown for three grid sizes of 0.5mm, 0.25mm and 0.125mm.
Fig 3: Measured (symbols) and predicted ignition delay (a) and flame LOL (b) plotted versus initial temperature.

Fig 4: Comparison of measured soot luminosity images with the predicted soot mass fraction contours for n-heptane reacting spray for ambient temperature=1000K, density=14.8kg/m³, O₂ mole fraction=0.21, and injection pressure=150MPa. Solid vertical lines at 0.017m in the computed images indicate the measured flame LOL. Green contour line represents the predicted OH mass fraction corresponding to 2% of the peak value.
Fig 5: Mixture fraction and temperature contours at different times (after start of injection) showing the temporal evolution of n-heptane spray flame. Colors indicate temperatures 1000-2500K. Contour lines represent mixture fraction or equivalence ratio between 0.15-3. Initial temperature=1000K. Dimensions are in m.

Fig 6: Heat release rate (J/s-m³) contours (left) and scatter plots in φ-T space (right) at different times after SOI. Heat release rates between -1x10⁹ to 1x10¹¹ for contours and between -1x10¹⁰ to 1x10¹² for scatter plots.
Fig 7: Integrated n-heptane vapor mass and heat release rate profiles with respect to time.

Fig 8: C$_2$H$_2$, OH, NO, and C$_6$H$_6$ mass fraction contours in n-heptane spray flame at t=0.0015s.

(a) NO  
(b) NO$_2$
Fig 9: Mass fraction contours for NO, NO$_2$, HCN, NH, N$_2$O, and NNH at 0.0015s in the constant volume reactor for n-heptane spray flame. Initial ambient temperature=1000K.

Fig 10: Peak temperature and total NO mass versus time for n-heptane (black) and 1-heptane (red) spray flames. Initial temperature is 1300K.
Fig 11: Dominant reaction paths for n-heptane (a) and 1-heptene (b) during ignition. Simulations are performed in a well-stirred reactor with initial $T=1300K$, $p=55$ atm and $\phi=1$. The red color indicates more dominant reactions. Percentage implies the relative amount of a species that is consumed through a given reaction. For example, in Fig. a, 66% of n-C$_7$H$_{16}$ is consumed through its reaction with OH to form C$_7$H$_{15}$.

Fig 12: Temporal profiles of temperature and NO mole fraction for well-stirred reactor simulations with n-heptane and 1-heptene at initial $T=1300K$, $p=55$ atm and $\phi=1$. 

Fig 12: Temporal profiles of temperature and NO mole fraction for well-stirred reactor simulations with n-heptane and 1-heptene at initial $T=1300K$, $p=55$ atm and $\phi=1$. 

Fig 11: Dominant reaction paths for n-heptane (a) and 1-heptene (b) during ignition. Simulations are performed in a well-stirred reactor with initial $T=1300K$, $p=55$ atm and $\phi=1$. The red color indicates more dominant reactions. Percentage implies the relative amount of a species that is consumed through a given reaction. For example, in Fig. a, 66% of n-C$_7$H$_{16}$ is consumed through its reaction with OH to form C$_7$H$_{15}$. 

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Fig 12: Temporal profiles of temperature and NO mole fraction for well-stirred reactor simulations with n-heptane and 1-heptene at initial $T=1300K$, $p=55$ atm and $\phi=1$.
Fig 13: Total amounts of HCN, N$_2$O, NNH and CH species in n-heptane and 1-heptane flames. Initial temperature is 1300K.
Fig 14: Scatter plots of HCN, N₂O and NNH in ϕ-T space for the n-heptane (left) and 1-heptene (right) flames at 1.4ms.
Fig 15: Benzene mass fraction contours for 1-heptene and n-heptane flames at 1.4 ms. Mass fractions are between 0.006 and 0.012. Dimensions are in m.

Fig 16: Integrated mass of benzene and pyrene for n-heptane (black) and 1-heptane (red) flames. Initial temperature is 1300K.
Fig. 17: Dominant reaction paths for benzene formation for n-heptane (a) and 1-heptene (b). Simulations are performed in a well-stirred reactor with initial $T=1300K$, $p=55$ atm and $\phi=1$. The effect of double bond in 1-heptene on the various reactions are indicated by the red color. Also AC$_3$H$_4$: allene; PC$_3$H$_4$: propyne; MCPTD: methyl-cyclo-pentadiene. Percentage implies the relative amount of a species formed though a given reaction. For example, in Fig. a, 79% of C$_6$H$_6$ is formed through the combined reactions between C$_3$ species.
Fig. 18: Integrated mass of acetylene (C\textsubscript{2}H\textsubscript{2}), propargyl (C\textsubscript{3}H\textsubscript{3}), 1,3-butadiene (C\textsubscript{4}H\textsubscript{6}) and allene (AC\textsubscript{3}H\textsubscript{4}) in n-heptane and 1-heptane flames.