NREL
Transforming ENERGY

Measuring Critical Fuel Properties for Simulations to Accelerate Fuel Qualification

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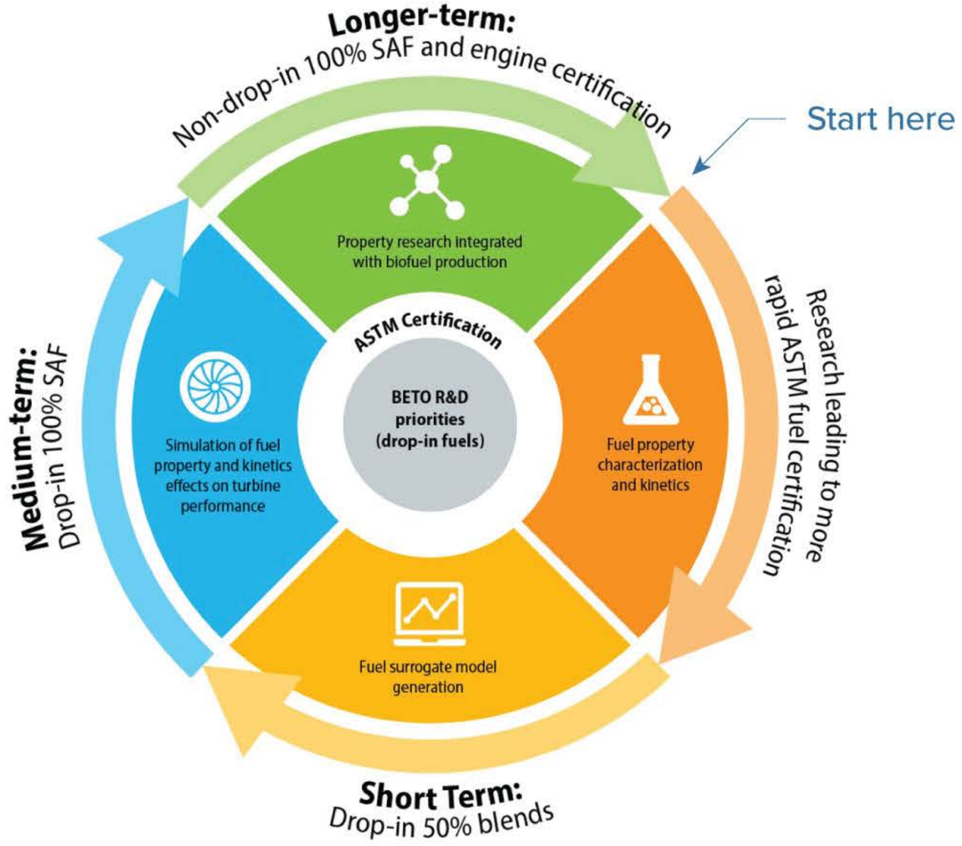
The SAF technology landscape

BETO VTO



Fuel production: BETO

Fuel property characterization: BETO and VTO

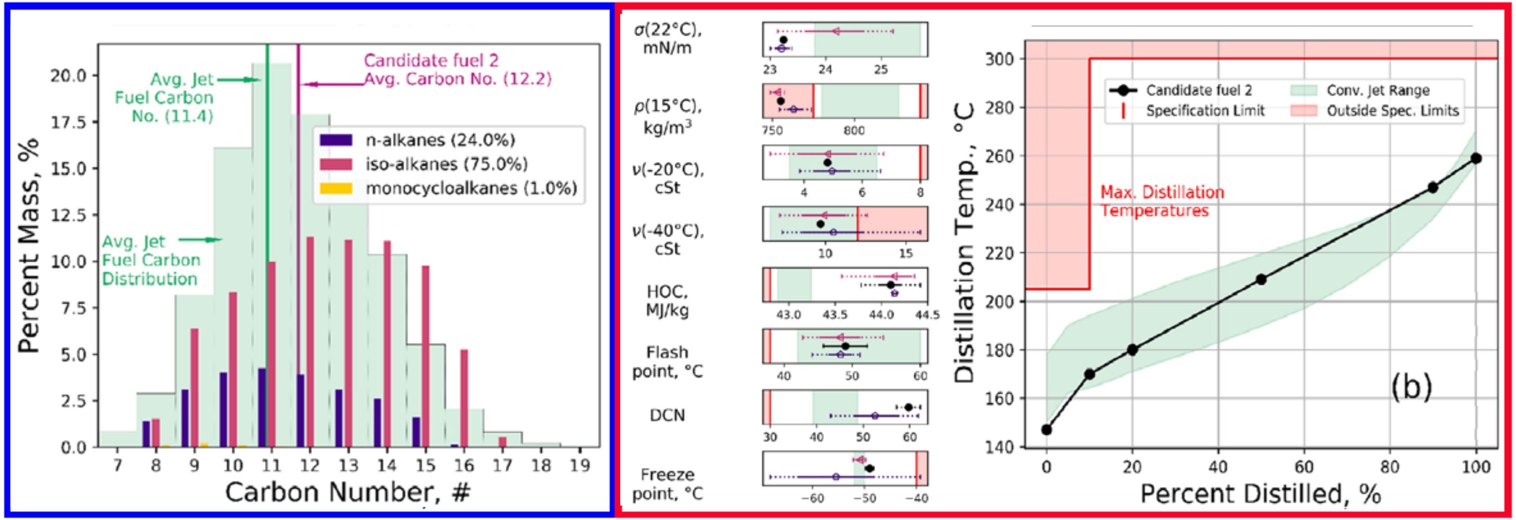
Fuel property mapping to turbine performance: VTO

Expanding boundaries of ASTM certification: VTO

De-risking qualification of new fuels (drop-in and marginally drop in): VTO and BETO

NREL Capability: Fast Track Properties

Compositional Comparison **Operability Comparison**



- NREL can (or will shortly) run entire list of Fast Track properties including simulated distillation and 2D GC (also true vapor pressure, heat of vaporization, …)
- For “pre-qualification” research to support BETO SAF production projects

Figure from: Heyne, et al., 2021 https://doi.org/10.1016/j.fuel.2020.120004

Actual T and P differ from those used in property measurements

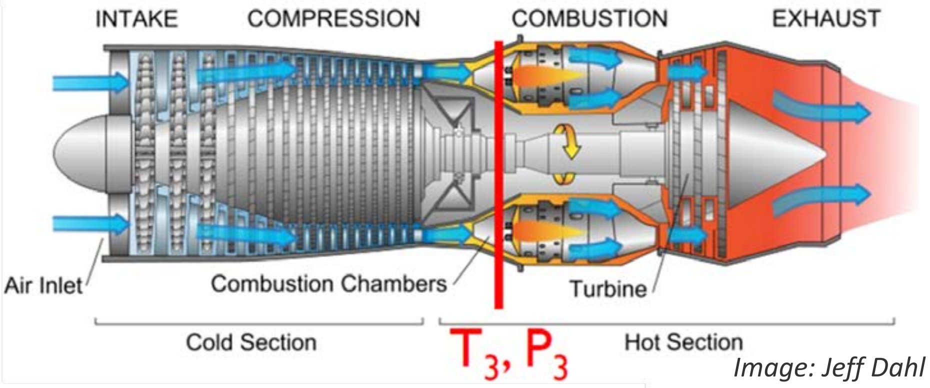
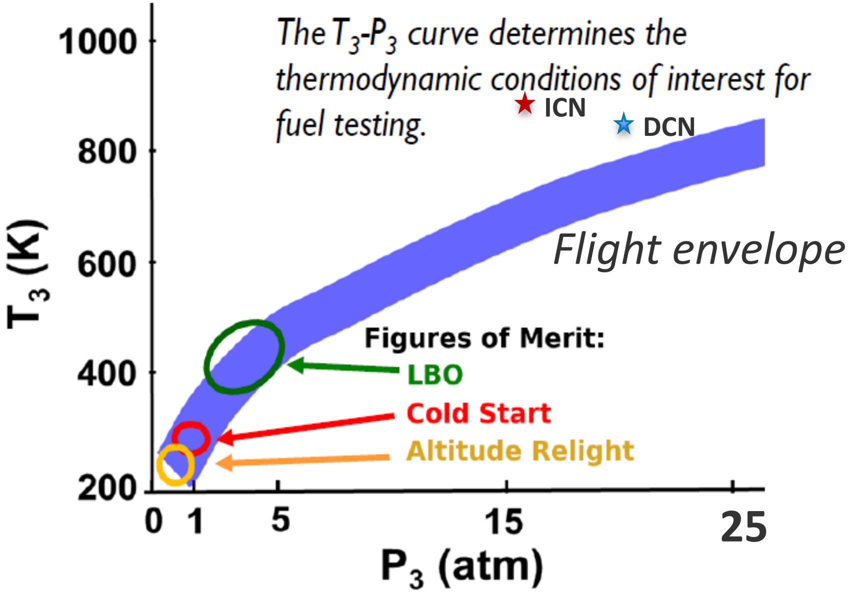


Image: Jeff Dahl



https://doi.org/10.2514/1.J055361

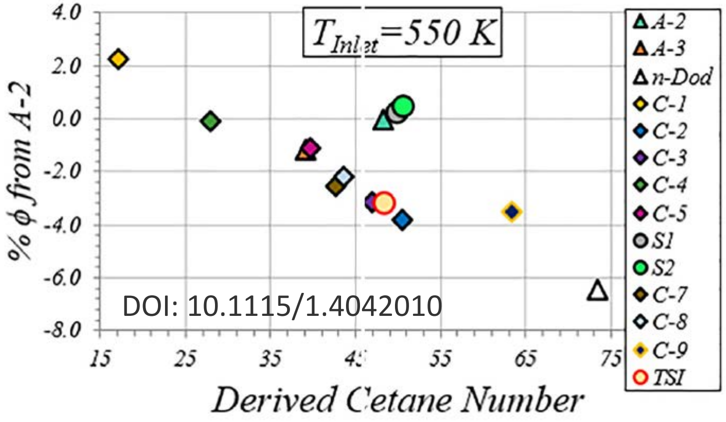
Experiments to Expand T and P Range

Property	Common Today	New Capability	Sample Volume
Density	-40 to 80°C / 1 atm	-10 to 200°C / 1 to 500 atm	2 mL
Viscosity	-40 to 40°C / 1 atm	-40C to 315°C / 1 to 1300 atm	5 mL
Surface tension	-10 to 40°C / 1 atm	-35 to 400°C / 1 to 60 atm	2 mL
Ignition delay – DCN/ICN	545°C / 21.4 atm 580°C / 17.5 atm	Up to 725°C / 2 to 50 atm	40 mL

All operational or planned to be operational in Q1 FY23

DCN vs ICN

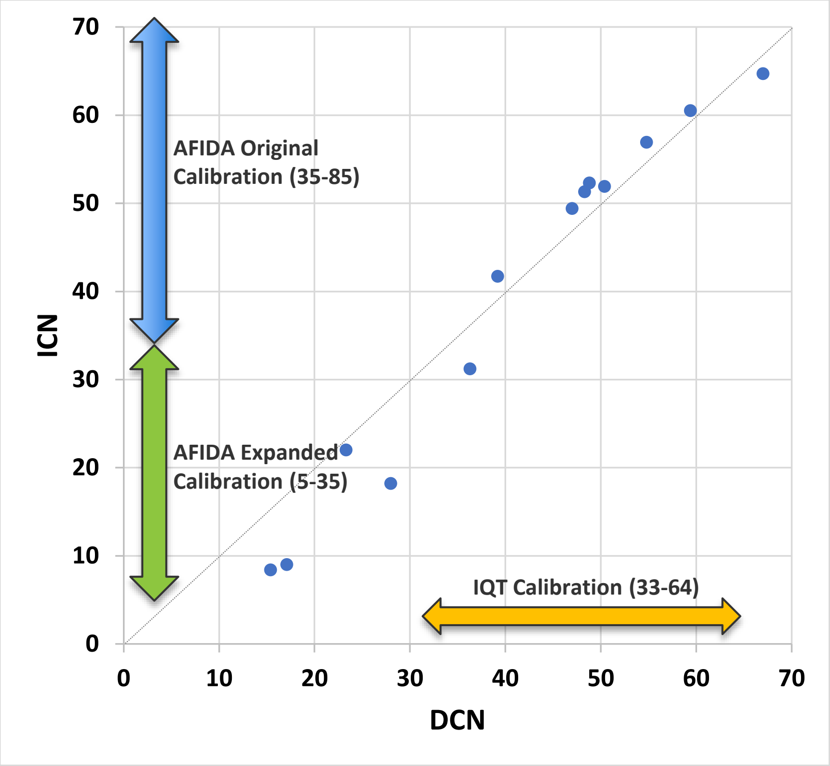
- Derived cetane number (DCN), measured in IQT at nominally 21.4 atm / 545°C / ϕ=3
  - Requires 140 mL of sample
  - Correlated with ϕ for lean blow out at higher temperatures
  - Perhaps related to cold start and relight
- Indicated CN (ICN) measured in AFIDA at nominally 17.5 atm / 580°C / ϕ=3
  - Requires 40 mL of sample
  - AFIDA easily programed to measure ignition delay at other T, P, and ϕ
- DCN/ICN comparison in collaboration with Josh Heyne and Ed Corporan



Fuel
A-1 (10264)
A-2 (10325)
A-3 (10289)
C-1 (13718)
C-2 (12223)
C-3 (12959)
C-4 (13217)
Commercial HEFA-SPK
Commercial HEFA-SPK
Commercial ATJ-SPK
50/50 A-2/HEFA-SPK
50/50 A-2/ATJ-SPK

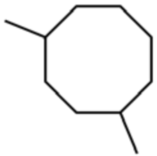
Jet fuel ICN / DCN comparisons

- Worked with AFIDA manufacturer to expand ICN calibration range down to 5 CN units
- Generally excellent agreement between ICN and DCN
  - ICN typically < DCN below 30
- Obtaining data over range of T, P and ϕ for these fuels
- Perhaps ignition delay at other conditions will be more predictive of performance in a gas turbine than CN (developed for diesel combustion)



Dimethyl cyclooctane – potential SAF blendstock

- Collaboration with Ben Harvey US Navy, NAWCWD
- Produced by sugar fermentation to isoprene, then catalytic conversion to DMCO   doi: 10.1039/c9gc02404b
- Exhibits both high mass density and energy density
- Volumetric energy density 10% greater than Jet A
- Some evidence can swell elastomers like aromatics
- NREL to perform additional property measurements and soot precursor pathways study (flow reactor)
- Status: project just started

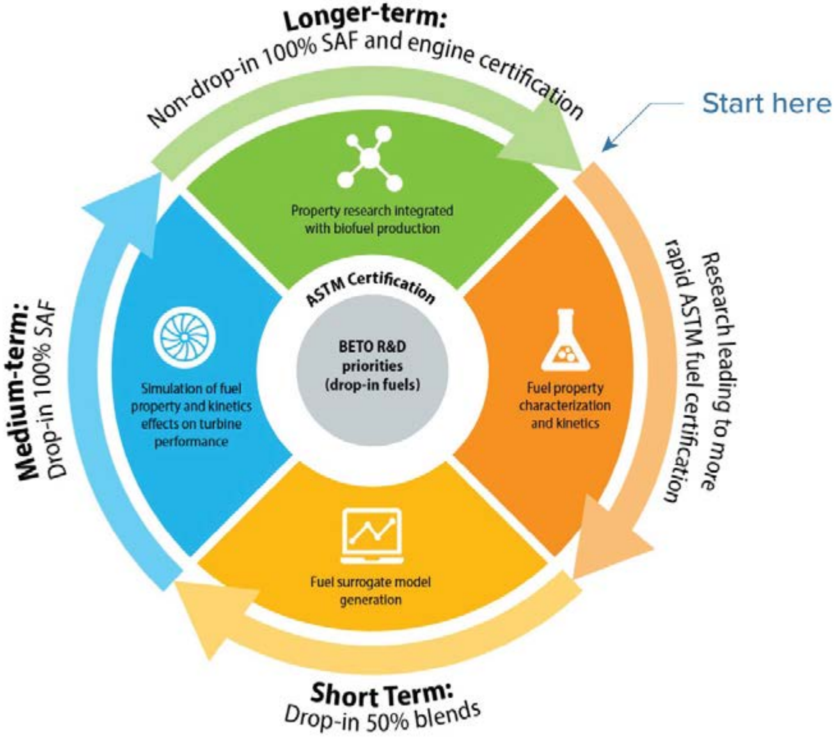


1,4-Dimethylcyclooctane

Density, kg/m^3	827
Energy density, MJ/kg	43.8
Volumetric energy, MJ/L	36.2
Freezing point, °C	<-78
DCN	18

SAF Research Vision Summary

- Close support of BETO biofuel production
  - Property measurements for SAF ASTM qualification
  - Mapping molecular structure to fuel properties
- Connecting fuel properties to engine performance
  - Measuring properties at operating conditions
  - Apply exascale-ready combustion simulations leveraging extensive SC investments
- De-risking scale up of low-carbon fuel production
- Move SAF technologies to TRL level allowing hand off to industry



Thank you!

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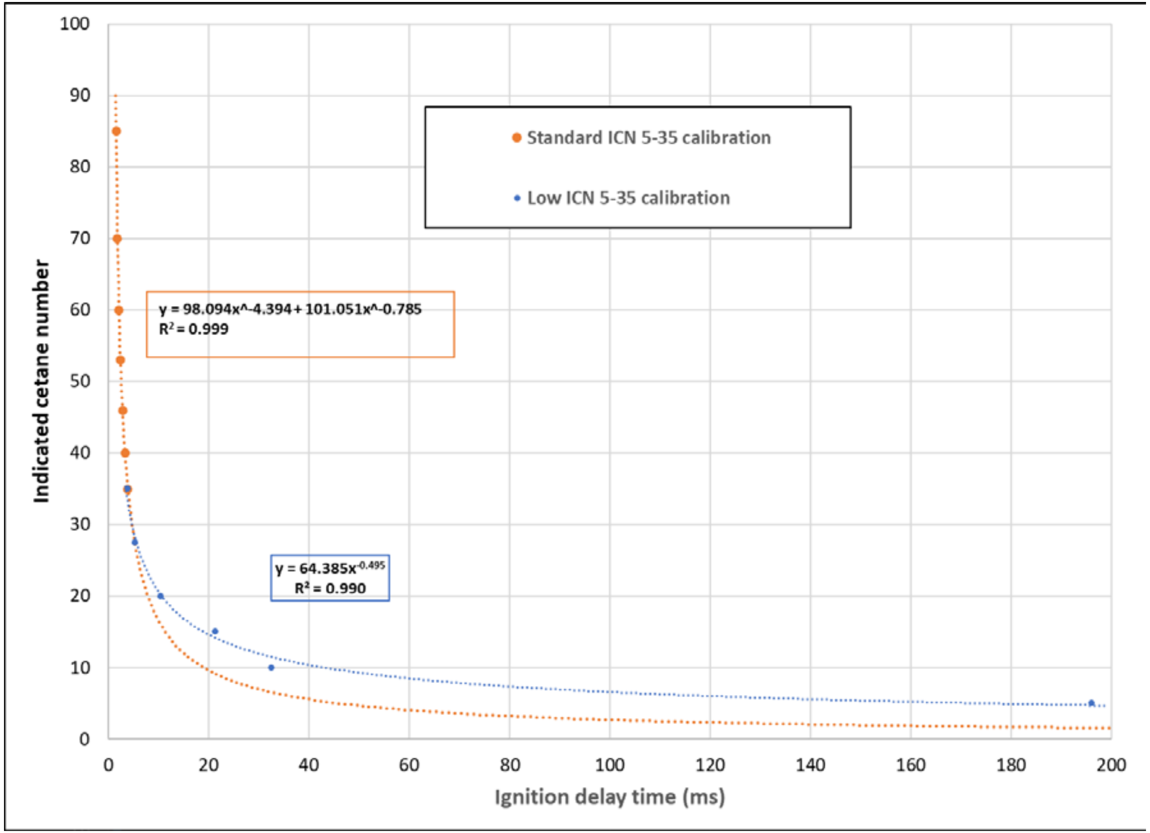
Backup Slides

ICN/DCN Results of Fuels from National Jet Fuel Combustion Program

NJFCP ID	DCN Edwards	DCN NREL	ICN NREL	Description
A-1 (10264)	48.8		52.3	JP-8
A-2 (10325)	48.3		51.3	Jet A
A-3 (10289)	39.2		41.7	JP-5
C-1 (13718)	17.1		9.0	ATJ from Gevo
C-2 (12223)	50.4		51.9	84% C14 iso-paraffins/16% 1,3,5 trimethyl benzene
C-3 (12959)	47.0		49.4	64% A-3/36% Amyris farnesane
C-4 (13217)	28.0		18.2	FT:ATJ Blend 60% Sasol IPK (FT-SPK)/40% C-1
Commercial HEFA-SPK		59.4	60.5	HEFA-SPK#1
Commercial HEFA-SPK		67.0	64.7	HEFA-SPK#2
Commercial ATJ-SPK		15.4	8.4	
NREL Blend		54.8	56.9	50/50 blend of A-2/HEFA-SPK#1
NREL Blend		36.3	31.2	50/50 blend of A-2/ATJ-SPK
Low CN fuel		23.3	22	Methylcyclohexane

Extended range indicated cetane number (ICN)

- ASTM D8183 Indicated Cetane Number (ICN) covers the range of (35-85)
  - Primary reference standard calibration using purified n-hexadecane/1-methlynaphthalene
  - Standard calibration PRFs (85, 70, 60, 53, 46, 40, 35)
  - $R^2 = 0.999$
- Low cetane calibration prepared from same quality standards
  - Low calibration PRFs (35, 27.5, 20, 15, 10, 5)
  - $R^2 = 0.990$



Ignition Delay for Jet A (A-2) at Different Conditions