FUEL EFFECTS ON COMPRESSION IGNITION

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Topic Motivation and Objectives

• Motivation
  ✓ Understand the fuel effects on spray at CI conditions as an additional dimension for model development and validation

• Objective
  ✓ Summarize and understand the available experimental and computational fuel effect studies
  ✓ Relevant studies on spray fuel effect
  ✓ Define a “Fuel” of interest for the ECN community

• Assumption:
  ✓ Variations of combustion chambers, boundary conditions, optical diagnostic techniques, definitions were not considered
Experimental Investigation of Spray Fuel Effects
Literature Referred


## Overview of Spray Fuel Effect Characterization

<table>
<thead>
<tr>
<th>Nozzle</th>
<th>Spray A</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single-hole, 90 µm, K 1.5 / 0.86</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Ambient temperature</th>
<th>700 – 1200 K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ambient density</td>
<td>15.2, 22.8, 45.6 kg/m³</td>
</tr>
<tr>
<td>Ambient oxygen</td>
<td>0%, 15%, 18%, 21%</td>
</tr>
<tr>
<td>Injection pressure</td>
<td>50, 100, 150 MPa</td>
</tr>
<tr>
<td>Institutions</td>
<td>CMT, SNL, IFPEN</td>
</tr>
</tbody>
</table>

### Fuels

<table>
<thead>
<tr>
<th>Fuels</th>
<th>Density [kg/m³]</th>
<th>CN</th>
</tr>
</thead>
<tbody>
<tr>
<td>D2 (No. 2 diesel)</td>
<td>843</td>
<td>46</td>
</tr>
<tr>
<td>JC (JP-8)</td>
<td>812</td>
<td>38</td>
</tr>
<tr>
<td>JW (World Average Jet A Blend)</td>
<td>806</td>
<td>46</td>
</tr>
<tr>
<td>JS (Fischer-Tropsch Fuel)</td>
<td>755.9</td>
<td>62</td>
</tr>
<tr>
<td>JP (Coal-Derived Fuel)</td>
<td>870.2</td>
<td>34</td>
</tr>
<tr>
<td>SR (Surrogate Fuel)</td>
<td>778.9</td>
<td>70</td>
</tr>
<tr>
<td>SME (soy ethyl ester)</td>
<td>877</td>
<td>51</td>
</tr>
<tr>
<td>nC12</td>
<td>750</td>
<td>80</td>
</tr>
<tr>
<td>PRF0</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>PRF20</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>PRF40</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>PRF60</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>PRF80</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>PRF100</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>B5 (5% esters)</td>
<td>833</td>
<td>53.1</td>
</tr>
<tr>
<td>JetA1</td>
<td>812</td>
<td>45.6</td>
</tr>
<tr>
<td>JetA1-surr.v1</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>JetA1-surr.v2</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>E5 (5% ethanol)</td>
<td>746</td>
<td>17</td>
</tr>
<tr>
<td>n-dodecane</td>
<td>745</td>
<td>73</td>
</tr>
<tr>
<td>G15</td>
<td>800</td>
<td>108</td>
</tr>
<tr>
<td>G33</td>
<td>835</td>
<td>110</td>
</tr>
<tr>
<td>G50</td>
<td>869</td>
<td>112</td>
</tr>
<tr>
<td>G50A</td>
<td>859</td>
<td>88</td>
</tr>
<tr>
<td>MD (Methyl decanoate)</td>
<td>871</td>
<td>48</td>
</tr>
</tbody>
</table>

### Graphs

1. **Liquid length vs. Temperature**
   - 0% O₂-900 K-22.8 kg/m³ -150 MPa
2. **Lift-off-length vs. Ignition delay**
   - R² = 0.9036
   - 15% O₂-900 K-22.8 kg/m³ -150 MPa
<table>
<thead>
<tr>
<th>Fuel type</th>
<th>Fuels</th>
<th>Fuel details</th>
<th>Density [kg/m³]</th>
<th>CN/DCN</th>
<th>LHV [MJ/kg]</th>
<th>C/H mass ratio</th>
<th>Aromatics volume %</th>
<th>Boiling temp. [°C]</th>
<th>Kinematic viscosity (40°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PRF fuel</td>
<td>PRF0</td>
<td>100% n-heptane, 0% iso-octane</td>
<td>684</td>
<td>55</td>
<td>44.6</td>
<td>5.25</td>
<td>0</td>
<td>98</td>
<td>0.51</td>
</tr>
<tr>
<td></td>
<td>PRF20</td>
<td>80% n-heptane, 20% iso-octane</td>
<td>685</td>
<td>46</td>
<td>44.5</td>
<td>5.27</td>
<td>0</td>
<td>99</td>
<td>0.54</td>
</tr>
<tr>
<td></td>
<td>PRF40</td>
<td>60% n-heptane, 40% iso-octane</td>
<td>686</td>
<td>36</td>
<td>44.5</td>
<td>5.29</td>
<td>0</td>
<td>99</td>
<td>0.57</td>
</tr>
<tr>
<td></td>
<td>PRF60</td>
<td>40% n-heptane, 60% iso-octane</td>
<td>688</td>
<td>29</td>
<td>44.5</td>
<td>5.30</td>
<td>0</td>
<td>99</td>
<td>0.59</td>
</tr>
<tr>
<td></td>
<td>PRF80</td>
<td>20% n-heptane, 80% iso-octane</td>
<td>689</td>
<td>21</td>
<td>44.5</td>
<td>5.32</td>
<td>0</td>
<td>99</td>
<td>0.62</td>
</tr>
<tr>
<td></td>
<td>PRF100</td>
<td>0% n-heptane, 100% iso-octane</td>
<td>690</td>
<td>13</td>
<td>44.4</td>
<td>5.33</td>
<td>0</td>
<td>99</td>
<td>0.65</td>
</tr>
<tr>
<td>Gasoline fuel</td>
<td>E5</td>
<td>European standard gasoline containing 5% of ethanol</td>
<td>746</td>
<td>17</td>
<td>42.8</td>
<td>-</td>
<td>-</td>
<td>27-225</td>
<td>-</td>
</tr>
<tr>
<td>JP</td>
<td>JC (JP-8)</td>
<td>a low cetane number fuel that can also be used to assess the use of aviation fuel using diesel engine hardware at diesel engine condition</td>
<td>812</td>
<td>38</td>
<td>43.2</td>
<td>6.19</td>
<td>11</td>
<td>266</td>
<td>~1.4</td>
</tr>
<tr>
<td></td>
<td>JW</td>
<td>an equal blend of five Jet-A fuel samples from different U.S. manufacturers, and with the same cetane number as D2</td>
<td>806</td>
<td>46</td>
<td>43.2</td>
<td>6.19</td>
<td>19</td>
<td>274</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>JS</td>
<td>a Fischer-Tropsch fuel characterized as fuel with minimal aromatics (0.4%) and high cetane number</td>
<td>756</td>
<td>62</td>
<td>44.1</td>
<td>5.49</td>
<td>0.4</td>
<td>276</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>JP</td>
<td>a coal-derived fuel, a low cetane number fuel with low 1.9% aromatics but high (&gt;90%) cyclopentane content</td>
<td>870</td>
<td>34</td>
<td>42.8</td>
<td>6.58</td>
<td>1.9</td>
<td>270</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>JetA1</td>
<td>European standard Jet fuel</td>
<td>812</td>
<td>46</td>
<td>43.5</td>
<td>-</td>
<td>-</td>
<td>187-300</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>JetA1-sur.v1</td>
<td>51.3% n-decane, 19.8% iso-octane, 28.9% n-propylbenzene</td>
<td>760</td>
<td>48</td>
<td>43.4</td>
<td>6.10</td>
<td>-</td>
<td>99-174</td>
<td>0.89</td>
</tr>
<tr>
<td></td>
<td>JetA1-sur.v2</td>
<td>47.5% n-decane, 17.6% iso-octane, 35.0% n-propylbenzene</td>
<td>770</td>
<td>46</td>
<td>43.3</td>
<td>6.27</td>
<td>-</td>
<td>99-174</td>
<td>0.89</td>
</tr>
<tr>
<td>Diesel fuel</td>
<td>D2 (No. 2 diesel)</td>
<td>an emissions-certification fuel with a cetane number of 46 and 47% aromatics</td>
<td>843</td>
<td>46</td>
<td>42.9</td>
<td>6.53</td>
<td>27</td>
<td>350</td>
<td>2.35</td>
</tr>
<tr>
<td></td>
<td>SR</td>
<td>a surrogate fuel, a mixture of 23% m-xylene (aromatics) and 77% n-dodecane</td>
<td>779</td>
<td>70</td>
<td>43.3</td>
<td>5.96</td>
<td>23</td>
<td>216</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>SME</td>
<td>soy ethyl ester</td>
<td>877</td>
<td>51</td>
<td>37.4</td>
<td>6.48</td>
<td>0</td>
<td>-</td>
<td>3.98</td>
</tr>
<tr>
<td></td>
<td>nC12 (SNL)</td>
<td>normal dodecane</td>
<td>752</td>
<td>87</td>
<td>44.2</td>
<td>5.54</td>
<td>0</td>
<td>216</td>
<td>1.5</td>
</tr>
<tr>
<td></td>
<td>B5</td>
<td>European standard Diesel fuel with 5% esters composition</td>
<td>833</td>
<td>53</td>
<td>42.5</td>
<td>-</td>
<td>-</td>
<td>187-343</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>n-dodecane (IFP)</td>
<td>normal dodecane</td>
<td>15</td>
<td>73</td>
<td>46.5</td>
<td>5.54</td>
<td>0</td>
<td>216</td>
<td>1.5</td>
</tr>
<tr>
<td></td>
<td>G15</td>
<td>Three fuels were blends of tri(propylene glycol) ether (TPGME) and n-hexadecane, identified as G15, G33 and G50, the last two digits indicating the percentage of TPGME in the blend, by volume</td>
<td>869</td>
<td>112</td>
<td>35.8</td>
<td>5.57</td>
<td>-</td>
<td>287</td>
<td>4.59</td>
</tr>
<tr>
<td></td>
<td>G33</td>
<td>Aromatic hydrocarbon, a 50/50 volume percent blend of TPGME and a diesel surrogate fuel, the latter composed of 77% n-dodecane and 23% m-xylene by volume.</td>
<td>859</td>
<td>88</td>
<td>35.5</td>
<td>6.25</td>
<td>-</td>
<td>287</td>
<td>3.43</td>
</tr>
<tr>
<td></td>
<td>MD (Methyl decanoate)</td>
<td>A different oxygenate chemical structure and was a surrogate for traditional biodiesel fuel</td>
<td>871</td>
<td>48</td>
<td>37.5</td>
<td>-</td>
<td>-</td>
<td>224</td>
<td>-</td>
</tr>
</tbody>
</table>
Experimental Results - Liquid Length vs. Temp

Higher density generally leads to longer liquid length:

- PRF < Gasoline < Jet < Diesel
- PRFs show shorter LL, while D2 and B5 have a longer LL
A strong correlation is observed between:

- LL and fuel density
- LL and boiling temperature

PRF: green
Gasoline: blue
Jet: red
Diesel: black
Viscosity seems to correlate with LL well

Heat of vaporization correlation is not expected

A sensitivity analysis would be useful to differentiate the relevant importance of all fuel properties
Experimental Results – Vapor Penetration Length

- Higher density generally leads to longer vapor penetration
  - SR is an outlier

0% O₂ - 22.8 kg/m³ - 150 MPa – 900K

PRF: green
Gasoline: blue
Jet: red
Diesel: black
## Experimental Results – Reacting Spray Penetration Length

### Graphs:
- **0-15% O<sub>2</sub> - 22.8 kg/m<sup>3</sup> - 150 MPa – 900K**

- Viscosity effect on liquid length doesn’t reflect on vapor penetration length
- Faster penetration of PRF0 due to higher CN – dilatation effect at reacting conditions
  - ✓ Higher CN leads to longer penetration

### Experimental Results

**Fuel type**: PRF fuel

<table>
<thead>
<tr>
<th>Fuel type</th>
<th>Fuels</th>
<th>Fuel details</th>
<th>Density [kg/m&lt;sup&gt;3&lt;/sup&gt;]</th>
<th>CN/DCN</th>
<th>LHV [MJ/kg]</th>
<th>C/H mass ratio</th>
<th>Aromatics volume %</th>
<th>Boiling temp. [°C]</th>
<th>Kinematic viscosity (40°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PRF0</td>
<td>PRF0</td>
<td>100% n-heptane, 0% iso-octane</td>
<td>684</td>
<td>55</td>
<td>44.6</td>
<td>5.25</td>
<td>0</td>
<td>98</td>
<td>0.51</td>
</tr>
<tr>
<td>PRF20</td>
<td>PRF20</td>
<td>80% n-heptane, 20% iso-octane</td>
<td>685</td>
<td>48</td>
<td>44.5</td>
<td>5.27</td>
<td>0</td>
<td>99</td>
<td>0.54</td>
</tr>
<tr>
<td>PRF40</td>
<td>PRF40</td>
<td>60% n-heptane, 40% iso-octane</td>
<td>686</td>
<td>38</td>
<td>44.5</td>
<td>5.29</td>
<td>0</td>
<td>99</td>
<td>0.57</td>
</tr>
<tr>
<td>PRF60</td>
<td>PRF60</td>
<td>40% n-heptane, 60% iso-octane</td>
<td>688</td>
<td>29</td>
<td>44.5</td>
<td>5.30</td>
<td>0</td>
<td>99</td>
<td>0.59</td>
</tr>
<tr>
<td>PRF80</td>
<td>PRF80</td>
<td>20% n-heptane, 80% iso-octane</td>
<td>689</td>
<td>21</td>
<td>44.5</td>
<td>5.32</td>
<td>0</td>
<td>99</td>
<td>0.62</td>
</tr>
<tr>
<td>PRF100</td>
<td>PRF100</td>
<td>0% n-heptane, 100% iso-octane</td>
<td>690</td>
<td>13</td>
<td>44.4</td>
<td>5.33</td>
<td>0</td>
<td>99</td>
<td>0.65</td>
</tr>
</tbody>
</table>
Experimental Results – ID/LOL vs. Temp

- Higher CN generally results in shorter ID and LOL

PRF: green
Gasoline: blue
Jet: red
Diesel: black

15% $O_2$ - 22.8 kg/m$^3$ - 150 MPa
A strong negative correlation is observed between ID/LOL and CN. PRF80 seems an outlier.

- PRF: green
- Gasoline: blue
- Jet: red
- Diesel: black

**Experimental Results – ID/LOL vs. CN**

15% O₂ - 22.8 kg/m³ - 150 MPa – 900 K
A negative correlation is observed between LOL / ID and CN

E5 is an outlier on ID
A strong positive correlation is observed between LOL and ID with various fuels.

- PRF: green
- Gasoline: blue
- Jet: red
- Diesel: black

**Experimental Results – LOL vs. ID**

- $15\% \text{ O}_2 - 22.8 \text{ kg/m}^3 - 150 \text{ MPa} - 900/1000 \text{ K}$
- $15\% \text{ O}_2 - 22.8 \text{ kg/m}^3 - 150 \text{ MPa} - 900/1000 \text{ K}$
- $15\% \text{ O}_2 - 22.8 \text{ kg/m}^3 - 150 \text{ MPa} - 900/1000 \text{ K}$

- $R^2 = 0.9036$
- $R^2 = 0.8368$
- $R^2 = 0.5008$
Experimental Results – Soot

At $T_{amb.} = 1000$ K, B5 (diesel fuel) forms more soot

- B5 (53) > JetA1 (46) > n-dodecane (73) > E5 (17)
- LOL, ID, fuel oxygen ratio, and aromatic content, affect the soot formation

PRF: green
Gasoline: blue
Jet: red
Diesel: black

Manin et al., SAE Int. J. Fuels Lubr. 2014.
Summary

• Liquid length:
  ✓ Higher density, boiling temperature and viscosity generally lead to longer liquid length, but their relevant importance needs to be further investigated.

• Vapor penetration length:
  ✓ Higher density generally leads to longer vapor penetration
  ✓ Viscosity doesn’t seem to have any effect
  ✓ Higher CN leads to longer spray penetration at reacting conditions

• Ignition delay and lift-off length
  ✓ Higher CN generally leads to shorter ID and LOL
  ✓ Strong negative correlations between ID/LOL and CN – PRF80 and E5 are outliers
  ✓ Strong positive correlation between LOL and ID was observed for a wide range of fuels

• Soot is affected by CN, fuel oxygen and aromatic contents etc.
Relevant Studies on Spray Fuel Effect
Literature Referred


## Injector and Fuel Specifications

<table>
<thead>
<tr>
<th>Outlet Diameter (µm)</th>
<th>Injector at Aramco</th>
<th>ECN Spray D</th>
</tr>
</thead>
<tbody>
<tr>
<td>176</td>
<td>180</td>
<td></td>
</tr>
</tbody>
</table>

| K-factor | 1.8 | 1.5 |

| Cd (Re = 12,000) | 0.94 | N/A |

| Description | Central axis, single-hole, solenoid driven, hydraulically lifted needle |

<table>
<thead>
<tr>
<th>Property</th>
<th>Units</th>
<th>ULSD - Diesel</th>
<th>RON60 Gasoline</th>
</tr>
</thead>
<tbody>
<tr>
<td>IBP</td>
<td>°C</td>
<td>167</td>
<td>41</td>
</tr>
<tr>
<td>T50</td>
<td>°C</td>
<td>257</td>
<td>67</td>
</tr>
<tr>
<td>FBP</td>
<td>°C</td>
<td>344</td>
<td>134</td>
</tr>
<tr>
<td>Density at 15.6 °C</td>
<td>g/mL</td>
<td>0.845</td>
<td>0.710</td>
</tr>
<tr>
<td>Kinematic Viscosity</td>
<td>cSt</td>
<td>2.49</td>
<td>0.58</td>
</tr>
<tr>
<td>Aromatics</td>
<td>Vol%</td>
<td>27.7</td>
<td>6.7</td>
</tr>
<tr>
<td>Olefins</td>
<td>Vol%</td>
<td>1.8</td>
<td>0.4</td>
</tr>
<tr>
<td>Saturates</td>
<td>Vol%</td>
<td>70.5</td>
<td>92.9</td>
</tr>
<tr>
<td>Sulfur</td>
<td>ppm</td>
<td>3.9</td>
<td>11.9</td>
</tr>
<tr>
<td>H/C Ratio</td>
<td>--</td>
<td>1.79</td>
<td>2.11</td>
</tr>
<tr>
<td>Cetane Number (CN)</td>
<td>--</td>
<td>44.2</td>
<td>33.9</td>
</tr>
<tr>
<td>AKI</td>
<td>--</td>
<td>n/a</td>
<td>56.8</td>
</tr>
<tr>
<td>Lower Heating Value</td>
<td>MJ/kg</td>
<td>42.87</td>
<td>44.15</td>
</tr>
</tbody>
</table>
Have our spray models considered the transient cone angle?

Fuel Effect on Spray Cone Angle

- Lower density gasoline fuel has a wider spray cone angle, leading to shorter vapor penetration
- Spray cone angle accounted for fuel effects is necessary

Have our spray models considered the fuel effect on transient cone angle?
Fuel Effect on Vaporizing Spray

- Different liquid length trend for diesel and gasoline at different ambient temperature
- Lagrangian-type of spray models can capture the interesting behavior – consistent model setup only with different fuel physical properties.

Is it a coincidence?

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Fuel Effect on Ignition Delay

• Difference becomes smaller at higher ambient temperatures
• TRF chemical kinetic model from Wang et al. CnF 2015 is capable of capturing both fuels
  ✓ ULSD – n-heptane
  ✓ RON60 Gasoline – n-heptane and iso-octane
• LES compared to RANS:
  ✓ Shorter ID at lower ambient temperature
  ✓ Similar ID at higher ambient temperature
• Suggesting TCI is more important for low CN fuels or for low reactive conditions that have a longer ID

Are the chemical kinetic and combustion models good enough to capture the fuel sensitivity?
Fuel Effect on Lift-Off Length

- With a well-mixed combustion model and a TRF mechanism, the sensitivity on LOL is not captured.
- Chemical mechanism certainly plays a role.
- A LES model improves the predictions suggesting a TCI model might be helpful.

Are the chemical kinetic and combustion models good enough to capture the fuel sensitivity?

15% $\text{O}_2$ – 6 MPa – 150 MPa
Fuel Effect on Soot

15% O₂ – 6 MPa – 150 MPa – 1000 K

Can soot models capture the fuel sensitivity?

- Much lower soot for gasoline compared to diesel
- LES+Hiroyasu might be able to reproduce soot cloud
- Quantitatively, a detailed soot model performs better in terms of soot lift-off length prediction

Experimental natural luminosity and line-of-sight integrated soot field from CFD

Fuel Effect on Injector Needle Motion

A HD 8-hole injector measured at Argonne APS by Chris Powell

- Diesel lift slope slightly shallower
- Diesel wobbles throughout injection
Fuel Effect on Needle Radial Motion

- Fuel physical properties has a significant effect on needle radial motion
Fuel Effect on Mass Flow Rate

- Radial motion is necessary to realistically examine the flow behavior
- Much higher orifice-to-orifice variation for gasoline
Fuel Effect on Flow Structure

- More cavitation for gasoline
- A jet-like structure for gasoline due to needle wobble motion
Fuel Effect on Plume-to-Plume Variability

- Plume-to-plume differences in liquid and vapor penetration
- Wider spreading angles at the beginning and end of the injection

Animation from Roberto Torelli at Argonne
Summary

• Spray
  ✓ Lighter fuel has a wider spray cone angle and shorter vapor penetration – spray cone angle needs to be properly accounted for
  ✓ Gasoline has a much shorter liquid length compared to diesel – Lagrangian-type of spray models seem doing well
  ✓ Ignition delay could be properly captured – TCI more important for longer ID
  ✓ Lift-off length prediction is more challenging
  ✓ Detailed soot model performs better

• In-nozzle flow:
  ✓ Fuel physical properties have effect on needle lift and radial motion
  ✓ Needle radial motion is necessary for realistic flow structure prediction
  ✓ Higher plume-to-plume variation and cavitation for gasoline
Acknowledgement

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• Tom Tzanetakis at Aramco Research Center - Detroit coordinated the HD spray experiments at MTU in collaboration with KAUST
• Might miss some experimental studies, please get in touch!
What would be a realistic “Fuel” variation for ECN7?

- A PRF blend seems a good option:
  - Simple, but vastly different to n-dodecane
    - Physical properties on light-end
    - Chemical properties can be tailored
  - Chemical mechanism is readily available
  - ...

- ECN7 fuel effect planning – PRF blends on Spray A, B, C, D
  - Experiments:
    - CMT, Spray A – 2012
    - SNL, Spray A – 2018
    - UNSW, Spray A – 2019
    - ...
  - Simulations:
    - UNSW - soon
    - Aramco – Detroit – in progress
    - ...

Thank you!
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Feedback and Future Directions

• Feedback:
  ✓ Different fuel blends – challenge chemistry, TRF, TRF-E
  ✓ Measurement techniques revisit to be consistent
  ✓ Empirical correlations revisit based on the wide range of fuels examined
  ✓ Work towards experiments and understanding real world fuels
  ✓ Broad topic of understanding fuel effects, methods, and related towards predictive soot modeling

• Future direction:
  ✓ PRF – as a starting point
  ✓ Combination of PRF, TRF, TRF-E
  ✓ Real world fuels
  ✓ Oxygenated fuels