FUEL TESTING APPROACHES FOR RAPID JET FUEL PRESCREENING
Project 65a

Lead investigator: Joshua Heyne, Washington State University
Project manager: Ana Gabrielian, FAA

October 15, 2025
Alexandria, VA

This research was funded by the U.S. Federal Aviation Administration Office of Environment and Energy through ASCENT, the FAA Center of Excellence for Alternative Jet Fuels and the Environment, project 65a through FAA Award Number 13-C-AJFE-WASU-035 under the supervision of Ms. Ana Gabrielian. Any opinions, findings, conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the FAA.

ASCENT

Project 65a

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Washington State University

PI: Joshua Heyne

PM: Ana Gabrielian

Cost Share Partner(s): DLR Germany, Air Company, Washington State University

Objective:

This project focuses on further development of low volume methods to determine properties of sustainable aviation fuels.

Project Benefits:

A tiered prescreening process for new alternative jet fuels using low fuel volumes that informs producers of risks to meeting ASTM D4054 approval criteria. This process increases the fidelity of information available to fuel producers at all stages of fuel readiness level.

Research Approach:

	Measured Property	Predicted Property
Tier α	Hydrocarbon Type Analysis (GCxGC)	LHV, Density, Surface Tension, Freeze Point, Viscosity, DCN, Flash point
	Distillation (ASTM D2887)	
Tier β	Density	LHV
	Viscosity	
	Surface tension	
	Freeze point	
	Flash point	
	DCN	

Major Accomplishments (to date):

- 22 journal articles have been sponsored in part by this project
  - 22 published
- **466 fuel samples have been received to date**
  - **65 samples since the last meeting**

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Publications

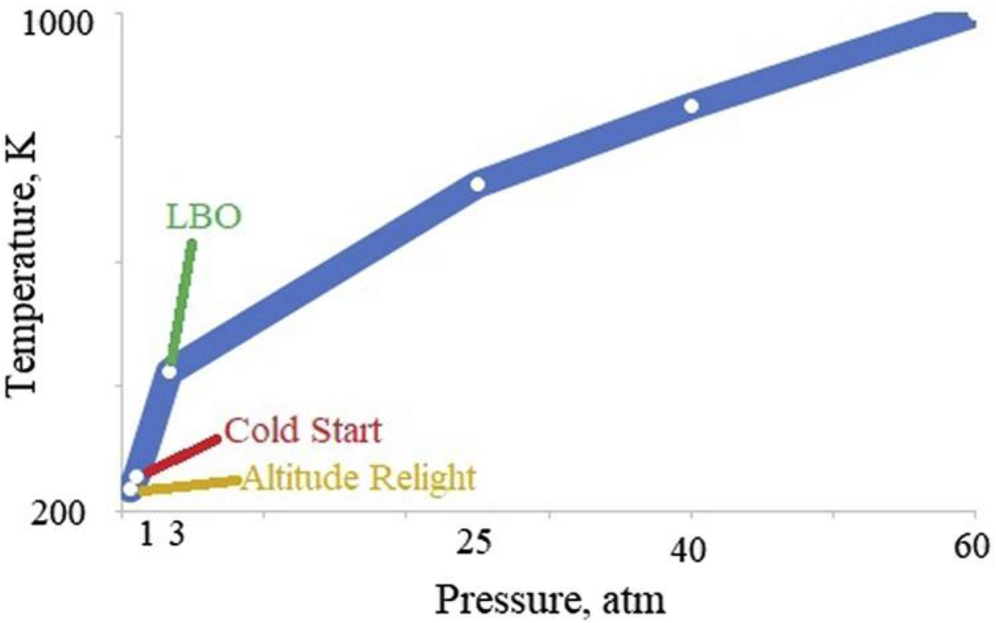
- "Geometric and Positional Isomer Effects on Ignition Behavior of Cycloalkanes: Implications for Sustainable Aviation Fuels" Z Yang, C Faulhaber, R Boehm, J Heyne, Energy & Fuels 2025
- "Measurement of Spray Chamber Ignition Delay and Cetane Numbers for Aviation Turbine Fuels" J Luecke, N Naser, Z Yang, J Heyne, RL McCormick, Energy & Fuels 2025
- "Upgrading of biocrude oil into sustainable aviation fuel using molybdenum carbide nanocatalysts" S Yu, H He, S Summers, Z Yang, B Si, R Gao, A Song, J Heyne, Y Zhang, H Yang, ScienceAdvances 2025
- "Freezing Point of Hydrocarbon Fuels from Single Species Concentrations" DC Bell, R Boehm, JS Heyne , Energy & Fuels 39 (9), 4221–4226, 2025
- "Assessing the effect of composition on dielectric constant of sustainable aviation fuel" Z Yang, D Bell, R Boehm, P Fischer Marques, J Boze, I Kosilkin, J Heyne, Fuel 2025
- "Dielectric Constant Predictions for Jet-Range Hydrocarbons: Evaluating the Clausius–Mossotti Relation and Correcting for Molecular Dipole Moments" C Faulhaber, D Bell, R Boehm, J Heyne, Energies 2024
- "Perspective on Fuel Property Blending Rules for Design and Qualification of Aviation Fuels: A Review" R Boehm, Z Yang, D Bell, C Faulhaber, E Mayhew, U Bauder, G Eckel, J Heyne, Energy & Fuels 2024
- "Volatility Measurements of Sustainable Aviation Fuels: A Comparative Study of D86 and D2887 Methods" Z Yang, D Bell, D Cronin, R Boehm, J Heyne, K Ramasamy, ACS Sustainable Chemistry & Engineering 2024
- "Quantifying Isomeric Effects: A Key Factor in Aviation Fuel Assessment and Design" C Hall, D Bell, J Feldhausen, B Rauch, JS Heyne, Fuel 2024
- "Quantitation of olefins in sustainable aviation fuel intermediates using principal component analysis coupled with vacuum ultraviolet spectroscopy" S Kosir, J Feldhausen, D Bell, D Cronin, R Boehm, J Heyne, Frontiers in Energy 2023
- "Measurements of Nitrile Rubber Absorption of Hydrocarbons: Trends for Sustainable Aviation Fuel Compatibility" C Faulhaber, C Borland, RC Boehm, JS Heyne, Energy & Fuels 2023
- "Maximizing Sustainable aviation fuel usage through optimization of distillation cut points and blending" Z Yang, RC Boehm, DC Bell, JS Heyne, Fuel 2023
- "Limits of identification using VUV spectroscopy applied to C8H18 isomers isolated by GC × GC" DC Bell, J Feldhausen, AJ Spieles, RC Boehm, JS Heyne, Talanta, 124451, 2023
- "Error quantification of the Arrhenius blending rule for viscosity of hydrocarbon mixtures" R Boehm, F Hauck, Z Yang, T Wanstall, JS Heyne, Frontiers in Energy Research, 2022
- "A Data Set Comparison Method Using Noise Statistics Applied to VUV Spectrum Match Determinations" DC Bell, RC Boehm, J Feldhausen, JS Heyne, Analytical Chemistry, 2022
- "Synthetic aromatic kerosene property prediction improvements with isomer specific characterization via GCxGC and vacuum ultraviolet spectroscopy" J Feldhausen, DC Bell, Z Yang, C Faulhaber, R Boehm, J Heyne, Fuel 326, 125002, 2022
- "Blend prediction model for the freeze point of jet fuel range hydrocarbons" RC Boehm, AA Coburn, Z Yang, CT Wanstall, JS Heyne, Energy & Fuels 36 (19), 12046-12053, 2022
- "Lignin-based jet fuel and its blending effect with conventional jet fuel" Z Yang, Z Xu, M Feng, JR Cort, R Gieleciak, J Heyne, B Yang, Fuel 321, 124040, 2022
- "Towards Fuel Composition and Properties from Two-dimensional Gas Chromatography with Flame Ionization and Vacuum Ultraviolet Spectroscopy" JS Heyne, DC Bell, J Feldhausen, Z Yang, RC Boehm, FUEL 312, 1-12, 2022
- "Threshold Sooting Index of sustainable aviation fuel candidates from composition input alone: Progress toward uncertainty quantification" RC Boehm, Z Yang, JS Heyne, Energy & Fuels 36 (4), 1916-1928, 2022
- "Lower heating value of jet fuel from hydrocarbon class concentration data and thermo-chemical reference data: An uncertainty quantification" RC Boehm, Z Yang, DC Bell, J Feldhausen, JS Heyne, FUEL 10, 2022
- "A GC × GC Tier α combustor operability prescreening method for sustainable aviation fuel candidates" Z Yang, S Kosir, R Stachler, L Shafer, C Anderson, JS Heyne, Fuel, 292, 120345, 2021

Major tasks since last meeting

- DCN observations
- Lubricity observations

Background on Lean Blow Out (LBO)

LBO is one of the three combustor figures of merit that aircraft Original Equipment Manufacturer (OEM) assess during the process of evaluation of new aviation turbine fuels



“Comparing Alternative Jet Fuel Dependencies Between Combustors of Different Size and Mixing Approaches” R Boehm, J Colborn, J Heyne, frontiers 2021

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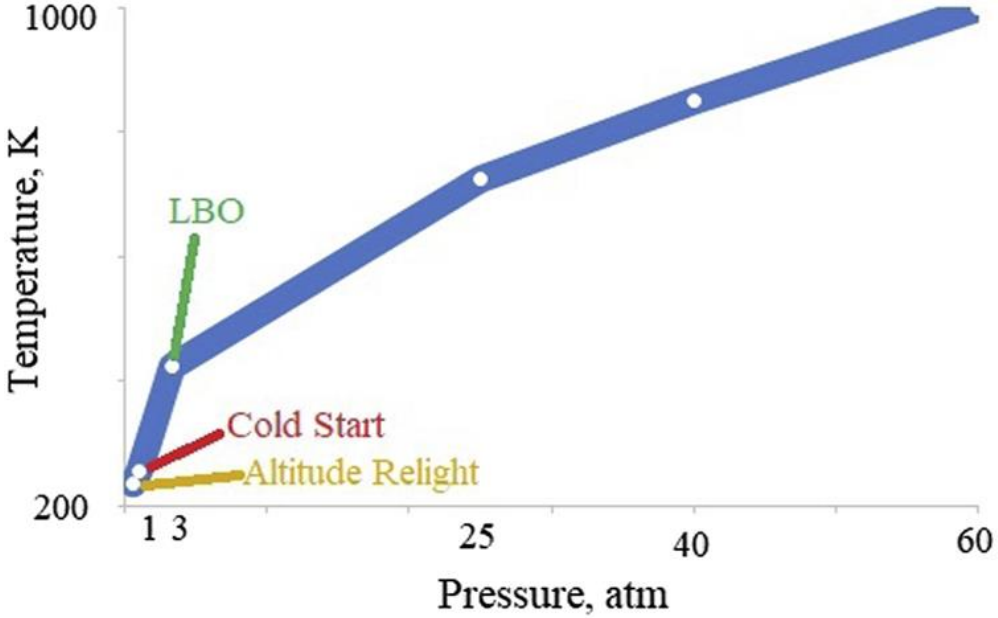

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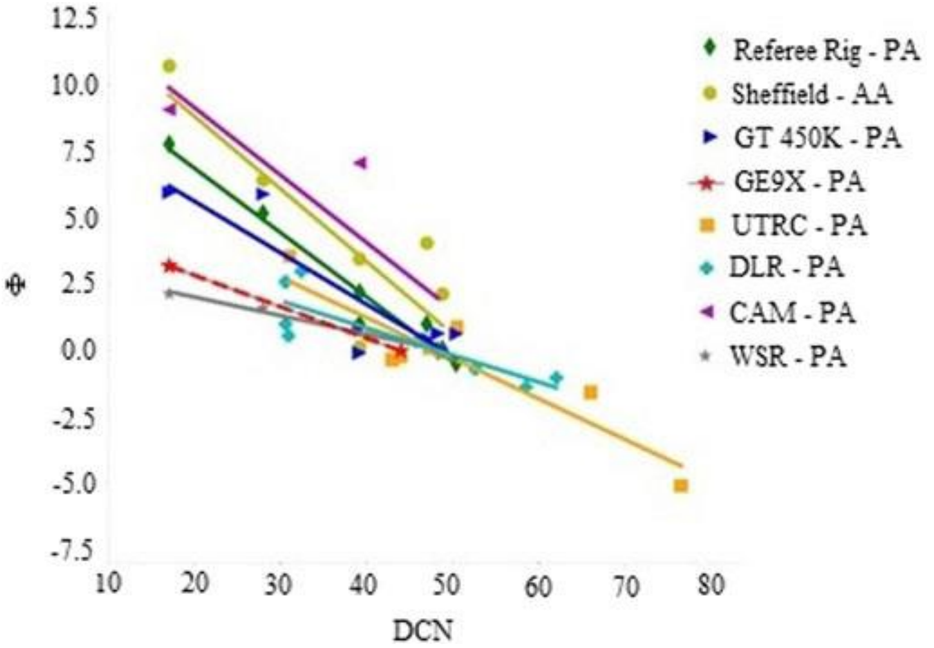
LBO requires a significant amount of fuel to run in an actual combustor. Most novel fuel producers does not make that much fuel

LBO limit as a function of Derived Cetane Number (DCN) for eight different rigs used within the National Jet Fuel Combustion Program (NJFCP).

LBO



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Why Derived Cetane Number (DCN) Matters for SAF Approval

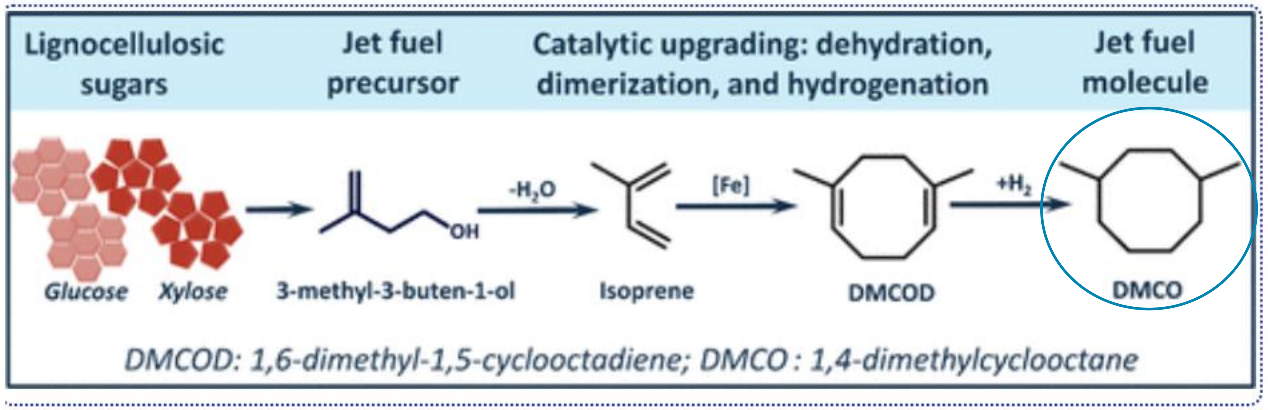
Ignition Quality Tester (IQT) from CFR Engines

- Jet fuel ignition quality must fall in ASTM D4054 DCN window: 35–60.
- Low DCN (slow ignition) → risk of lean blowout (LBO) at altitude.
- High DCN (fast ignition) → hardware durability issues.
- OEMs cautious: Cycloalkane behavior historically uncertain.
- This study helps reduce uncertainty by quantifying cis/trans effects

The IQT measure Ignition Delay (ID) and DCN could be calculated based on equation below:

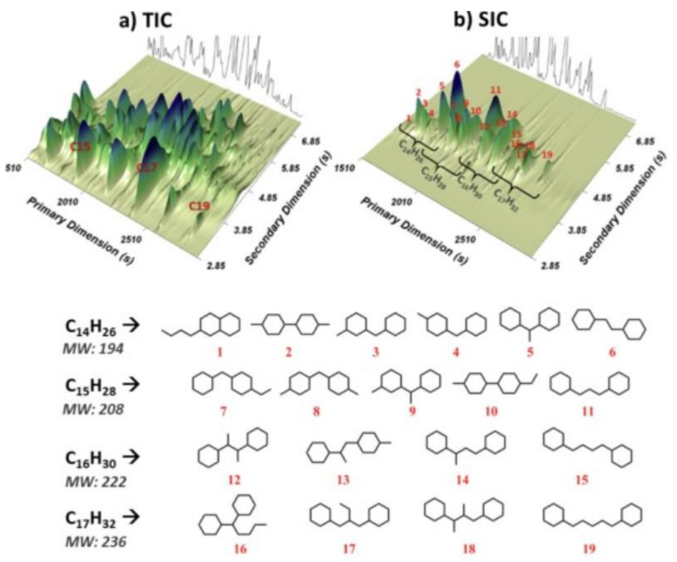
$$DCN = 4.460 + 186.6/ID$$

Many Novel Alternative Jet Fuel are Rich in Cycloalkanes



https://pubs.acs.org/doi/10.1021/acssuschemeng.1c03772

CycloSAF
- Going through ASTM D4054 process right now, process make primarily cycloalkanes



Lignin jet fuel (LJF)
- First continuous process developed, process make primarily polycycloalkanes

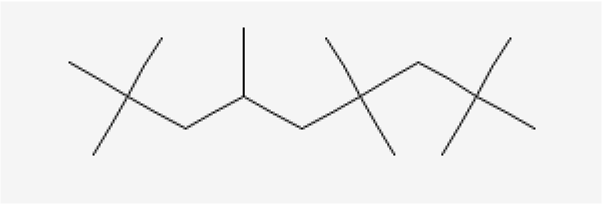
https://www.sciencedirect.com/science/article/pii/S0016236122008985

However →

Due to limited research and historical uncertainty regarding cycloalkane behavior in combustion, OEMs and regulatory bodies continue to limit the cycloalkane content within certain D7566 annexes and specifications.

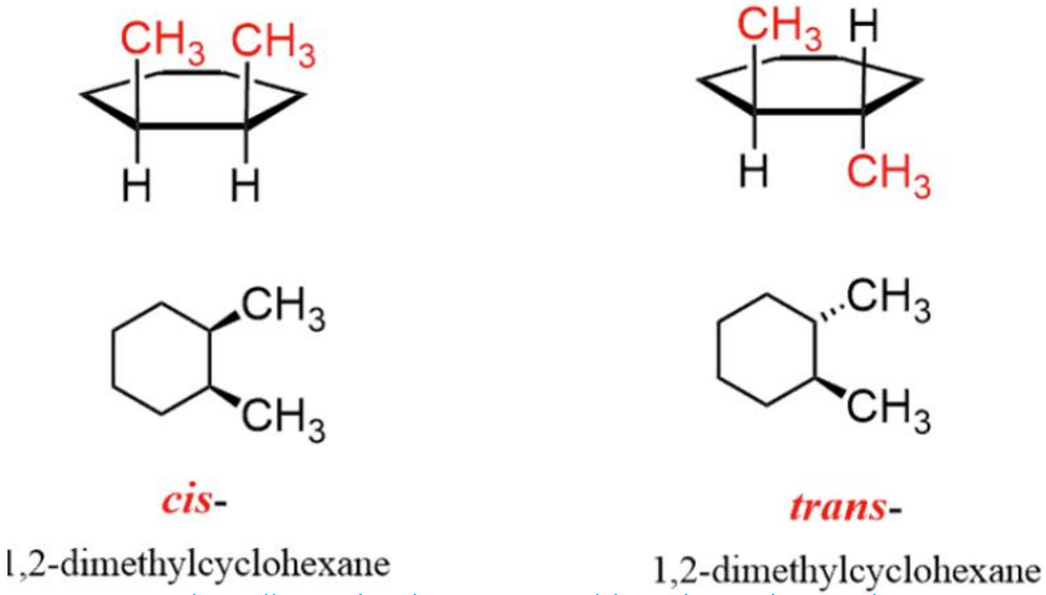
Cycloalkanes Behave Different than Iso- and N-alkanes

n-alkanes



iso-alkanes

Predominately hydrocarbon group in HEFA-SPK

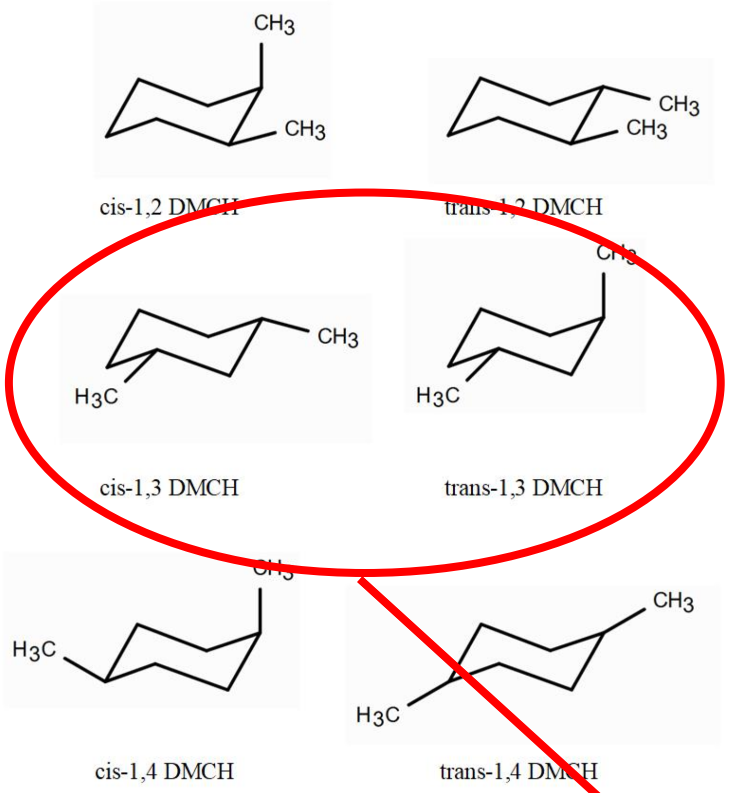


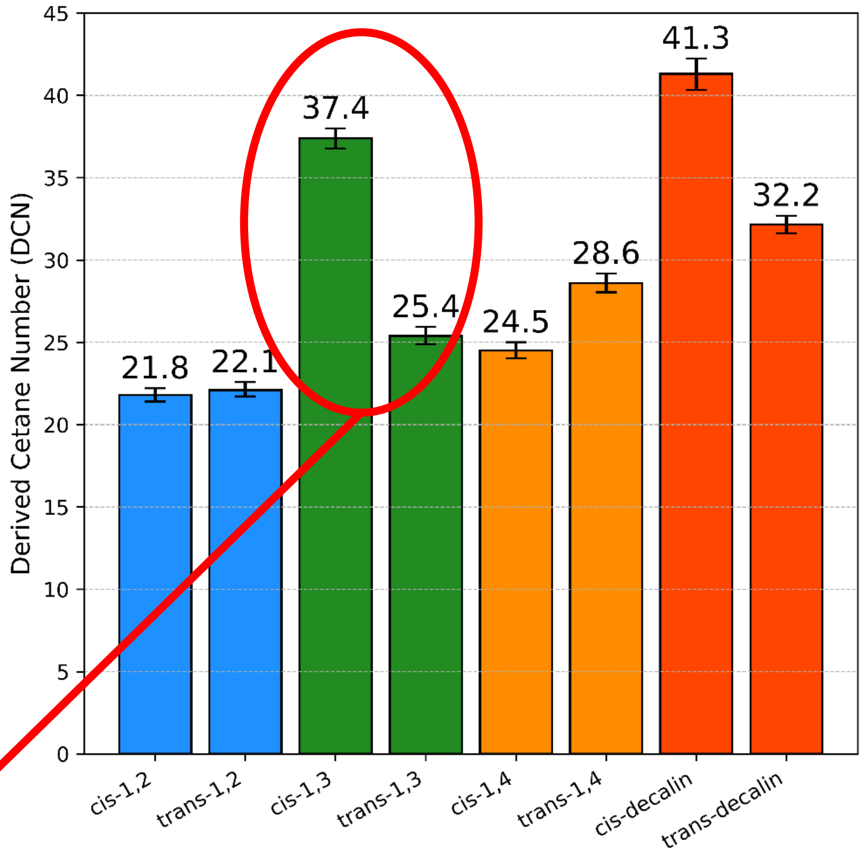
https://www.chemistrysteps.com/cis-and-trans-isomers/

- The **cyclic ring structure** of cycloalkanes restricts free rotation.
- This leads to **two possible configurations** at substituents:
  - **Cis** → substituents on the same side of the ring.
  - **Trans** → substituents on opposite sides of the ring.

These small geometric changes could lead to large differences in ignition reactivity.

DCN measurement of Dimethylcyclohexane (DMCH)



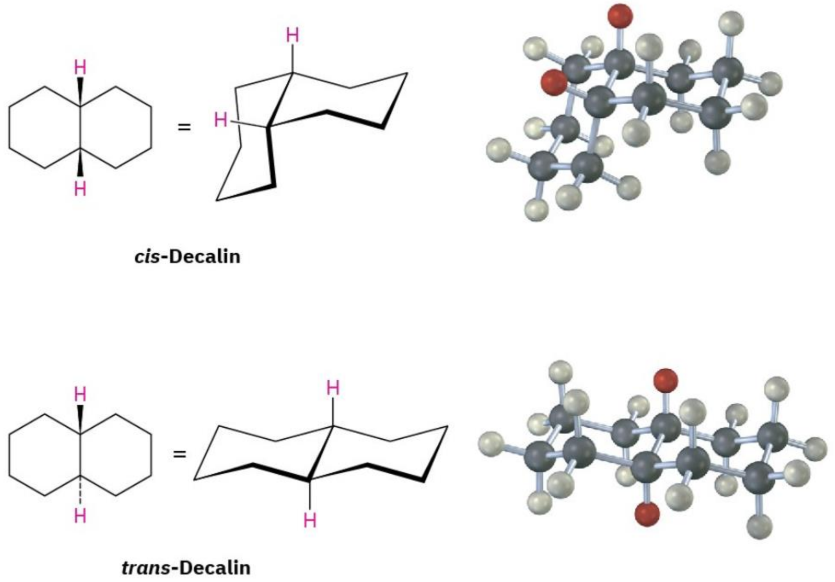


Cis/Trans structure controls ignition reactivity in jet fuel

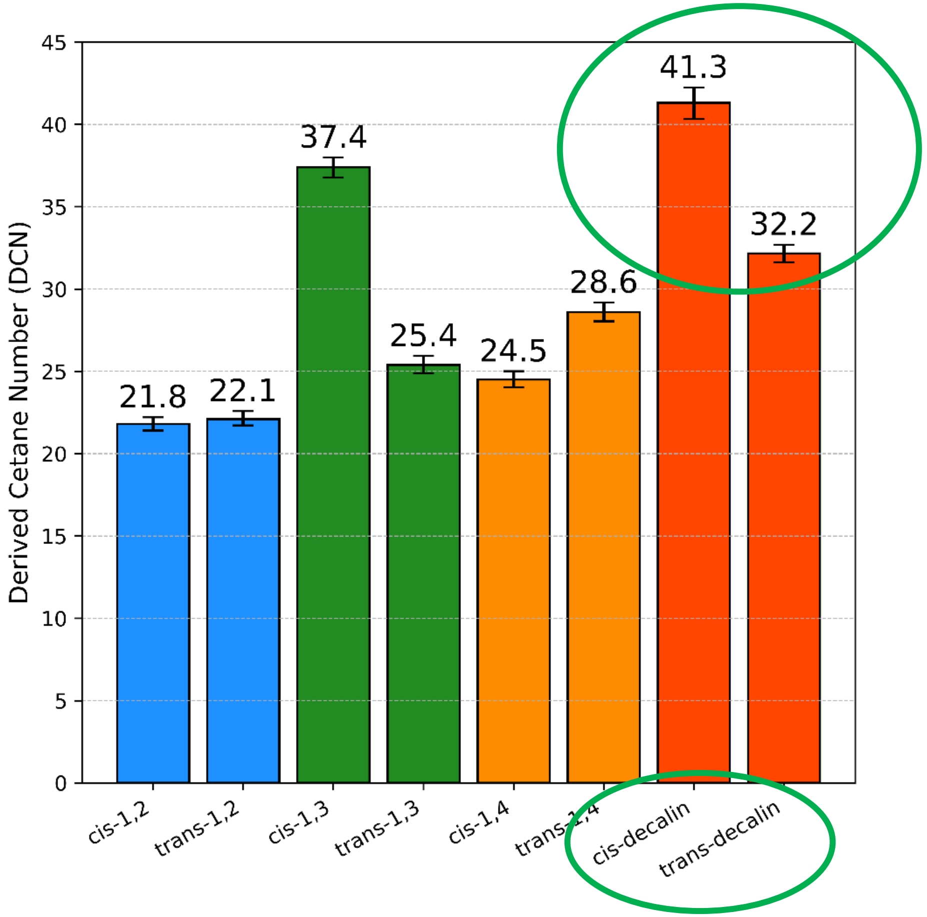
Cis-1,3-DMCH ignite quick than tran-1,3-DMCH just because of different **configurations**

12 DCN difference between cis- and trans-1,3-DMCH

Why does cis and trans- isomer cause difference in ID and DCN



https://ncstate.pressbooks.pub/organicchem/chapter/4-9-conformations-of-polycyclic-molecules/

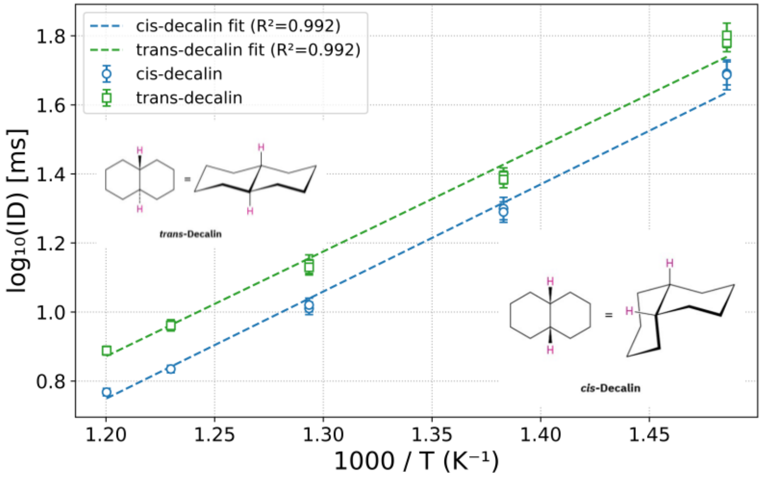


We want to adjust IQT testing conditions to investigate why cis- and trans-decalin exhibit different ignition delays.

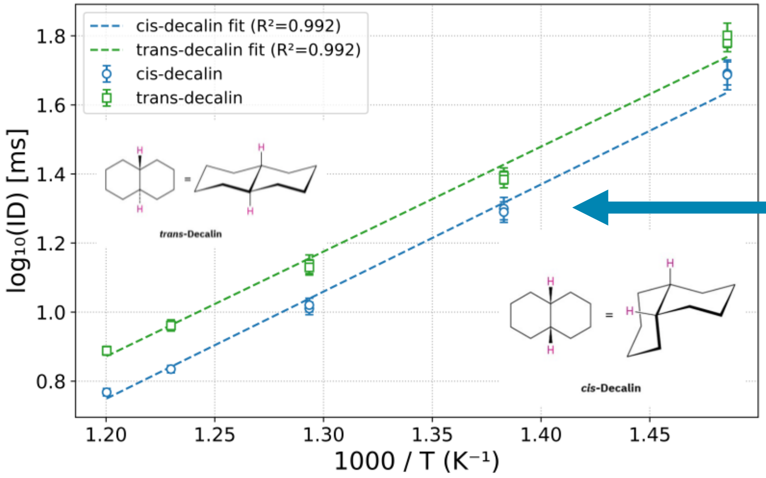
Two key kinetic “knobs” we can vary:

- Pressure
- Temperature

Temperature and Pressure Dependence of Decalin Isomers



Temperature and Pressure Dependence of Decalin Isomers



- Although both exhibit similar slopes, the cis isomer consistently displays shorter ID times across the entire temperature range studied.
- Cis = flexible geometry, enables fast 1,5-H shifts → earlier radical formation.
- Trans = rigid geometry, limited to 1,6-H shifts → slower ignition.

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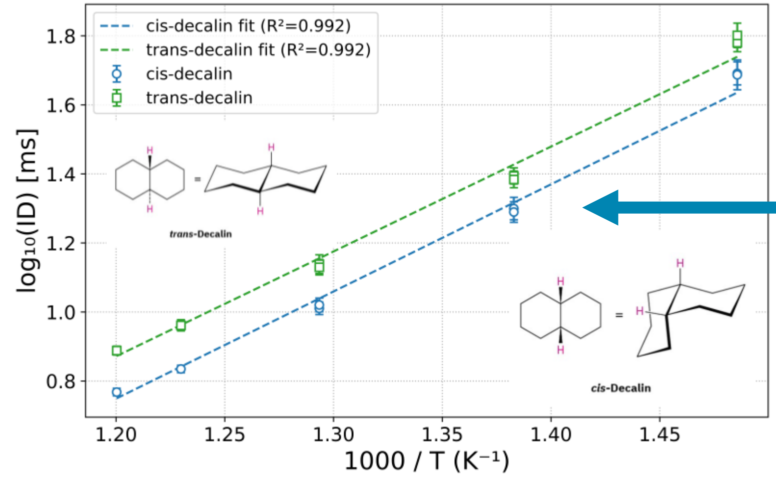

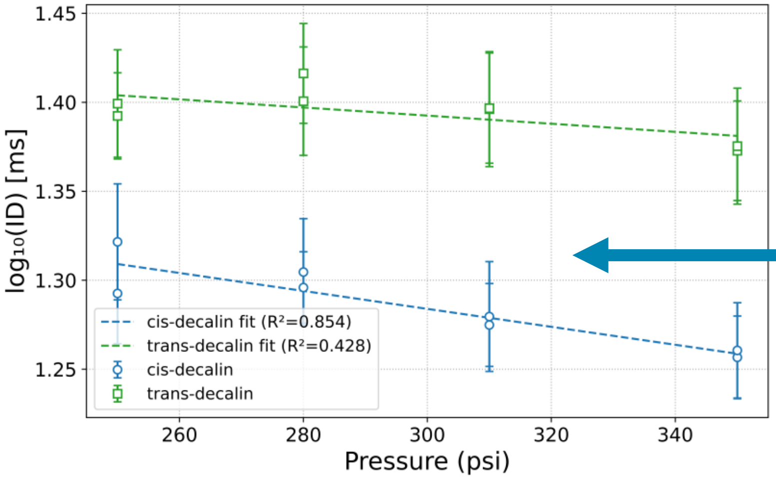

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Cis-decalin also exhibits stronger pressure dependence ($R^2 = 0.854$), while trans-decalin shows weak sensitivity to pressure changes ($R^2 = 0.428$).

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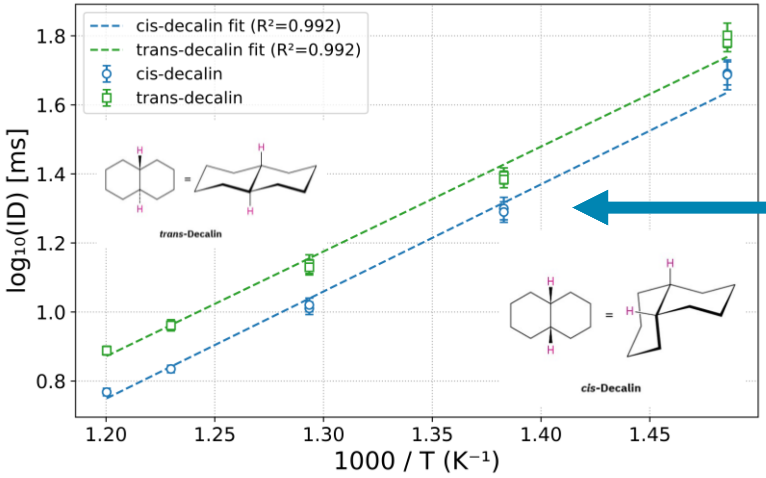

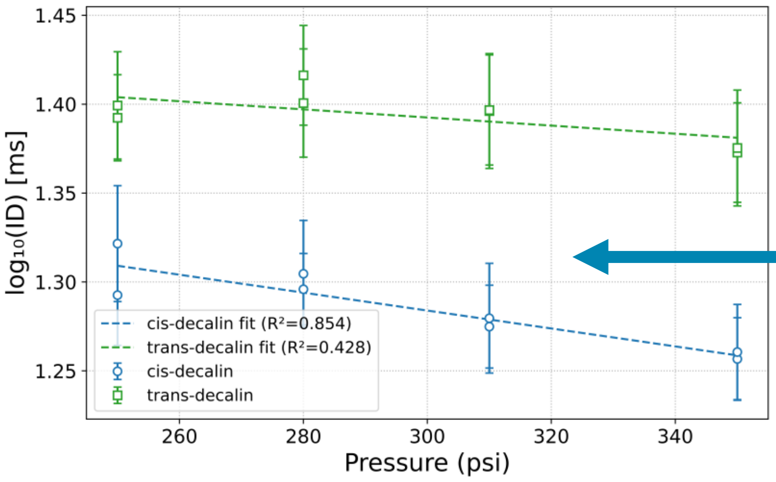

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→

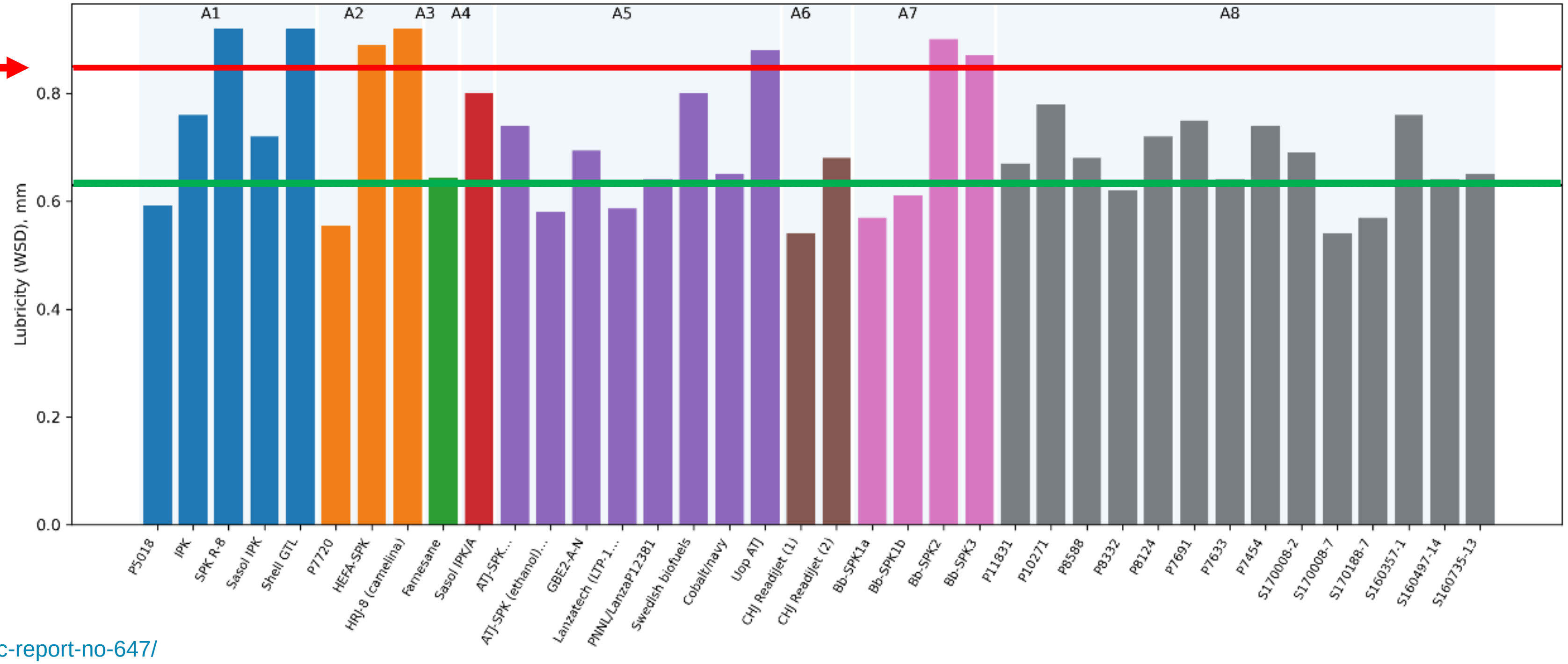
This differential response implies that cis-decalin benefits significantly from pressure assisted stabilization of radical intermediates, which is consistent with unimolecular reaction pathways that involve third-body collisions.

Why Lubricity Matters in SAF

- Boundary lubrication is critical in fuel pumps & controls.
- Petroleum Jet A has natural polar species (S/N/O compounds) → good lubricity.
- Neat SAFs (HEFA, FT, ATJ) lack these → lubricity deficit.
- ASTM requires blends or additives to protect pumps.

Spec limit (D7566)

Jet A average*

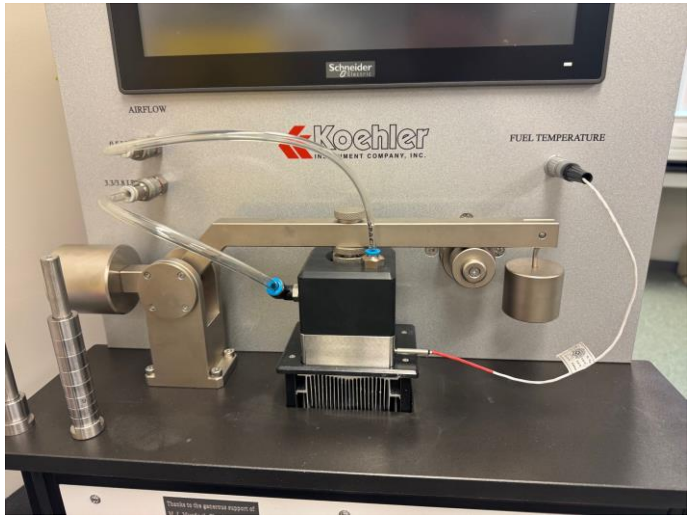


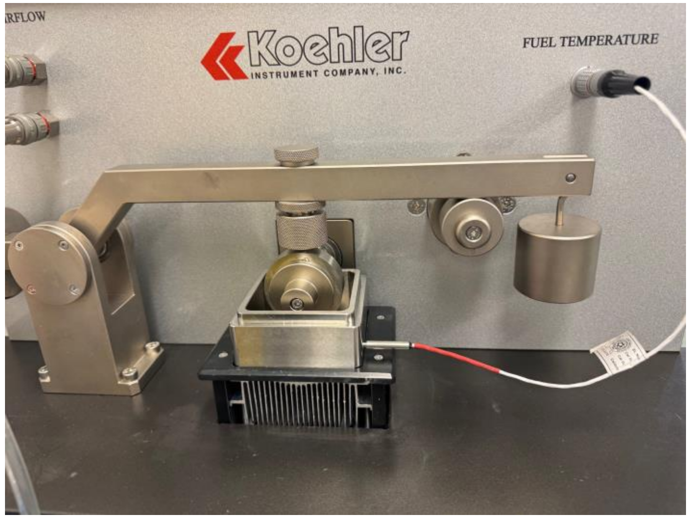
Currently, all SAF are blended with Jet A to restore natural lubricity

But OEM are looking into 100% synthetic aviation fuel

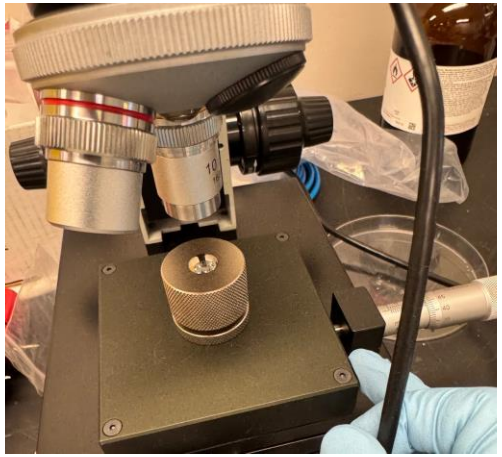
*CRC report 647, WORD FUEL SAMPLING PROGRAM, https://crcao.org/crc-report-no-647/

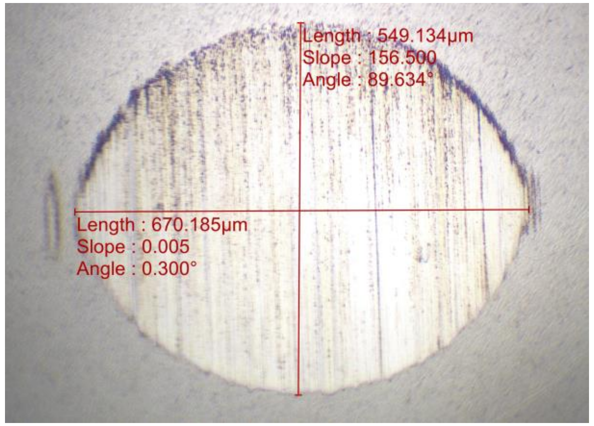
Ball-on-Cylinder Lubricity Evaluator (BOCLE)





BOCLE method (ASTM D5001): measure **wear scar diameter (WSD)**.





12.2.1 Calculate the wear scar diameter as follows:

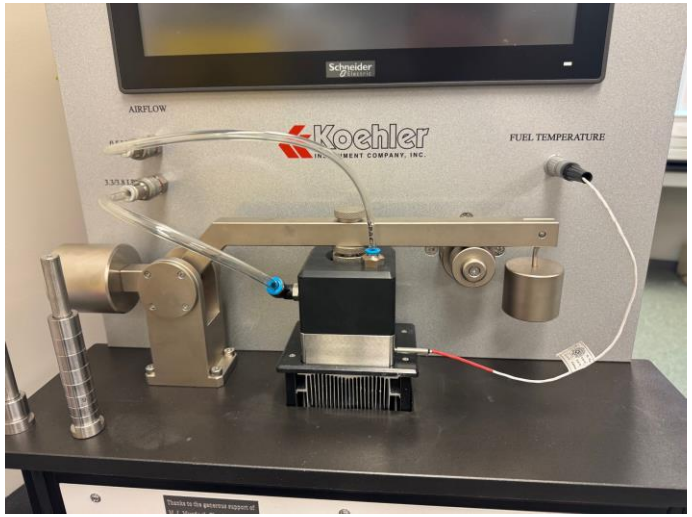
$$WSD = (M + N)/2 \quad (1)$$

where:

WSD = wear scar diameter, mm,
M = major axis, mm, and
N = minor axis, mm.

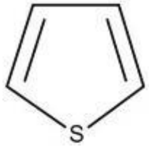
Testing the Role of Sulfur Species

- Doped HEFA-SPK with defined sulfur species:
  - Aliphatic thiol (1-dodecanethiol)
  - Aromatic sulfurs (thiophene, dibenzothiophene, benzo[b]thiophene)
- Goal: Is lubricity controlled by sulfur **type** or just total sulfur?

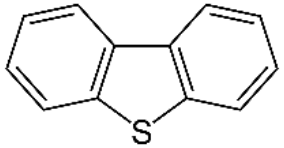


Ball-on-Cylinder Lubricity Evaluator (BOCLE)

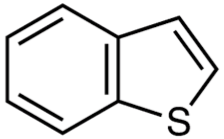
1-dodecanethiol



thiophene

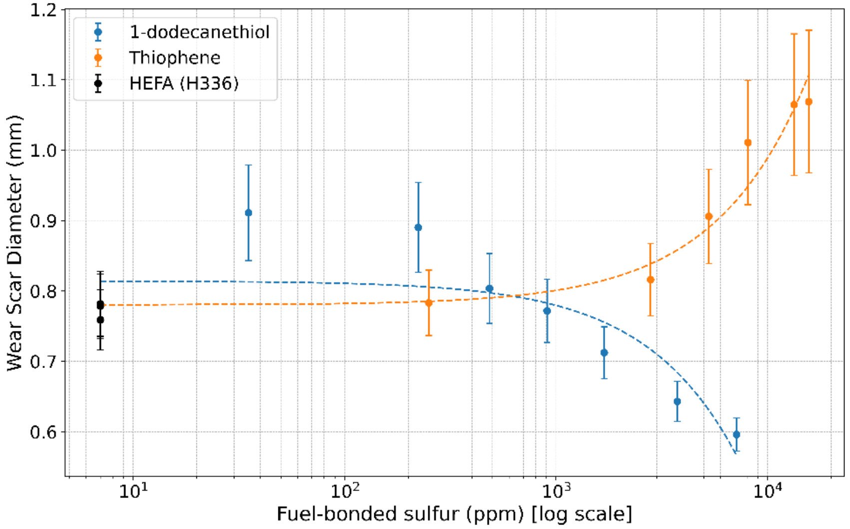


dibenzothiophene



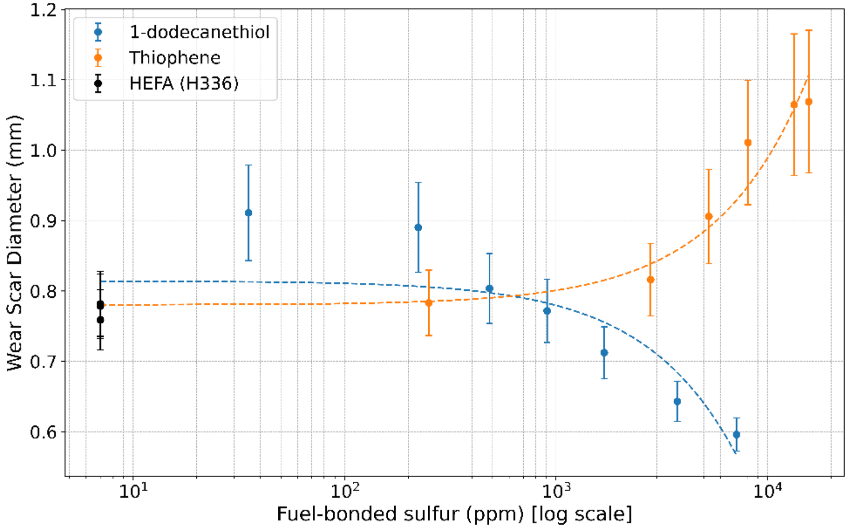
benzo[b]thiophene

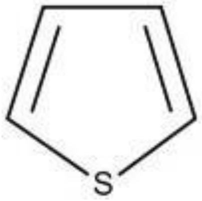
Not All Sulfur Improves Lubricity

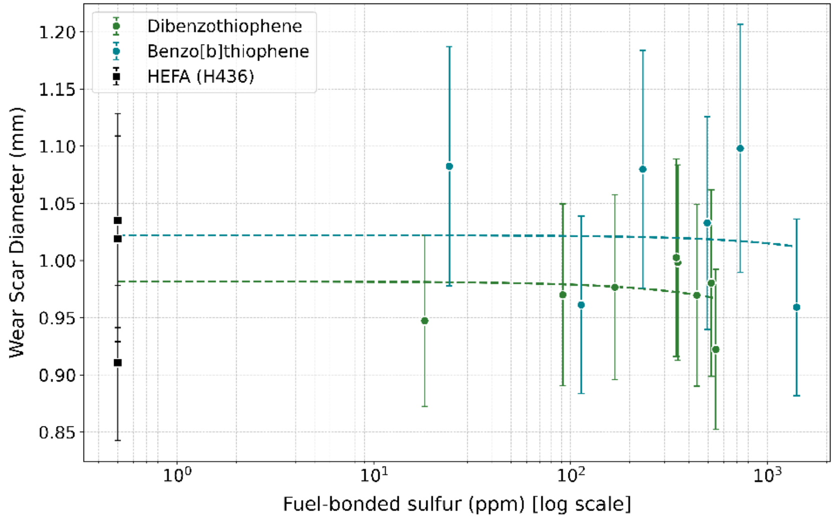


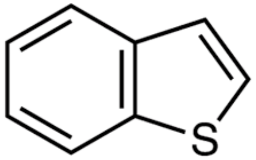
- Sulfur containing compounds react differently toward lubricity

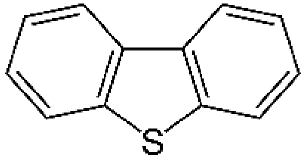
Not All Sulfur Improves Lubricity











- Sulfur containing compounds react differently toward lubricity

- 1-dodecanethiol → strong improvement, WSD ↓ with sulfur ppm.
- Thiophene → neutral or worse (high concentration degrades lubricity).
- Dibenzothiophene & benzo[b]thiophene→ negligible benefit

Summary

- Summary statement
  - DCN difference between cycloalkanes
    - Cycloalkane-rich fuels have been limited due to **uncertainty in ignition quality**.
    - Data shows **isomerism explains much of the variability**.
    - Adding more confidence in OEM and other stakeholders
  - Sulfur effect on lubricity
    - Current blending rules (ASTM D7566) mask lubricity deficits
    - For future 100% synthetic fuels, polar species or additives will be essential.
    - Data informs ASTM discussions on neat SAF lubricity specs
- Next steps
  - Continue prescreening for novel SAF producers
  - Finish sulfur effect on SAF lubricity paper
  - Continue effect on Solid Phase Extraction (SPE) for polar compounds in jet fuel

Acknowledgements

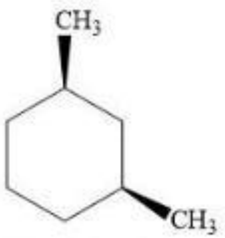
- U.S. Federal Aviation Administration Office of Environment and Energy

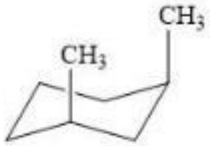
Participants

- Zhibin Yang
- Joshua Heyne
- Randall Boehm
- Alexander Kelly
- Patricia Garcia-Alfaro

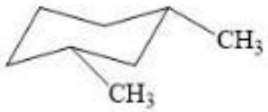
Back up

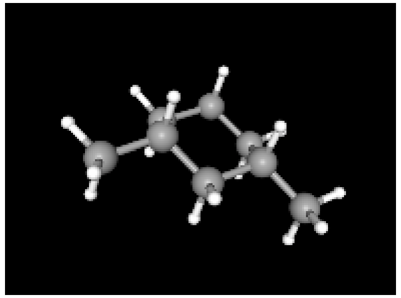
DCN Measurements of isomers of dimethylcyclohexanes

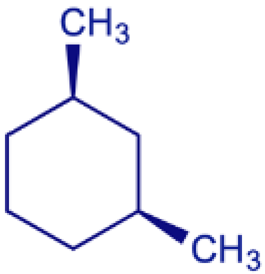




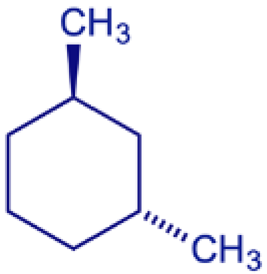
cis-1,3-dimethylcyclohexane



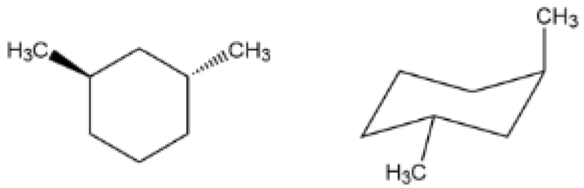




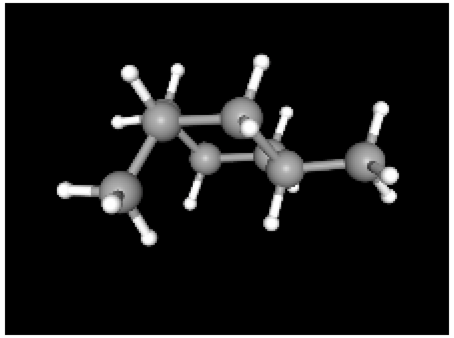
1,3-*cis*
more stable



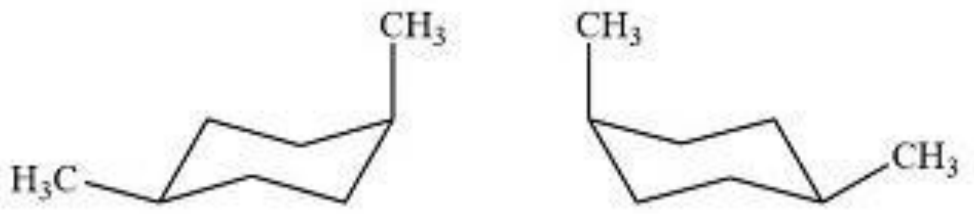
1,3-*trans*



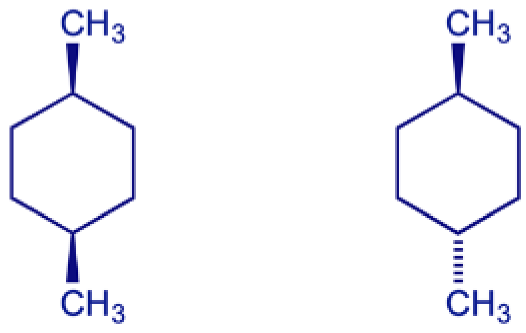
Trans-1,3 dimethyl cyclohexane



DCN Measurements of isomers of dimethylcyclohexanes

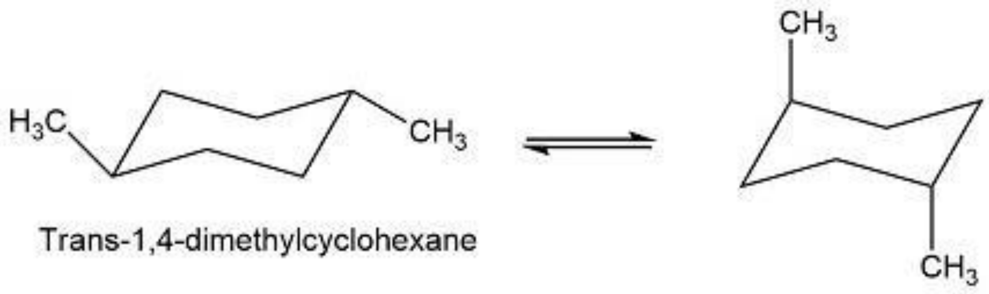


cis-1,4-dimethylcyclohexane



1,4-*cis*

1,4-*trans*
more stable



Trans-1,4-dimethylcyclohexane

Lab Expansion

- Current capabilities
- less than full capability due to:
  - Personnel familiarization
  - Incomplete supply or accessory list
  - Equipment not working properly

Fuel Property	Test Method
Mercaptan sulfur	D3227
Lubricity(BOCLE)	D5001
Hydrogen content	D7171
Trace metal	D7111
Copper content	D6732
Thermal conductivity vs T	D2717
Peroxides	D3703
FAME	IP 585
Particulate matter	D5452
Corrosion of copper	D130
Vapor pressure vs T	D6378
Electrical conductivity	D2624

Fuel Property	Test Method
Total aromatics	D1319
Total sulfur	D5453
Smoke point	D1322
Total acidity	D3242
Halogens	D7359
Distillation curve	D86
Distillation curve	D2887
Flash point	D3828
Thermal stability	D3241
LHV	D4809
Density vs T	D7042
Viscosity vs T	D7042
Freeze point	D5972
Nitrogen (fuel bound)	D4629
Specific heat vs T	E1269
Surface tension vs T	D1331
Dissolved water	D6304
Dielectric constant vs T	D924
Total olefins	D2710
Derived cetane number	D6890

Lab has been undergoing an expansion of capabilities

- Recent awards, contracts, and donations from:
  - The Murdock Charitable Trust
  - Alaska Airlines
  - United Airlines
  - CleanJoule

Equipment on order

Fuel Property	Test Method
Vapor pressure vs T	D6378
Halogens	D7359

Equipment current in the lab

Fuel Property	Test Method
Mercaptan sulfur	D3227
Peroxides	D3703
Lubricity(BOCLE)	D5001
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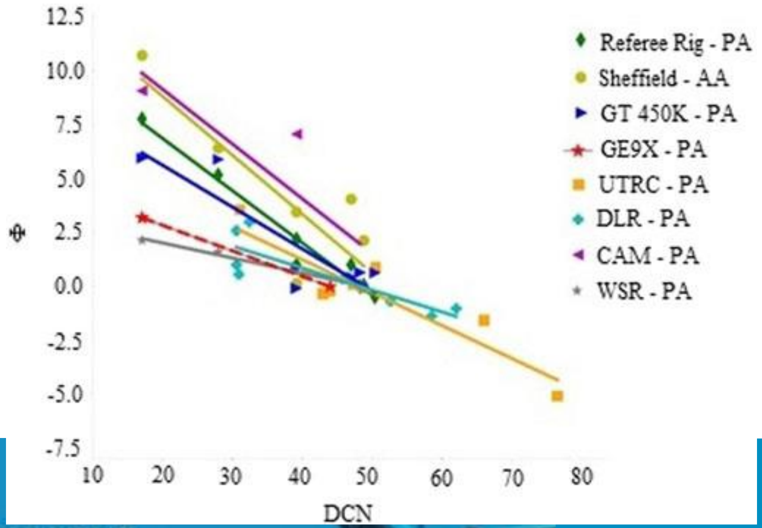
Dissolved water	D6304
Dielectric constant vs T	D924
FAME	IP 585

IQT and DCN Measurement

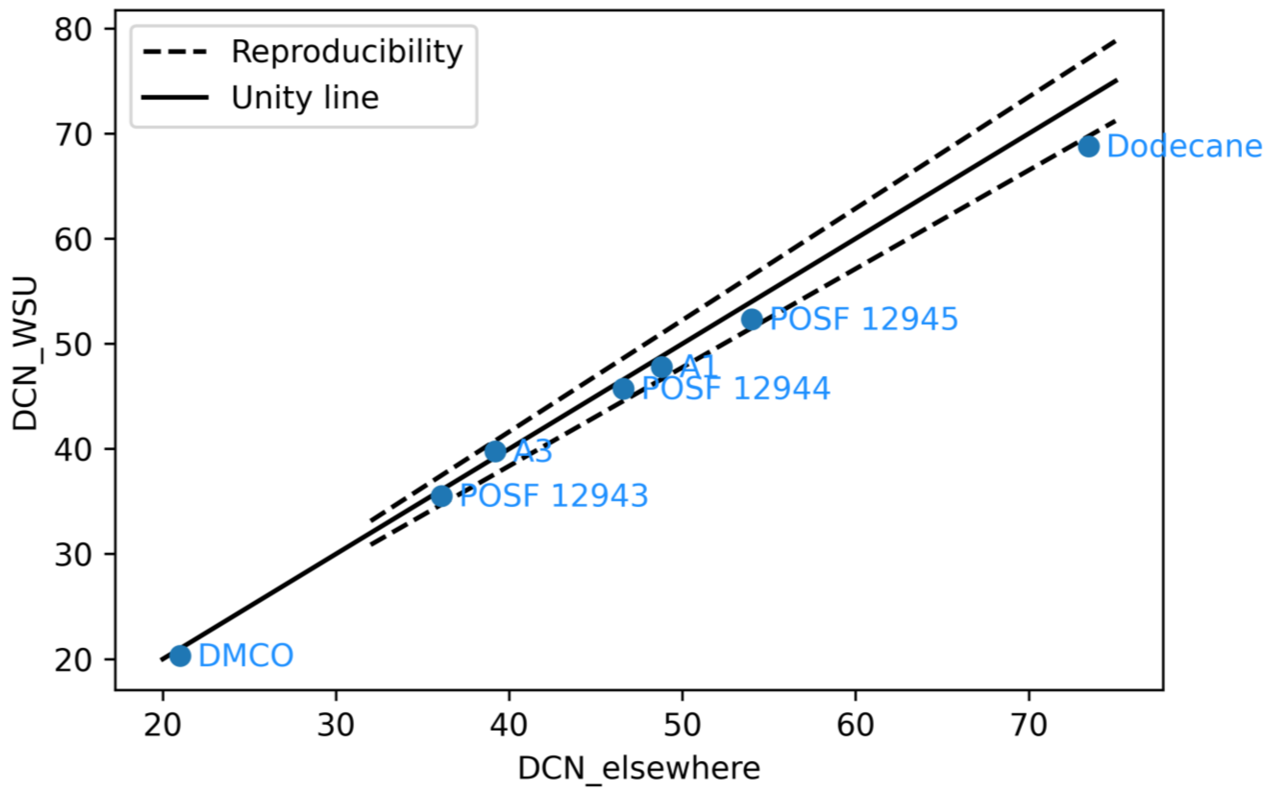
Historically operators have asked for around 150 to 200 mL of material to complete a derived cetane number test

LBO limit as a function of DCN for eight different rigs used within the NJFCP.



“Comparing Alternative Jet Fuel Dependencies Between Combustors of Different Size and Mixing Approaches” R Boehm, J Colborn, J Heyne, frontiers 2021

Low-volume DCN Measurement



This using only 15 mL of fuel, the historical volume needed is between 150 to 200 mL

Roughly a 10 X reduction in volume required to get a meaningful test result

IQT improvement throughout the years

- fuel injection systems tolerances