Generation of Comprehensive Surrogate Kinetic Models and Validation Databases for Simulating Large Molecular Weight Hydrocarbon Fuels

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Princeton, NJ 08540
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Overview

• Objective
• Threshold Sooting Index (TSI) approach
• Model Gas Turbine Combustor
• Related Studies of Coal-based Jet Fuel
• Summary
Objectives

• Apply and extend recent work done at Penn State using the Threshold Sooting Index (TSI) as a direct means to evaluate in-combustor soot expected from surrogate fuel component mixtures and matching this property with real fuel behavior.

• Experimentally investigate and further validate this approach to provide needed information on proposed surrogate components, their mixtures, and real fuels.
The Threshold Sooting Index (TSI) was developed by Calcote and Manus\textsuperscript{1} to rank the sooting tendency of pure hydrocarbon fuels.

Recent work at Penn State has extended that approach to the characterization of real jet fuels\textsuperscript{2} and the development of a coal-based jet fuel (JP-900) that is equivalent to JP-8.

\textsuperscript{1}H.F. Calcote and D. Manos, Combust. Flame, 49 (1983) 289-304.
Threshold Sooting Index

Threshold sooting index (TSI) for diffusion flames is defined as:

\[ \text{TSI} = a \left( \frac{\text{MW}}{\text{SP}} \right) + b \]

where SP is the smoke point and MW the molecular weight of the fuel. The constants \( a \) and \( b \) scale the TSI from 0 to 100, and are dependent on the apparatus used for smoke point measurement. The TSI rating of ethane and methylnaphthalene were assigned to be 0 and 100, respectively.

For multi-component fuels \( \text{TSI}_{\text{mix}} = \sum x_i \text{TSI}_i \)
Application of the TSI Model to Various Fuels

\[ TSI = 3.18 \left( \frac{MW}{SP} \right) \]

\[ R^2 = 0.970 \]

\[ rmse = 3.3 \]

Total of 80 data points from our work and other workers taken from literature.
## Properties of JP-900 Candidate Fuels

<table>
<thead>
<tr>
<th>ID</th>
<th>Description</th>
<th>BP, °C</th>
<th>H, wt %</th>
<th>Composition, wt %</th>
<th>SP, mm</th>
<th>MW, g/mol</th>
<th>TSI</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>P</td>
<td>N</td>
<td>MA</td>
<td>DA</td>
</tr>
<tr>
<td>EI-001</td>
<td>HDT LCO</td>
<td>152-373</td>
<td>11.18</td>
<td>24.84</td>
<td>10.34</td>
<td>54.25</td>
<td>10.57</td>
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<tr>
<td>EI-002</td>
<td>HDT (RCO/LCO 1:1)</td>
<td>163-376</td>
<td>10.04</td>
<td>7.68</td>
<td>10.47</td>
<td>55.33</td>
<td>26.34</td>
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<tr>
<td>EI-003</td>
<td>HDT RCO</td>
<td>165-377</td>
<td>9.02</td>
<td>0.55</td>
<td>11.31</td>
<td>50.20</td>
<td>37.94</td>
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<tr>
<td>EI-004</td>
<td>SAT LCO</td>
<td>138-341</td>
<td>12.98</td>
<td>41.27</td>
<td>48.01</td>
<td>8.47</td>
<td>2.25</td>
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<tr>
<td>EI-005</td>
<td>SAT (RCO/LCO 1:1)</td>
<td>116-358</td>
<td>12.60</td>
<td>18.00</td>
<td>78.41</td>
<td>3.59</td>
<td>0.00</td>
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<tr>
<td>EI-006</td>
<td>SAT RCO</td>
<td>119-369</td>
<td>12.60</td>
<td>8.71</td>
<td>91.25</td>
<td>0.05</td>
<td>0.00</td>
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<tr>
<td>EI-031</td>
<td>HDT (RCO/LCO 1:1)</td>
<td>180-270</td>
<td>8.68</td>
<td>1.05</td>
<td>2.52</td>
<td>52.89</td>
<td>43.54</td>
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<tr>
<td>EI-032</td>
<td>HDT (RCO/LCO 1:1)</td>
<td>180-300</td>
<td>8.68</td>
<td>2.51</td>
<td>1.83</td>
<td>37.45</td>
<td>58.20</td>
</tr>
<tr>
<td>EI-033</td>
<td>HDT (RCO/LCO 1:1)</td>
<td>180-320</td>
<td>8.47</td>
<td>1.49</td>
<td>1.96</td>
<td>40.02</td>
<td>56.53</td>
</tr>
<tr>
<td>EI-034</td>
<td>HDT (RCO/LCO 3:1)</td>
<td>180-270</td>
<td>8.75</td>
<td>0.78</td>
<td>2.22</td>
<td>64.60</td>
<td>32.39</td>
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<tr>
<td>EI-035</td>
<td>HDT (RCO/LCO 3:1)</td>
<td>180-300</td>
<td>8.68</td>
<td>1.22</td>
<td>1.93</td>
<td>55.51</td>
<td>41.33</td>
</tr>
<tr>
<td>EI-036</td>
<td>HDT (RCO/LCO 3:1)</td>
<td>180-320</td>
<td>8.81</td>
<td>1.47</td>
<td>1.76</td>
<td>52.95</td>
<td>43.81</td>
</tr>
<tr>
<td></td>
<td>JP-8</td>
<td></td>
<td>78.01</td>
<td>9.83</td>
<td>8.73</td>
<td>3.43</td>
<td>23.9</td>
</tr>
<tr>
<td></td>
<td>JP-8+100</td>
<td></td>
<td>78.23</td>
<td>6.23</td>
<td>12.1</td>
<td>3.43</td>
<td>24.4</td>
</tr>
</tbody>
</table>

- P - Paraffin
- N - Naphthene
- MA – Monoaromatics
- DA - Diaromatics
Relationship Between TSI and $MW/SP$ Ratio for Prototype JP-900 Fuel Mixtures

$$TSI = 3.52(MW/SP) - 7.42$$

$$R^2 = 0.9962$$
TSI Variations with Tetralin Concentration

Points are experimental measurements, TSI = 3.37(MW/SP)-1.47. Solid line is predicted via TSI = \( \sum x_i S_i \). Dotted line is TSI_{max} = 24.
Model Gas Turbine Combustor
## Model Gas Turbine Combustor Operating Conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet Air Flow Rate-g/s (lbm/s)</td>
<td>20-200 (0.04-0.44)</td>
</tr>
<tr>
<td>Inlet Air Temperature-K (°F)</td>
<td>300-800 (80-980)</td>
</tr>
<tr>
<td>Inlet Air Velocity-m/s (ft/s)</td>
<td>57-90 (187-295)</td>
</tr>
<tr>
<td>Fuel Flow Rate</td>
<td></td>
</tr>
<tr>
<td>Natural Gas-g/s (lbm/s)</td>
<td>1.2-12 (0.003-0.03)</td>
</tr>
<tr>
<td>Liquid Fuel-ml/s (Gal/min)</td>
<td>0.53-9.50 (0.0085-0.15)</td>
</tr>
<tr>
<td>Chamber Pressure-MPa (psia)</td>
<td>0.2-2 (29.4-294)</td>
</tr>
<tr>
<td>Degree of Swirl</td>
<td>Variable</td>
</tr>
<tr>
<td>Fuel Injection Location</td>
<td>Variable</td>
</tr>
<tr>
<td>Chamber Length-mm (in)</td>
<td>235 (9.25), 350 (13.78)</td>
</tr>
</tbody>
</table>
Schematic of Apparatus and Flow System

Natural Gas
Choked Inlet
Fuel and Atomization Air
Air Swirler
Fuel Injector
Combustion Chamber
Quartz Section
Quartz Window
Exhaust

200 mm
622 mm
38 mm
235 mm
Cutaway View of Combustion Chamber

- Cooling Air
- Main Air
- Fuel
- Atomization Air
- Viewing Window
- P.T. Ports
- Combustion Chamber
- Quartz Cylinder
- Outer Chamber
- Exhaust Gases

Dimensions:
- 9.5 mm, 20 mm, 45 mm, 50 mm, 51 mm, 114 mm
Soot Refractive Index at 514.5nm
n = 1.57 - i 0.56
Diagnostics Capabilities

- Critical System Temperatures and Pressures
- Exhaust Gas Analyzers

<table>
<thead>
<tr>
<th>Species</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO (ppm)</td>
<td>0-1000</td>
</tr>
<tr>
<td>CO₂ (%)</td>
<td>0-20</td>
</tr>
<tr>
<td>NO (ppm)</td>
<td>0-1000</td>
</tr>
<tr>
<td>NOₓ (ppm)</td>
<td>0-1000</td>
</tr>
<tr>
<td>O₂ (%)</td>
<td>0-25</td>
</tr>
<tr>
<td>HC (ppm)</td>
<td>0-30,000</td>
</tr>
</tbody>
</table>

- OH*/CH* Chemiluminescence Imaging
- OH Planar Laser-Induced Fluorescence (PLIF)
- Raman Scattering
- Particle Imaging Velocimetry
- Phase Doppler Particle Analyzer (PDPA)
Image of a Typical Flame for a Practical Fuel (JP-8)

Swirler Type: 45°
Chamber Length: 235 mm
Equivalence Ratio: 0.75

Chamber Pressure: 0.5 MPa (73 psia)
Inlet Temperature: 675 K (750 ºF)
Air Mass Flowrate: 53.7 g/s (0.118 lbm/s)
(Atomization Air Flow: 8%)
Image of a Typical Flame for a Pure Hydrocarbon (n-Heptane)

Equivalence Ratio: 0.45

Inlet Temperature : 675 K (750 °F)
Air Mass Flowrate: 52.8 g/s (0.116 lbm/s) (Atomization Air : 8%)
Chamber Pressure: 0.425 MPa (62 psia)
Measurements of Soot Volume Fraction for JP-8 and Coal-based Fuels (X-610 & EI-173)

$T = \sim 550K$

$P_{ch} = \sim 0.51$ MPa
Comparison of NO$_x$ Emissions

- $\triangle$ - Ethylene
- $\times$ - Natural Gas
- $\Diamond$ - n-Heptane
- $\Box$ - Kerosene (JP-8)
- $\circ$ - HDT-LCO-RCO

Concentration, corrected to 15% O$_2$ (ppmvd)

Overall Equivalence Ratio
Summary

• Using the TSI approach described, a direct means exists to evaluate expected in-combustor soot from proposed surrogate fuel component mixtures.

• Furthermore, the TSI approach provides a basis for comparing the soot behavior of proposed surrogates with real fuels.

• Experimental investigations will further validate this approach under high pressure combustion conditions to provide needed information on soot formation for proposed surrogate components, their mixtures, and real fuels.