DOE Bioenergy Technologies Office (BETO)

2019 Project Peer Review

Analysis for Engine Optimized Sustainable Drop-In JET High Performance Fuels (HPF)

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7th March 2019, Denver Colorado

Goal statement

Develop framework to:

1. Identify one or more High Performance fuels (HPF) that will offer at least a 5% increase in total energy content as measured by either energy density (MJ/L) or specific energy (MJ/kg) or a combination thereof with corresponding performance operational benefits relative to an average conventional jet fuel and devise a more meaningful energy content goal for future.
2. Identify one or more combinations of renewable blendstocks in which the renewable content of the final HPF is at least 30%.
3. Identify up to three new alkyl cycloalkane jet fuel blending mixtures and identify the major fuel component molecules and evaluate how such a mixture behaves in the Pareto model.

Key milestones

Phase I	FY 2018				FY 2019			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Develop a blending optimization tool (JudO) to evaluate high performance jet fuel molecules for drop-in operability and high performance								
Produce a list of high performance jet fuel molecules								
Estimate economic operational benefits that can be derived from the potential use of high performance jet fuels								

Phase II	FY 2018				FY 2019			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Determine structure-function property of alkyl cycloalkanes								
Advance HPF JudO optimization tool and Pareto modeling								
Perform economic benefits of HPFs for NAS-wide fleet								
Identify up to three alkyl cycloalkane jet fuel mixtures and evaluate how mixtures behave in Pareto model.								
Produce mixtures of identified cycloalkanes and perform jet fuel operability testing on a pre-screening level								

Project Budget Table

	Original Project Cost (Estimated)		Project Spending and Balance	
Budget Period (FY18)	**DOE Funding**	**Project Team Cost Shared Funding**	**Spending to Date**	**Remaining Balance**
SNL	$63K	$63K	100%	0
Activity 1	Which molecules & structures can confer these performance benefits?			
UDayton	$167K	$167K	100%	0
Activity 2	What performance increases can we achieve with advanced drop-in Sustainable Alternative Jet Fuel (SAJFs)?			
Georgia Tech	$70K	$70K	100%	0
Activity 3	What is the value of these fuels to the aviation industry?			

Quad chart overview

Timeline

Project start date	01-10-2018
Project end date	09-30-2018
No cost extension till	12-31-2018
New funding	02/2019-09
Percent Complete	Phase 1:100% , Phase 2: 0%

	Total Costs Pre FY17	FY 17 Costs	FY 18 Costs (K)	Total Planned Funding (FY 19-Project End Date) (K)
DOE Funded		NA	$300	$840
Project Cost Share (BETO)	NREL	NA	-	$250
	PNNL	NA	-	$250
	SNL	NA	$63	$120
	UDayton	NA	$167	$120
	GeorgiaTech	NA	$70	$100

Barriers addressed

- Ct-J. Identification and Evaluation of Potential Bioproducts
- At-A. Analysis to Inform Strategic Direction.
- At-B. Analytical Tools and Capabilities for System-Level Analysis
- At-E. Quantification of Economic, Environmental, and Other Benefits and Costs

Partners

UDayton: 55% (FY18)
GeorgiaTech: 23%

Additional Partners: NREL, PNNL (FY19)

Project overview

Funding mechanism

- This is a seed project to explore and devise framework for evaluation of high performance jet fuels
- Foundations laid by the DOE – AFRL – NASA coordinated JET workshop on "Jet fuels & Engine co-opTimization" held at NASA Glenn (Sept. 2017)
- Initial funding of $100k (Jan-Jun), followed by addition of $200k

Changes to project team

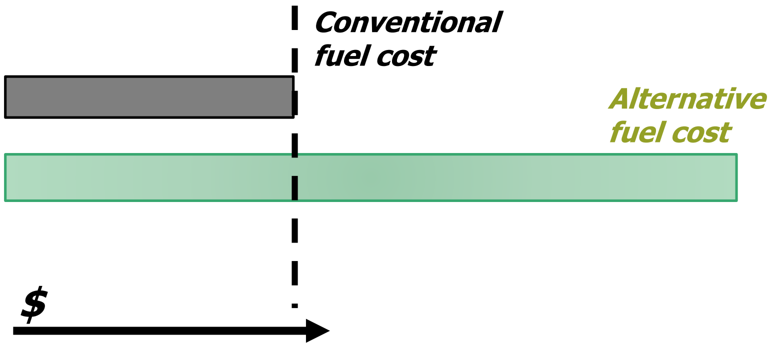
- SNL added fuels researchers to lead HPF molecule discovery efforts
- PNNL and NREL added to 2nd phase of the project

Progress, accomplishments and changes

- Results from milestones lead to no-cost extension till Dec 2018, and review (22nd Jan 2019) to define next steps.
- Further funding approved Feb 2019 for SNL, PNNL, NREL, Udayton and Georgia Tech

Project overview
The problem: cost discrepancy with value uncertainty

Fuel cost

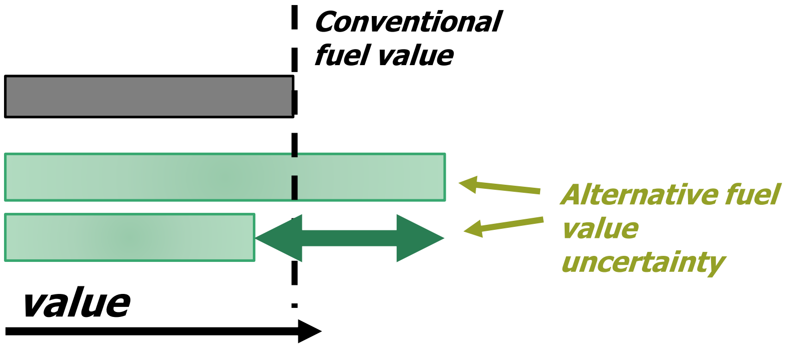


Alternative jet fuels are more expensive

"Every dollar a barrel increase in oil prices result in $425 million dollars in airline expenses"

(Davidson et al., 2016)

Fuel value



High performance alternative jet fuels add value

What is the value gained with HPF fuels?
Can this value be objectively monetized?
Can we maximize monetized benefits to minimize the cost discrepancy?

1 Approach (technical)

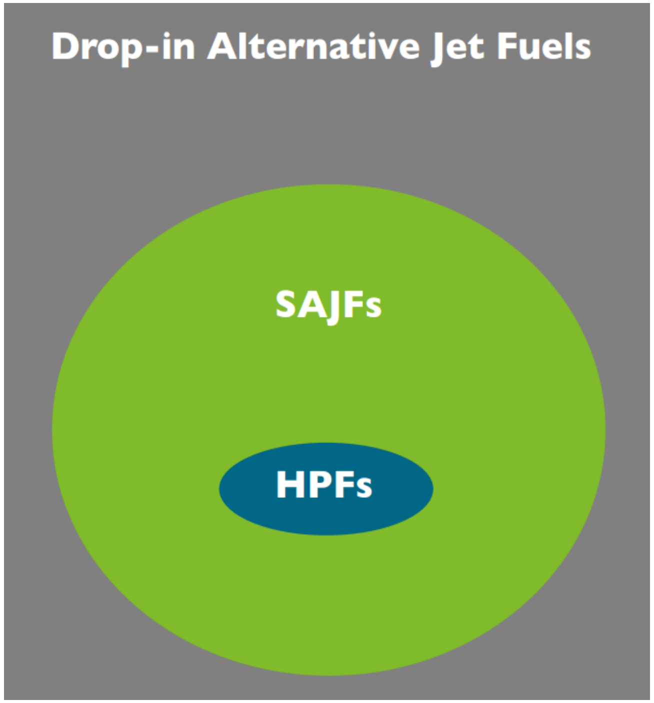
Foundational questions frame approach

- What performance increases can we achieve with advanced drop-in Sustainable Alternative Jet Fuel (SAJFs)?
- Which molecules & structures can confer these performance benefits?
- What is the value of these fuels to the aviation industry?

1 Approach (technical)
Defining HPFs to enable goals

HPFs:

- are ‘drop-in’ fuels and are a subset of SAJFs
- offer higher CO_2 and PM emissions reduction
- are highly compatible with jet engine hardware and combustion for better operability
- offer superior performance due to higher energy content and thermal stability



HPFs need to be net price-competitive for their successful commercial deployment

1 Approach (technical)

HPF value proposition: operability & performance

Operability:

- Bulk properties: DCN*, T_b, T_f, η, P_{vap}, σ, T_{10}
- Essential for SAJF approval (ASTM D4054)

Required for safety

Performance:

- Specific energy, MJ/kg
- Energy density, MJ/L
- Thermal Stability
- Emissions

Adds value to consumer

*DCN – Derived cetane number

1 Approach (technical)
Performance benefit overview

Focus of this project

Specific Energy, MJ/kg

- Every mission will benefit from an increase
  - Better specific fuel consumption
  - More payload
  - CO2 emission reductions

Energy Density, MJ/L

- Benefits by improving the mechanism that jet fuel is purchased as $/gallon
- Volume limited flights
- Military applications

Thermal Stability

- Potential for increase thermodynamic cycle efficiencies
- Maintenance costs
- Lower fuel usage, CO2 and PM emissions

Emissions

- New International Civil Aviation Organization (ICAO) emissions regulations for CO2 and PM
- Non-attainment regions

2 Approach (management)

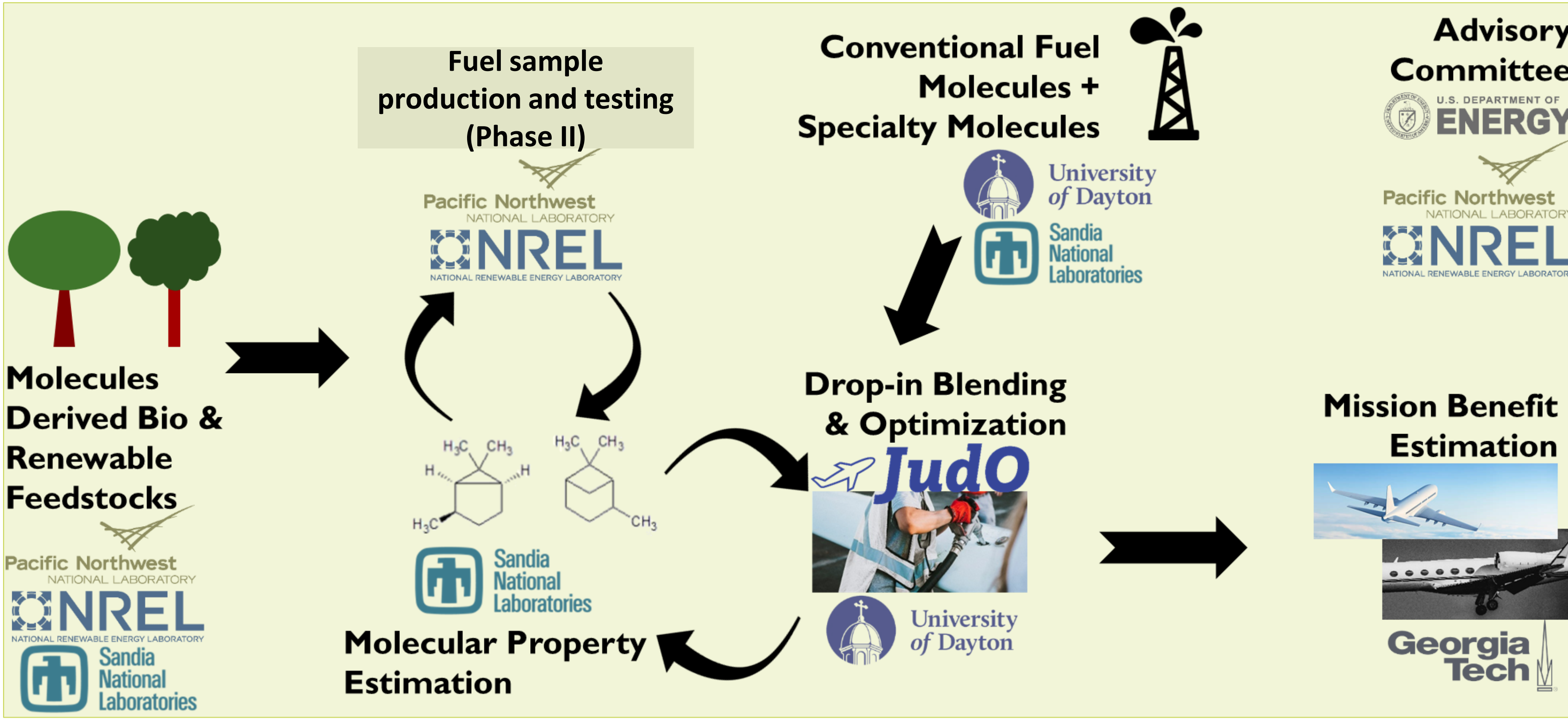
- What performance increases can we achieve with advanced drop-in Sustainable Alternative Jet Fuel (SAJFs)?
  PI – Josh Heyne (UDayton)

- Which molecules & structures can confer these performance benefits?
  PI – Anthe George (SNL)

- What is the value of these fuels to the aviation industry?
  PI – Russell Denney (Georgia Tech)

- Collaborations and involvement from AFRL, BOEING, DOD, NASA, NavAir, NREL, PNNL, and many others including airlines, jet engine and fuel producers

2 Approach (management)



2 Approach (management)

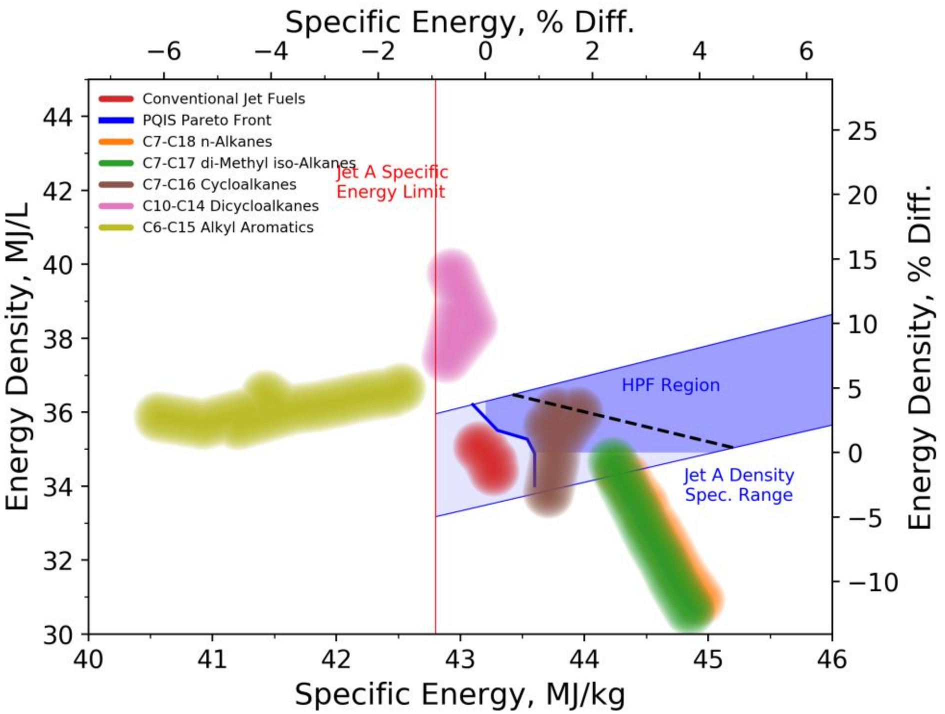
- Bi-weekly results update meetings
- Team face-to-face meeting
- Meetings open to all labs and stakeholders (attendance up to ~20 in some meetings – (attendees include members from AFRL, Boeing, DOD, NASA, NavAir, national laboratories, among others)
- Communications with airlines, engine manufacturers, and fuel producers
- Conference attendances
- Briefings, presentations & outreach to ABLC, CAAFI, AIAA

3 Technical progress
What performance increases can we achieve with HPFs?

Developing blend calculator (JUDO) for optimization of HPF for operability and performance

- Identifies upper bounds for blending based on ASTM specification, previous SAJF approvals, and NJFCP learnings
- Can be used to explore HPF fuels and their limits as well as 'what if' scenarios for processes
- Reproduces to first order the previous evaluation results from evaluation and approvals

SEED Plot
(**S**pecific **E**nergy – **E**nergy **D**ensity)



JudO
Jet Fuel Blend Optimizer

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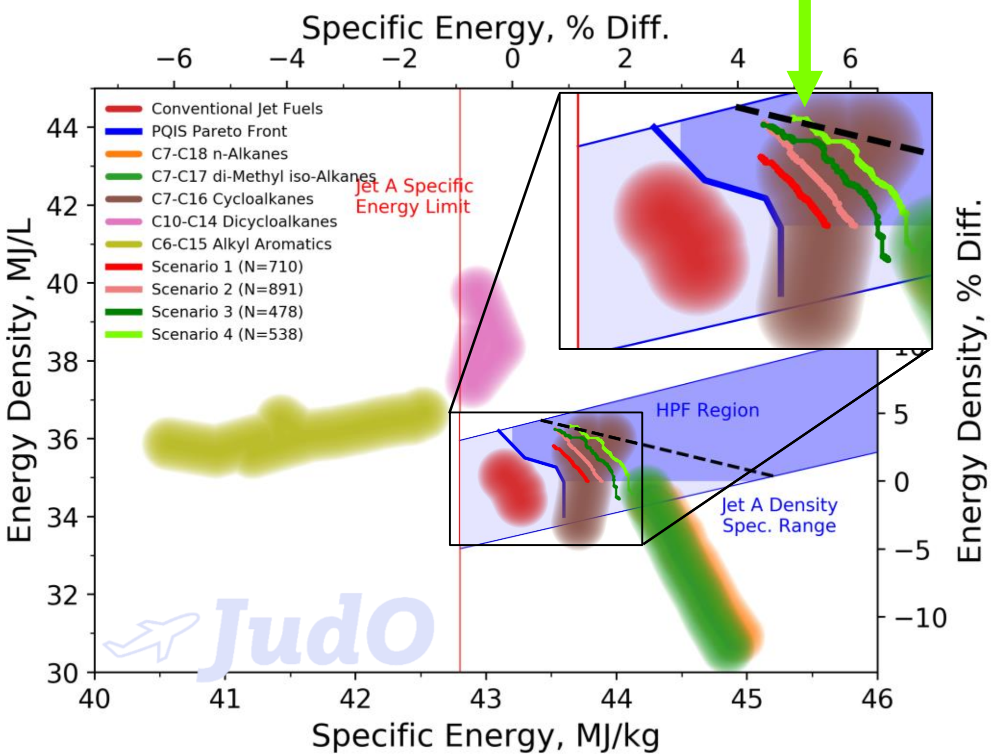
3 Technical progress
What performance increases can we achieve with HPFs?

Aromatic removal and including novel cycloalkanes can increase the combine energy density and specific energy beyond 5%



	Molecule Set	Constraint	Key
1	Conventional Fuel Molecules	Aromatics [8-25%v]	(red)
2	Conventional Fuel Molecules	Aromatics, relaxed	(light red)
3	Scenario 1 + Novel Cycloalkanes	Aromatics [8-25%v]	(dark green)
4	Scenario 2 + Novel Cycloalkanes	Aromatics, relaxed	(light green)

- Novel cycloalkanes and the removal of aromatics can provide a significant benefit to a fuel's specific energy
- This proves a direct specific fuel consumption benefit

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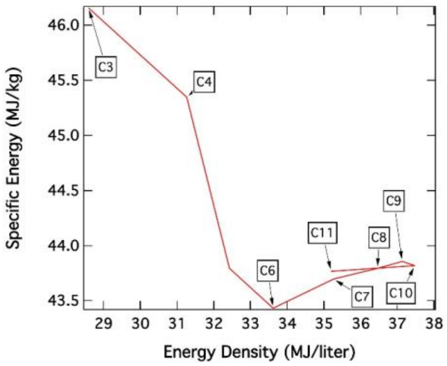
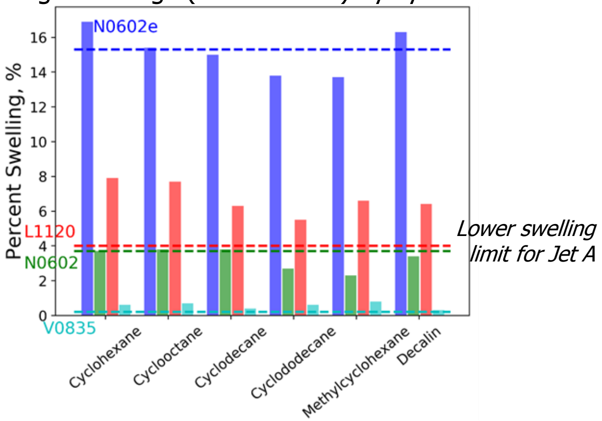
3 Technical progress
Cycloalkanes as substitutes for aromatics in HPFs

- Unstrained cycloalkanes:
  - High energy density; moderate specific energies
  - Many properties in the jet fuel spec range
  - Can provide similar seal swelling to aromatics
- Multiple scenarios are explored to develop optimized blends

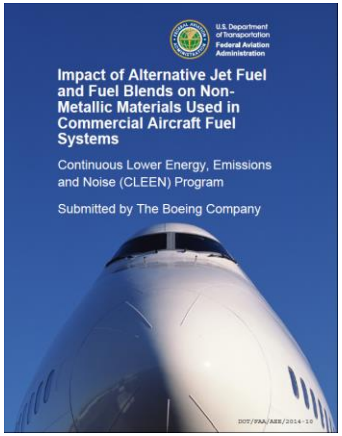


Energy density versus specific energy by varying cyclic C no.

Swelling of O-rings (colored bars) by cycloalkanes



Cycloalkanes in a 30%v blend with an IPK swell within the Jet A range
Current HPF optimizations have 40-60% cyclic compound composition



Authored by UDRI (John Graham) and Boeing

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3 Technical progress
Which molecules and structures can perform as HPFs?

n- and iso-alkanes

- highest specific energy and lowest energy density

Aromatics

- poor emission and specific energy characteristics

Monocyclic alkanes

- meet specific energy and energy density specs

Fused dicyclic alkanes

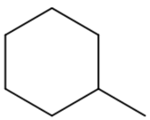
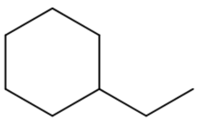
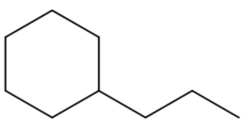
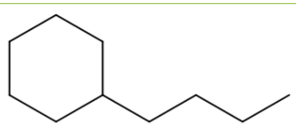
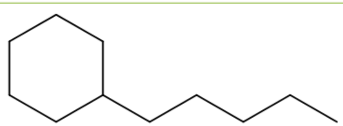
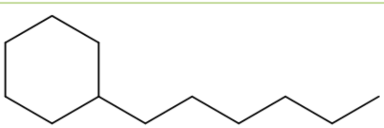
- could replace the need for aromatics for swelling

Strained molecules

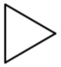
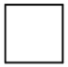
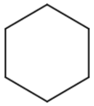
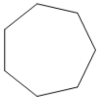
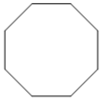
- greatest potential for performance benefits

3 Technical progress
Structure property relationships enhance understanding of new HPFs

Energy Density increases with alkyl chain length while specific energy remains approximately constant

	mass energy density MJ/kg	volumetric energy density MJ/l
	43.36	33.17
	43.40	34.04
	43.41	34.29
	43.42	34.54
	43.59	34.83
	43.41	34.92

Energy Density decreases with increasing number of carbon atoms in cyclic compounds whilst specific energy increases

	mass energy density MJ/kg	volumetric energy density MJ/l
	46.16	28.59
	45.34	31.26
	43.82	34.45
	43.35	33.17
	43.67	35.27
	43.8	35.45

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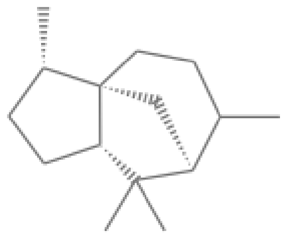
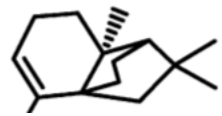
3 Technical progress

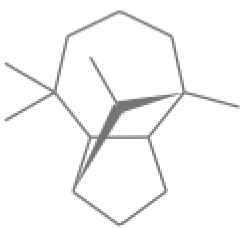
Bio-derived structures can reshape the research space



alpha-cedrane

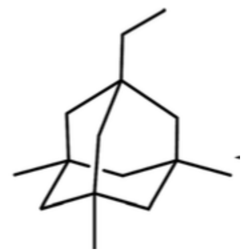


Alpha-neoClovene (hydrogenated)

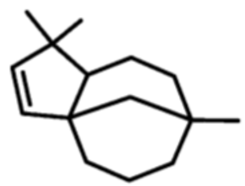


longifolane

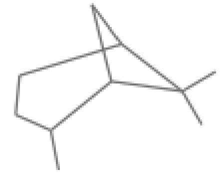
Example structures evaluated



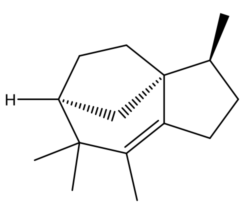
1-ethyl-3,5,7-trimethyladamantane



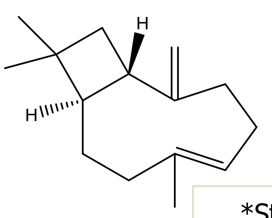
clovene (hydrogenated)



pinane



Epi-isoziaene (hydrogenated)

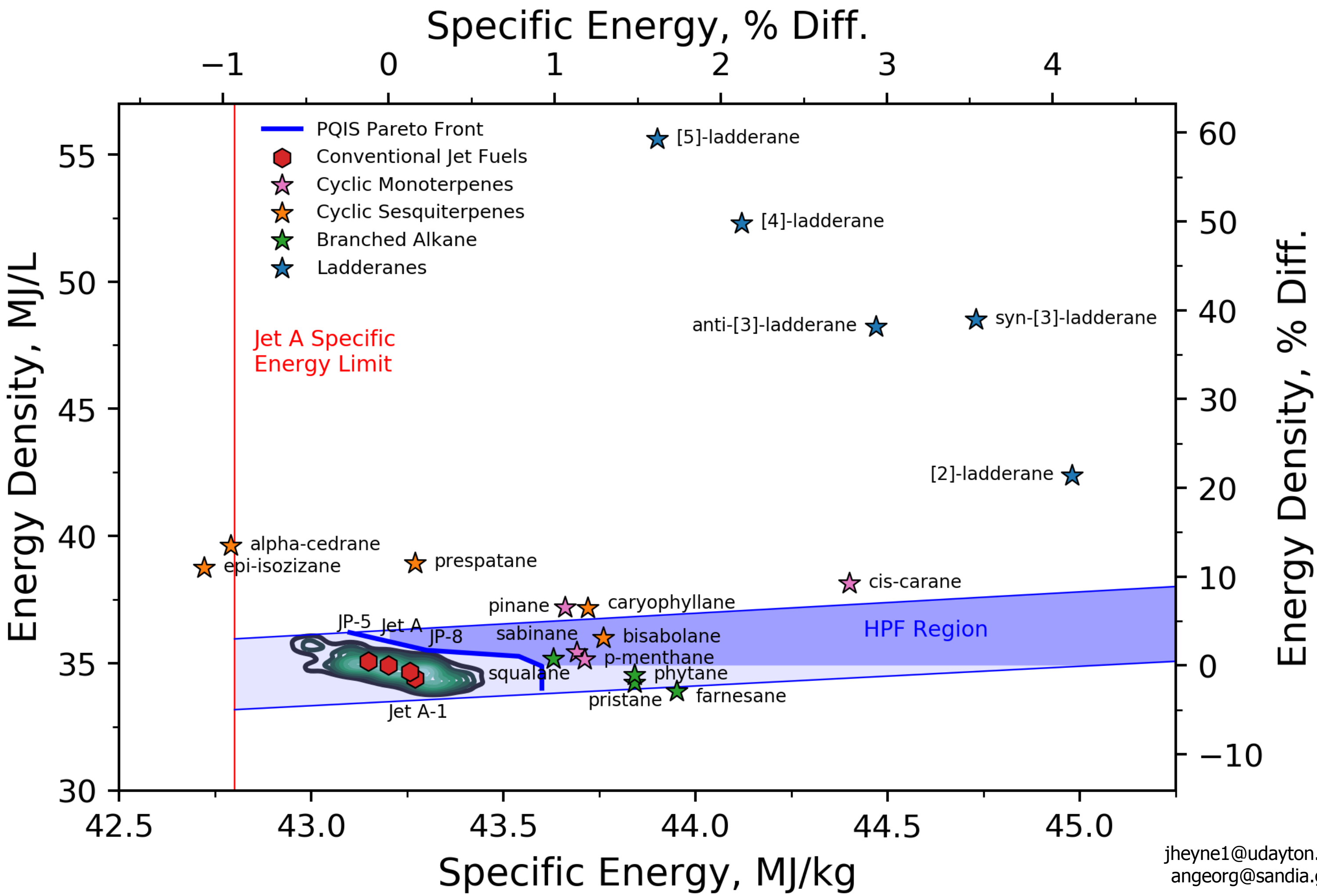


Beta-carophyllene

*Structures evaluated are saturated analogues
Structures shown example structures evaluated

3 Technical progress

Ab initio quantum chemistry calculations show high energy content



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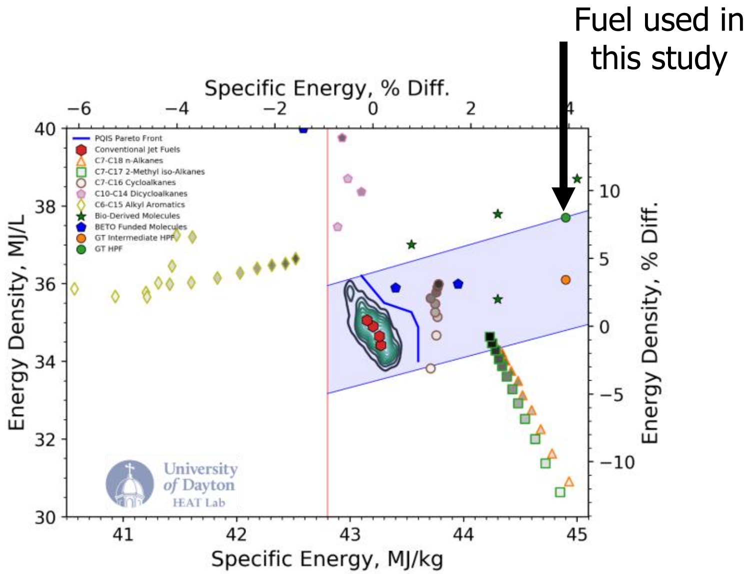
3 Technical progress
What is the value of HPFs to the aviation industry?

Energy density based performance benefits

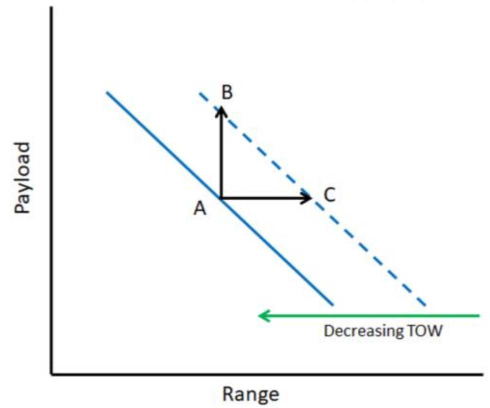
Option A. same payload for same range, lower fuel and take-off weight (TOW):

- Purchase less fuel
- Fewer flight restrictions due to high, hot or short runways
- Reduced thrust takeoffs, which can save fuel and/or engine life



Option B. carry lower fuel weight but additional payload for same range and same TOW:

- Potential increased revenue from cargo



Option C. carry same payload at same TOW for increased range:

- Potential increased revenue from new routes

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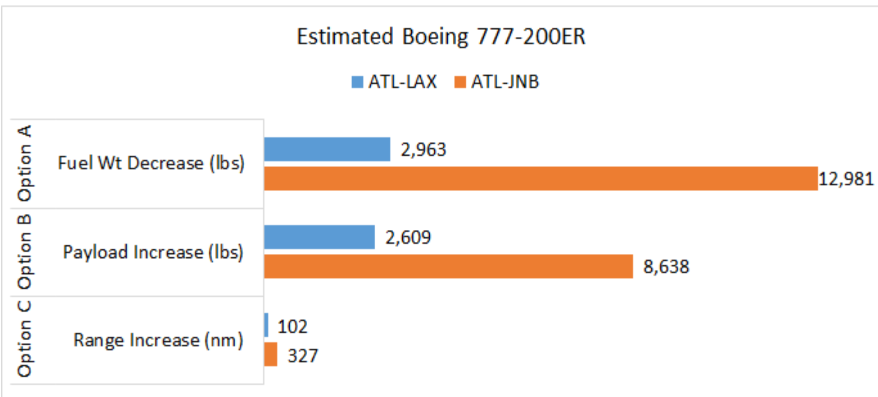
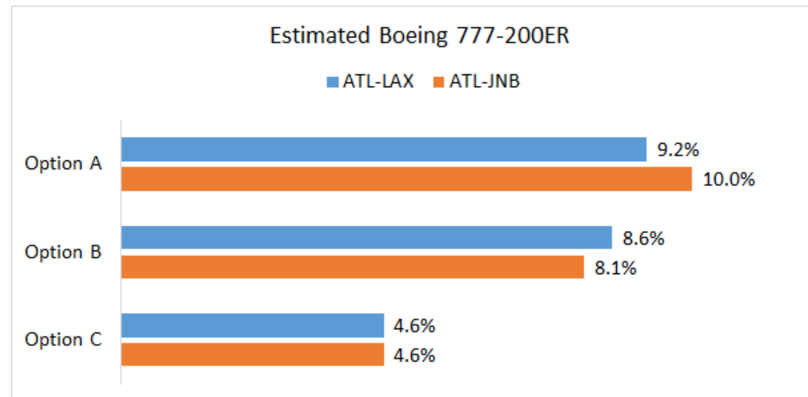
3 Technical progress
Maximum performance benefits of notional HPF

Boeing 777-200ER Performance Analysis

Mission performance benefits



Value to the airline



- Three aircraft classes (50-, 150-, and 300-passenger) were analyzed over a range of fuel properties
- Performance depends on the specific flight combination of aircraft and mission, and HPF fuel properties analyzed
- Break-even fuel price is very sensitive to the assumptions made about additional aircraft operating costs and revenues

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4 Project relevance
Strong stakeholder inter-ties and addresses BETO gaps

Stakeholders

- Air Force Research Lab
- Dept. of Defense
- NASA
- Jet engine and fuel industry

JET HPF Program

Core BETO Programs

- Analysis & Sustainability
- Agile Biofoundry
- BETO Core Conversion
- Co-Optima
- BETO MYP
- BETO FOA

5 Future work

- Refine operability and performance optimization of HPF fuel blends by addition of DCN, surface tension, and low temperature viscosity constraints for optimization
- Model development and calculation of further HPF properties (e.g. for surface tension and viscosity of new structures)
- Refine estimates of monetized HPF benefits for fleet-wide domestic operations
- Explore fuel efficiency benefits of highly thermally stable HPFs
- Evaluate potential of cycloalkanes as HPFs in terms of properties and production routes

Summary

- A framework for evaluating HPFs has been developed
- Multi-objective optimization indicates that monocycloalkanes can significantly improve fuel performance
- Bio-derived terpenes have the potential to confer benefits similar to conventional monocycloalkanes
- Break-even HPF prices have been determined for three aircraft with various usage scenarios

Additional Slides

Reference summary

Overview	▪ Develop a framework to offset HPF cost discrepancy with value by asking: ▪ What performance increases can we achieve with advanced drop-in Sustainable Alternative Jet Fuels? ▪ Which molecules & structures can confer these performance benefits? ▪ What is the value of these fuels to the aviation industry?
Approach	▪ Establish framework to evaluate performance using energy density and specific energy as metrics ▪ Build blend calculator (JudO) to determine and establish effect of blending HPFs to meet 'drop-in' requirements for operability ▪ Develop methodologies for predicting properties ▪ Evaluate suites of molecular classes to understand effect of structure and bioderived molecules on specific energy and energy density ▪ Quantify value of HPF to aviation industry in terms of increased range, payload and reduced fuel ▪ Develop sample HPF fuels and test them for energy, blending and operability requirements
Technical progress	▪ A framework for evaluating HPFs has been developed ▪ Multi-objective optimization indicates that monocycloalkanes can significantly improve fuel performance ▪ Bio-derived terpenes have the potential to confer benefits similar to conventional monocycloalkanes ▪ Break-even HPF prices have been determined for three aircraft with various usage scenarios
Relevance	▪ Establish framework for off-setting HPF cost-discrepancy with value, thereby enabling development of commercially viable technologies for energy-dense, fungible, cost-competitive 'drop-in' jet fuels
Future work	▪ Addition of DCN, surface tension, and low temperature viscosity constraints for optimization tool ▪ Calculation of additional properties for bio-derived molecules of interest ▪ Domestic fleet-wide analysis of achievable HPF benefits ▪ Sample production of HPF fuels and their prescreen testing

Presentations and publications

Presentations

Improvement in Jet Aircraft Operation with the Use of High-Performance Drop-in Fuels, Lily Behnke, Joshua S. Heyne, Robert D. Stachler, Giacomo Flora, Steven Zabarnick, Anthe George, Alexander Landera, Ray Bambha, Russell K. Denney, Mohan Gupta, AIAA-2019-0993 , AIAA SciTech,1/7/19-1/12/19 San Diego, CA

Engine Optimized Sustainable Drop-in JET High Performance Fuels (HPF), Anthe George, Russell Denney, Joshua Heyne, Mohan Gupta, ABLC GLOBAL 2018, The Advanced Bioeconomy Leadership Conference, San Francisco, CA, 10-11-2018

Publications:

Improvement in Jet Aircraft Operation with the Use of High-Performance Drop-in Fuels Lily Behnke, Joshua S. Heyne, Robert D. Stachler, Giacomo Flora, Steven Zabarnick, Anthe George, Alexander Landera, Ray Bambha, Russell K. Denney, Mohan Gupta, Report to AIAA

Properties Calculator and Optimization for Drop-in Alternative Jet Fuel Blends, Giacomo Flora, Shane Kosir Lily Behnke, Robert Stachler, Joshua Heyne, Steven Zabarnick, Mohan Gupta, Report to AIAA

Engine Optimized Sustainable Drop-in JET High Performance Fuels (HPF) Joshua S. Heyne, Robert D. Stachler, Giacomo Flora, Steven Zabarnick, Anthe George, Alexander Landera, Ray Bambha, Chris Shaddix, Russell K. Denney, Dimitri Mavris, Ph.D, Mohan Gupta,

Risk registry table

	Risk Identified		Mitigation Strategy	Status
Risk ID	Risk Description	Severity (H/M/L)	Mitigation Response	Active/ Closed
JudO Tool				
1	Credibility of JudO optimization tool	H	JudO tool is being continuously tested against ASTM pre-approved AJFs for blending determination	Active
Molecules Property-Structure relationship				
2	Accuracy in theoretically determined molecular property values and trends	L	Comparing values and trends against the laboratory data	Active
Economic Benefit Assessment				
3	Validating the benefit analysis	M	Working with stakeholders for guidance	Active
Meeting 'drop-in' operability requirements for HPFs				
4	Achieving targeted energy content while meeting all requirements for 'drop-in' fuel	M	Developed plans for Tier-Alpha and Tier zero pre-screening testing of sample HPF fuels	Active
Realization of HPF Framework				
5	Achieving targeted performance gains of drop-in HPFs while meeting BETO MSFP and LCA goals	H	Analysis will be initiated once the HPF pathways are identified through Lab work	To be started
Program Coordination and Sharing of Information				
6	Frequency of communication and real-time data sharing	M	Exercising norms of communication and data sharing on a regular impromptu basis	Active