

CAAFI Prescreening

Motivation, process, and an example

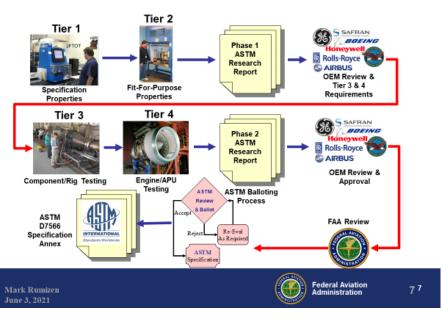
Joshua Heyne (jheyne I @udayton.edu) | 3 June 2021 | CAAFI mini-symposium



Alt. fuel evaluation and qualification route:

The motivation for the National Jet Fuels Combustion Program (NJFCP)

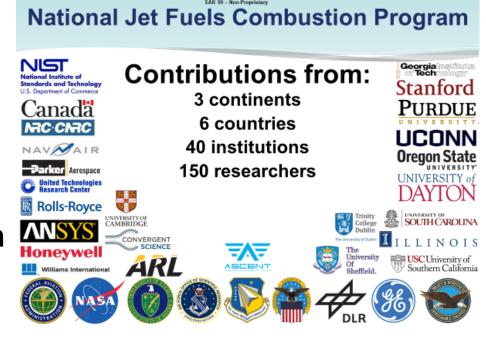
ASTM D4054 Evaluation Process



- Each Tier increases volume required and testing costs
 - Previous evolutions require 5 years and tens of thousands of gallons
- NJFCP's mission: 'streamline the evaluation process for alt.

fuels'

- Focused on Engine
 Operability
 - Lean blowoutAltitudeCold ignitionrelight
- Maximize variance in
 - . fuels,
 - 2. conditions, and
 - 3. geometry

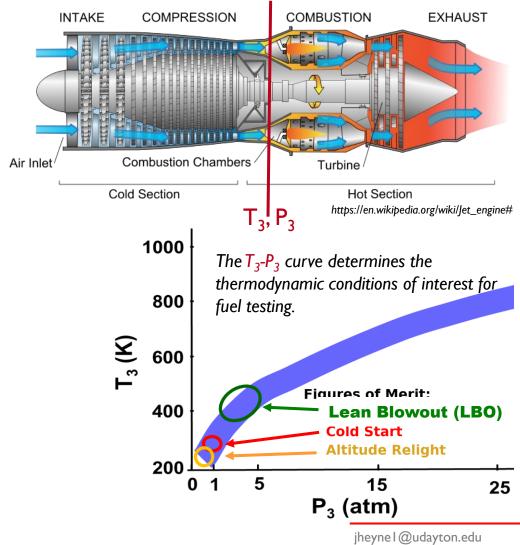


NJFCP Accomplishments

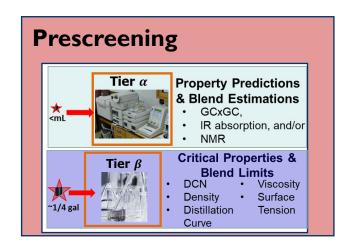
A novel combustor stabilization mechanisms was discovered

- Evaluation of ~12 fuels across dozens of experimental devices
- Analysis suggests bounding of ~8 properties can account for ~90% of all observed variance
 - Remaining variance is attributed to coupling of mass transfer and autoignition propensity
 - One unexplained observation remains.
- Referee Rig operability limits at relevant conditions match all known OEM hardware trends
- CFD matches operability trends for several fuels and conditions
- Process for custom chemical kinetics developed

Gas Turbine Engine Schematic



NJFCP Outcomes and Learnings



Tier	Measured Property	Predicted Property	Vol. (mL)	No. tested
O	GCxGC	LHV, Density, Surface tension, Freeze point, Viscosity, DCN, Flash point	ı	61
α	Distillation			
	Density	cosity face ten. LHV sh point	10	38
	Viscosity			
O	Surface ten.			
P	Freeze point			
	Flash point			
	DCN		140	8

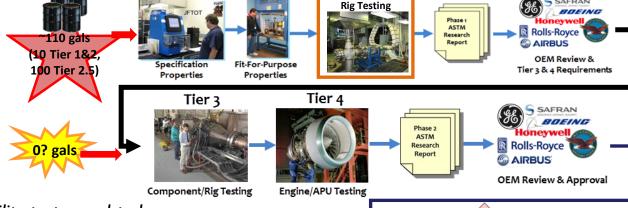
Tier 2

Guide compositions to meet properties most likely to eclipse Tier 3 and 4 operability tests with minimal volume requirements

Volumes needed for

	various testing Tiers	
•	$\mathcal{O}(gal)$	Tier
← Prescreenin	~10-6	α
	~10-1	β
	~10²	1 & 2
← Referee	~10²	2.5
Rig	~10 ³	3 & 4

Proposed ASTM D4054



Tier 2.5

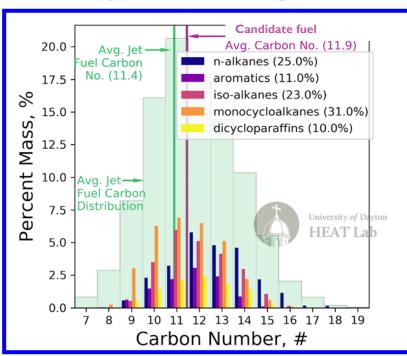
Referee compusior

- Elimination and/or minimization of operability tests (Tier 3 and 4)
- There is no evidence that operability tests need to be done at OEM facilities.
 - That does not mean there isn't reason to do so, however.

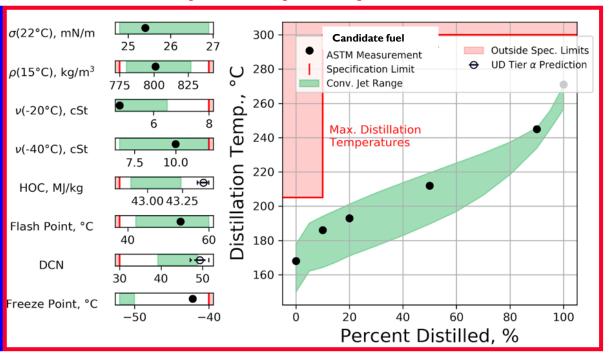
Prescreening example

Tier α and β prescreening dash-board

Compositional Comparison



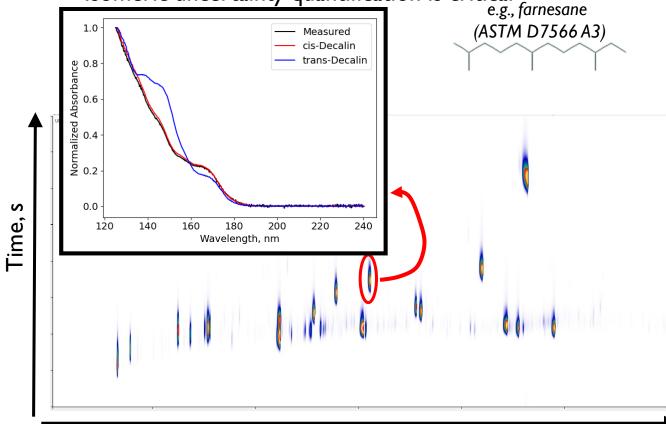
Operability Comparison



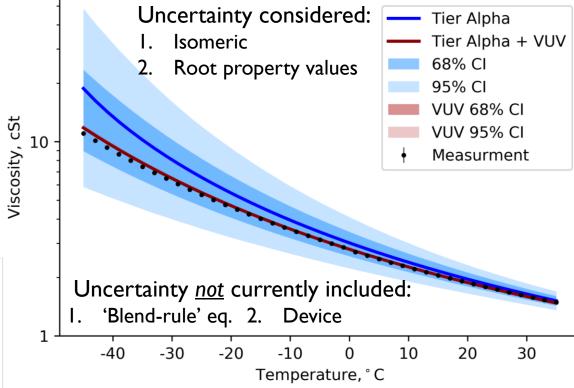
VUV identification with GCxGC separation

- ~2/3 of samples arrive in with <3 mL
 - Critical properties are predicted
- SAFs can have 'strange' and very specific isomeric structures

Isomeric uncertainty quantification is critical



Time, min

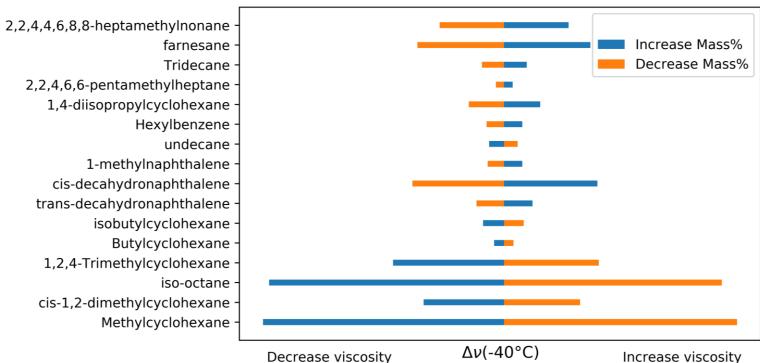


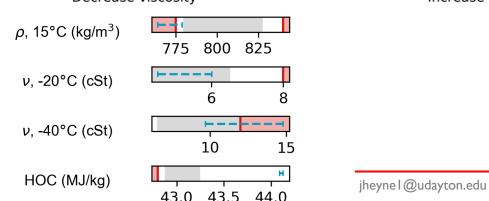
- 3-5k molecules and their associate properties are leveraged for predictions
- Blind Tier α predictions are compared with the **VUV** identification

Sensitivity analysis by property and specific analyte (or group)

- Some distillation cuts or process can have several properties off.
- Sensitivity analysis can illuminate which analyte(s) or hydrocarbon type(s) can facilitate compliance.

 Both property predictions and the associated sensitivity analysis can be done in the absence of sample but with some composition information





Conclusions

- ~8 different labs and companies have sent samples
- Some labs have changed/iterated methods significantly
- Technology development is useful at I-3 mL
 - Expansion to additional simultaneous diagnostics would clarify and
 - Physical property measurements at very low volumes

- Three learnings a year+ in:
 - Distillation maters!
 - 160-240°C works well but could be dilated depending on feedstock-process
 - Depending on the hydrocarbon types, lighter or heavier cuts could be more compatible.
 - Trace materials are important (N and O)
 - Single component fuels will undergo more scrutiny.
- SAFs per expectation can be very strange

Thank you!

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NJFCP Fuels

Category A: conventional fuels

A-1: 'Best' case

A-2: 'Average' case

A-3: Worse' case

Category C: fuels that characterize alternative fuels with extreme properties

