An Improved Metric for the Sooting Propensity of Fuels

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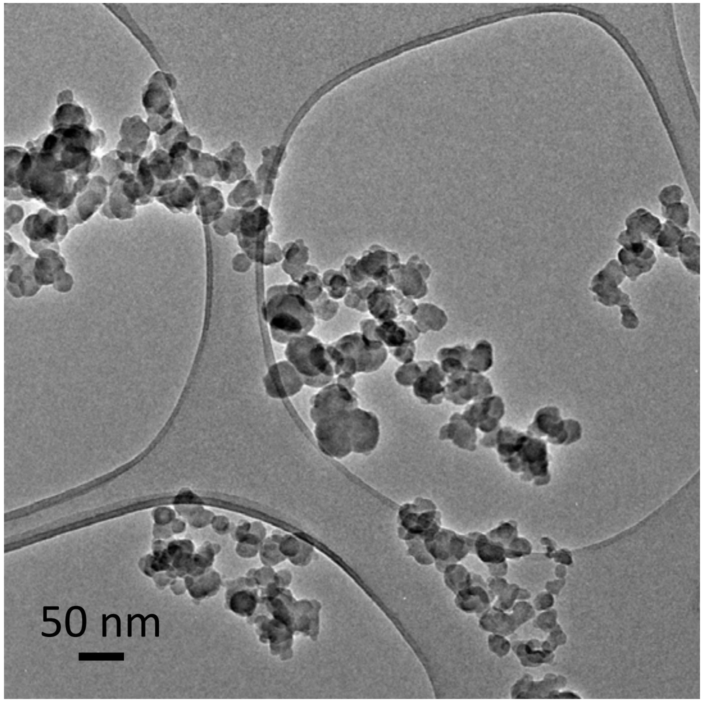
Background

- 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.

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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]

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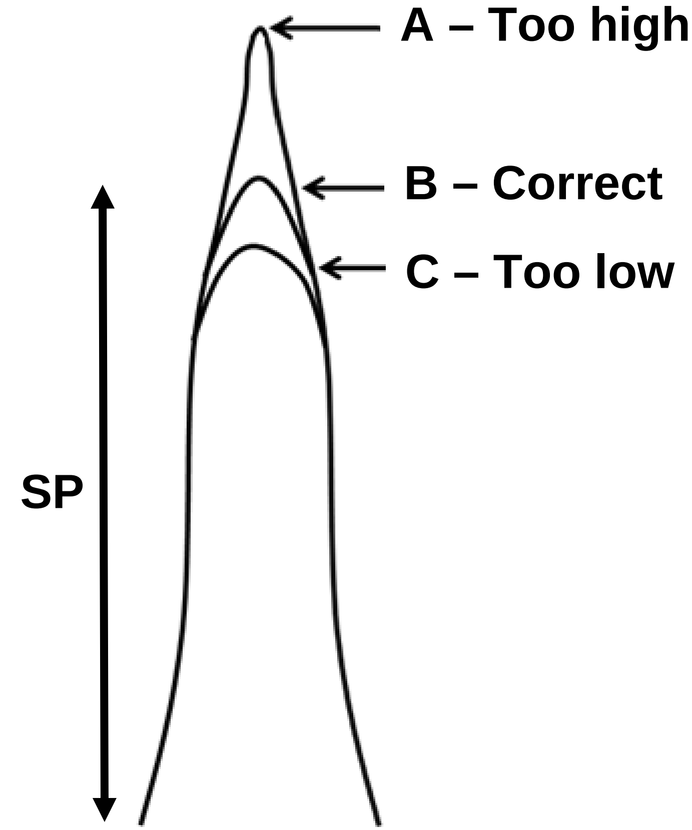
The Smoke Point test

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

$$TSI = a\left(\frac{\mathrm{MW}}{\mathrm{SP}}\right) + b$$



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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:

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

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

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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:

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

- Is this really an improvement?

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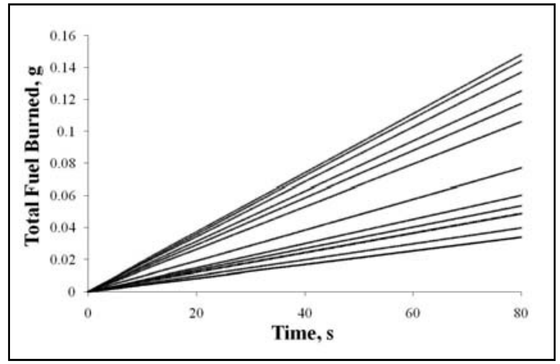
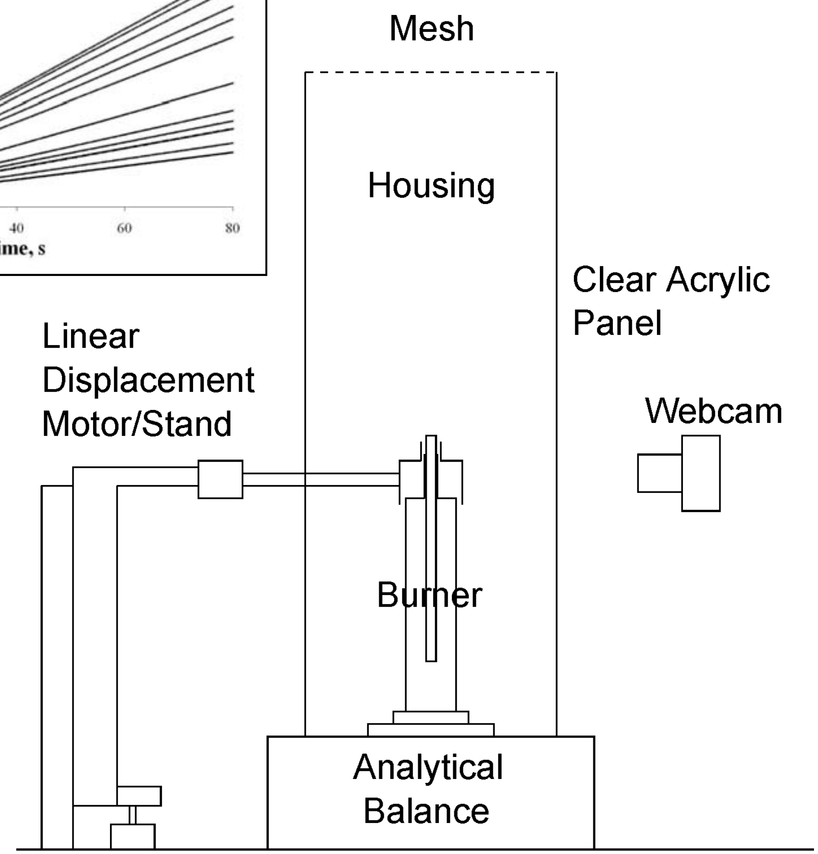
Understanding the Smoke Point

- 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





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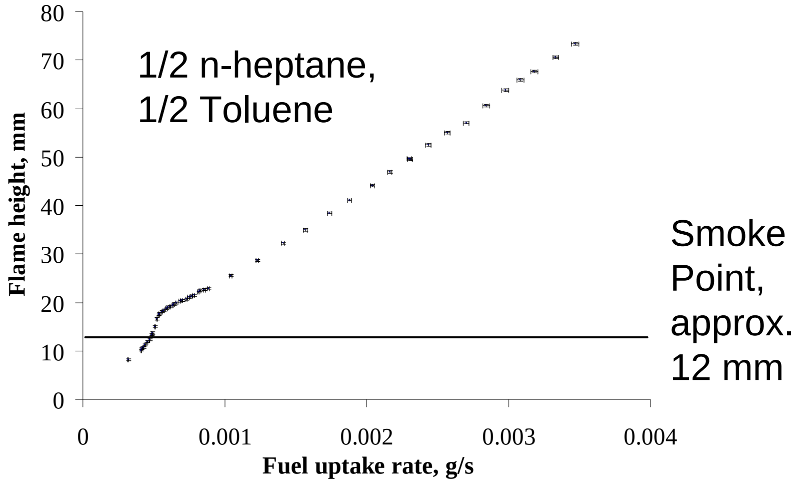
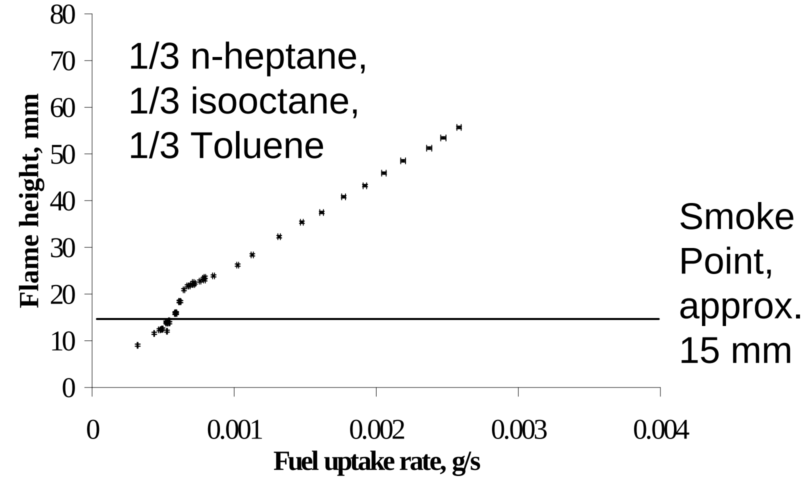
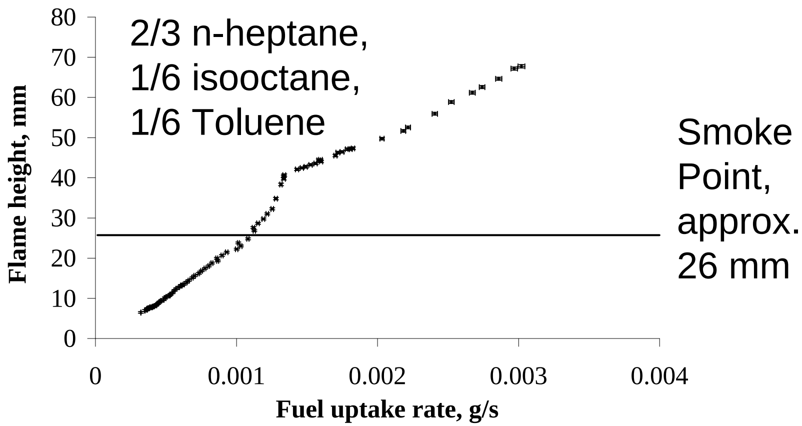
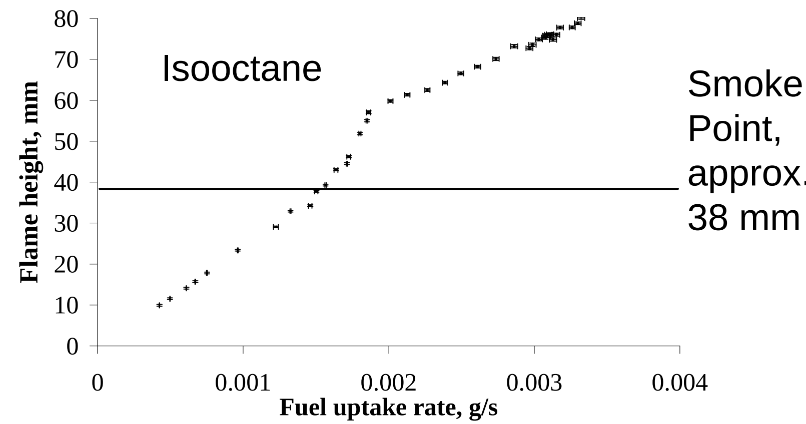
Flame height vs Fuel Uptake Rate









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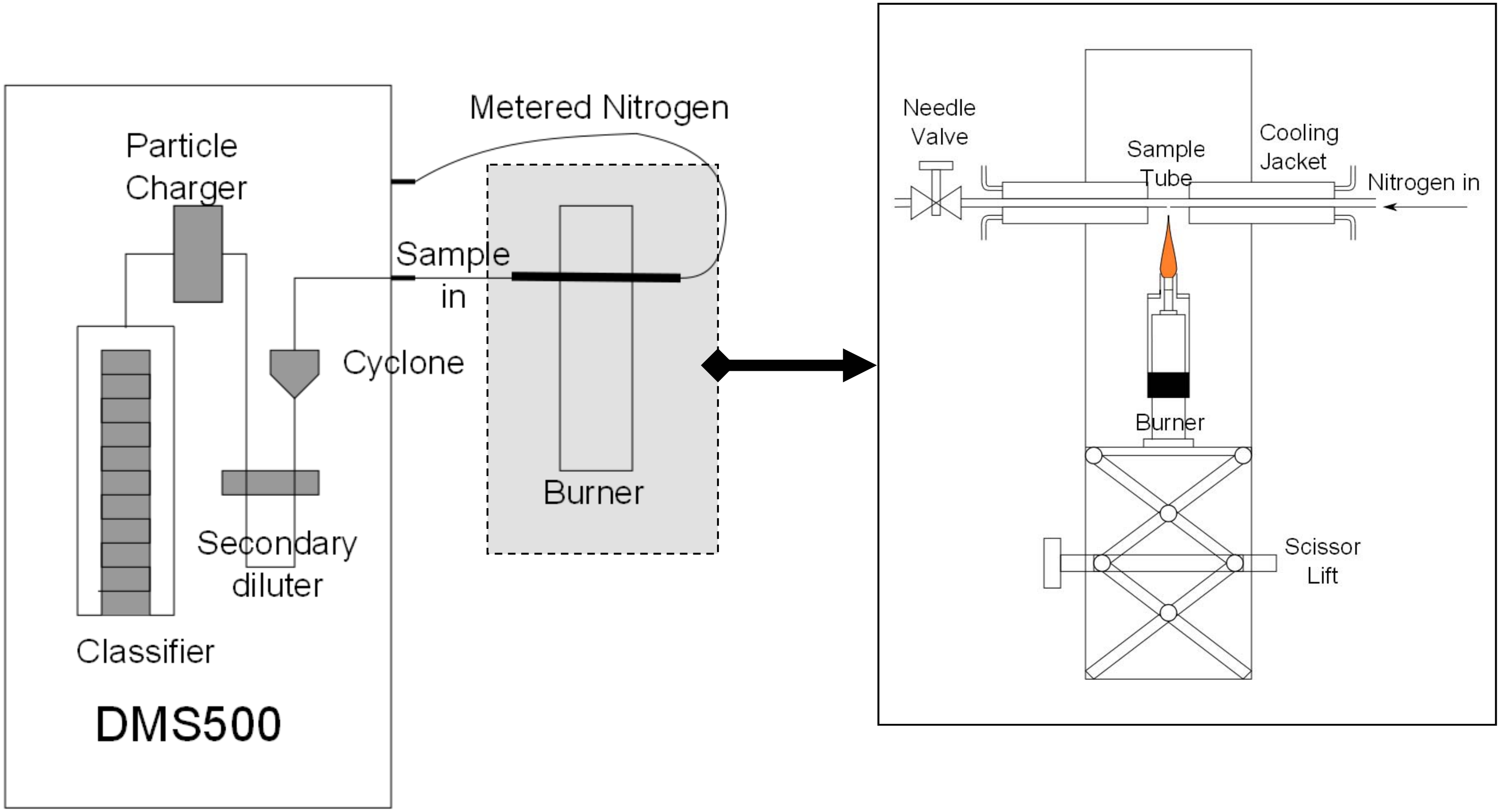
PSD measurement Apparatus



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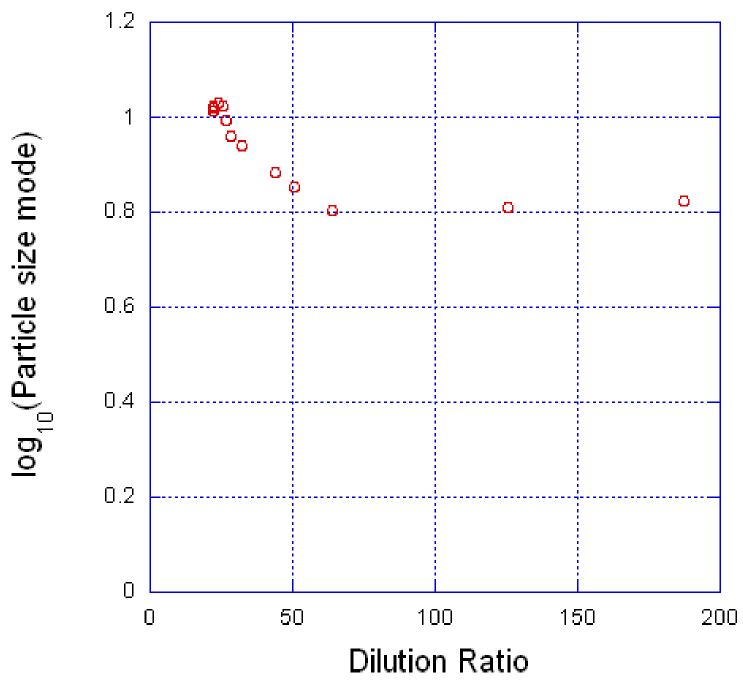
Sample Dilution



- 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

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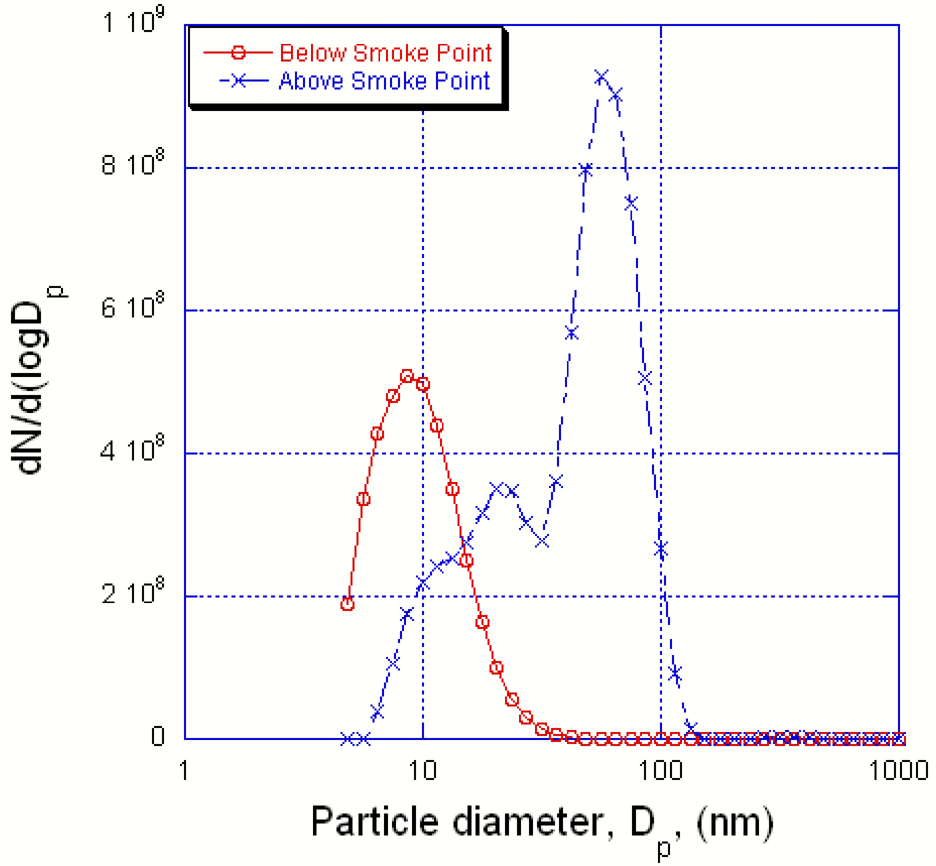
PSD above smoking & non-smoking flames



- 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

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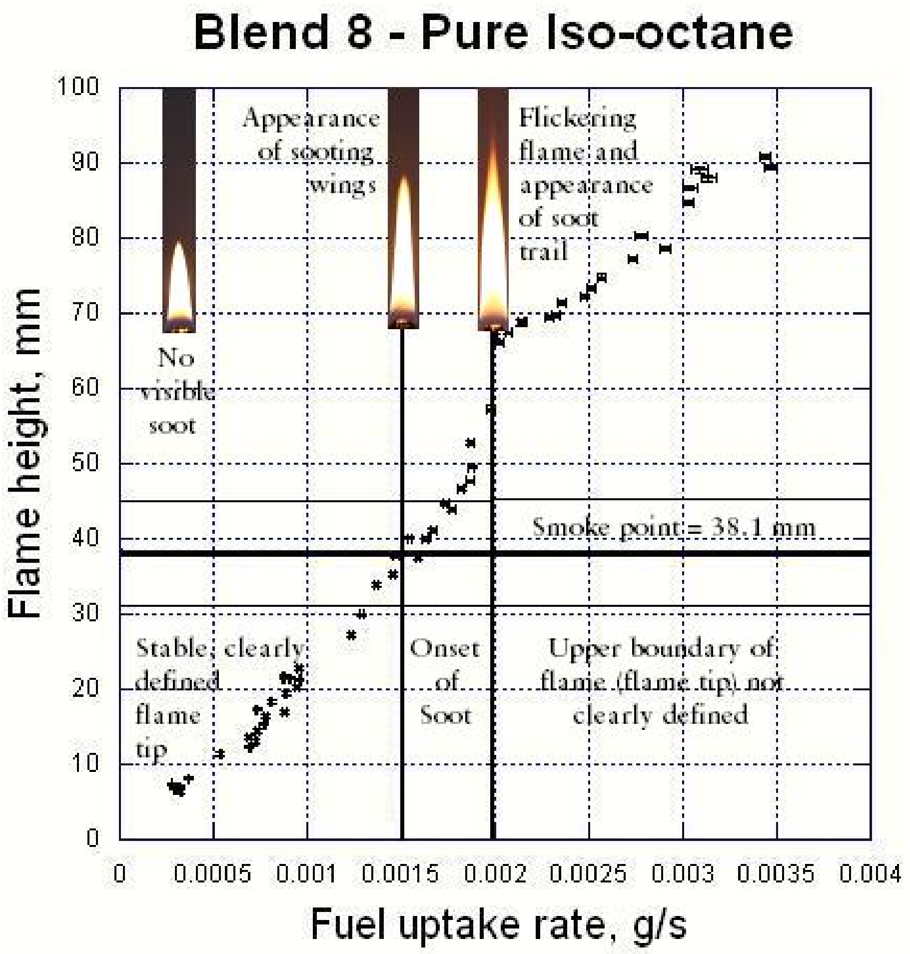
Findings

- 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!



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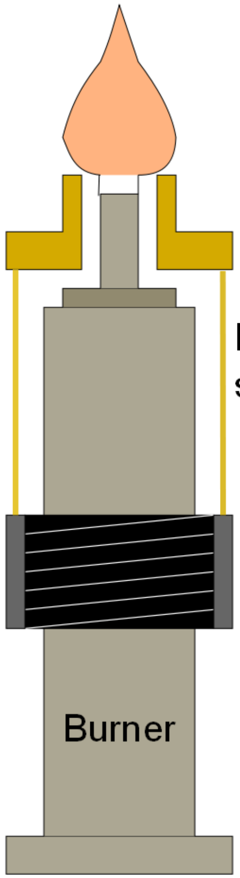
Lightweight Burner Design



- **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

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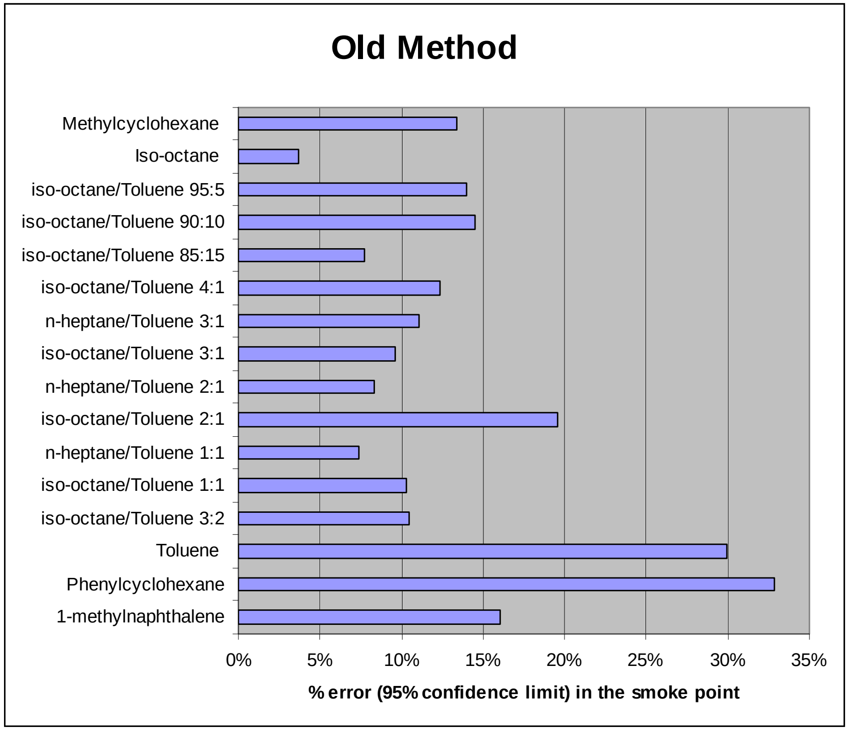
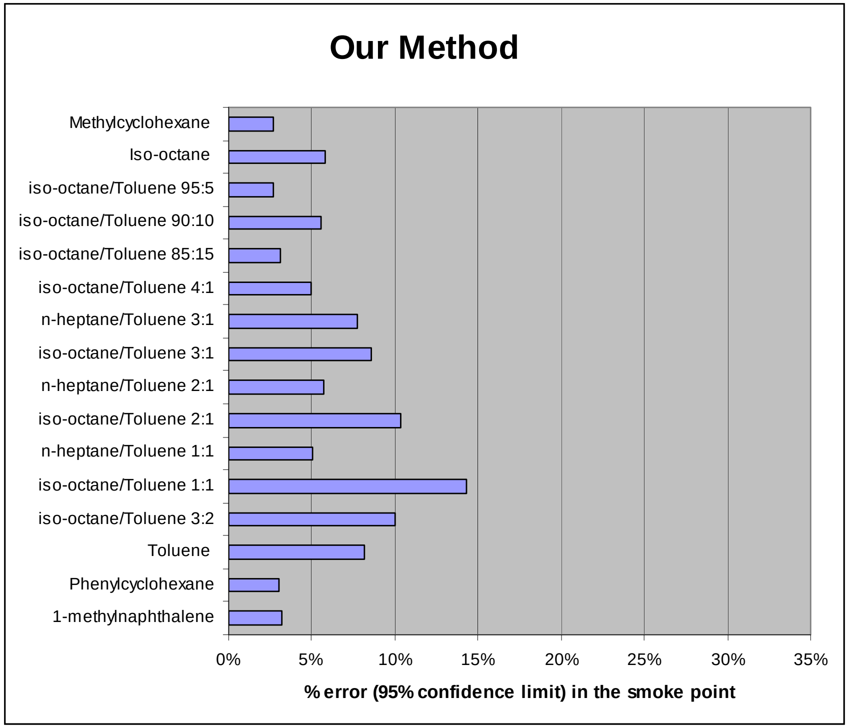
Testing a New Method

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





Experimental uncertainty in raw data has been halved!

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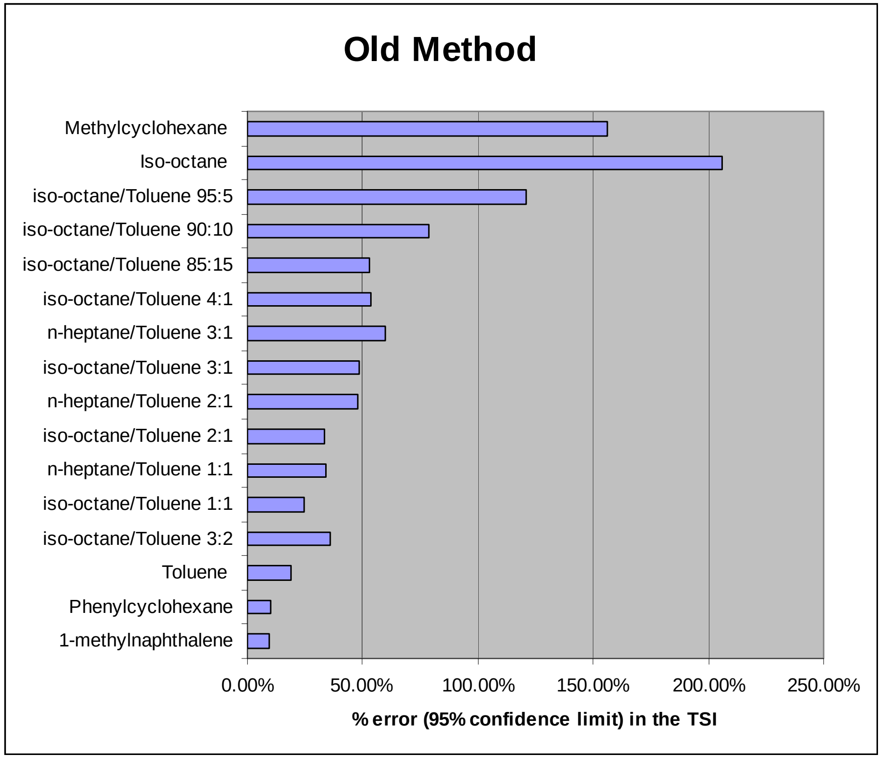
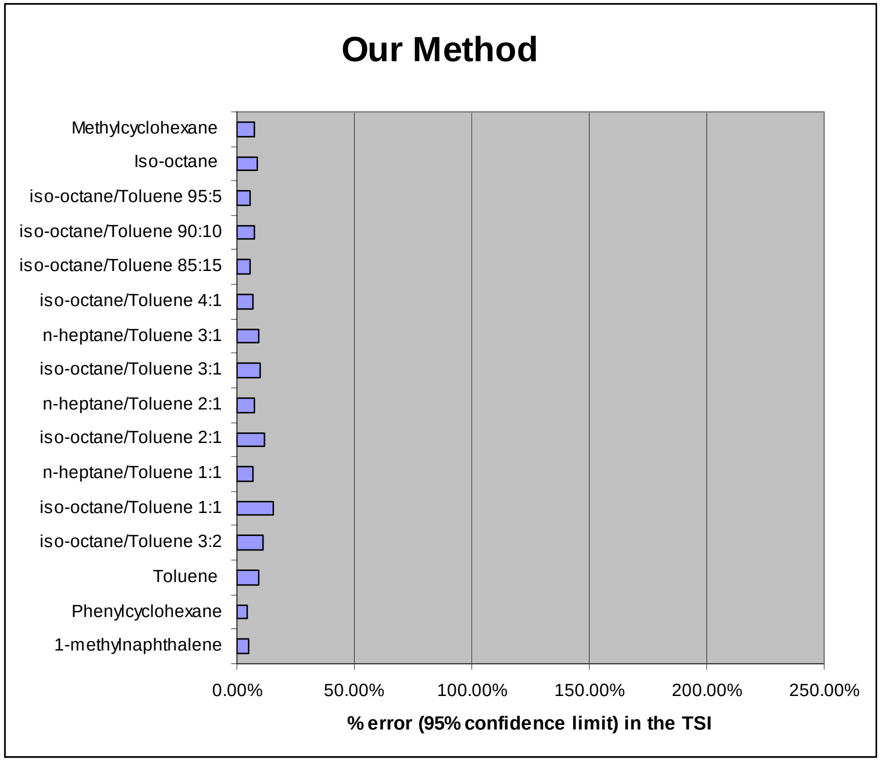
Error in the TSI





$$TSI = a\left(\frac{\mathrm{MW}}{\mathrm{SP}}\right) + b$$

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

Includes error in determining coefficients *a* and *b*

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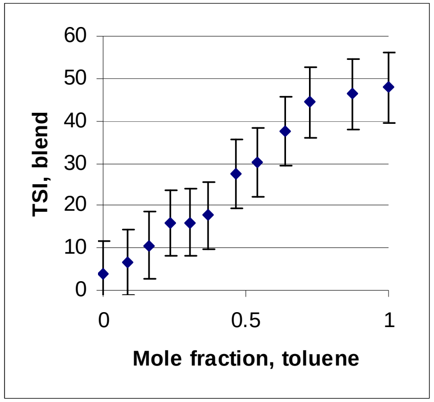
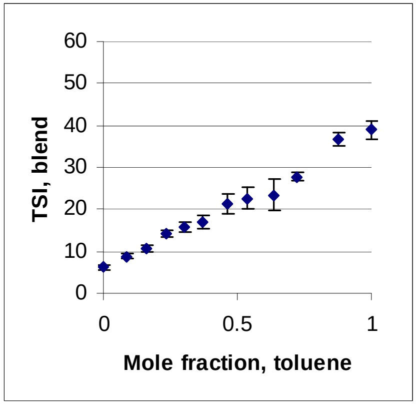
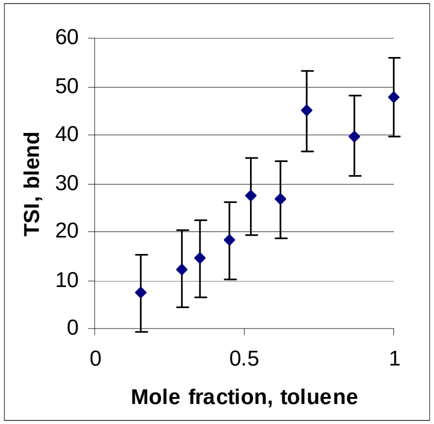
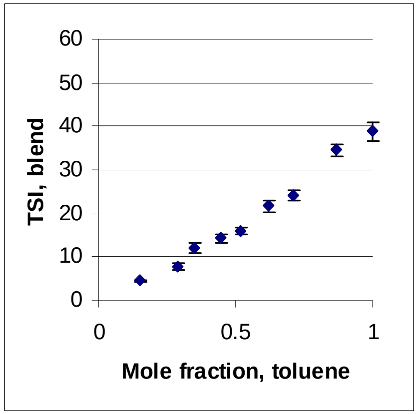
Conversion to TSI – Linear Blending?

	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:

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

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

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