

DOE Bioenergy Technologies Office (BETO)
2021 Project Peer Review

Opportunities in BioJet

Anthe George
Sandia National Laboratories
in collaboration with Georgia Tech, LANL, NREL, PNNL, U. Dayton

March 22, 2021



Overview

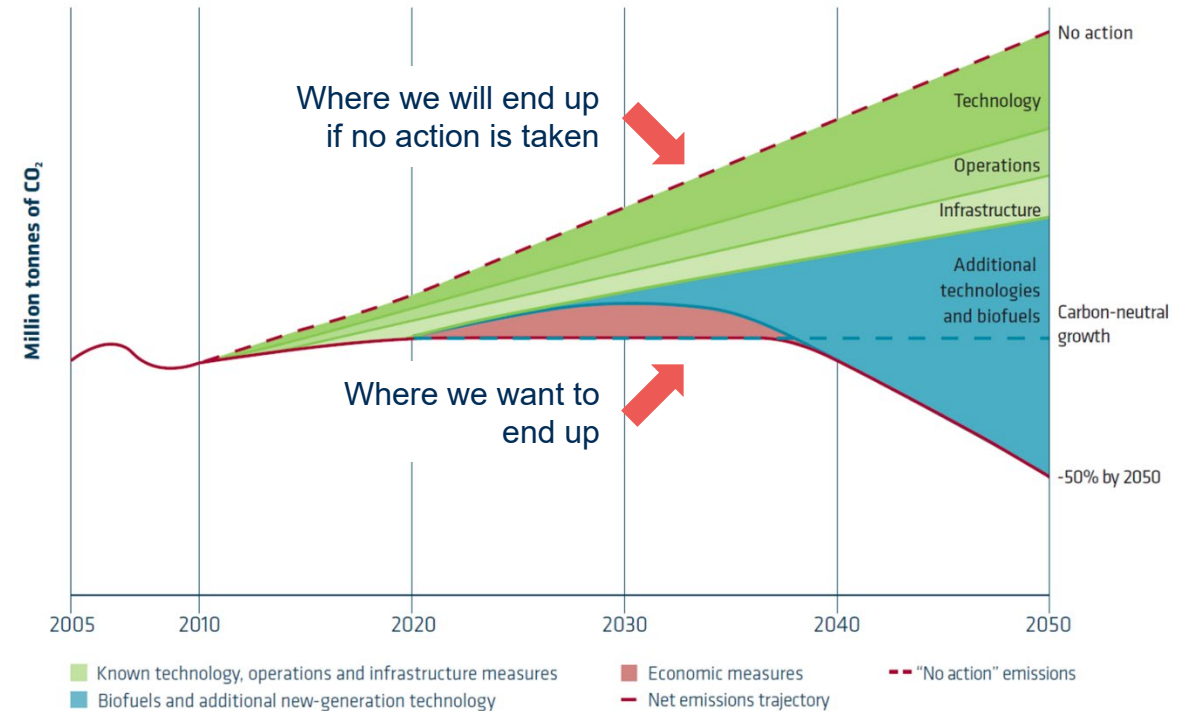
Sustainable aviation fuel [SAF] deployment is critical for meeting industry targets



- **Substantial growth** in air travel by 2050
- **ICAO/Industry Goal:** Aviation CO₂ emissions impact to be returned to 2005 levels by 2050
- International Air Transport Association (IATA) in 2009 set a goal of 50% reduction in CO₂ emissions relative to 2005 levels
- Up to 75% of the emissions growth by 2050 is offset by SAF and/or carbon off-sets
- Electrification will be limited; viable feedstocks and SAFs need to be developed and deployed

*SAF –Sustainable aviation fuels

IATA Technology Roadmap 2013



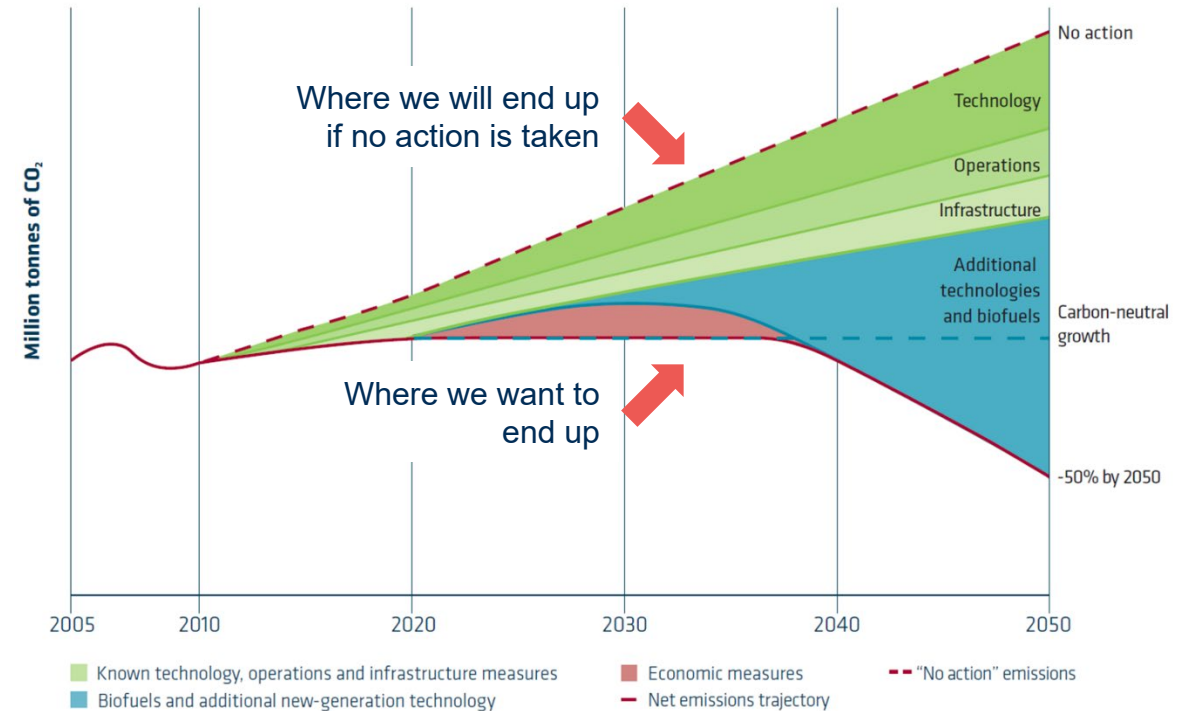
Overview

This project aims to remove technical and analysis barriers to SAF deployment



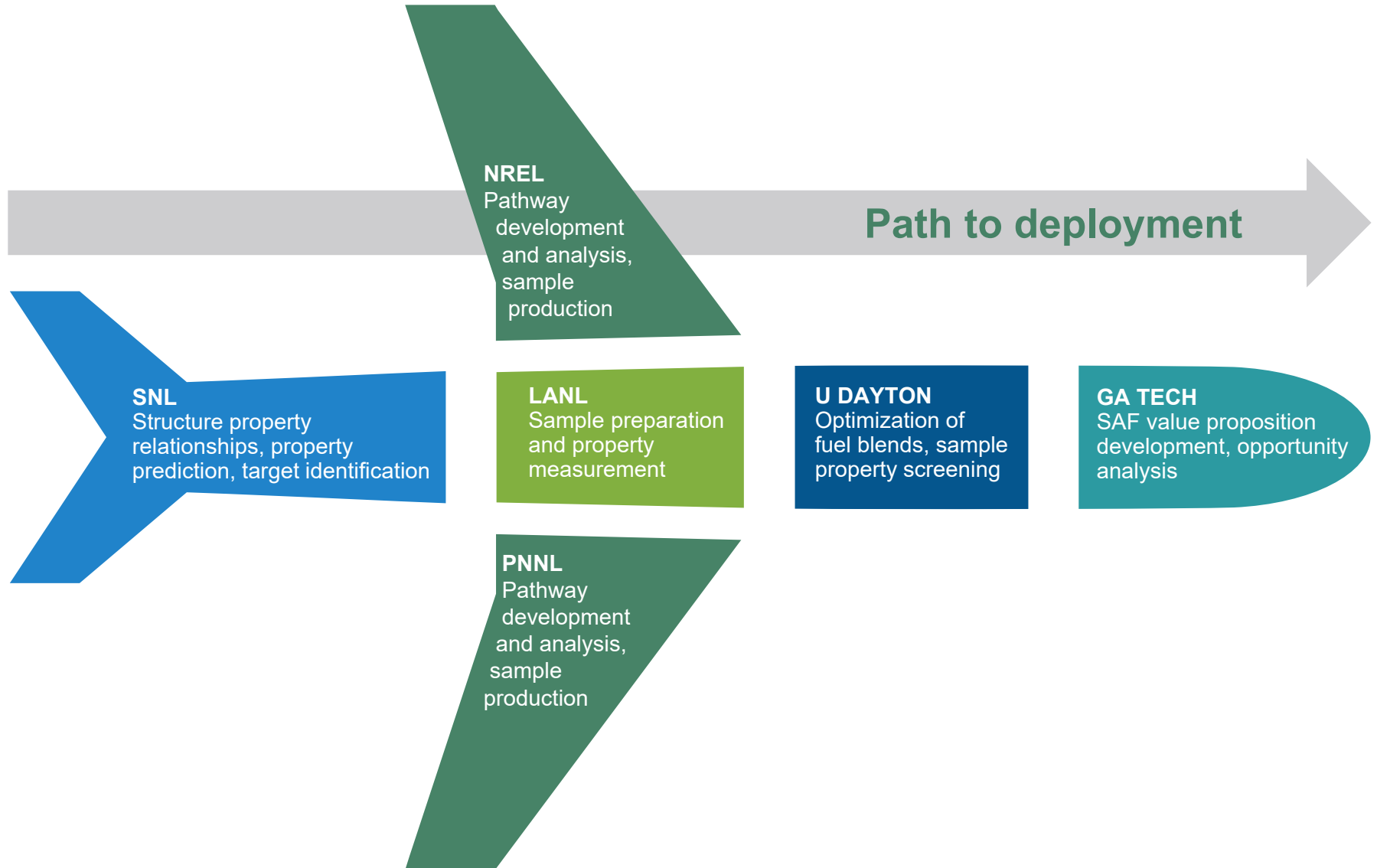
- **Goal:** Address key roadblocks to deploying new sustainable aviation fuels
 - What molecules and blends are optimal?
 - How can we reduce costs associated with SAF?
 - What is the value proposition of these SAF to industry?
- **Outcome:** Provide foundational knowledge needed by stakeholders for SAF deployment
- **Relevance:** Technology to meet aggressive international aviation targets for CO₂ reductions and BETO's biofuel goals

IATA Technology Roadmap 2013



1. Management

A team of national labs and academia driving towards common goals



1. Management

Strong co-ordination and communication ensure objectives are met



- Structured meetings, centralized information sharing and stakeholder engagement keep the project organized and on track
- Tiered meetings
 - Annual kick off meeting
 - Monthly report-outs
 - Regular sub-group meetings
- Box platform for data sharing and collection
- Slack channels for impromptu topical discussions
- Information dissemination via conferences, outreach and scientific reports and publications



1. Management

Strong co-ordination and communication ensure objectives are met



Key relationships with broad spectrum of stakeholders

- Airlines of America
- Atlanta Hartsfield Jackson Intl. Airport
- Delta and other airlines
- Port of Seattle
- FAA Office of Environment and Energy
- ICAO Committee on Aviation Env. Protection
- General Electric
- Boeing
- CAAFI
- Colonial and Plantation pipelines (upcoming)

Strong ties to other DOE offices and programs: BETO and beyond



Co-Optimization of
Fuels & Engines



1. Management

Risks to technical challenges are identified and mitigated



Risks

Computational models are not fully predictive for important properties

Predicted biofuel cost cannot be reduced to achieve parity with incumbent



Risk mitigation

Selected fuels are measured to verify actual properties, and discrepancies are used in model improvements

System modeling is used to identify selected biofuel/ conventional blends and ratios that increase overall value

2. Approach

BETO Sustainable Aviation Fuel Workshop report guides approach



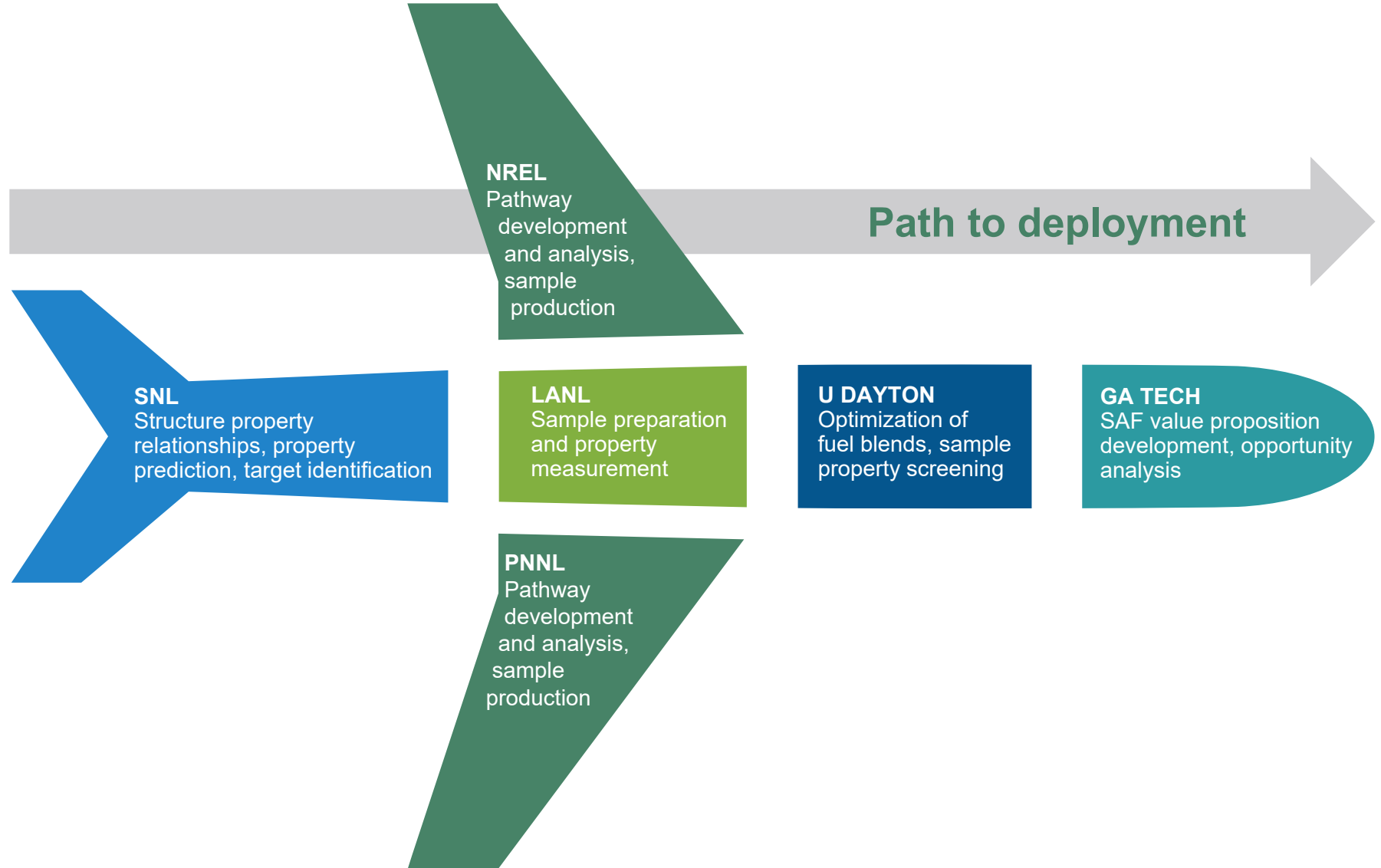
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2. Approach

Complementary capabilities result in a natural work flow

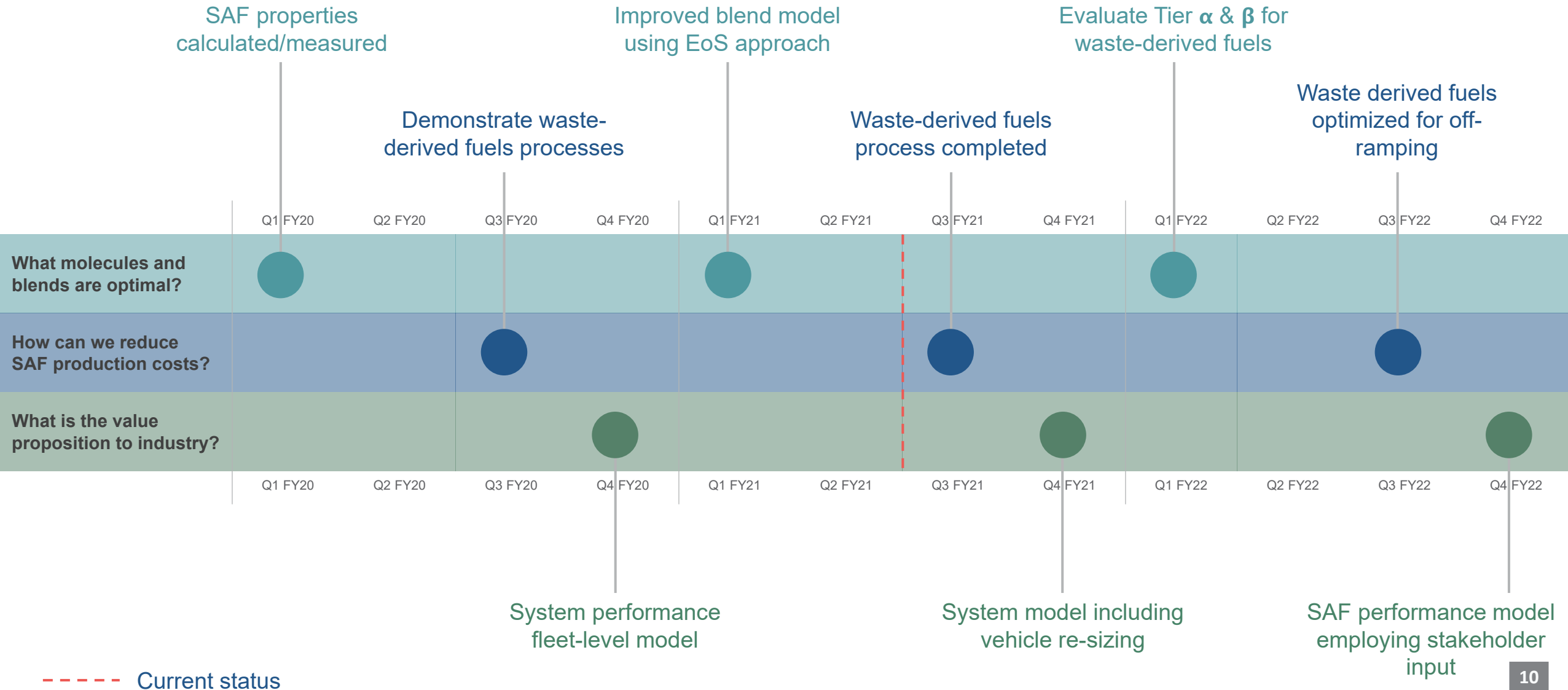


- **Property modeling**
- **SAF screening**
- **Blend optimization**
- **Pathway development**
- **Systems analysis**



2. Approach

High-level milestones enable targeted progress



2. Approach

Metrics and Go/No-Go decisions for main technical challenges ensure progress



Technical Metric

Candidate SAFs must meet defined performance and operability metrics to be considered for further investigation.



Go/No-Go Decision Points

Identify at least one candidate that is compliant with physical density and low temperature viscosity specs and has 4% higher composite energy than conventional jet fuel.



3. Impact

Advancing technical state-of-the-art and giving stakeholders deployment options



- Fuel developers will be able to answer “what if” questions regarding innovative new molecules and blends
 - Optimization of fuel composition to meet physical property specifications will be possible
 - Stakeholders will be able to compare operational benefits from different fuel choices in a streamlined manner
- Novel SAFs will be poised to enter the ASTM D4054 process for approvals ranging from 10% to 50% blend ratios with conventional fuel

- Presentations and publications are targeted for impact with relevant stakeholders and the broader scientific community
 - Commercial Alternative Aviation Fuel Initiative (CAAFI) community via webinars and committee meetings
 - Publications in leading journals [PNAS, FUEL and AIAA SciTech];
 - Presentations and contributions at ACS, CRC, the EU Commission, international research institutions and other workshops

3. Impact

Example 1: we are off-ramping our outcomes to other DOE programs and stakeholders



Connecting to other DOE offices that leverage our project developments



U.S. DEPARTMENT OF
ENERGY

Office of
Science

JBEI

Joint BioEnergy Institute

Research | [Open Access](#) | Published: 12 November 2020

Conversion of poplar biomass into high-energy density tricyclic sesquiterpene jet fuel blendstocks

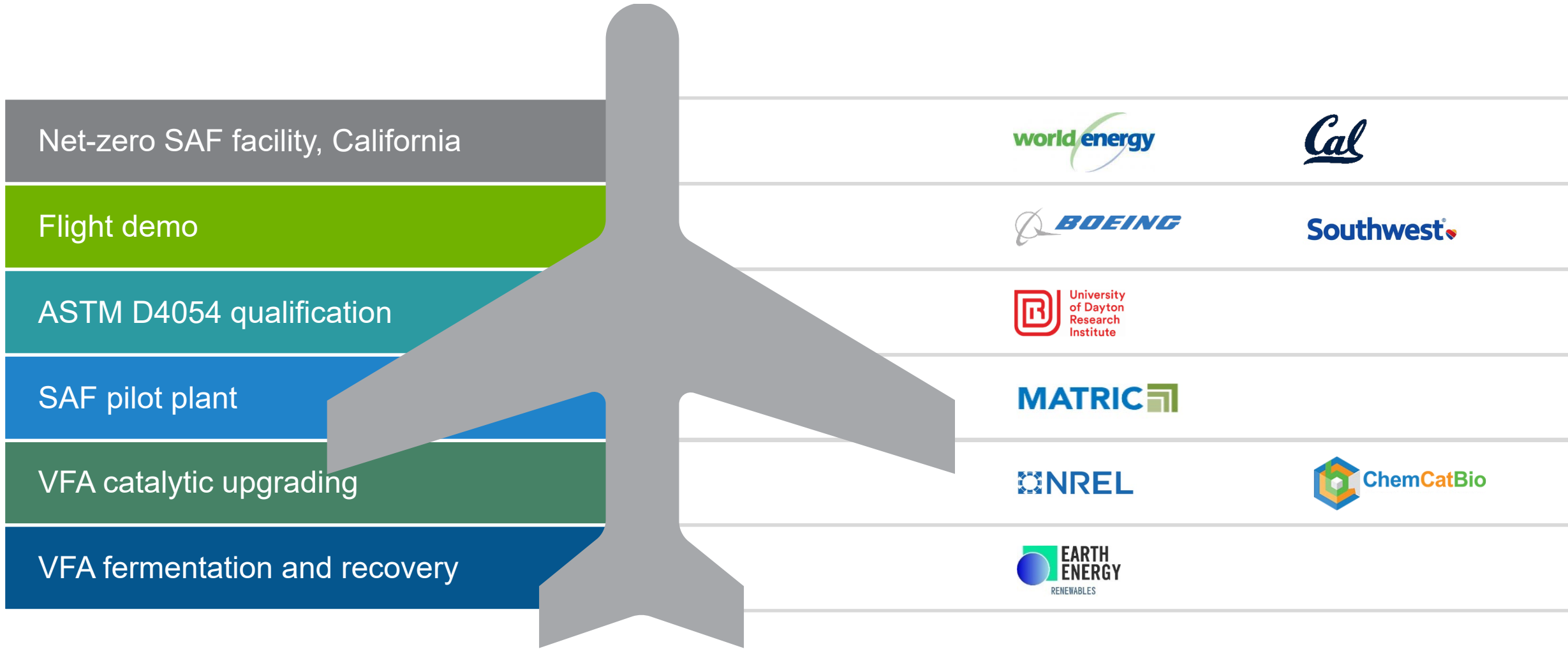
[Gina M. Geiselman](#), [James Kirby](#), [Alexander Landera](#), [Peter Otoupal](#), [Gabriella Papa](#), [Carolina Barcelos](#), [Eric R. Sundstrom](#), [Lalitendu Das](#), [Harsha D. Magurudeniya](#), [Maren Wehrs](#), [Alberto Rodriguez](#), [Blake A. Simmons](#), [Jon K. Magnuson](#), [Aindrila Mukhopadhyay](#), [Taek Soon Lee](#), [Anthe George](#) & [John M. Gladden](#)
✉

[Microbial Cell Factories](#) **19**, Article number: 208 (2020) | [Cite this article](#)

781 Accesses | 1 Citations | [Metrics](#)

3. Impact

Example 2: we are off-ramping our outcomes to other DOE programs and stakeholders



- Off-ramping results to BETO SCUBA FOA with industry for first “waste-to-jet” scale-up

4. Progress and outcomes

Structure-property and blend work is on track to meet FY21 goals



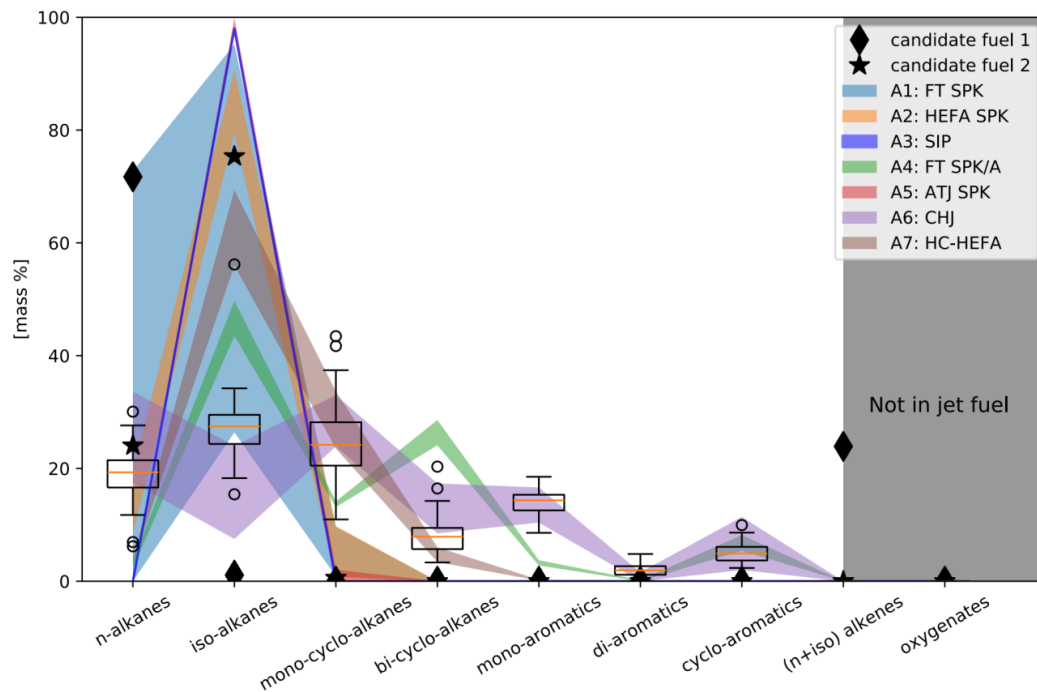
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4. Progress and outcomes

Tier α and Tier β criteria are used to prescreen candidate SAFs



Tier α : GC/GC measurements of fuel composition are analyzed to predict the most likely range of physical property parameters on the basis of a hydrocarbon property database and blending rules



Tier β : Laboratory measurements compared with Jet-A specifications for important operational parameters

- Viscosity
- Surface tension
- Distillation curve
- Liquid density
- Flash point
- DCN
- Swelling

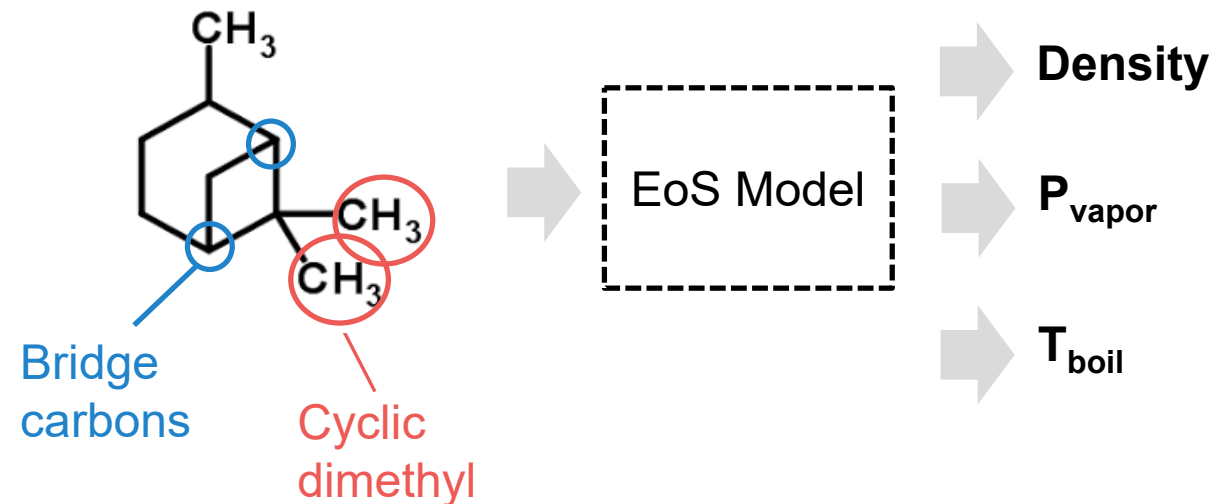
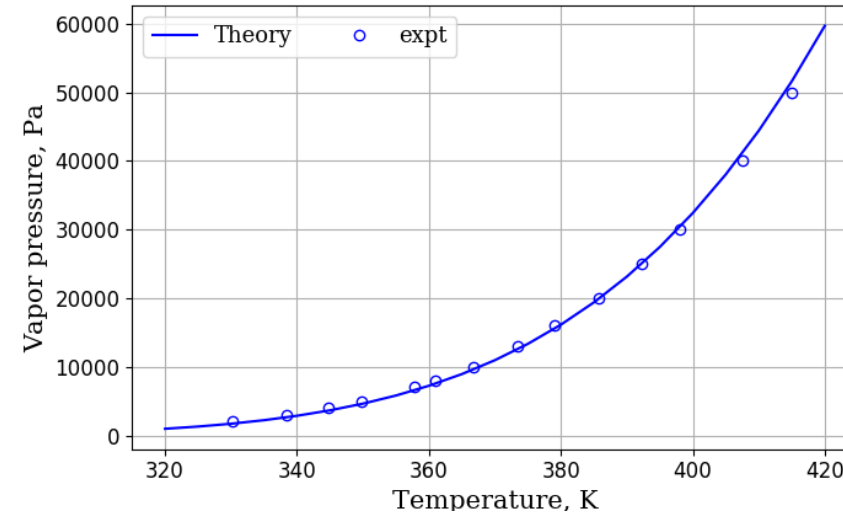
4. Progress and outcomes

Neat fuels: properties are predicted and structure-function relationships developed



A workhorse for property modeling:
Equations of State [EoS]

- Focused on 3 chemical classes and screened >60 fuels
 - Cycloalkanes
 - Branched alkanes
 - Terpenes
- Identified molecules in all families meeting operational specs and conferring performance advantages
- Employed EoS modeling to improve blending rules used in fuel optimization



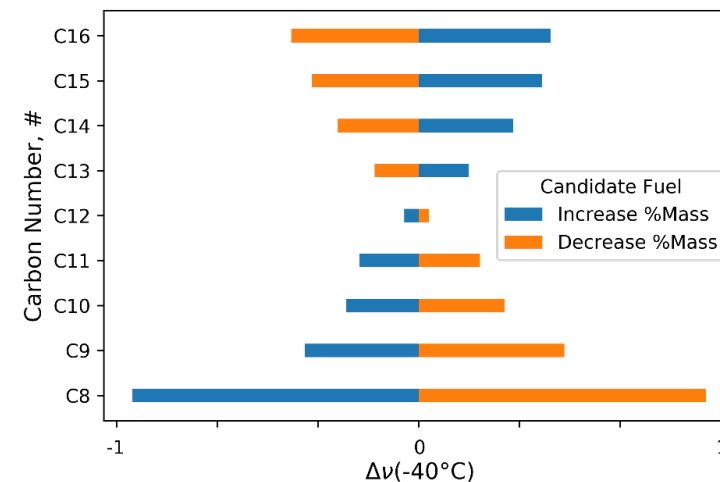
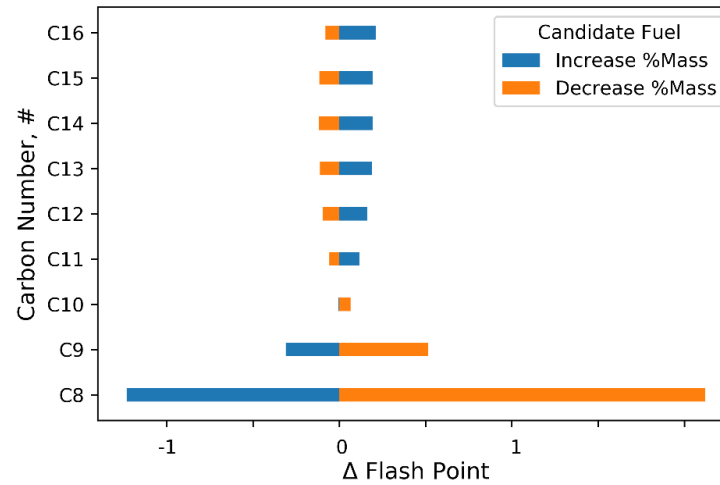
4. Progress and outcomes

Blended fuels: tools allow blends to be analyzed and optimized to meet specifications

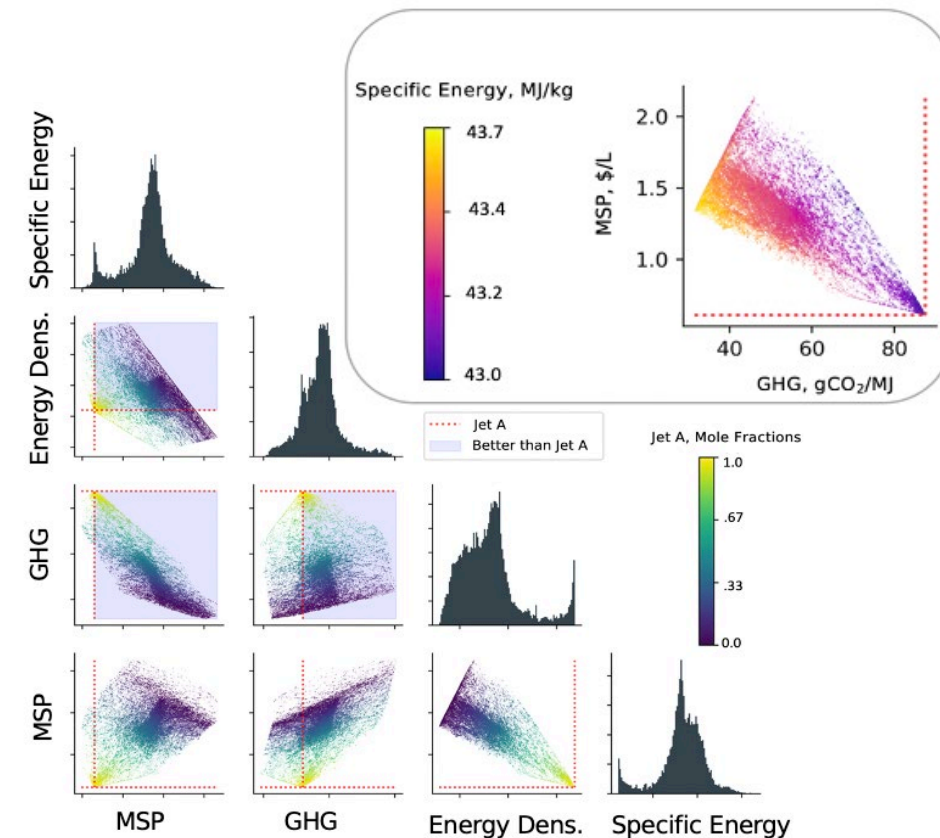


Software tools to evaluate SAF blend components

- A best practice for viscosity blend modeling with neat components
- A method for evaluating the sensitivity of operability properties to SAF carbon-number composition
- Four dimensional Pareto to evaluate drop-in SAF candidates on the basis of MSP, GHG, and energy content



4-D Pareto modelling

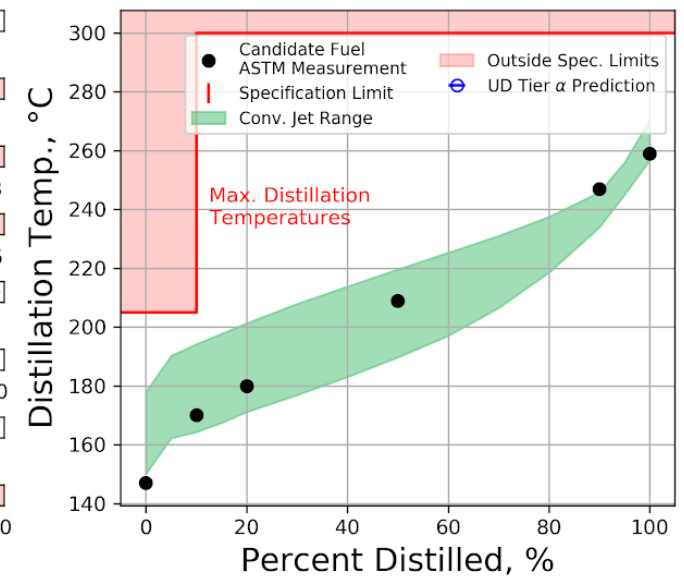
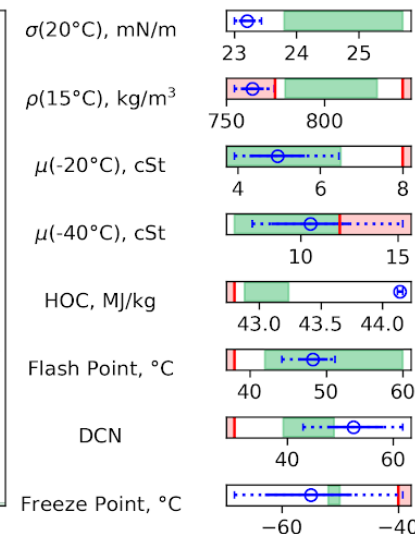
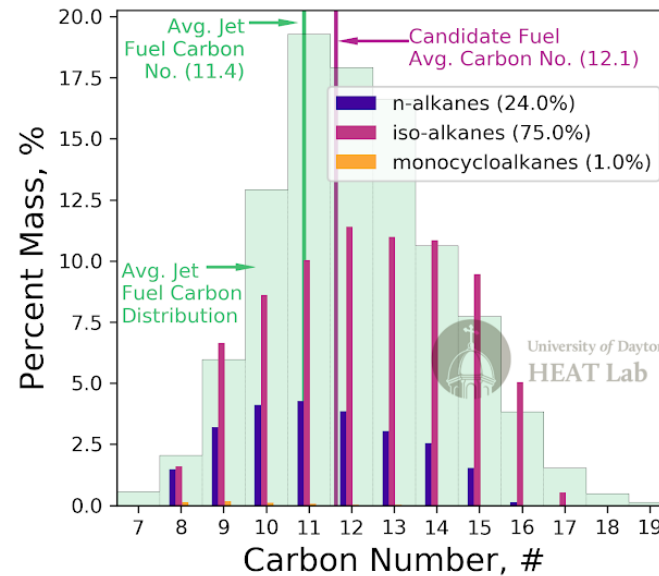


4. Progress and outcomes

Prescreening fuels for certification / blend optimization enables rapid “in / out” down-selection



- More than a dozen DOE BETO funded fuels have been evaluated for Tier α and β properties which are critical to the approval and evaluation process (ASTM D4054)
- Panel plots have been sent to labs for all fuels ‘prescreened’

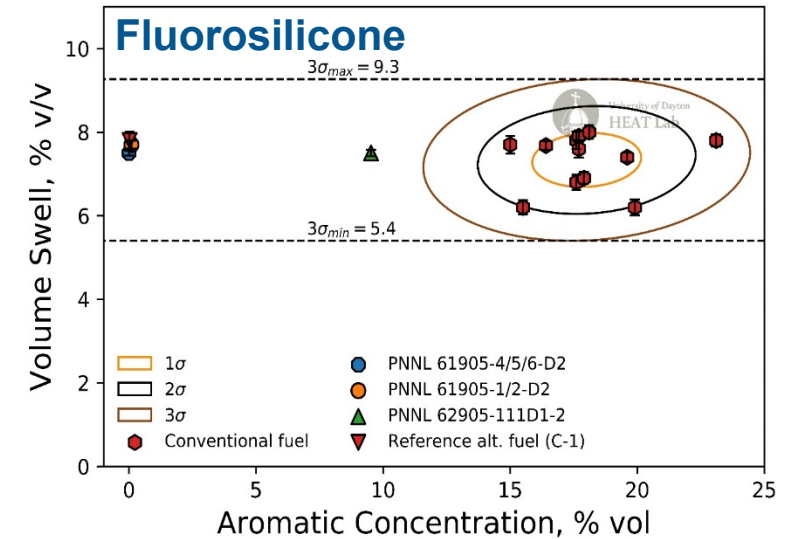
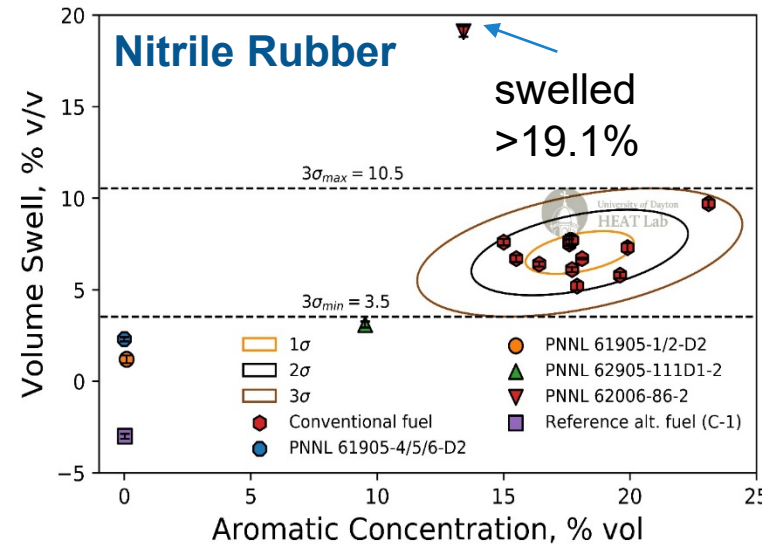


4. Progress and outcomes

SAF seal-swelling evaluated to ensure materials compatability



- PNNL fuels tested with nitrile rubber: none fell within the 3σ range for conventional fuel
- PNNL fuels tested with fluorosilicone: fuels fell within the 3σ range for conventional fuel

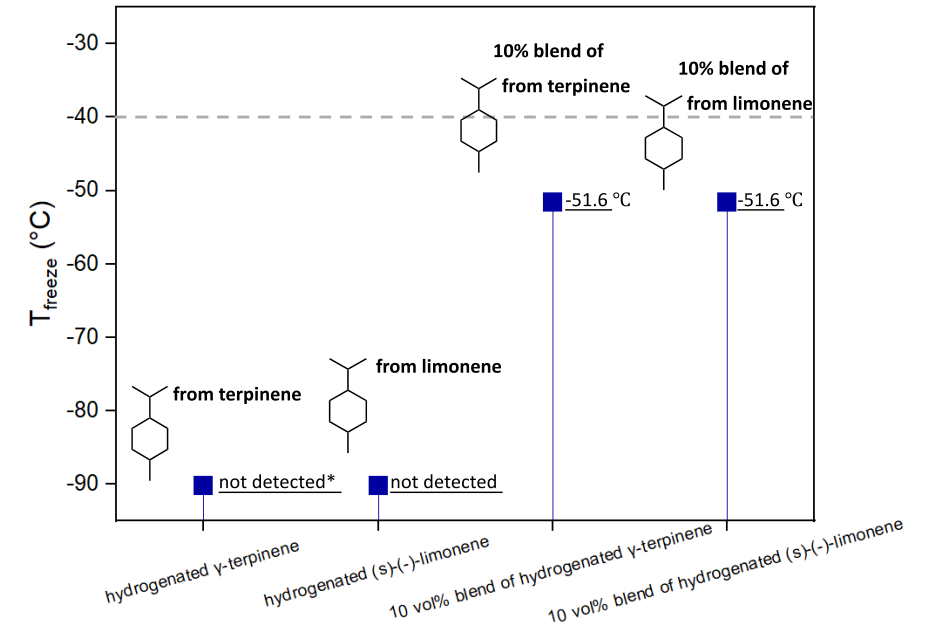
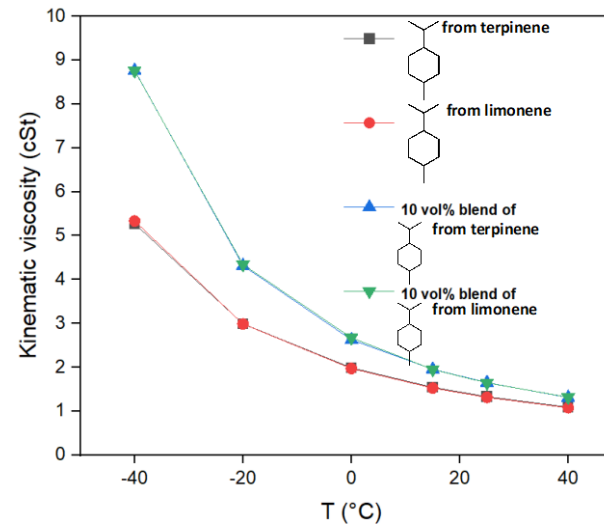
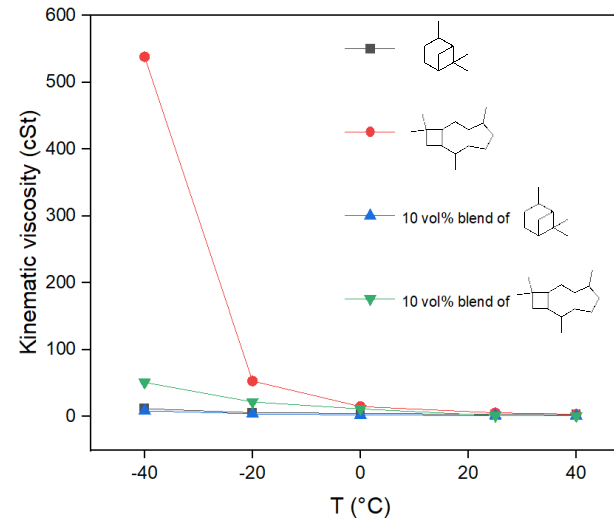


4. Progress and outcomes

Several terpene candidates were screened for operability parameters



- Hydrogenation was optimized for several terpenes; properties screened on 25-50mL scale
- Fuel property measurements provide validation data for modeling efforts within consortium
 - Multicyclic terpenes tested have poor cold flow properties; monocyclics were acceptable
 - Monocyclic terpenes can have excellent freezing points, much lower than petroleum jet fuel



4. Progress and outcomes

Waste-to-jet conversion work is on track to meet FY21 goals



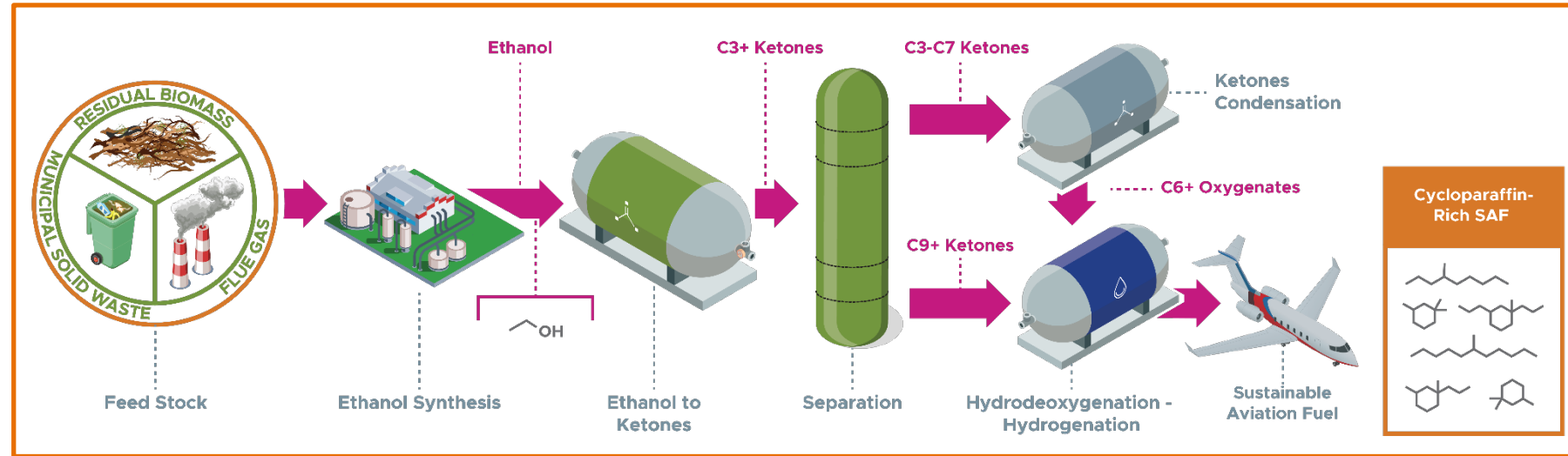
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4. Progress and outcomes

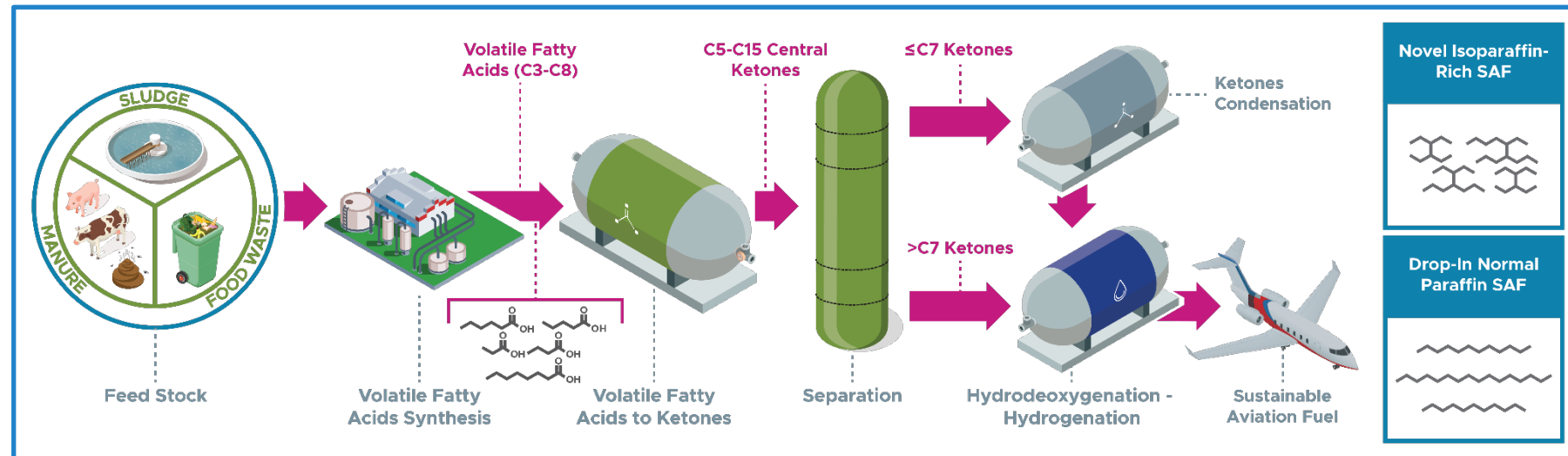
We are pursuing two feedstock approaches for waste-to-jet fuel synthesis



- Waste feedstocks to SAF via ethanol intermediate
- Cycloalkanes and paraffins



- Waste feedstocks to SAF via volatile fatty acid intermediate
- Branched paraffins

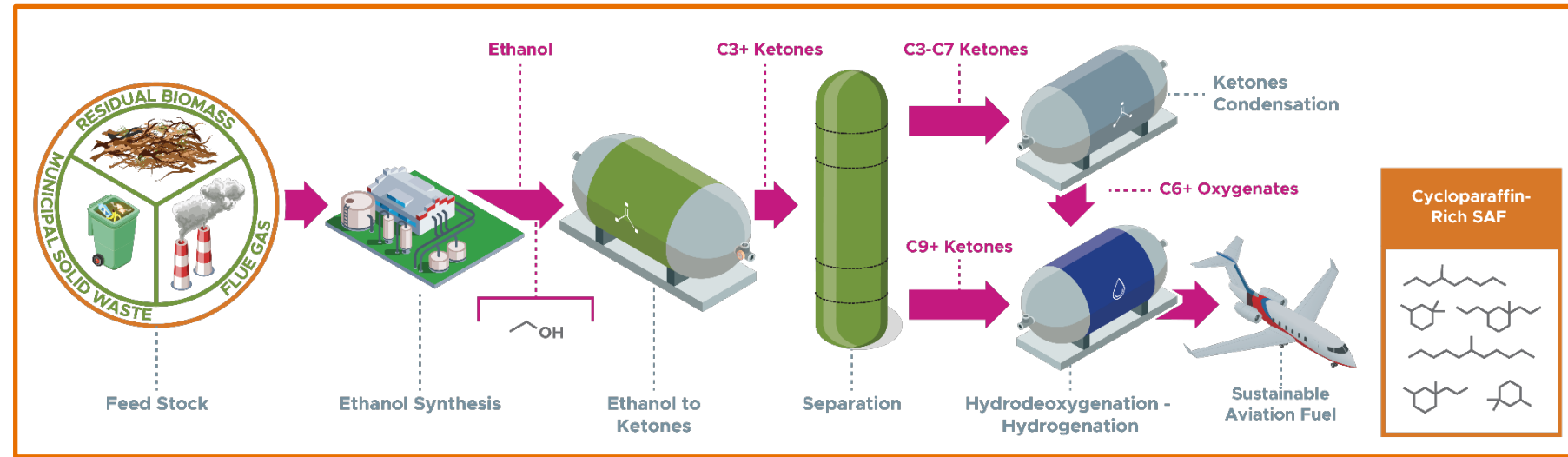


4. Progress and outcomes

Waste derived SAFs from ethanol intermediate



Goal: to optimize cycloalkane production and product properties and demonstrate the potential fuel costs and GHG savings



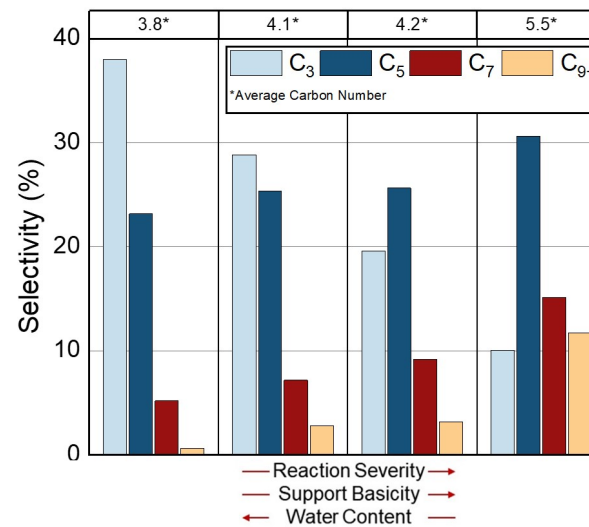
4. Progress and outcomes

Flexibility of ethanol-to-jet catalytic step produces desired jet fuel fraction

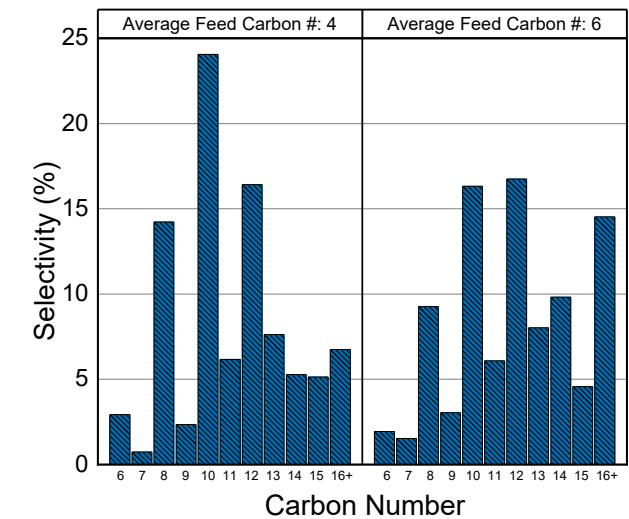


- Developed tunable system to produce molecules in target jet range
- Flexible with variable operating conditions (temperature, pressure, feed composition impurities)

Ethanol to C3+ Ketones



C3+ Ketones to jet fuel range hydrocarbons (aldol condensation followed by hydrogenation)

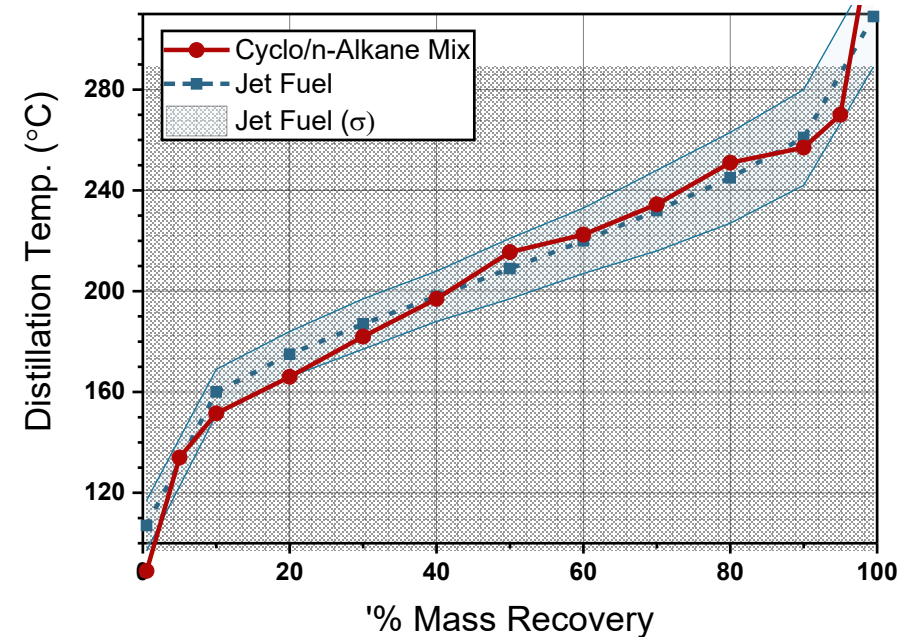


4. Progress and outcomes

Neat and blended ethanol-derived fuel samples meet ASTM requirement



- Cycloalkane/ alkane mixture (neat) simulated distillation curve falls in the conventional jet fuel range
- Fuel properties of the cycloalkane/ alkane mixture was analyzed as neat, 10% & 30% blend in Jet-A
 - Jet-A blended samples at both 10% and 30% levels meet the D7566 requirement
 - Viscosity of the neat sample is outside the range due to the presence of higher carbon number compounds



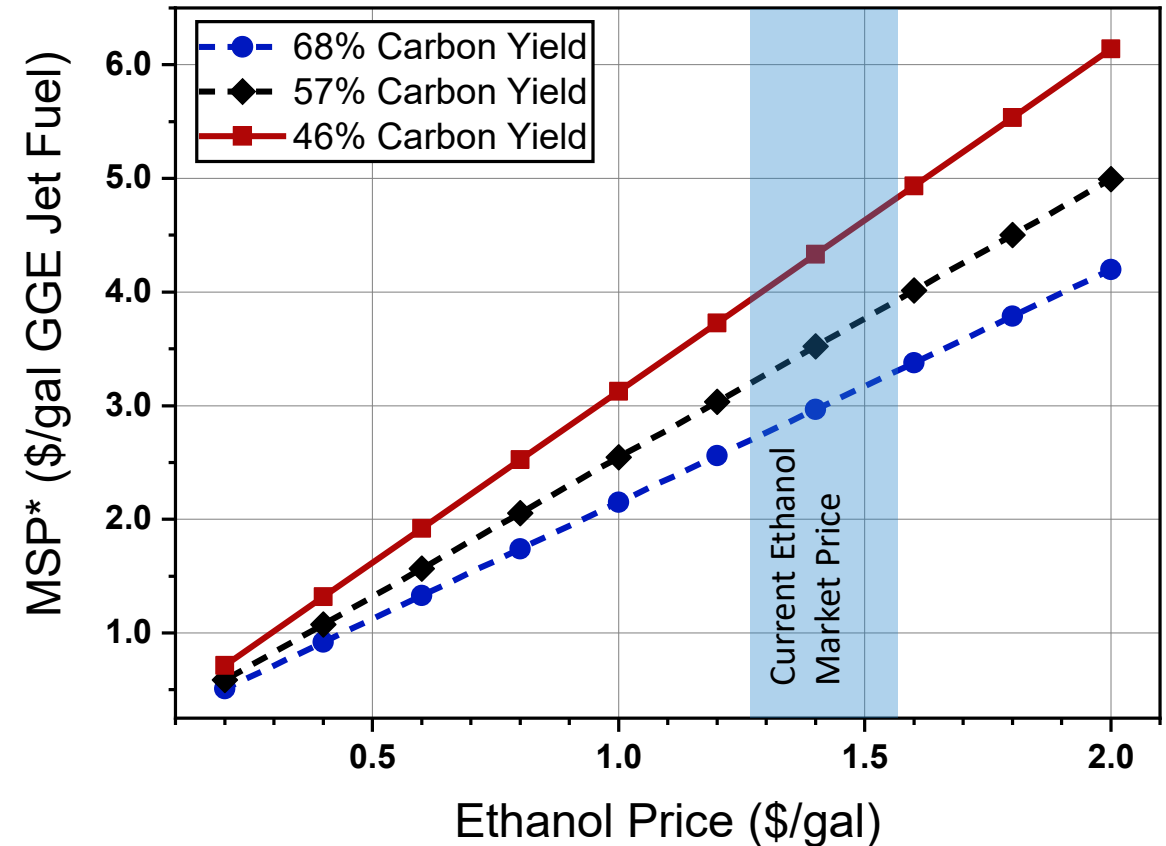
Sample ID	Viscosity, 40 °C mm ² /s	Density, 15 °C g/mL	LHV MJ/kg	Flash Point °C	Freeze Point °C
D7566 (Standard)	Max 12	0.775-0.84	Min 42.8	Min 38	Max -40
PNNL (Neat)	23.2	0.806	43.64	59	< -90
PNNL+ Jet A (10 %)	9.7	0.797	43.15	52	-50.9
PNNL+ Jet A (30 %)	11.0	0.798	43.27	56	-53.4

4. Progress and outcomes

Alcohol feedstock cost is the dominant factor in the final fuel price



- Feedstock cost is the dominant factor in the final fuel price
- Carbon yield level at 46% is based on the current experimental results
- Remaining carbon ends up in naphtha and CO₂
- H₂ generated from ketone formation recycled for the final hydrogenation of products
- Process can potentially be price competitive, particularly if low-cost waste sources are leveraged

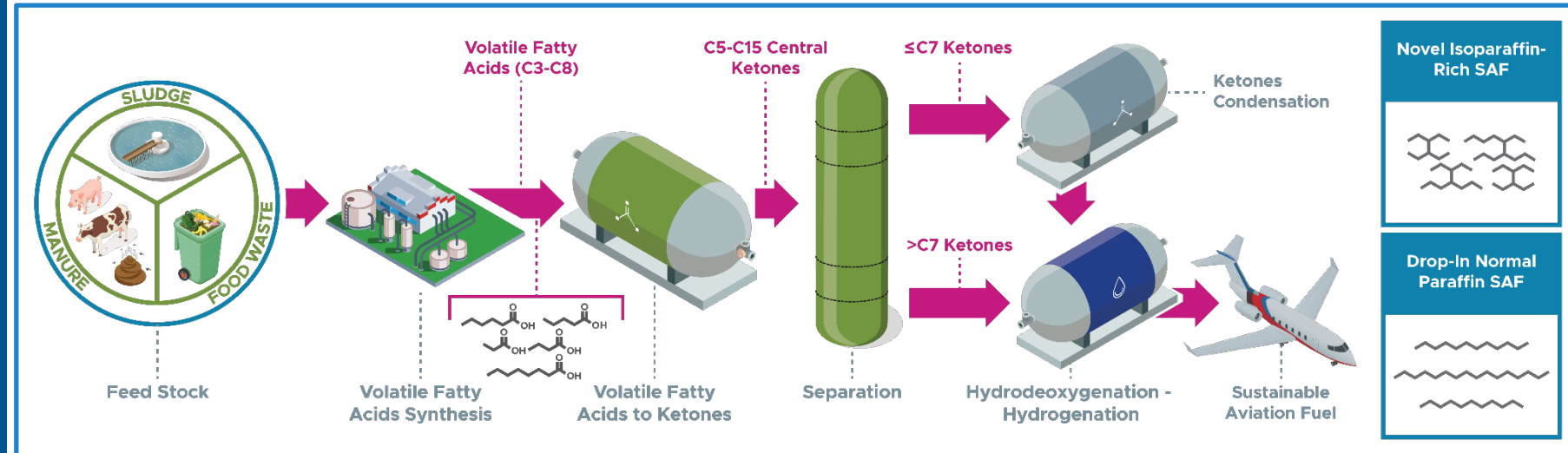


4. Progress and outcomes

Sustainable aviation fuels from wet waste volatile fatty acids



Goal: to de-risk the fuel properties of VFA-SAF to inform conversion R&D and demonstrate the potential fuel costs and GHG savings



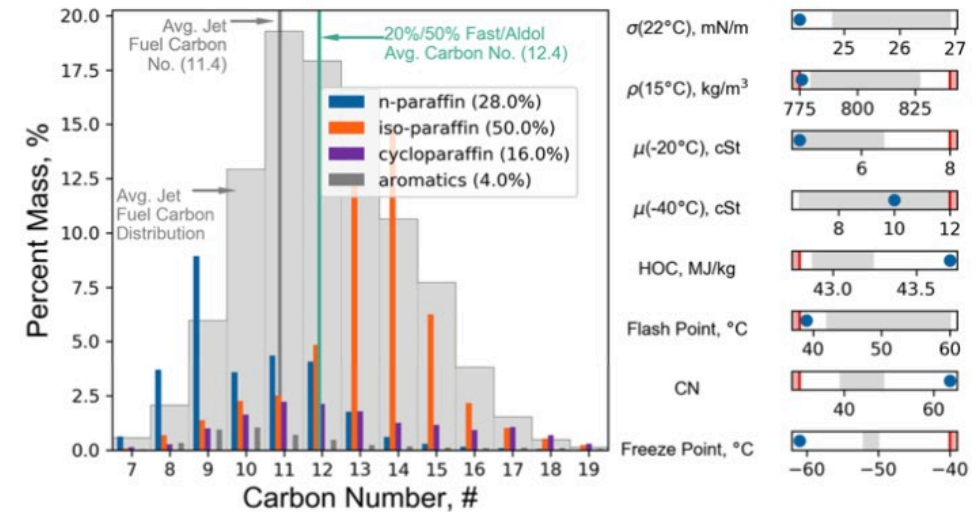
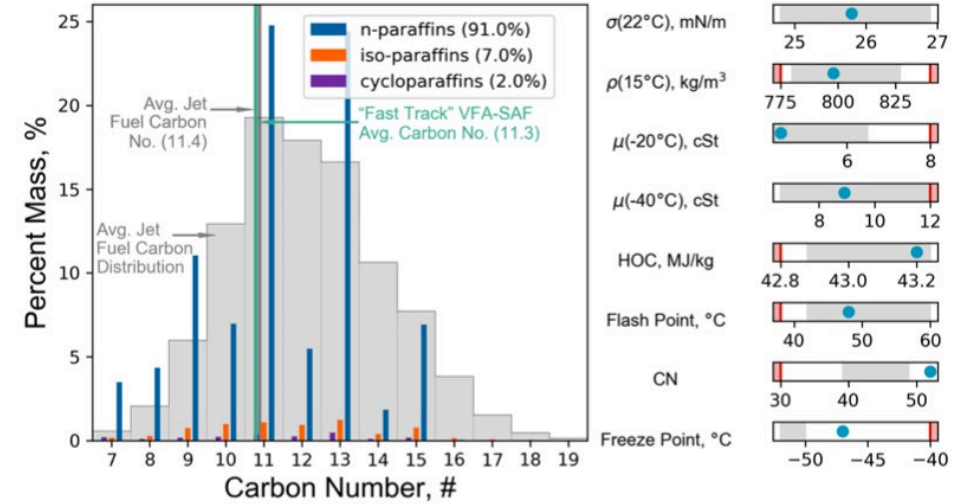
Fast Track VFA-SAF 10% Blend

4. Progress and outcomes

All fuel properties for 10% fast-track blends meet specifications



- Validated 10% Fast Track fuel properties for VFA-SAF normal paraffins, as well as potential for 70% blend with novel VFA-SAF mix
- Fast Track 10% VFA-SAF blend meets ASTM D7566
- Novel 70% VFA-SAF blend meets ASTM D7566



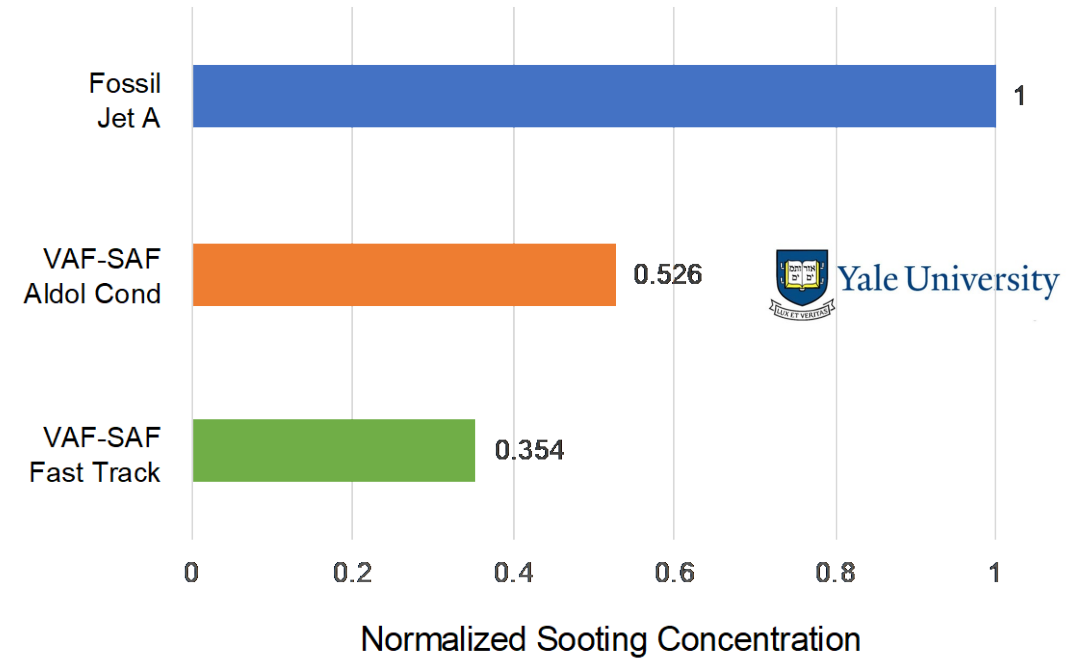
4. Progress and outcomes

Improved specific energy and sooting properties were demonstrated



Demonstrated exceptionally high specific energy of neat VFA-SAF, as well as significantly reduced sooting

Fuel	POSF	Formula	nHOC, MJ/kg
VFA-SAF Fast Track	N/A	$C_{9.1}H_{20.0}$	44.5
VFA-SAF Aldol Cond	N/A	$C_{13.5}H_{28.8}$	44.1
Conventional Jet A	10325	$C_{11.4}H_{22.0}$	43.0
Syntroleum FT-SPK	5018	$C_{11.8}H_{25.6}$	44.1
Dynamic Fuels HEFA-SPK	7272	$C_{12.4}H_{26.7}$	43.9
Sasol FT-SPK	7629	$C_{10.8}H_{23.4}$	43.7
UOP HEFA-SPK	10301	$C_{12.0}H_{25.9}$	43.9
Gevo ATJ	11498	$C_{12.6}H_{27.2}$	43.9
Lanzatech ETJ	12756	$C_{11.7}H_{25.4}$	43.9

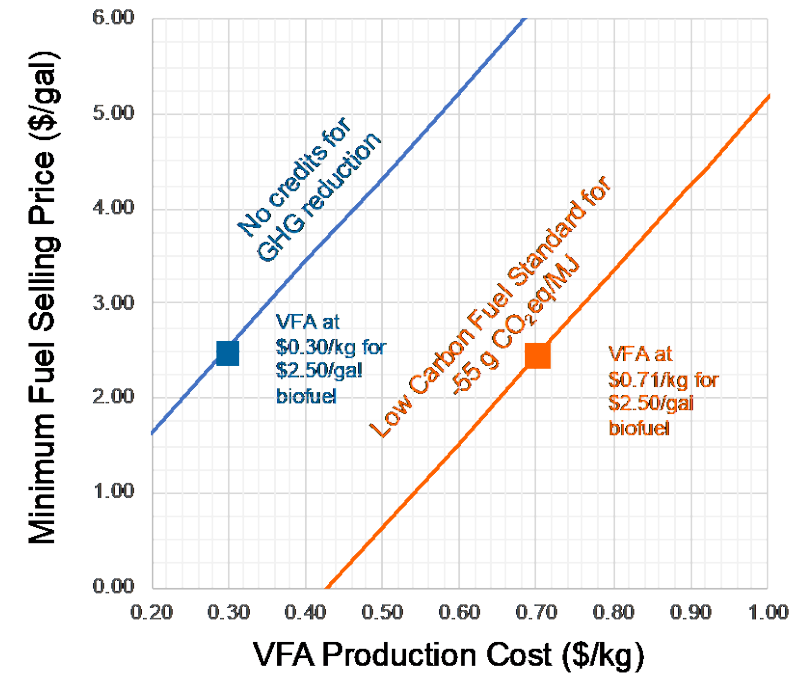
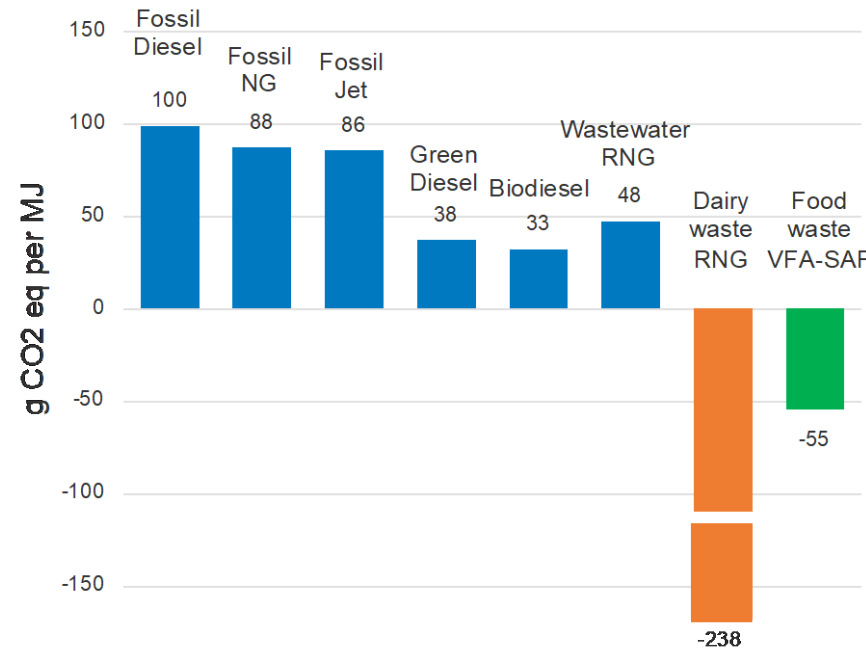


4. Progress and outcomes

Sustainable aviation fuels from wet waste volatile fatty acids



- Potential for negative life cycle carbon intensity for VFA-SAF derived from waste
- Potential for under \$4/gal VFA-SAF without LCFS
- LCFS credit up to \$3.70/gal based on GHG



4. Progress and outcomes

System modeling work is on track to meet FY21 goals



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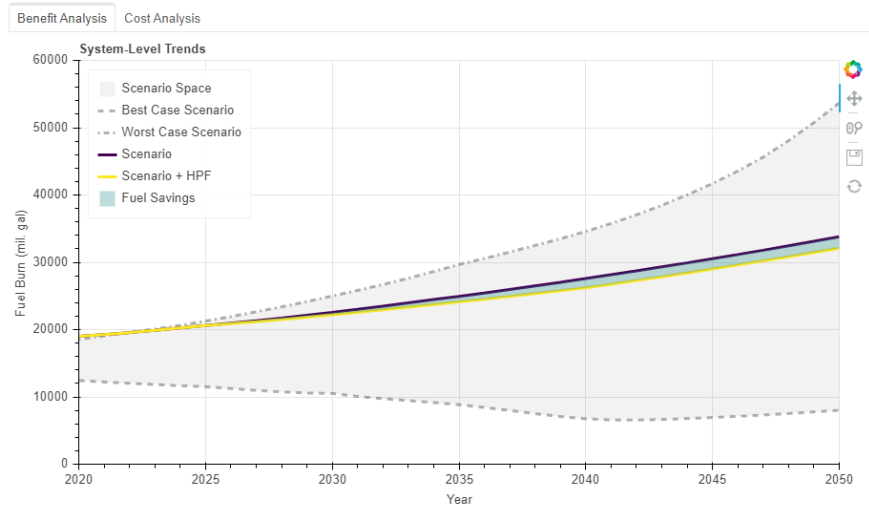
4. Progress and outcomes

Dashboard provides stakeholders easy visualization of system analyses



Fleet-level analysis

Fuel burn

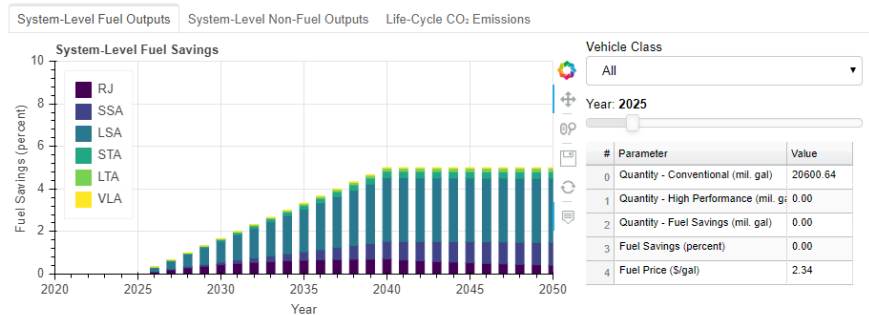


Inputs for SAF scenario

Scenario Selection | HPF Adoption | HPF Properties | HPF Vehicle-Level Efficiency Gains

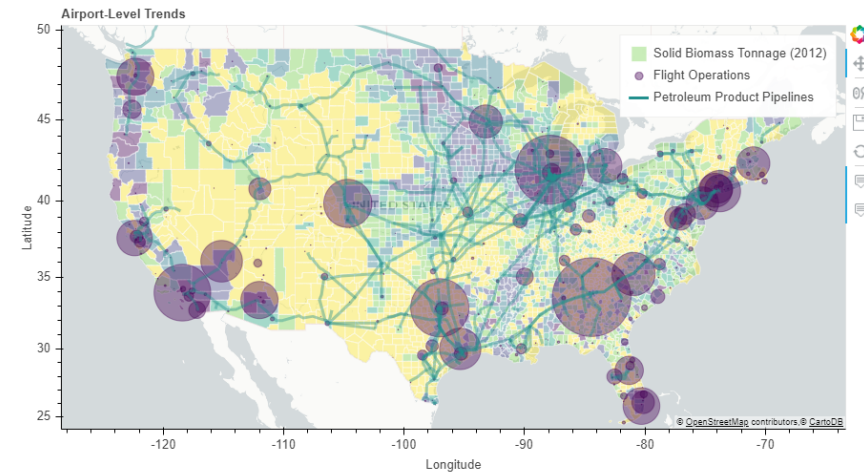
Scenario:

Fuel savings and monetized benefits



Lead: Kirby, Georgia Tech

Airport-level analysis

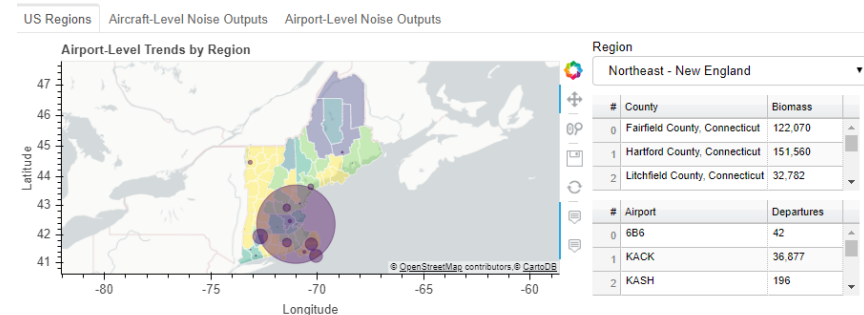


US Operations | Range Distributions

Year: 2025

Vehicle Class:

Filters for plotting flight operations



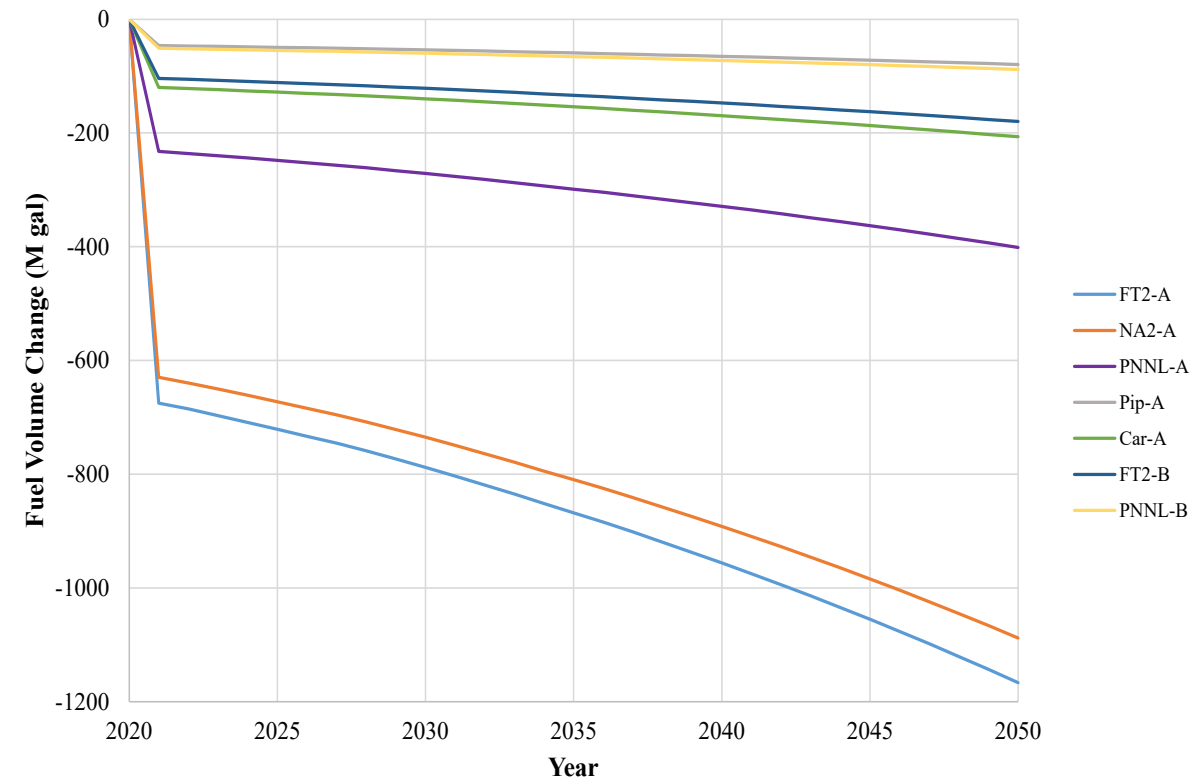
4. Progress and outcomes

Benefits of new biofuels to flight operations are being analyzed



- Six biofuels analyzed; lower and upper bounds of actual fuel energy density identified
- Some fuels show significant performance benefits, >1 billion gallons saved by 2050
- Fuel savings can be significant
 - reduce emissions, noise, operational costs
 - increase payload and/or passengers

Fleet-level fuel savings

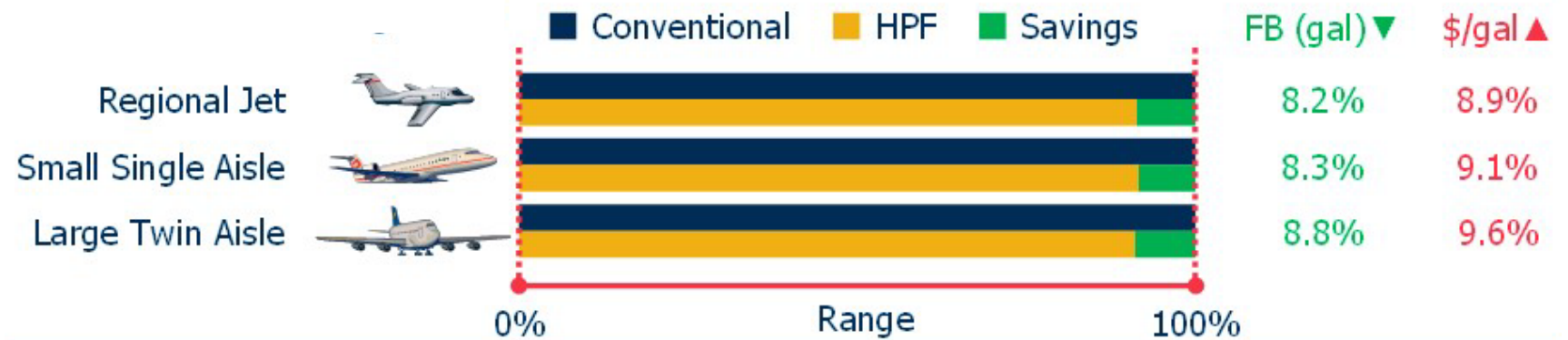


4. Progress and outcomes

Benefits of new biofuels to flight operations show impact of increased energy density



- Increased energy density evaluated for cost savings
- SAF with 3.9% increase in specific energy and 8.6% increase in energy density evaluated
- Largest jet showed greatest fuel savings of 8.8%. Can increase break even fuel price 9.6%



Summary

Management, approach, impact, progress and outcomes



Management

- Team of six partners working towards removing roadblocks to SAF deployment
- Strong co-ordination and communication ensure objectives are met
- Risks for technical challenges are identified and mitigated

Approach

- Built models to identify promising SAFs, neat and in blends; conduct screening
- Developed low-cost feedstock routes and analyzed value proposition to industry
- Established metrics and Go/No-go points to ensure progress

Impact

- Advancing technical state-of-the-art and giving stakeholders deployment options
- Off-ramping activities to other DOE programs and stakeholders
- Disseminating technical results in high impact publications

Progress & outcomes

- Models developed and > 60 fuels screened for operation and performance properties
- Two low-cost production routes to cycloalkanes / paraffins can be tuned for properties
- Fleet-level analysis determined fuel savings with improved energy density

Quad chart overview



Timeline

- Year 1: October 1, 2019 to September 30, 2020
- Year 2: October 1, 2020 to September 30, 2021
- Year 3: October 1, 2021 to September 30, 2022

	FY20	Active Project
DOE funding	LANL, NREL, PNNL, SNL, UDayton, GTech \$250k each partner	\$1250 / yr

Partner labs

- LANL, NREL, PNNL, SNL, UDayton, Georgia Tech

Barriers addressed:

ADO-H Materials Compatibility, and Equipment Design and Optimization

At-A Analysis to Inform Strategic Direction

Ft-A Feedstock Availability and Cost

Ot-B Cost of Production

Project goal

- Address key roadblocks to deploying new sustainable aviation fuels

End-of-project milestones

- Identify the technical targets and projected production capacity of at least one waste-to-biojet pathway in line with the DOE cost targets of \$2.50/GGE by 2030
- Quantify the potential impact of optimized biojet fuel blend production to the airline industry based on supply chain constraints

Funding

- Annual operating plan

Additional slides



Acronyms and Symbols



ACS	American Chemical Society
ATJ	Alcohol-to-jet
CRC	Coordinating Research Council
DCN	Derived cetane number
ETJ	Ethanol-to-jet
EoS	Equation of State
FAA	Federal Aviation Administration
FT-SPK	Fischer-Tropsch Synthetic Paraffinic Kerosene
GC/GC	Two dimensional gas chromatography
GGE	Gallons gasoline equivalent
GHG	Greenhouse gas
HDO	Hydrodeoxygenation
HEFA	Hydroprocessed Esters and Fatty Acids
HTL	Hydrothermal liquefaction
IATA	International Air Transport Association
ICAO	International Civil Aviation Organization
LCA	Lifecycle analysis
MESP	Minimum ethanol selling price
MSP	Minimum selling price
PNAS	Proceedings of the National Academy of Sciences
SAF	Sustainable aviation fuel
TEA	Techno-economic analysis / lifecycle analysis
VFA	Volatile fatty acid
YSI	Yield sooting index

ν	viscosity
μ	kinematic viscosity
σ	surface tension or standard deviation
ρ	density



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Heyne J., High Value Drop-in Aviation Fuels: From Molecule Selection to Mission Benefits, Panel Title: Fuel quality matters, DOE BETO/ PNNL HTL Workshop, virtual, November 2020.

Heyne J., Prescreening of HTL SAFs: Rapid low-volume, lowcost testing, Panel Title: Sustainable Aviation Fuel Certification, DOE BETO/ PNNL HTL Workshop, virtual, November 2020.



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