An Improved Metric for the Sooting Propensity of Fuels

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Background

• We all know soot is bad for health and the environment

• Two key questions:
  – What kind of soot do different fuels produce under different circumstances?
  – How much soot do they produce?

Soot agglomerate from the soot trail of a toluene laminar diffusion flame above its smoke point. Sample taken by R Watson; image by C Ducati.
The Threshold Sooting Index (TSI)

- Standard metric for the sooting propensity of a fuel
- Can be obtained from laminar diffusion or premixed flames
- Usually obtained from the ‘smoke point’ or the ‘critical equivalence ratio’ [Calcote & Manos]
- Typically given by correlations of the form:

  \[ TSI = b \pm ax \]

  (where \( a \) and \( b \) are empirical coefficients and \( x \) is a simple function of the measured parameter).

- Shown to correlate well with soot emissions from real combustors [Yang, Boehman & Santoro]
The Smoke Point test

- ASTM D1322 criterion is the most commonly used
- Identifies smoke point with a specific flame morphology
- Highly subjective
- Smoke point converts to TSI using:

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

• Choose two reference fuels based on literature data. For example:
  – TSI (methylnaphthalene) = 100
  – TSI (methylcyclohexane) = 5

• Use your apparatus to determine the smoke point of these reference fuels experimentally.

• Determine the apparatus-dependent coefficients $a$ and $b$ by simultaneous solution:

$$a = \frac{TSI_1 - TSI_2}{\left(\frac{MW_1}{SP_1}\right) - \left(\frac{MW_2}{SP_2}\right)} \quad b = \frac{TSI_1 \left(\frac{MW_2}{SP_2}\right) - TSI_2 \left(\frac{MW_1}{SP_1}\right)}{\frac{MW_2}{SP_2} - \frac{MW_1}{SP_1}}$$

• In practice, the error margin in the TSI is typically at least 15% and can be much higher – not good!
Alternative method

• Use the fuel uptake rate at the smoke point to characterise sooting propensity instead [Olson & Pickens]
• Uptake rate was thought to be less sensitive to flame height around the smoke point, meaning that readings might be more reproducible
• The following equation was suggested:

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

• Is this really an improvement?
Understanding the Smoke Point

- Used ASTM burner with modified housing to measure fuel uptake rate vs flame height
- Flame height from video camera & MATLAB image analysis
- Uptake rate from analytical balance readings
Flame height vs Fuel Uptake Rate

1/2 n-heptane, 1/2 Toluene
Smoke Point, approx. 12 mm

1/3 n-heptane, 1/3 isoctane, 1/3 Toluene
Smoke Point, approx. 15 mm

2/3 n-heptane, 1/6 isoctane, 1/6 Toluene
Smoke Point, approx. 26 mm

Isooctane
Smoke Point, approx. 38 mm

1/2 n-heptane, 1/2 Toluene

1/3 n-heptane, 1/3 isoctane, 1/3 Toluene

2/3 n-heptane, 1/6 isoctane, 1/6 Toluene

Isooctane
PSD measurement Apparatus

DMS500

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Sample Dilution

- Effects of oxidation, surface reaction and coagulation mitigated by diluting the sample with nitrogen
- Dilution ratio was adjusted using a needle valve, which decreased the sample line vacuum
- PSD was found to be independent of dilution when the dilution ratio was higher than about 50-100
PSD above smoking & non-smoking flames

- Very difficult to get repeatable results because of high particle number concentration gradients; needs precise positioning and a very stable flame
- Clear shift from single mode (volatiles?) to multi-mode PSD when a soot trail is visible
Findings

• Fuel uptake rate vs flame height curve always showed a distortion just above the smoke point
• Relationship is still almost linear at the smoke point itself
• Lowest sensitivity to flame height occurs just prior to the appearance of a soot trail - Measure uptake rate here instead!
Lightweight Burner Design

- **Our Method**: Need to measure fuel uptake rate at incipient formation of soot trail by weighing burner
- Burner mass must not exceed the balance rating
- Lightweight burner was designed for quick and easy measurements, with rapid changeover of fuels
Testing a New Method

Smoke point errors estimates based on 9 measurements between at least two different experimentalists

Experimental uncertainty in raw data has been halved!
Error in the TSI

<table>
<thead>
<tr>
<th>Compound</th>
<th>Old Method % Error (95% confidence limit)</th>
<th>Our Method % Error (95% confidence limit)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methylcyclohexane</td>
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<tr>
<td>Iso-octane</td>
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<td>n-heptane/Toluene 3:1</td>
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<td>iso-octane/Toluene 3:1</td>
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<tr>
<td>Toluene</td>
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<tr>
<td>Phenylcyclohexane</td>
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<td>1-methylnaphthalene</td>
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</tbody>
</table>

In the Old Method:

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

In the Our Method:

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

Includes error in determining coefficients \( a \) and \( b \)
Conversion to TSI – Linear Blending?

ASTM Method

Our Method

Isooctane + toluene

n-heptane + toluene

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Conclusions

• Much better TSI reproducibility is achieved by basing it on fuel uptake rate at the point of incipient soot trail formation instead of the smoke point
• The best correlation for TSI seems to be:

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

• Confirmed that TSIs blend almost linearly with mole fraction, although there might be slight curvature


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