Soot Formation Benefits of Sustainable Aviation Fuels Characterized with a Yield-Based Approach to Sooting Tendency

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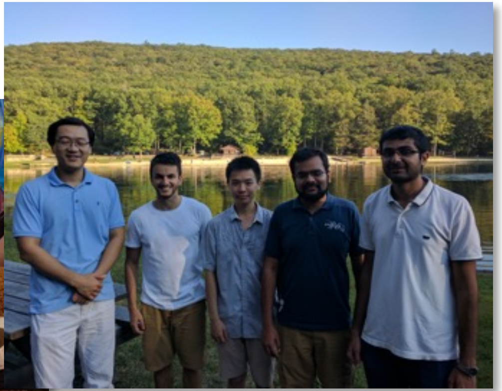

Photos: Charles McEnally, Yuan Xuan, Hyunguk Kwon

Acknowledgements

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- Nabila Huq and Derek Vardon (National Renewable Energy Laboratory) – synthesis of alkanes representative of SAF
- Harrison Yang and Joshua Heyne (University of Dayton) – characterization of jet fuel composition

Sustainable Aviation Fuels

- Sustainable aviation fuels (SAF) are jet fuels derived from renewable sources such as biomass and wastes instead of petroleum

- Their purpose is to reduce the impact of aviation on climate change

- They are also likely to reduce emissions of soot particles given that they typically contain fewer aromatics than petroleum-derived jet fuels

Aviation Causes of Climate Change

Climate Agent	Mechanism	Radiative Forcing (mW/m^2)	Ref.
CO_2	• Absorption of IR radiation from earth	+35	[1]
Soot	• Absorption of sunlight	+9.5	[2]
Aircraft–Induced Clouds (AIC)	• Absorption of IR radiation from earth • Nucleate from soot particles	+50	[1]

Particulate reductions present greater opportunity than CO_2 reductions

[1] B. Kärcher, *Nature Comm.*, **2018**, 9, 1824; [2] M.E.J. Stettler, *Environ. Sci. Technol.*, **2013**, 47, 10397

Fuel Composition Affects Soot

Sooting tendency is a fuel property that quantifies the effects of fuel composition on soot

Photo: Charles McEnally

Engine Emissions Measurements

1. Large fuel volumes required

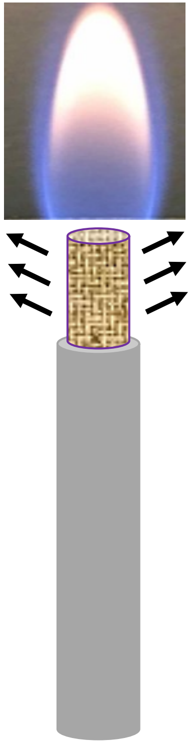
2. The local optimum for specific hardware may not be the global optimum

➢ A bench-scale sooting tendency metric is needed during fuel development

Photos: https://commons.wikimedia.org/wiki/File:KC135_refueling.jpg

Smoke Point Sooting Tendency

- Smoke point = height of the flame at the threshold of smoking
- Sooting tendency ~ 1/(SP)
- Larger SP = less sooty fuel
- Jet Fuel specifications (ASTM D1655) require SP > 18



Issues with Smoke Point

The measurement is subjective: the tester has to determine when the flame is at the smoke point

More Issues with Smoke Point

- Requires a large sample volume
  - 10 mL to satisfy ASTM D1322
  - Large volume required to saturate the wick
- Narrow dynamic range
  - Isocetane: maximum fuel flow is insufficient to reach SP
  - Benzene: SP = 8 mm; naphthalene: SP = 6 mm
- Difficult to simulate from first principles

Yield-Based Sooting Tendency

- Smoke point was created because soot was impossible to measure in the 1920's

- Soot measurement is easy today (e.g., laser extinction, color-ratio pyrometry, etc.)

1. Generate a fuel-doped methane/air flame
2. Measure maximum soot concentration $F_{v,max}$
3. Sooting tendency ~ $F_{v,max}$

Methane
Nitrogen
Test fuel, (usually) 1000 ppm

Photo: Charles McEnally

Yield Sooting Index (YSI)

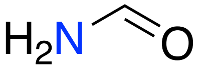
- $F_{v,max}$ depends on uninteresting experimental details (dopant concentration, burner dimensions, soot diagnostic, etc.)

- Rescale $F_{v,max}$ to an index (analogous to an octane rating)
  - Yield Sooting Index (YSI) = $A * F_{v,max} + B$
  - A, B are constants for a given experimental set
  - They are chosen so that YSI(n−heptane) = 36.0 and YSI(toluene) = 170.9
  - Scale constructed so that YSI(benzene) ≈ 100 and the YSI of a fuel that produces no soot ≈ 0

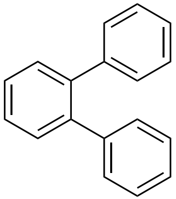
YSI Overcomes the Issues with SP

- Small sample volume: [dopant] = 1000 ppm
  - ❖ Typically less than 100 μL

- Wide dynamic range: can change [dopant] as needed
  - ❖ Minimum YSI = −3.1 (formamide)



  - ❖ Maximum YSI = +1340 (1,2-diphenylbenzene)

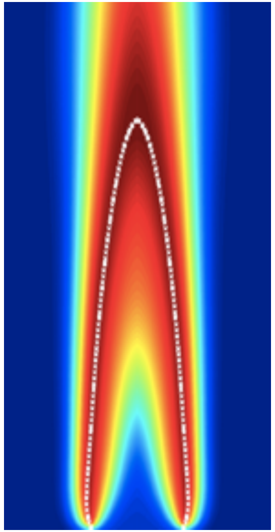


- Results can be simulated from first principles
  - ❖ One flame with well-defined boundary conditions
  - ❖ Simplified computations with perturbation methods

First Principles Prediction of YSI

Experiment

CFD



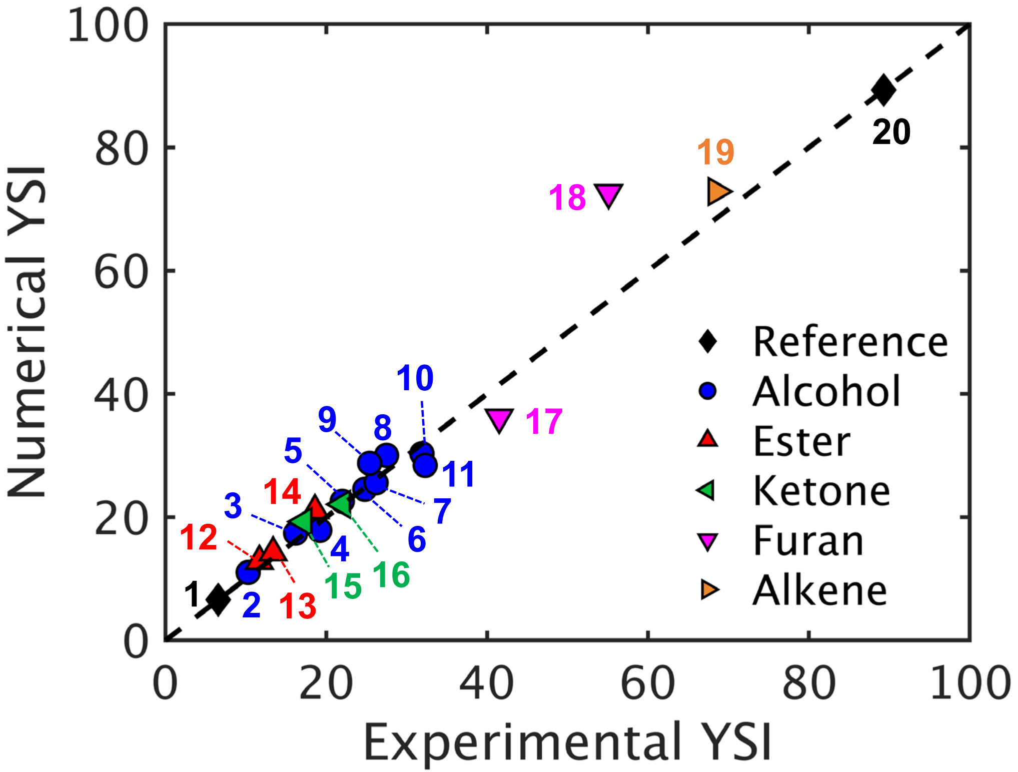
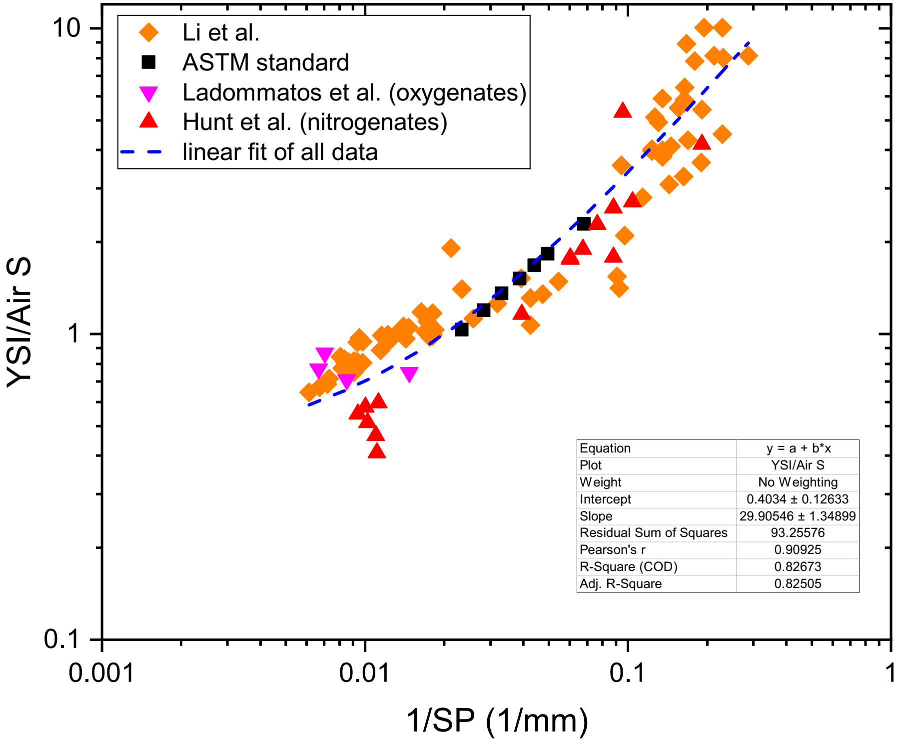


Photo: Charles McEnally; image: Yuan Xuan; figure: Kwon, *Fuel*, **2020**, 276, 118059

YSI Correlates with Smoke Point

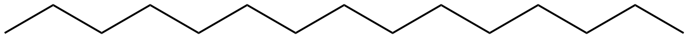
This correlation can render an equivalent SP for a measured YSI



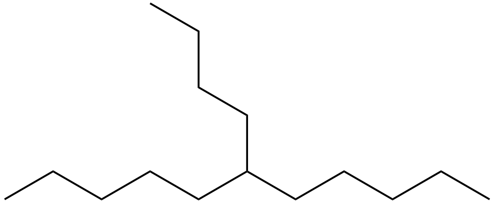
Li, *Combust. Sci. Technol.*, **2012**, 184, 829; ASTM D1322-18, **2018**; Ladommatos, *Fuel*, **1996**, 75, 114; Hunt, *Ind. Eng. Chem.*, **1953**, 45, 602

Demonstration – Jet Fuel Alkanes

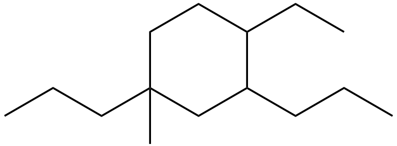
A. Linear C15 alkane



B. Branched C15 alkane



C. Cyclic C15 alkane



B and C synthesized by Nabila Huq and Derek Vardon, National Renewable Energy Laboratory

Results – Jet Fuel Alkanes

Fuel	YSI (smaller is better)	Equivalent SP (larger is better)
Linear C15 alkane; $C_{15}H_{32}$	82.3	86.4
Branched C15 alkane; $C_{15}H_{32}$	87.9	75.3
Cyclic C15 alkane; $C_{15}H_{32}$	145.7	32.4
POSF 10325 (typical Jet A); $C_{11.4}H_{22.0}$	150.0	20.5

POSF 10325 characterized by Harrison Yang and Joshua Heyne, University of Dayton

Conclusions and Future Work

- The sooting tendencies of sub-mL quantities of sustainable aviation fuels can be characterized with a yield-based approach

- We are building an inventory of current and future SAF in collaboration with the DOE Biojet Consortium, and will evaluate the sooting benefits of these fuels