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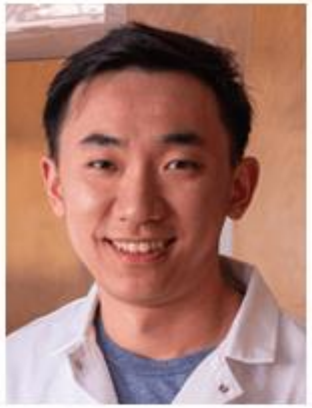

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Assis. Research Prof.

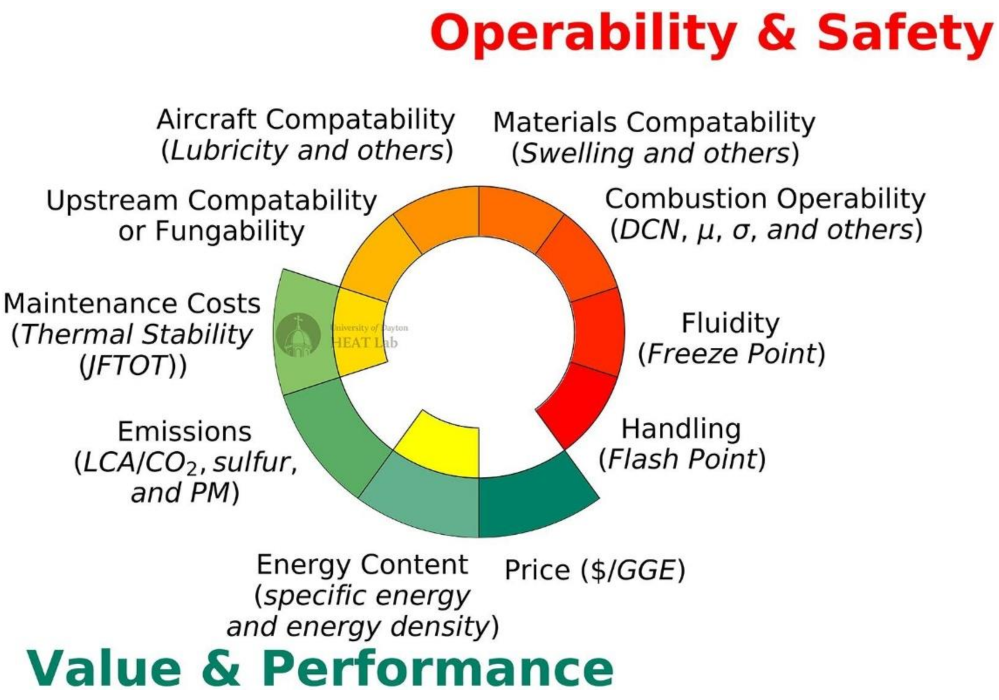
David Bell, Ph.D.
Post-doc

Conor Faulhaber
Graduate student,
Alaska Airlines Fellow

ICAO

Developing 100% drop-in compositions that minimize sooting

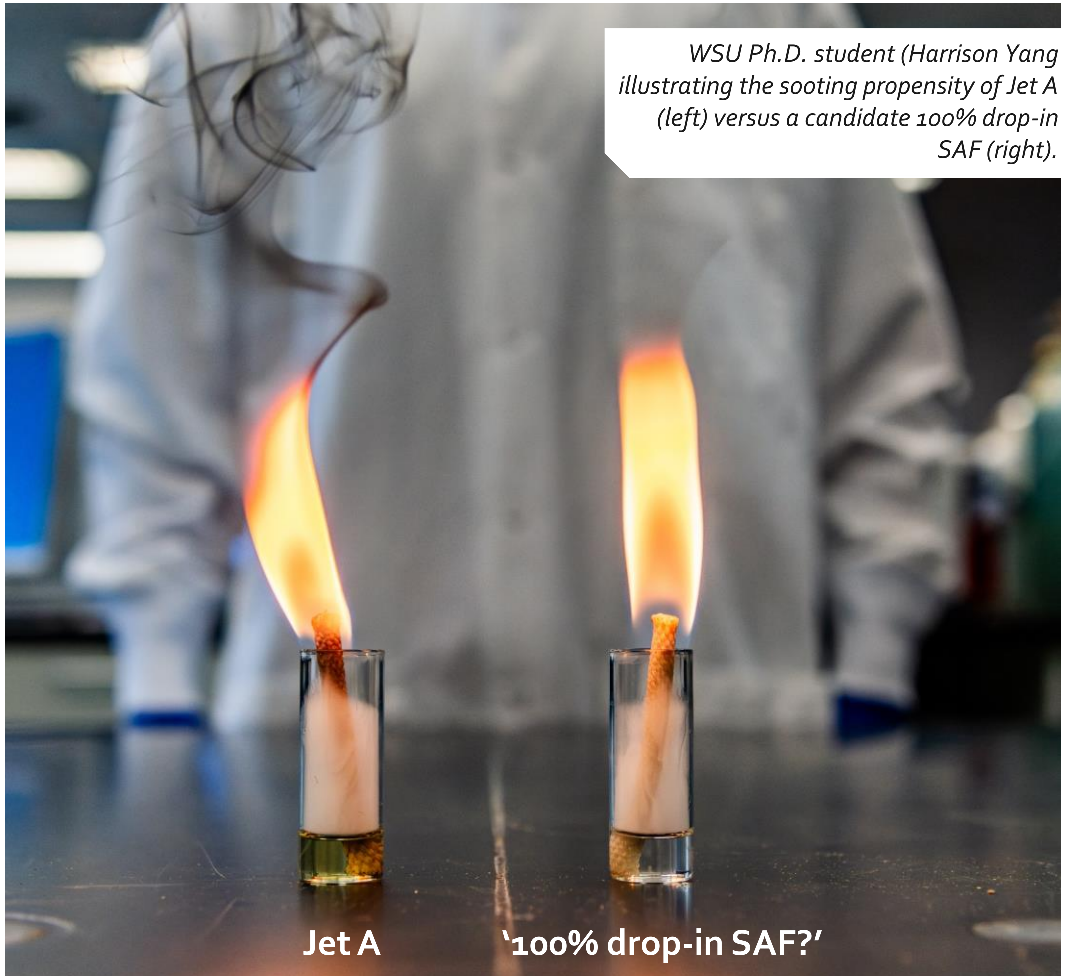
- Experimentally:
  - 36 pieces of equipment
  - 100s of purchased and sourced materials
  - Papers on individual properties
- Computationally:
  - Jet Fuel Blend Optimizer (JudO) software
  - ~35 different properties*
  - >1,200 molecules with necessary properties (>20k molecules with some properties)



*Boehm, Yang, Bell, Faulhaber, Mayhew, Bauder, Eckel, Heyne, Perspective on Fuel Property Blending Rules for Design and Qualification of Aviation Fuels: A Review, *Energy & Fuels,* **2024**. DOI: 10.1021/acs.energyfuels.4c02457

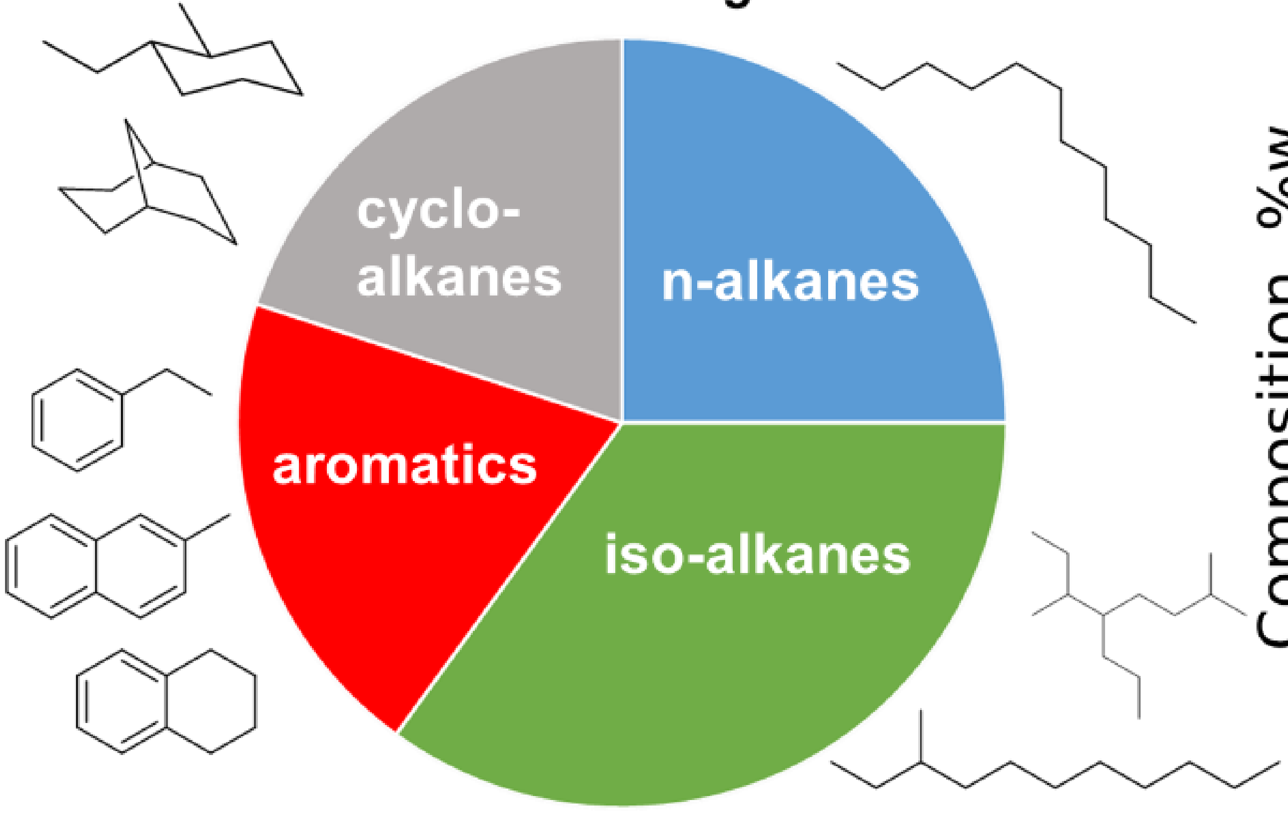
Testing SAF candidate materials

- Received and tested >320 unique samples from roughly 40 institutions globally
  - < 1 mL to liters of material
- Established a prescreening protocol for tiered testing
- Producers are typically well aware of nvPM emissions early in their technology development process.

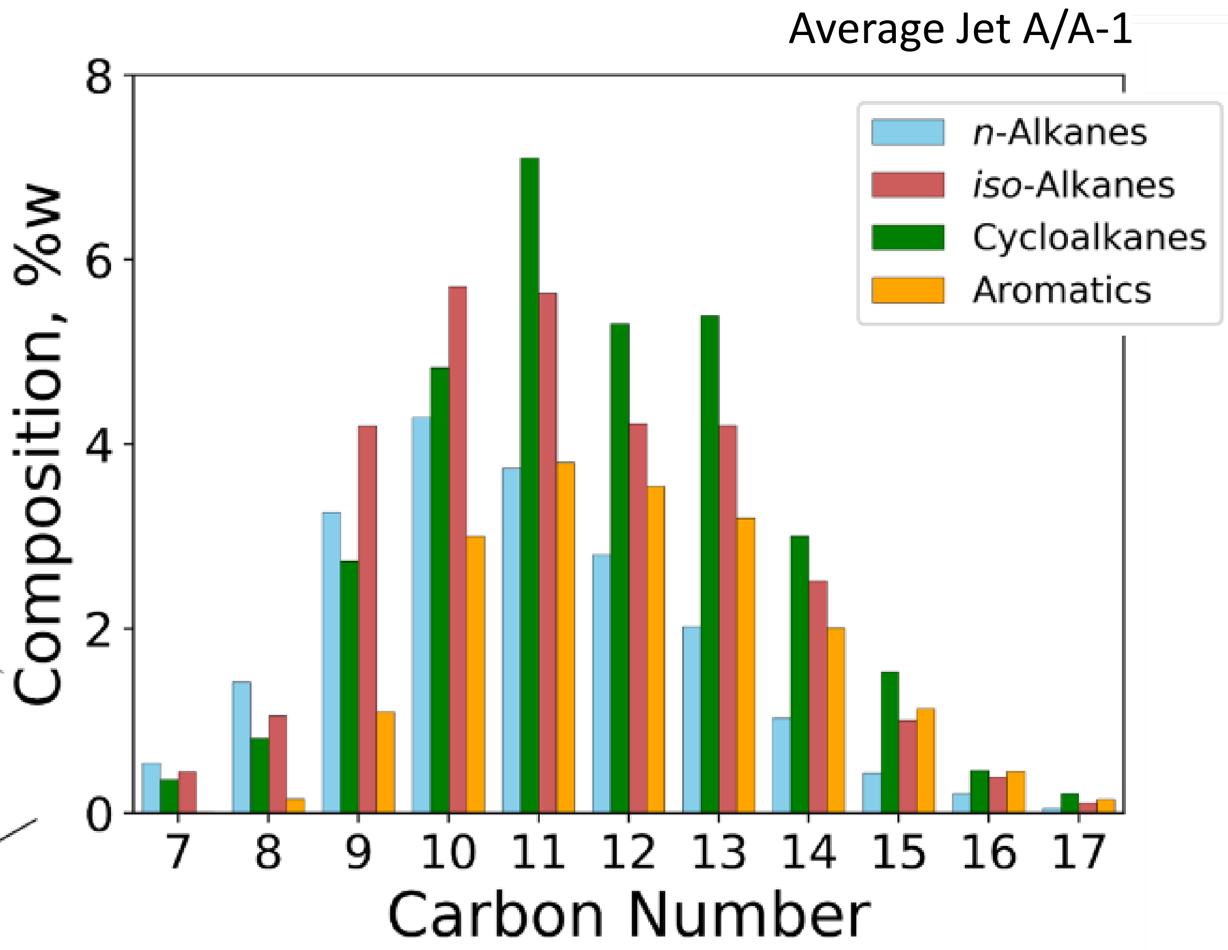


WSU Ph.D. student (Harrison Yang illustrating the sooting propensity of Jet A (left) versus a candidate 100% drop-in SAF (right).

Ideal Carbon Length C8-C16



fractions vary



Aromatics are limited to 25%

Olefins and heteroatoms are limited (not allowed)

- Olefins (<1%) (gum formation)
- S, N, O containing (limited allowance)

Holladay, Abdullah, Heyne, Sustainable Aviation Fuel: Review of Technical Pathways, DOE BETO Report, 2020.

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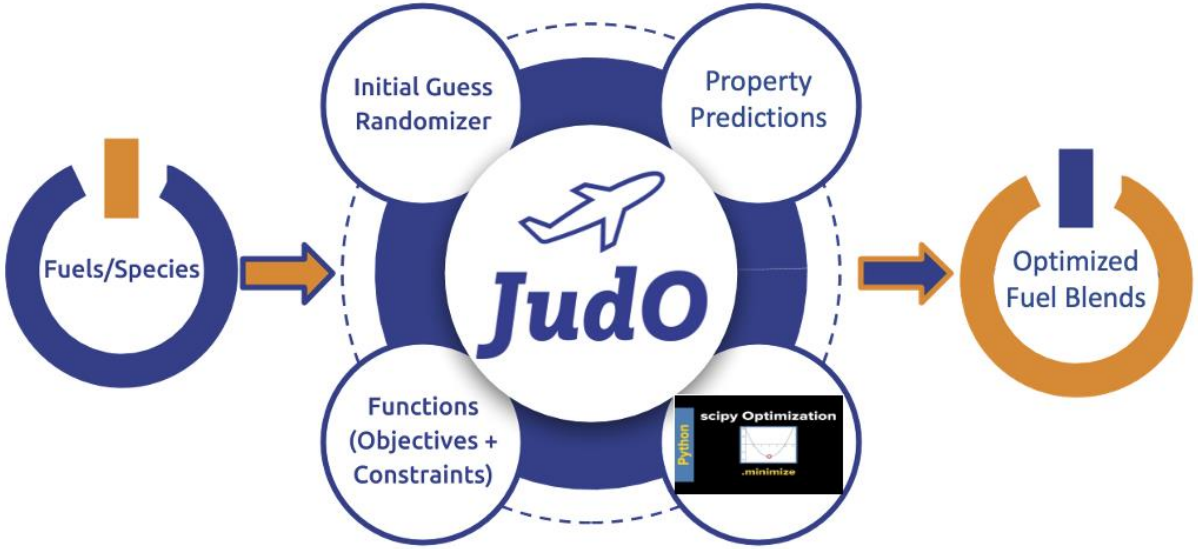
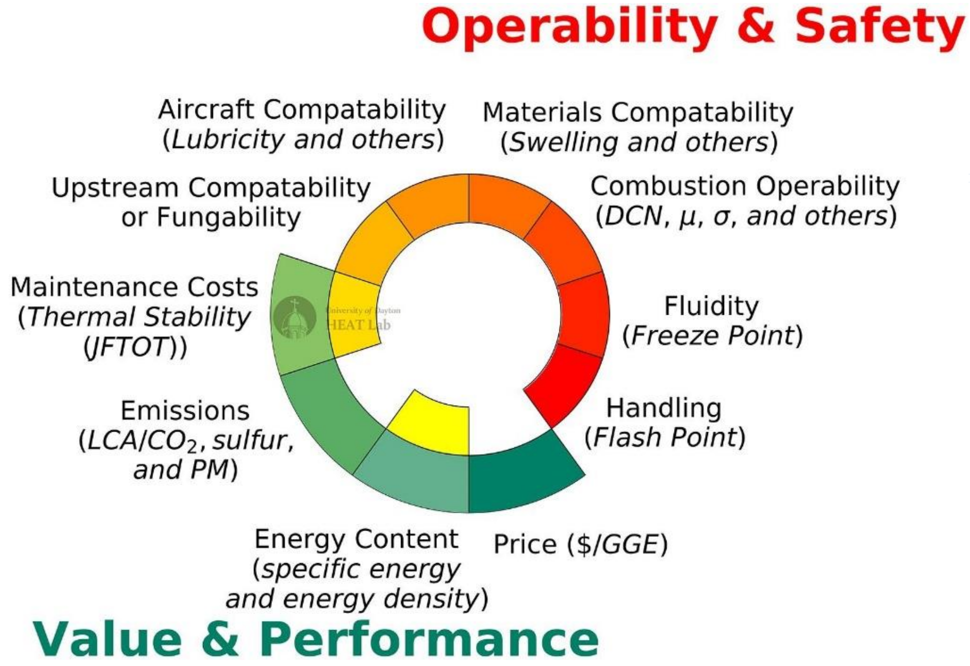
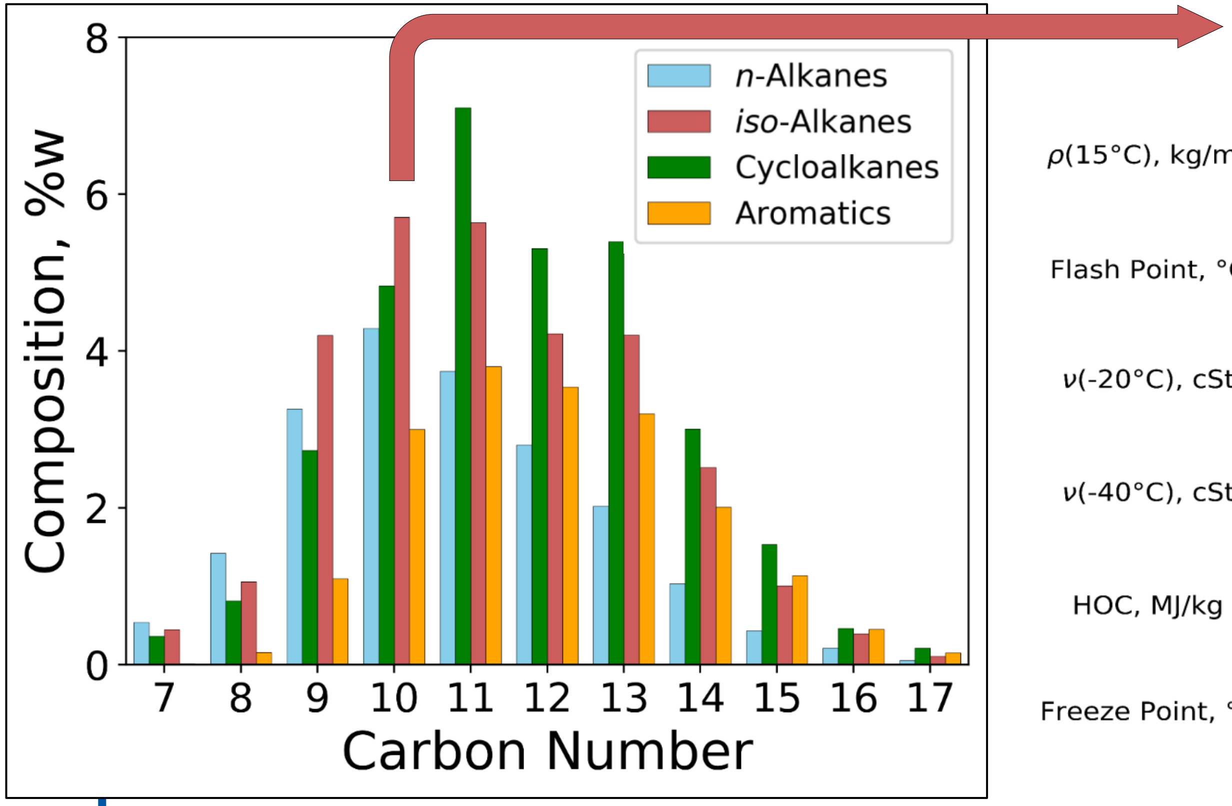
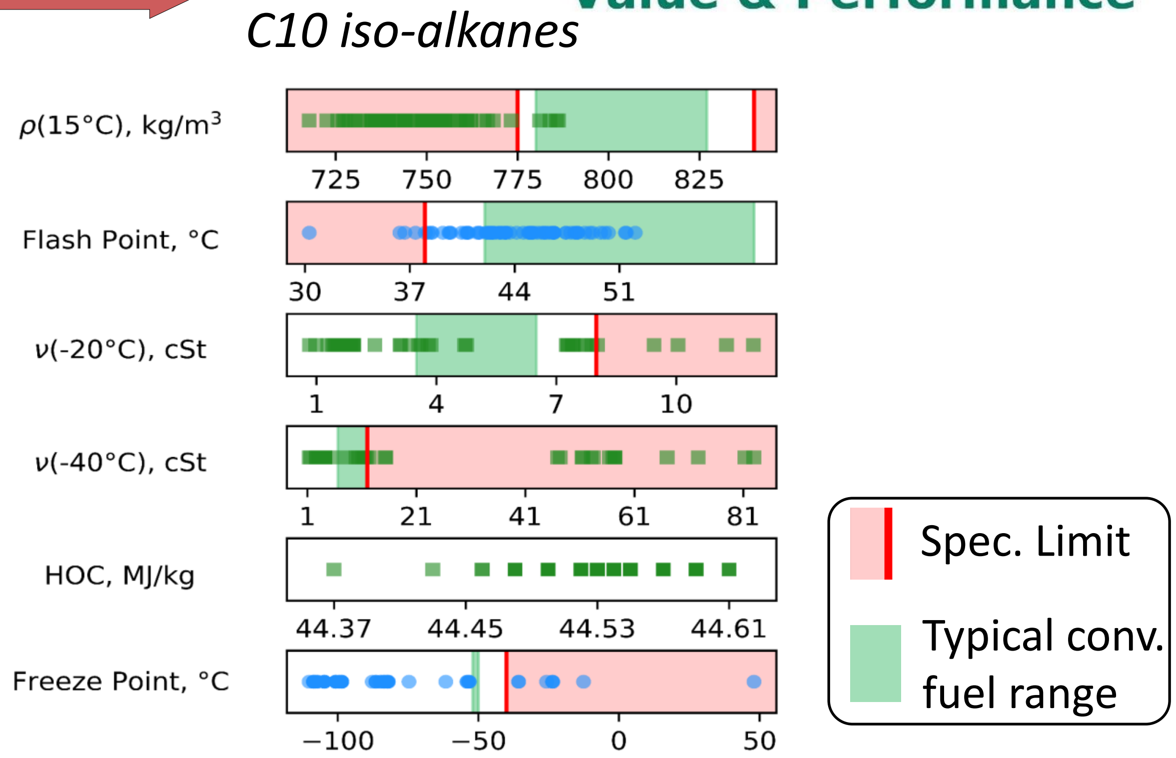

Fuels/Species
Initial Guess Randomizer
Property Predictions
JudO
Functions (Objectives + Constraints)
scipy Optimization
Python
.minimize
Optimized Fuel Blends


Operability & Safety
Aircraft Compatability (Lubricity and others)
Materials Compatability (Swelling and others)
Upstream Compatability or Fungability
Combustion Operability (DCN, μ, σ, and others)
Maintenance Costs (Thermal Stability (JFTOT))
Fluidity (Freeze Point)
Emissions (LCA/CO_2, sulfur, and PM)
Handling (Flash Point)
Energy Content (specific energy and energy density)
Price ($/GGE)
Value & Performance

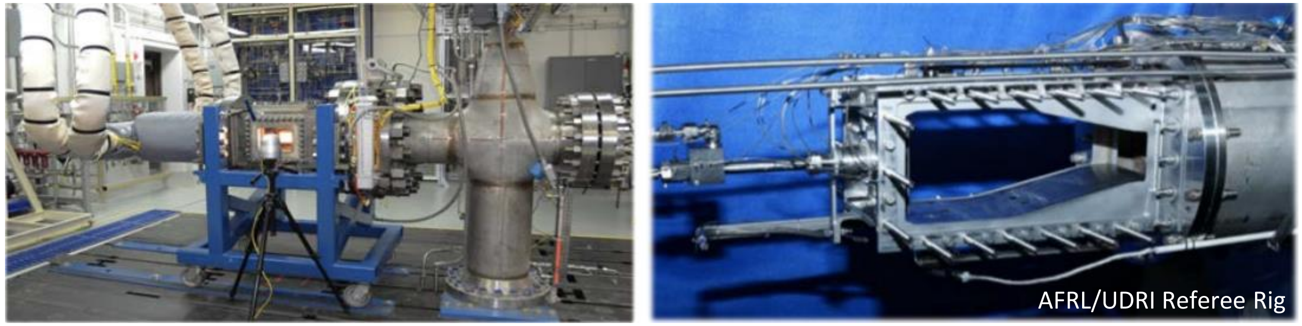

Composition, %W
Carbon Number
n-Alkanes
iso-Alkanes
Cycloalkanes
Aromatics
0
2
4
6
8
7
8
9
10
11
12
13
14
15
16
17


C10 iso-alkanes
ρ(15°C), kg/m^3
725 750 775 800 825
Flash Point, °C
30 37 44 51
ν(-20°C), cSt
1 4 7 10
ν(-40°C), cSt
1 21 41 61 81
HOC, MJ/kg
44.37 44.45 44.53 44.61
Freeze Point, °C
−100 −50 0 50
Spec. Limit
Typical conv. fuel range

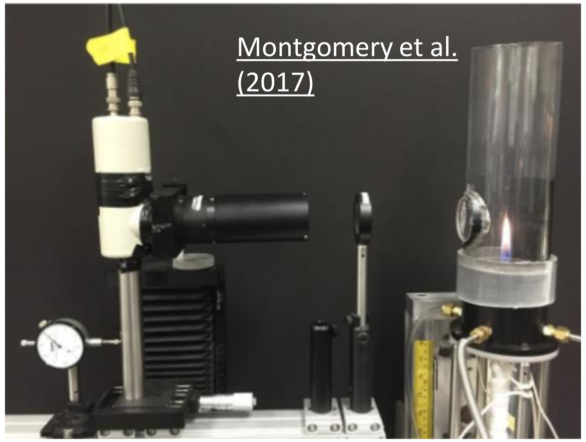
Background: Measuring Sooting


Voigt et al. 2020 NASA trailer plane following DLR A320

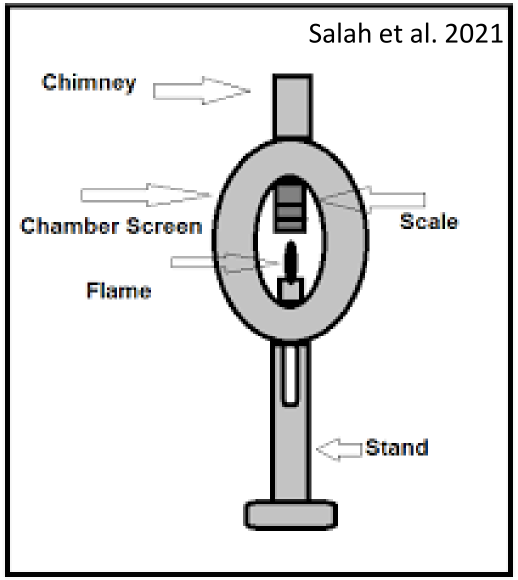
Full-scale engine testing: Ideal, but prohibitively costly during development of novel fuels


AFRL/UDRI Referee Rig

Referee Rig Testing/Emissions Indices (EI): Still expensive and complex, but realistic for producers further along in R&D

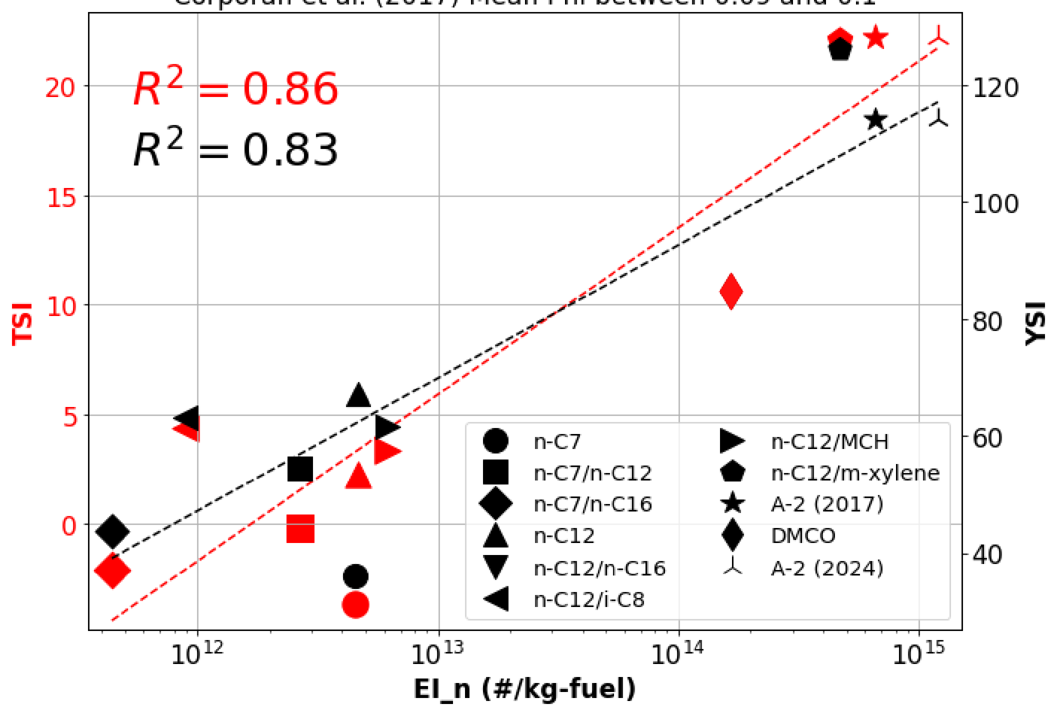

Montgomery et al. (2017)

Yield Sooting Index (YSI): Cheaper with established prediction methods



Salah et al. 2021

Threshold Sooting Index (TSI): Simple to measure and predict

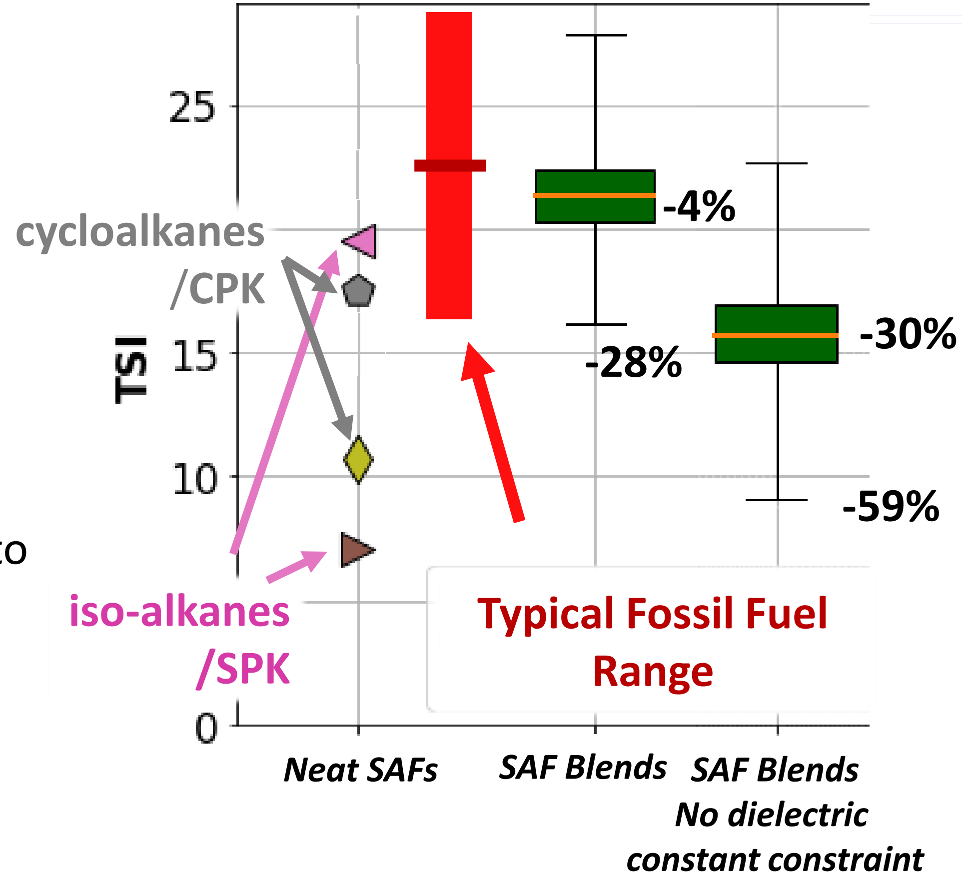


Most of our research uses TSI to evaluate the sooting propensity of jet fuel

What do we know…

- Renewable vs. fossil carbon has no impact on and emissions reduction:
  - The comments below also apply to the concept of Low Carbon Aviation Fuel (LCAF).
- **‘Drop-in’ solutions can lower sooting potential:**
  - *There are many drop-in solutions available that have the potential to lower the sooting propensity of aviation fuels.*
  - Current SAF technologies have demonstrated a **28% reduction in the Threshold Sooting Index (TSI) vs. avg. fossil jet**, which is a metric used to quantify sooting behavior.
  - The incorporation of additional or novel molecules in solutions has shown promise, with a potential reduction of up to **60%** in TSI.
- Non-drop-in solutions and their potential for emission reduction:
  - HEFA (or SPK) has approximately a **67%** reduction in TSI versus.
- Relationship between aromatic molecular weight and sooting propensity:
  - There is a general trend indicating that lower molecular weight aromatics tend to have lower sooting propensities.
  - This suggests that selecting and utilizing lower molecular weight aromatic compounds in aviation fuels could potentially contribute to reduced sooting and improved emissions performance.

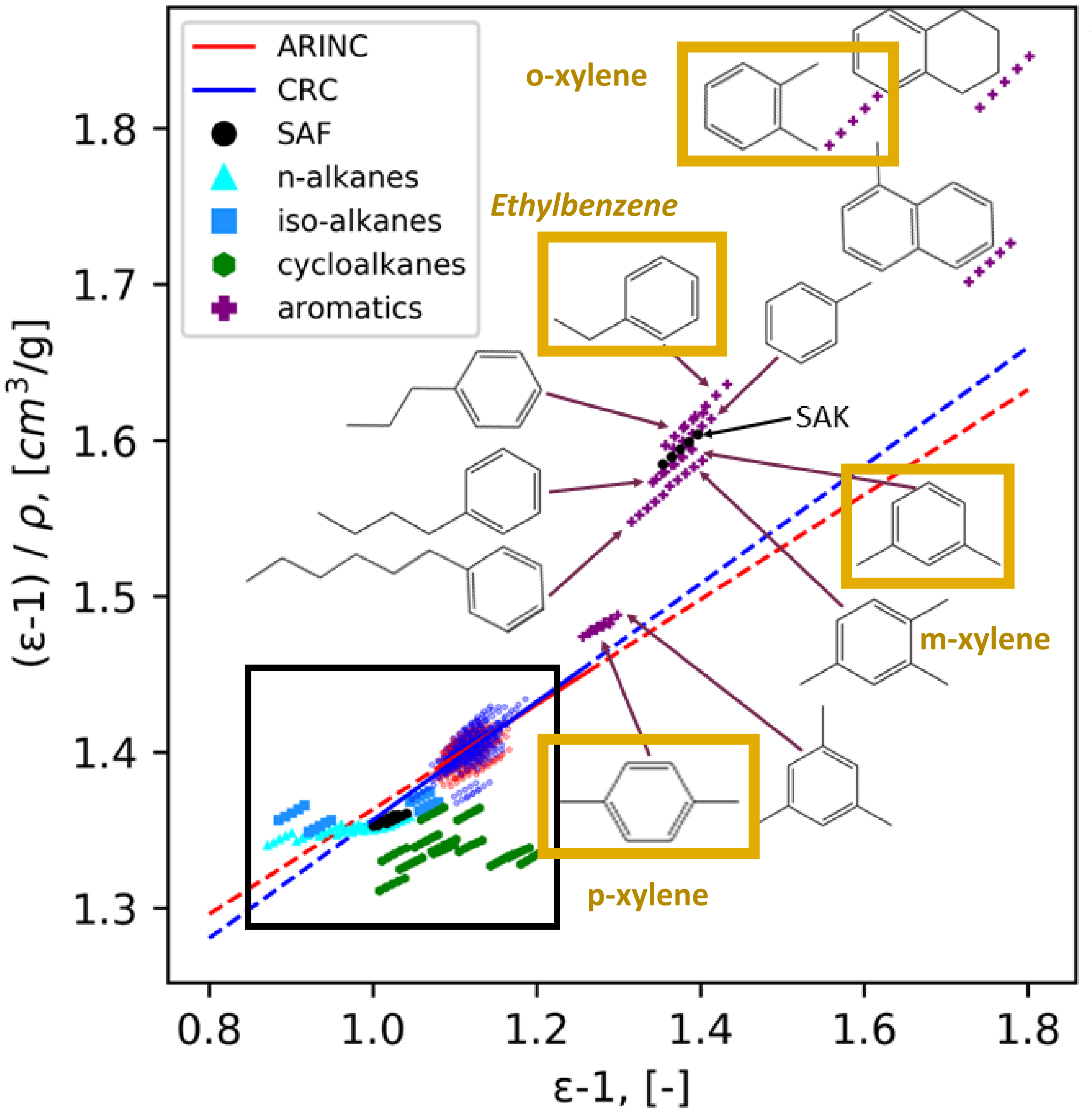
Illustrative preliminary results
restrictive dielectric constant scenario
but not all properties



What we do not know…

Four isomers (C_8H_{10}) with wide-ranging dielectric properties. Three (xylenes) have the same TSI (54.3). Ethylbenzene has a TSI of 46.8.

1. **What is the bottle-neck for 8% aromatics** and defining drop-in:
   - What are the specific limitation impacting the ability to go lower than 8% aromatics?
2. **Effective understanding across various scales and conditions:**
   - How can we accurately and consistently translate fuel compositions and performance from small-scale laboratory tests and predictions to larger-scale applications?
3. **How low can 'drop-in' go? …** evaluating the need for a new Jet-X specification:
   - If we continue to illuminate the physical limits of drop-in fuels, how close can we get to the desired properties and performance?
   - At potential future low blending limits, does the need for a new specification matter, or are the existing standards adequate?



Yang, Bell, Boehm, Boze, Kosikin, Heyne, Assessing the Effect of Composition on Dielectric Constant of Sustainable Aviation Fuel. *in revision*.