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RENEWABLE ENERGY**

Sustainable Aviation Fuel

Review of Technical Pathways



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Acknowledgments

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Abstract

The 106-billion-gallon global (21-billion-gallon domestic) commercial jet fuel market is projected to grow to over 230 billion gallons by 2050 (U.S. EIA 2020a). Cost-competitive, environmentally sustainable aviation fuels (SAFs) are recognized as a critical part of decoupling carbon growth from market growth. Renewable and wasted carbon can provide a path to low-cost, clean-burning, and low-soot-producing jet fuel. Research shows an opportunity to produce fuel in which aromatics are initially diluted with the addition of renewable iso-alkanes, aromatics are later fully replaced with cycloalkanes, and finally high-performance molecules that provide mission-based value to jet fuel consumers are introduced. Key to this fuel pathway is sourcing the three SAF blendstocks—iso-alkanes, cycloalkanes, and high-performing molecules—from inexpensive resources. When resourced from waste carbon, there are often additional benefits, such as cleaner water when sourcing carbon from wet sludges or less waste going to landfills when sourcing the carbon from municipal solid waste or plastic waste. Jet fuel properties differ from gasoline and diesel, so research will be most successful if it begins with the end result in mind.

List of Acronyms

ASTM	ASTM International
ATJ	alcohol-to-jet
BETO	Bioenergy Technologies Office
Btu	British thermal unit(s)
CAAFI	Commercial Aviation Alternative Fuels Initiative
Co-Optima	Co-Optimization of Fuels & Engines
CORSIA	Carbon Offsetting and Reduction Scheme for International Aviation
DCN	derived cetane number
DOE	U.S. Department of Energy
EERE	Office of Energy Efficiency and Renewable Energy
FAA	Federal Aviation Administration
FT	Fischer-Tropsch
GHG	greenhouse gas
HEFA	hydroprocessed esters and fatty acids
HTL	hydrothermal liquefaction
ICAO	International Civil Aviation Organization
LCA	life-cycle analysis
MFSP	minimum fuel selling price
MSW	municipal solid waste
NASA	National Aeronautics and Space Administration
NJFCP	National Jet Fuels Combustion Program
NREL	National Renewable Energy Laboratory
OEM	original equipment manufacturer
PNNL	Pacific Northwest National Laboratory
R&D	research and development
SAF	sustainable aviation fuel
SPK	synthetic paraffinic kerosene
syngas	synthesis gas
TEA	techno-economic analysis
USDA	U.S. Department of Agriculture

Executive Summary

Airlines have committed to carbon-neutral growth in international commercial aviation beginning in 2021 and U.S. airlines have set a goal to reduce carbon dioxide (CO₂) emissions by 50% in 2050 compared to 2005 levels (Airlines for America 2020; IATA 2020). U.S. airlines have improved efficiency by 130% compared to 1978 levels (Airlines for America 2020). Additional efficiency improvements in planes and engines are not likely to be enough. Meeting the 2050 goal will require fuels that have a lower carbon footprint, referred to as sustainable aviation fuel (SAF)—defined by the International Civil Aviation Organization (ICAO) as alternative aviation fuels that “(i) achieve net GHG [greenhouse gas] emissions reduction on a life cycle basis; (ii) respect the areas of high importance for biodiversity, conservation and benefits for people from ecosystems, in accordance with international and national regulations; and (iii) contribute to local social and economic development, and competition with food and water should be avoided” (ICAO 2018).

One challenge for providing SAF is that the size of the jet fuel market is large and growing. Global demand is expected to increase from 106 billion gallons in 2019 to 230 billion gallons in 2050 (U.S. EIA 2020a). The domestic market in 2019 was 26 billion gallons, exceeding 3 quadrillion British thermal units (3 quads) (U.S. EIA 2019). This market could consume several hundred million tons of biomass per year, which is consistent with the current availability of biomass in the United States (340 million tons) (Langholtz, Stokes, and Eaton 2016).

A second challenge is that the price of SAF today is higher than petroleum-based Jet A fuel. Fuel price is a hurdle because fuel is 20%–30% of the operating cost of an airline (IATA 2018). Research and development (R&D) can help bring the cost down.

Unlike light-duty vehicles, the low energy density of even the best batteries severely limits opportunities for electrification.¹ While many are working on electrification, efforts are for smaller aircraft and airlines will have no alternative for some time but to use SAF to operate in a GHG-emission-constrained future.

Part I of this report provides an overview of commercial jet aviation fuel: how it compares to fuels for cars and trucks, its composition, its specification, and its certification process.

Jet fuels consist of *n*-alkanes, iso-alkanes, cycloalkanes, and aromatics. Aromatics do not burn as cleanly as alkanes, resulting in higher particulate emissions, and have lower specific energy. The *n*-alkanes are acceptable but do not meet fluidity and handling properties, limiting their blend potential. The iso-alkanes have high specific energy, good thermal stability, and low freezing points. Cycloalkanes bring complementary value to iso-alkanes, providing the same functional benefits as aromatics by enabling fuels to meet the density requirement and potentially providing the seal-swelling capacity provided today from aromatics. Combined, iso-alkanes and cycloalkanes offer the potential to add value to a fuel by enabling high specific energy and energy density and minimizing emission characteristics. The U.S. Department of Energy (DOE) is evaluating the hypothesis that improved fuel energetic properties (i.e., specific energy and energy density) may provide increased range, higher payload capacity, or fuel savings.

Original equipment manufacturer (OEM)-led ASTM D4054 fit-for-purpose testing generally costs several million dollars and can require years to be approved (ASTM 2018). A fast-track approval process has been accepted for fuels in which the SAF blending component is limited to 10% and consists of the same types of molecules that are in petroleum-based jet fuel. A clearinghouse annex has also been proposed to reduce cost and time for approval. The Bioenergy Technologies Office (BETO), Federal Aviation Administration, and U.S. Department of Defense are investing in prescreening and testing protocols that need only small quantities (milliliters to liters) to provide feedback about a candidate fuel blend fit-for-purpose. To date, there are six

¹ Jet fuel has an energy density equal to 43 MJ/kg, while lithium-ion batteries in today’s electric vehicles have an energy density equal to 0.72 MJ/kg (200 Wh/kg). The amount of weight severely limits battery use in large passenger aircraft.

ASTM International (ASTM) D7566-approved SAFs for use in up to 10% to 50% blends. The SAF initially composed of *n*- and iso-alkanes now include all four hydrocarbon families listed previously and are produced from synthesis gas (syngas); fats, oils, and greases; sugars; and alcohols.

Part I finishes by summarizing the learnings from three BETO-supported workshops. These include the Alternative Aviation Fuel Workshop held in Macon, Georgia, in 2016, which focused on SAF production; the JET workshop held in Cleveland, Ohio, in 2017, which focused on high-performance fuels; and the Trilateral Biojet Workshop held in Richland, Washington, in 2018, which focused on jet fuel R&D collaborations between Canada, the United States, and Mexico. Some of the key learnings from these workshops include:

- The aviation industry seeks to reduce its GHG emissions significantly, decoupling airline growth from carbon growth.
- The current cost of SAF is high. Airlines are willing to support SAF development by purchasing some fuel at a higher price, but for SAF to scale, prices need to be reduced.
- OEM-led ASTM D4054 approval and evaluation process is expensive and time-consuming. Developing new engines is even more onerous regarding timescale and cost, and hence a program coupling fuel development and engine development R&D would not help overcome industry barriers.
- Existing engines can use fuels that have a much higher heat of combustion than Jet A, and specific energy (i.e., heat of combustion) increases can deliver greater range, higher payload capacity, or decreased fuel consumption.
- More sources of low-cost feedstock are required as fats, oils, and greases are not currently available in enough volume to meet SAF demand.
- The use of cover crops to increase availability of oil seeds while improving soil quality as well as use of other lipid-rich streams, such as manures and sludges, may increase availability. Processes for their conversion will need to be approved through ASTM.
- Techno-economic analysis (TEA) and life cycle analysis (LCA) are inconsistent across the SAF industry, but the consistent message from most models is that the main cost drivers are feedstock costs, yields, and plant capital recovery.
- Current policies are skewing renewable fuels towards diesel and away from the jet market.

Part II provides insights resulting from a study of the aviation fuel industry, challenges of and successes with the approved pathways, and BETO capabilities and R&D portfolio. The insights focus on reducing cost and optimizing the value proposition for SAF. SAF in the future may include strained or otherwise novel molecules that are not found in conventional fuels, if the molecules can be produced at low cost. Research shows an opportunity to produce fuel in which aromatics are initially diluted with the addition of renewable iso-alkanes, aromatics are later fully replaced with cycloalkanes, and finally high-performance molecules that provide mission-based value to jet fuel consumers are introduced. To accomplish this transition and reduce costs to improve the value proposition, efforts in the following areas will be helpful:

- Understanding properties of cycloalkanes and production routes from biomass
- Developing process-intensification strategies as a means of reducing capital cost
- “Solving another problem” as a means of improving the value proposition
- Reducing cost and improving value of low-value process streams of currently approved pathways
- Understanding scaling requirements that make sense to the industry as a means of reducing cost.

Examples of work could include the following:

- In the near term (0–5 years), research can help further reduce the cost of existing approved pathways to iso-alkanes and synthetic paraffinic kerosene molecules. Research could include low-cost routes to cycloalkanes, including alkylated cyclohexanes, and understanding the properties of molecules with various ring structures available from catalytic, biological, thermal, and hybrid approaches.
- Public–private partnerships and collaborations across agencies may accelerate cost reductions by ensuring a diverse set of stakeholders are involved early in the solution to ensure it can address barriers for industrywide use.
- In the longer term, as SAF volumes increase, aviation fuels may provide better performance and reduced emissions (i.e., soot).
- Use of nontraditional raw materials including carbon oxides, methane, deconstructed plastic, and other waste materials may keep cost in parity with conventional fuels.

BETO’s R&D capabilities and feedstock/technology portfolio provide tools for meeting the technical needs to overcome hurdles preventing SAF deployment, including cost reduction.

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Introduction

Commercial aviation is responsible for about 13% of transportation greenhouse gas (GHG) emissions (U.S. EIA 2020b, 202). Airlines have committed to carbon-neutral growth for international commercial aviation beginning in 2021 and reducing carbon dioxide (CO₂) emissions by 50% in 2050 compared to 2005 levels (Airlines for America 2020; IATA 2020). While airlines are squeezing efficiency through improved aircraft and flight logistics, decoupling carbon growth will require non-fossil-sourced fuels, which in this report will be referred to as sustainable aviation fuel (SAF).²

In 2018, about two million gallons of SAF were produced. An additional 300 million gallons of renewable diesel was also produced using the same technology.³ This is not enough for airlines to meet their CO₂ reduction goals, which is 50% GHG reduction by 2050.

Purchasing fuel is a primary operating cost for airlines, a cost only exceeded by labor (IATA 2018). SAF will need to be cost-competitive, but although costs must be reduced, SAF does not need to mimic petroleum. A better fuel via bio-derivatives can be made and still meet international specifications (i.e., ASTM International, or ASTM).

This report presents ways to lower costs and improve the benefits of aviation fuel through targeted SAF production. Part I provides background information needed for decision makers, program and technology managers, and biofuel researchers:

- Chapter 1. Jet Fuel Markets
- Chapter 2. Jet Fuel Specifications
- Chapter 3. Jet Fuel Certification
- Chapter 4. Workshop Learnings

Given the preceding background, in Part II insights in consideration of one possible value chain is provided:

- Chapter 5. R&D – Fuel Molecules
- Chapter 6. R&D – Cost Reduction
- Chapter 7. Summary and Insights

The appendices provide more information.

² Aircraft are more efficient than ever, and flight plans are being optimized for fuel efficiency. Electrification is not an option for commercial flight for decades, if not longer. Fuel that has a low carbon footprint is the sole option.

³ Another 600 million gallons of renewable diesel used in the United States is under consideration for ASTM approval for jet fuel (U.S. EPA 2019).

Part I – Background



1 Jet Fuel Markets

1.1 Jet Fuel Versus Ground Transportation Fuel Markets

The ground transportation fuel market (motor gasoline and diesel) is 183 billion gallons per year (Figure 1). The market is highly segregated with a diversity of producers, sellers, and customers, each with various needs. Gasoline is blended with ethanol by up to 10% by volume, depending on the geographic location, climate, time of year, and other reformulated blendstock for oxygenate blending requirements, and this can have a significant impact on price. Gasoline is sold in different grades to a multitude of customers (more than 280 million vehicles were on the road in 2019 [Hedges & Company 2020]) whose seasonal driving practices alter demand. Marketplace transactions for gasoline sales are generally at smaller volumes and for the short term, allowing for greater price variability.

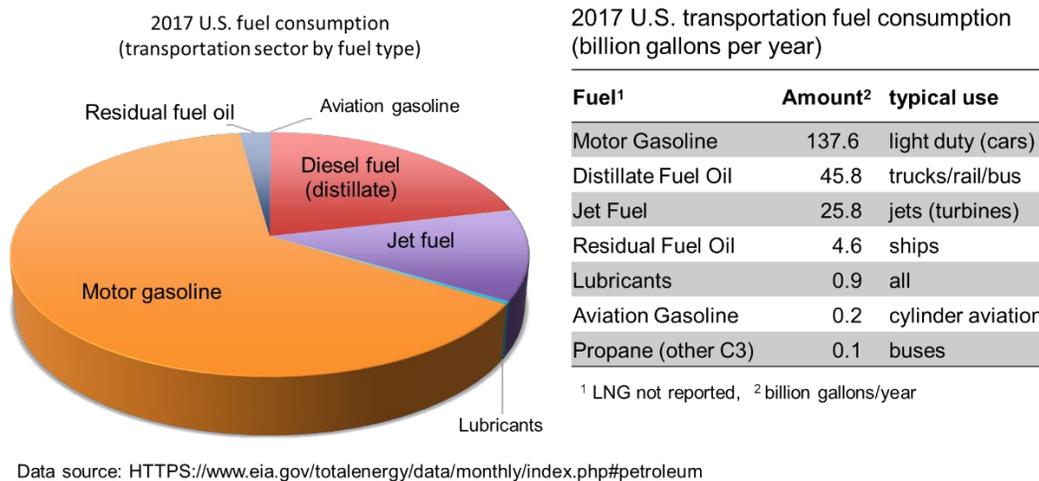


Figure 1. U.S. transportation fuel consumption (billions of gallons per year) (U.S. EIA 2017)

Note: LNG = liquid natural gas

The supply chain for gasoline uses blending terminals at central locations where the hydrocarbon fuel from refineries is blended with ethanol and other additives. These central locations confer a brand name to the final product that is shipped to service stations and is where the fuel is tested for quality. Gasoline is generally shipped via pipeline or rail to blending terminals and then transported to individual service stations in smaller quantities by truck.

The demand for motor gasoline is expected to decrease in the coming decades because of higher-efficiency drivetrains, increasing electrification of the light-duty fleet, and societal changes such as increased use of ride sharing.

The jet fuel market is different from the gasoline market in size, consumers, property variance, and demand locations. The domestic market size is 26 billion gallons per year. The global market size exceeds 81 billion gallons (Airlines for America 2018). Passenger demand is projected to double over the next 20 years (IATA 2016).⁴ In contrast to the gasoline market, the jet fuel market has a smaller number of customers⁵ (individual airlines and a modest number of fuel suppliers), who purchase the bulk of their fuel using negotiated long-term purchase agreements, and some small-volume customers (such as corporate fleets and private airplane owners) who purchase fuel at retail prices. Airlines are very price-sensitive because jet fuel accounts for approximately

⁴ This is also consistent with projections from the U.S. Energy Information Administration.

⁵ Two hundred and ninety International Air Transport Association airlines represent 82% of traffic, while several thousand smaller airlines comprise the rest.

20%–30% of their operating costs. Some studies have suggested that a price increase of \$1.00 per barrel of crude oil results in roughly \$425 million of additional expense for the airline industry (Davidson et al. 2014). Large airlines, having significant bargaining power, negotiate offtake agreements with fuel providers for long periods—often years—because these agreements can be made at lower fuel prices and significantly reduce exposure to market volatility. In general, the price of jet fuel correlates to that of ultra-low-sulfur diesel, which is often used as a reference point for supply contracts (Airlines for America 2018). Jet fuel prices at the Gulf Coast are usually lower because production exceeds demand in that part of the country.

Despite the sensitivity of bottom-line revenue to fuel prices, the renewable jet fuel demand curves for large airlines can potentially be more elastic with respect to price because airline customers have voluntarily shown a willingness to incur extra costs to assist new fuel introductions into the market. In addition to airlines, fixed-base operators at airports can also be significant fuel purchasers. Fixed-base operators purchase fuel in bulk and resell it at airports to small corporate and private customers at retail prices, which can be three times the spot price for jet fuel. As a result, there can be substantial differences in price for the same Jet A fuel between what a large airline pays through a large and/or long-term offtake agreement and the price a corporate customer and private airplane owner pay.

Unlike gasoline, jet fuel specifications do not vary by climate, time of year, or location, and thus blending, quality assurance, and quality control to meet applicable fuel specifications are done first at the refinery, with subsequent downstream validations. The jet fuel supply chain is different from that of gasoline because of the large volume requirements for jet fuel delivered to airports. Generally, shipment is by pipeline or barge from refineries to terminals, and from there to storage near airports (Figure 2). Airlines buy fuel from multiple suppliers because not every fuel supplier operates at every airport. Many airlines also purchase fuel directly from refineries, take the title of the fuel at the refinery gate, and ship it to where it is needed in order to avoid disruption of the fuel supply (ASTM 2018). Maintaining resilient jet fuel production and transport (pipelines) will be critical, particularly as fuel consumption doubles over the next 20 years. SAF offers resiliency in terms of feedstock and may help with fuel transport resiliency if biojet fuel facilities are located near the airports they serve. Port authorities that operate airports, such as SeaTac in Washington State, have announced their support of being a fuel aggregator and having fuel produced on land the ports own (Stephanie Meyn, personal communications; Biojet Workshop 2018).

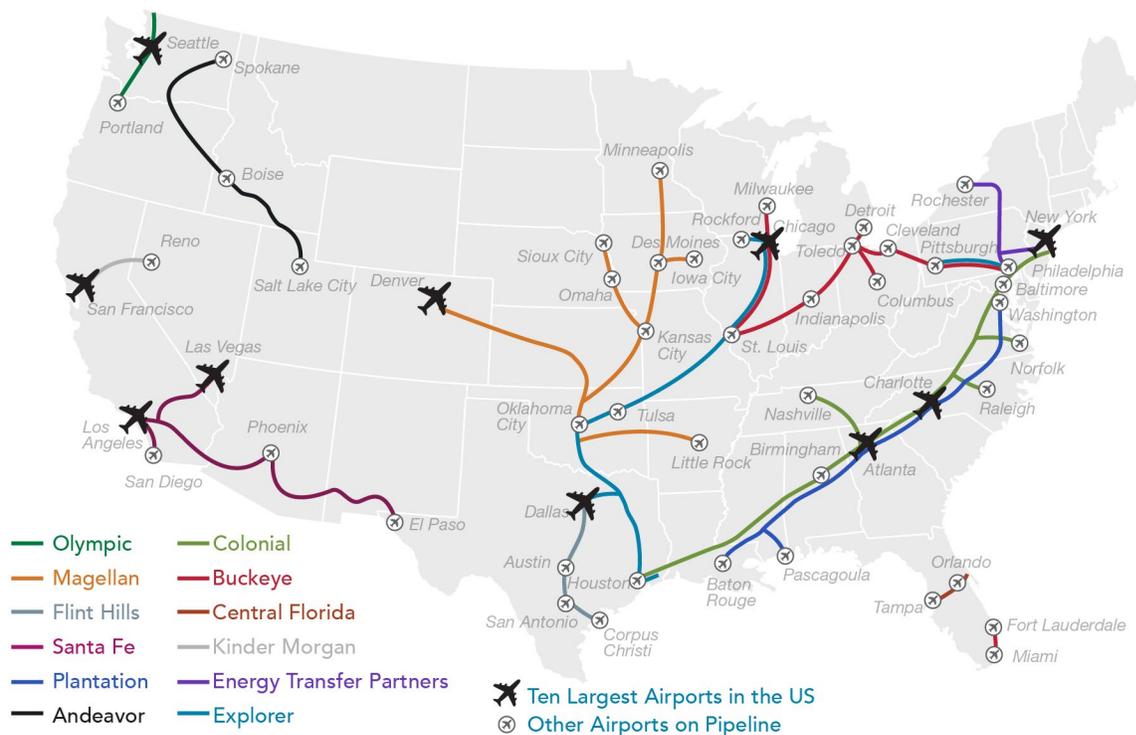


Figure 2. Major U.S. refined products pipelines carrying jet fuels (Airlines for America 2018) and the 10 largest airports by traffic volume

1.2 How Is Jet Fuel Similar to and Different from Other Transportation Fuels?

Gasoline, jet, and diesel fuels are mostly blended mixtures of several hundred different hydrocarbon molecules. Molecules in gasoline fuel range from those containing 4 carbon atoms to those containing 12 carbon atoms. Gasoline has an initial boiling point at atmospheric pressure of about 35°C and a final boiling point of about 200°C. Molecules in jet fuel range from those containing 8 carbon atoms to those containing 16 carbon atoms. Jet fuel has an initial boiling point at atmospheric pressure of about 125°C and a final boiling point of about 290°C. Molecules in diesel fuel range from those containing 8 carbon atoms to those containing 23 carbon atoms. Diesel has an initial boiling point at atmospheric pressure of about 150°C and a final boiling point of about 380°C.

As shown in Figure 3, jet fuel is the middle distillate product between gasoline and diesel. There is significant overlap in the boiling point range of gasoline and jet fuel, and almost complete overlap in the boiling point range between jet fuel and diesel. These overlaps have several implications from the perspective of fuel producers.

First, if a process produces molecules that have a broad range of boiling points spanning those of gasoline, jet, and diesel, then collection of the jet fuel fraction through distillation will need to be done in a manner in which neither the gasoline nor diesel stream is compromised, which can affect the amount of jet fuel recovered. Otherwise, the gasoline fraction is left with only light volatile components (4–8 carbons in length) and the diesel fraction is composed of a distribution with the heaviest fractions.

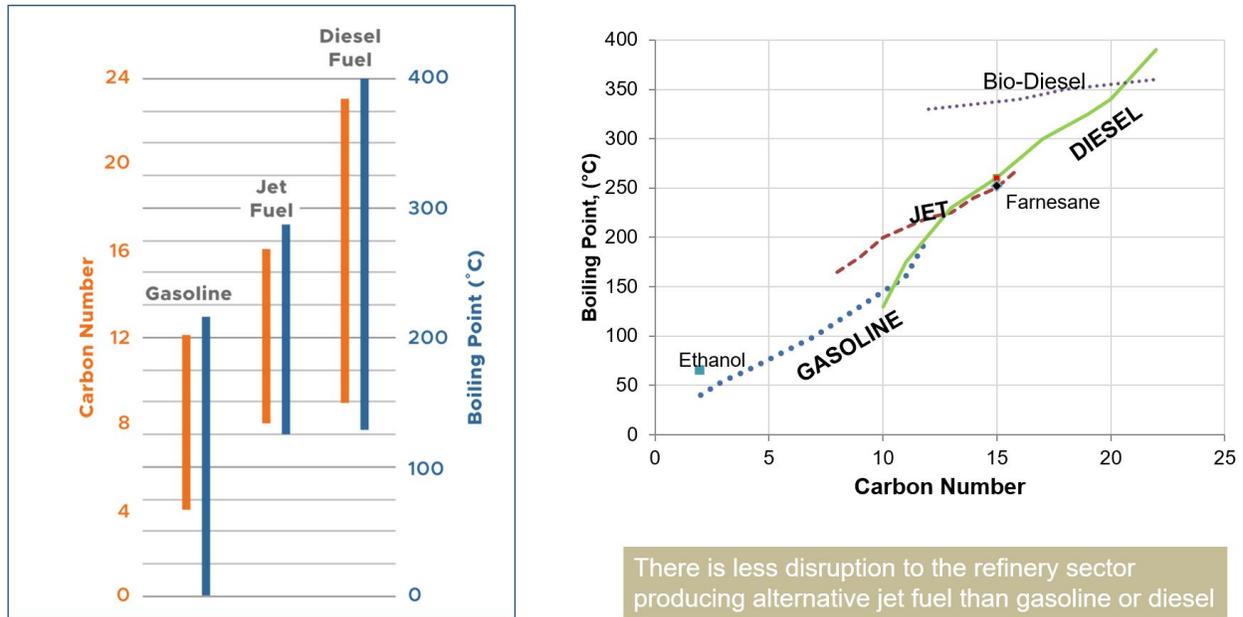


Figure 3. Carbon numbers and boiling points for gasoline, jet, and diesel fuels

Second, the almost complete overlap of the boiling point ranges of jet fuel and diesel allows a refinery to select which product to make depending on market conditions and other incentives. For example, if the market value of diesel is higher than that of jet fuel, then a refinery would be incentivized to produce diesel rather than jet fuel. This would be particularly true if a refinery can have good control of the boiling point range and does not have to distill out the lower-value heavy components. Today, biorefiners are producing renewable diesel at the expense of renewable jet fuel.

Third, if all jet fuel were replaced with SAF (in a long-term scenario), refiners would still have a home for all the fractions they produce. Today, many refineries do not produce jet fuel. Figure 4 shows 2018 domestic biofuel production. U.S. production of renewable diesel exceeded 300 million gallons. SAF, made with the same technology, was two million gallons. While there is some difference in production cost, the difference in renewable diesel production and SAF production is driven by policy.

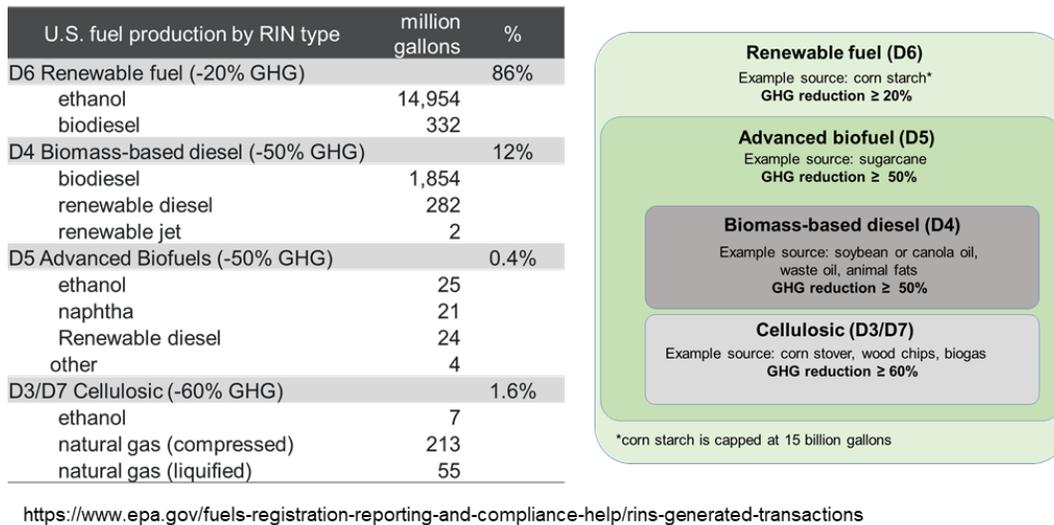


Figure 4. U.S. renewable fuel production in 2018 (U.S. EPA 2019)

Note: RIN = renewable identification number

1.3 Why Invest in SAF?

Jet fuel is purchased by a small group of buyers who negotiate long-term contracts, or at least yearly contracts, and are exceptionally price-conscious. Those same purchasers, such as United Airlines and FedEx, have voluntary goals to decouple passenger growth and carbon emission growth (United Airlines 2018; FedEx 2012). They view SAF as being critical to their future. Hence, there is a strong market pull for SAF.

The fuels are delivered to airports via pipelines, stored in common tankage, and delivered to planes through hydrant systems at major airports. SAFs, as discussed in Chapter 2, are delivered as fully fungible fuels, and once they enter the airport storage are in the same storage and delivery systems as all other jet fuels. Hence, SAF fits into current infrastructure.

The jet fuel market, although smaller than gasoline and diesel fuel markets, still exceeds 26 billion gallons (3.4 exajoules of energy, or greater than 3 quadrillion British thermal units, or Btu). Market growth is expected to double over the next 20 years, while gasoline markets are not expected to grow. U.S. Department of Energy (DOE) investment today addresses current and future market needs.

The jet fuel market matches biomass availability. The amount of biomass available today—about 340 million tons according to the *2016 Billion-Ton Report*—could provide roughly 21 billion gallons, about the size of the jet fuel market (Langholtz, Stokes, and Eaton 2016). As biomass availability is expected to increase, so too does the size of the jet fuel market.

Unlike cars, the commercial jet fleet currently cannot be fully electrified with battery technologies. SAF will continue to be important into the 21st century.

2 Jet Fuel Specifications

The material in this chapter covers the general requirements for SAF in terms of performance, operability, and infrastructure compatibility (drop-in). The information is useful background to researchers considering fuel properties desired in SAF.

Jet fuel specifications are defined in ASTM D1655, *Standard Specification for Aviation Turbine Fuels* (ASTM 2019a). ASTM has defined the steps for qualification and approval of new aviation turbine fuels in ASTM

D4054, *Standard Practice for Evaluation and Approval of New Aviation Turbine Fuels and Fuel Additives* (ASTM 2019b). Finally, there is a specification for SAF, ASTM D7566, *Standard Specification for Aviation Turbine Fuels Containing Synthesized Hydrocarbons* (ASTM 2019c). A fuel meeting these specifications is fully fungible. Maintaining jet fuel properties is critical. Meeting the specifications outlined in ASTM D7566 Table 1, Parts 1 and 2, and the associated D7566 annex ensures the necessary performance and operability requirements are met (ASTM 2019c).

2.1 Properties: Performance, Operability, and Drop-In Requirements

The categorical description of jet fuels and associated properties vary based on perspective. The following describes a jet fuel and its properties from the perspective of value, safety, and compatibility. The categorical requirements for jet fuel are then (1) performance (value added), (2) operability (safety), and (3) drop-in (infrastructure compatibility). A drop-in fuel is deemed to be equivalent to conventional jet fuel, can be used in current engines and infrastructure, and is fully fungible. These requirements are essential for safety, general usage, and execution of commercial and military missions.

2.1.1 Performance

Performance attributes in this report refer to properties that add to the value proposition of a fuel in the context of a mission. In a broader sense, performance can also be used to describe life cycle carbonaceous emissions, costs, or other associated valued effects throughout the supply chain. The functional performance of gas-turbine aviation fuels is defined by the ability of a fuel to service the Brayton cycle of an engine. Performance properties are those that can provide the most direct financial incentives to fuel end-use consumers. These properties include:

- Specific energy (energy per unit *mass*), expressed as MJ/kg
- Energy density (energy per unit *volume*), expressed as MJ/L
- Emissions, including particulate matter
- Thermal stability (inhibition of fuel to degrade or coke under thermal stress).

These performance properties enable mission payload-range requirements and maintenance of an acceptable limit of fuel degradation and, as discussed later, limit the range, payload, and cycle efficiency of fuel in a mission. The ratio of the number of hydrogen atoms to the number of carbon atoms in a molecule largely determines the specific energy of the fuel. Fuels with higher ratios have higher specific energies in the absence of bond strain. The fuel's liquid density mostly determines the energy density of fuel because liquid densities change more than specific energies.

Other properties of the fuel are also key to performance, such as a low freeze point, which allows long-range flights to use more optimum flight profiles, and clean-burning fuels, which may reduce maintenance cost.

2.1.2 Operability

Operability limits apply to the safe use of fuel under specific engine conditions. The determination of an SAF's operability limits is the focus of high volumetric and capital cost expenditures as part of the ASTM D4054 evaluation and approval process. Properties associated with operability limits are in the ASTM D1655 specification, documented in the previous D4054 approval process, and under investigation through the National Jet Fuels Combustion Program (NJFCP), which is trying to streamline the process of securing ASTM approval of SAFs for commercial uses. Historically, the operability limits of an SAF are part of the certification process at original equipment manufacturer (OEM) facilities. The conditions of such tests ensure the safe usability of fuel under the most severe conditions, such as cold-soaked altitude relight with its associated low temperature and pressure.

2.1.3 Drop-In

Drop-in limits refer to a fuel's ability to be used in conjunction with existing aircraft and handling hardware with *no changes to fuel and aircraft infrastructure*. For example, novel SAFs that meet drop-in requirements must have the ability to be used seamlessly with existing operations and handling because an aircraft can be in service for decades (i.e., they must be fully fungible). Nonetheless, non-drop-in characteristics of fuel are conceptually possible. However, non-drop-in fuels would have to meet additional requirements as well as all those associated with SAFs. These would be on top of those for the additional fueling infrastructure.

Most of the performance characteristics and operability limit effects described here are associated with fuel bulk properties. However, both bulk and trace fuel property limits are needed to meet drop-in requirements. Performance, operability, and drop-in limits are listed in Table 1 and Table 2. Additional properties and specification requirements are listed in ASTM D4054 and D7566, and the D1655 documentation. The impacts of some of these properties on engine operability remains an open research issue that the NJFCP is currently investigating.

Table 1. Performance Properties

Property	Units, {qualitative}, [quantitative]	Description/Relevance
Specific energy	{Energy/mass}, [MJ/kg]	Enables fuel efficiency by lowering takeoff weight, critical for mass-limited missions
Energy density ^a	{Energy/volume}, [MJ/L]	Most important metric for volume-limited missions or military operations involving refueling
Thermal stability	Variable	Limits ability of fuel to sustain elevated temperatures in the engine and fuel injector
Emissions/sooting ^a	Variable	Particulate emissions

^a Not included as part of the ASTM D1655 specification

Table 2. Operability and Drop-In Requirements

Property	Units, {qualitative}, [quantitative]	Description/Relevance
Viscosity	{length ² /time}, [mm ² /s]	Important for flow performance, particularly at cold temperatures
Density	{mass/volume}, [kg/m ³]	Used in calculating fuel tank volumes
Freeze point	{temperature}, [°C]	Inhibits freezing of the fuel in flight at an altitude
Flash point	{temperature}, [°C]	Safe handling
Distillate temperature	{temperature}, [°C]	Enables sufficient volatility of a fuel
Derived cetane number (DCN) ^a	unitless	Important for lean blowout limit stability
Minimum aromatic concentration ^a	{percent}, [%]	Ensures proper swelling of certain O-rings and seals that have been previously exposed to fuels with high aromatic content
Surface tension ^a	{force/length}, mN/m	High values can inhibit spray break-up and atomization

^a Not currently included as part of the ASTM D1655 specification

Bulk properties most important for approval and performance are in the ASTM D1655 specification sheet for Jet A and Jet A-1 for conventional fuels. Bulk properties are determined by the mean mass or volumetric composition of fuel and typically are not influenced heavily by contaminants or molecules in low concentrations, the latter of which must not be ignored.

2.1.4 Other Properties

Trace composition properties typically relate to auxiliary yet critical functions of the fuel as a working fluid while being pumped and stored in an aircraft or storage facility. Deleterious trace properties will result in seizing up of mechanical parts, leaking fuel, corrosive behavior, or other antagonistic issues.

All told, these specifications tend to be tighter and less malleable than those used in marine or ground transportation applications because of the significantly higher safety issues, capital intensity of aircraft and engines, and the broad range of performance requirements that aviation transportation imposes on the fuel compared to other applications. The nuanced testing of SAFs for bulk and trace properties is an example of these more stringent specifications. Chapter 3 illustrates some of these nuanced and extensive testing requirements.

2.1.5 Fuel Properties Derived from Bulk Versus Trace Composition

Jet fuel properties are derived from both the bulk composition and trace components of the fuel. A list of bulk and trace properties is provided in Table 3.

Bulk fuel properties primarily address performance and operability requirements of a fuel. Thermodynamic and mission efficiencies are determined by the thermal stability and energy content (MJ/kg and MJ/L), respectively. Safety and operability limits are primarily determined by a fuel's viscosity, density, reactivity (DCN), surface tension, flash point, and freeze point.

Table 3. Fuel Properties Derived from Either Bulk or Trace Components

Bulk Composition	Trace Composition
Energy content	Lubricity
Combustion character	Stability
Distillation range	Corrosivity
Density	Cleanliness
Fluidity	Electrical conductivity

Trace properties must not impair the performance, combustion operability, or drop-in nature of the fuel. Trace properties are associated with material and component wear such as pumps (lubricity), corrosion, thermal stability, and conductivity, which typically affect aircraft operability. Both the bulk and trace property requirements of jet fuel need to be understood and considered even at the bench scale, when costs associated with separation and cleanup can still be mitigated.

2.2 Molecular Families in Jet Fuel

Four hydrocarbon families compose an acceptable alternative to conventional jet fuel: aromatics, cycloalkanes, iso-alkanes, and *n*-alkanes (Figure 5). Other molecular families—oxygenated molecules, heteroatom-containing molecules, unsaturated hydrocarbons (olefins), and metals—are unacceptable for various reasons, including poor thermal stability, freeze point, and specific energy properties. Conventional fuels are composed of molecules with approximately 7 to 18 carbons, and most of the composition stems from molecules with 9 to 15 carbons and an average of 12 carbons.

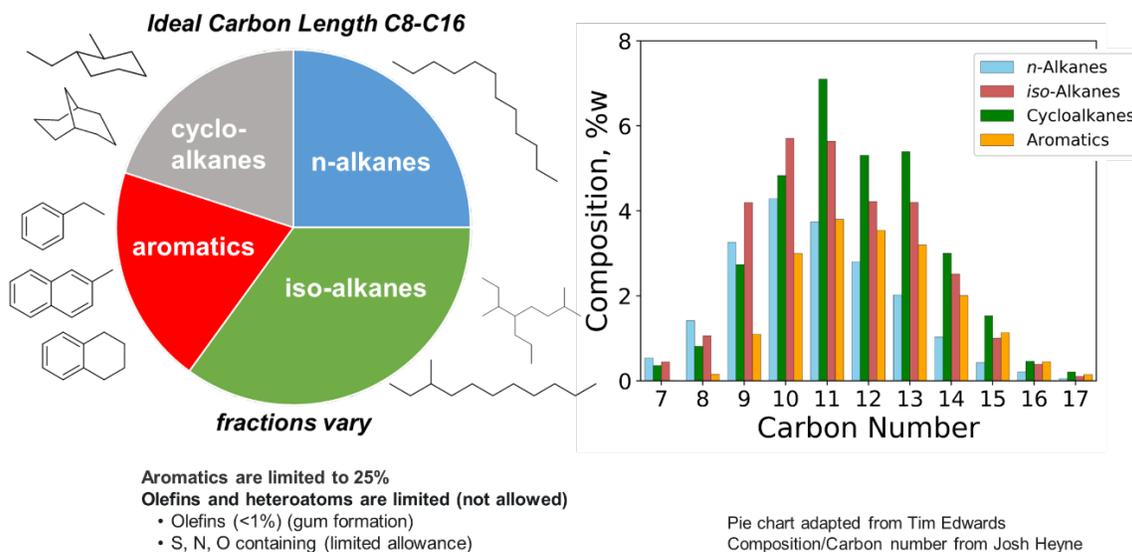


Figure 5. Composition of an average Jet A (POSF 10325) (Edwards 2017). *n*-Alkanes, iso-alkanes, cycloalkanes, and aromatics are approximately normally distributed across the carbon number range. A molecule with 11 to 12 carbons is approximately average.

Conventional fuel variance can be bounded by the difference between JP-8 and JP-5 fuels, which are conventional aviation fuels that meet ASTM D1655 but have different underlying specifications. JP-8-type fuels are generally “lighter” in molecular composition because lower-carbon-number molecules compose a larger fraction of the total fuel. Conversely, JP-5-type fuels are “heavier” due to the U.S. Navy’s requirement for a higher flash point and because a fuel’s average molecular weight scales proportionally.

Table 4 reports select properties of a best-, average-, and worst-case conventional fuel. While the differences in conventional fuel properties seem small, combustion operability testing on them has yielded significantly different results, particularly regarding cold-ignition experiments. Qualitative jet fuel rankings are based on fuel performance and observed operability limits under NJFCP (Edwards 2017).

Table 4. Comparison of Three Jet A Fuel Compositions and Properties (Edwards 2017)

	Best-case operability (JP-8 POSF 10264)	Average (Jet A POSF 10325)	Worst-case operability (JP-5 POSF 10289)
Composition, wt%:			
<i>n</i> -alkanes	26	20	13
iso-alkanes	37	30	19
monocyclic alkanes	19	25	30
bicyclic alkanes	3	7	17
aromatics	14	19	20
Properties:			
hydrogen to carbon ratio (H/C)	2.01	1.94	1.90
specific energy (MJ/kg)	43.2	43	42.9
density (kg/m ³)	780	803	827

	Best-case operability (JP-8 POSF 10264)	Average (Jet A POSF 10325)	Worst-case operability (JP-5 POSF 10289)
energy density (MJ/L)	33.7	34.5	35.5
avg. molecular weight (g/mol)	152	159	166
viscosity (cSt)	3.5	4.6	6.5
flash point (°C)	42	48	60

2.2.1 *n*-Alkanes and iso-Alkanes

The *n*- and iso-alkane families of molecules typically compose approximately 55%–60% of conventional jet fuel. Table 5 summarizes the performance and operability effects of these molecules. They tend to have higher specific energy, lower energy density, and higher thermal stability than the remaining molecular families. The blending of these molecules is limited by the density specification despite their otherwise high-performance characteristics. *n*-Alkanes are known to have the highest DCN of hydrocarbons that have similar carbon numbers, and all *n*-alkanes violate either the freezing point or flash point specifications of ASTM D1655. Increasing isomeric branching of *n*-alkanes generally lowers the freeze point, which is a positive attribute (+), and lowers the DCN, which is a negative attribute (–), while raising the vapor pressure, which is a positive for ignition (+) but negative for flash point (–).

Table 5. Fuel Properties – Molecular Structure Relationship

		<i>n</i> - Alkanes	Iso-Alkanes Weakly Branched	Iso-Alkanes Strongly Branched	Cycloalkanes Monocyclic	Cycloalkanes Fused Bicyclic	Aromatics
Performance	Specific energy	++	++	++	+	0	–
	Energy density	–	–	–	+	++	++
	Thermal stability	+	+	+	+	+	
	Sooting	++	++	++	+	+	--
Operability	DCN	++	+	–			–
	Density	–	–	–	+	++	+
	Freeze point	–	+/-	+	+	+	+
	Sooting	++	++	++	+	+	--

2.2.2 Aromatics

Aromatics in conventional jet fuel are mostly composed of alkyl aromatics with smaller amounts of tetralins and naphthalenes (multi-ring aromatics). The attributes can be positive (+) or negative (–). Collectively, this group of molecules has low specific energy (–), high energy density (+), and contributes most significantly to sooting (– –). Early SAF testing indicated that aromatics contribute significantly to the ability of other nitrile O-rings to swell. The key is that the contribution of aromatics results in the current misperception of their need in all SAF blends. Aromatics are necessary only to ensure the swelling of nitrile O-rings and seals that have been previously exposed to fuel that had a high aromatic content. Seals that have not previously been exposed to fuel do not require aromatics for acceptable performance, as demonstrated using 100% hydroprocessed esters and fatty acids (HEFA) fuel in Boeing 777 aircraft. Additionally, aromatics are well established as the most significant contributor to incipient soot production and particulate matter emissions. Ground and altitude emissions of particulate matter are a growing concern in the aviation community because they contribute

heavily to ground air quality, contrails, and environmental forcing. This concern could be addressed in part by understanding the minimal aromatic content required and blending aromatics to the minimum. Alternatively, there is evidence that certain cycloalkanes can provide seal swelling (FAA 2013). Research to validate the seal swelling requirements is needed as the International Civil Aviation Organization (ICAO) will begin regulating the emission of particulate matter in forthcoming requirements (ICAO 2019).

2.2.3 Cycloalkanes

Cycloalkanes comprise a diverse spectrum of molecules and properties, discussed here in the context of monocyclic, fused bicyclic, and strained molecules. Each of these cycloalkane classes is associated with higher energy densities than typical Jet A fuel; however, the properties across this group can vary significantly and it remains an area of needed research. Nominally, average Jet A fuel is approximately 25/7/0 wt% monocyclic/fused bicyclic/strained. The monocyclic portions of conventional fuels are mostly composed of six-member rings with alkyl chains and branches stemming from the central ring. Monocyclic alkanes can have a density (+), freeze point (+), flash point (+), and specific energy (+) exceeding conventional fuel requirements. Alkylated monocyclic alkanes could be the only molecular subfamily capable of being a drop-in fuel, ignoring the aromatic requirement and pending an acceptable DCN. Monocyclic alkanes with larger ring structures (>7 carbons) and smaller ring structures (3–5 carbons) remain an area of continued exploration in the properties they possess and biofeedstocks that could feed into their production.

Fused bicyclic alkanes in Jet A fuel are composed of decalin moieties (Figure 6), often with additional carbons of varying alkyl lengths and branching. These fused bicyclic molecules are characterized by high energy densities (++), specific energies near Jet A averages (~), and superior thermal stabilities (++). Additionally, decalin and monocyclic alkanes have shown similar swelling capabilities near those of Jet A fuel with aromatics, making them a potential replacement for the aromatic concentration minimums previously mentioned (Graham et al. 2011).

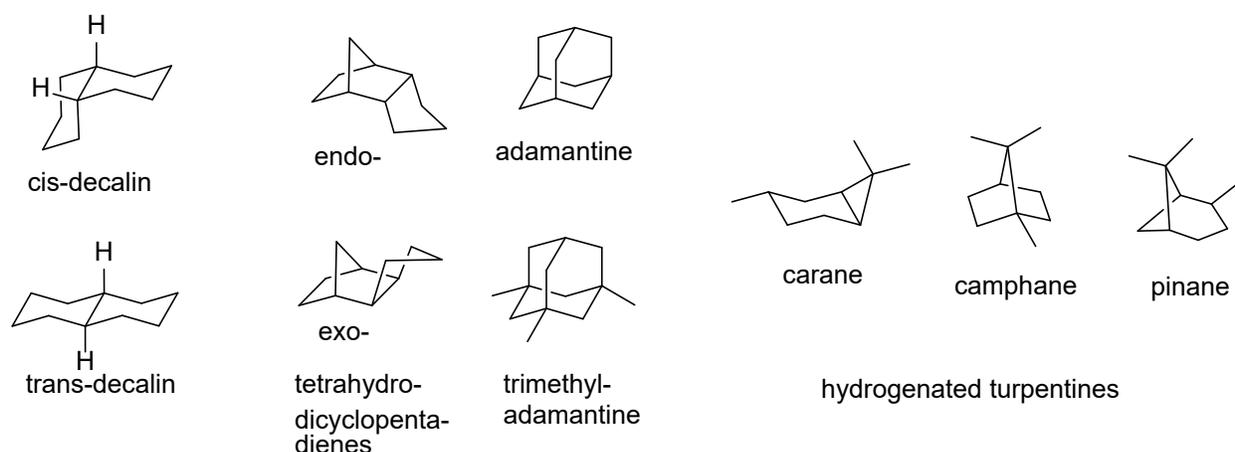


Figure 6. Various examples of fused and strained molecules

Strained cycloalkanes remain an active area of research. This class of cycloalkanes is not found in conventional fuels and may have thermal stability issues. It may be difficult to predict the properties of strained cycloalkanes. Each of these would pose unique challenges to obtaining the approval of a novel SAF and advancement of technologies to enable their research exploration.

Variation in conformation and level of branching can impact the fuel properties of fused and strained cycloalkanes. Examples of these property challenges can be found in the property variance between apparently similar molecules shown in Figure 6:

- Freeze points of endo- versus exo-tetrahydrodicyclopentadiene (+84°C and –90°C, respectively)

- DCNs of trans- versus cis-decalin⁶ (32.0 and 41.6, respectively)
- Specific energies of alkyl adamantines versus adamantine (approximately -2% and +3% difference from an average Jet A fuel, respectively).

The opportunity for a novel SAF with high performance lies in the reduction and removal of aromatics, and with the addition of molecules with high energy densities and specific energies. (However, it should be noted that in some optimization scenarios the low specific energy, high energy density JP-10 is preferred in concentrations around 2%.)

2.2.4 Blended Fuels

Fuels typically consist of blends of molecules rather than single compounds or even single classes of compounds.⁷ The properties of blended fuels are based on the bulk properties of the blended molecules and minor/trace molecules (including inorganics, metals, etc.). Molecules from four chemical families—*n*-alkanes, iso-alkanes, cycloalkanes, and aromatics components—meet the requirements codified by ASTM when blended, which is the subject of Chapter 3. Because a single molecule or family of molecules will be blended with other molecules, only the finished fuel needs to meet the fuel specifications.

2.3 Beyond Current Fuels – High Performance

Fuel performance can be measured by the usefulness of a fuel in the utilitarian function of a flight (see Chapter 2.1), as well as its performance regarding another metric (Figure 7). The utilitarian performance of a fuel—what an airline is likely willing to pay more for—can be predicted by at least the specific energy and energy density of a fuel. High-performance fuel refers to any fuel composition, pathway, or effect that has advantageous characteristics relative to a conventional fuel and is not limited to strained or novel molecules.

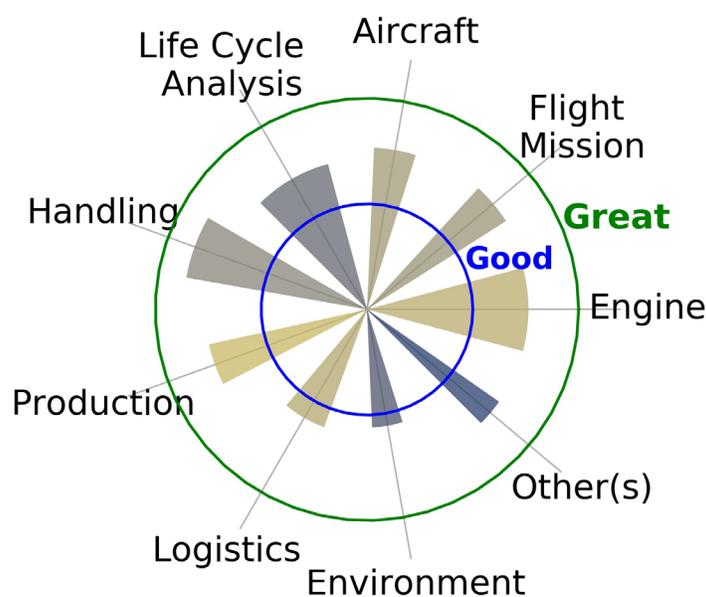


Figure 7. Performance metrics of a fuel can be clumped into nine categories that are dependent on the mission of the flight. Other nonutilitarian performance benefits could be achieved by increasing the value proposition to some other stakeholder. For example, Figure 7 illustrates several other possible performance metrics that a hypothetical

⁶ The cis and trans forms of decalin can adopt relatively low-strain chair configurations but have different strains relative to C–H interactions. Other ring structures could also have very different DCNs.

⁷ In the Co-Optimization of Fuels & Engines (Co-Optima) initiative, fuel components are referred to as blendstocks.

high-performance fuel could achieve. Costs associated with logistics or handling can conceptually be reduced. Alternatively, environmental benefits can be realized with fuels that have low aromatic content. Recent work, however, focuses on the direct utilitarian performance metrics with additional discussions of costs.

Specific energy and energy density improvements have the potential to be used by an aircraft or airline immediately. All flights benefit from increases in specific energy, as the flight can achieve the mission at a lower total weight and hence reduce fuel burn. On payload-limited flights or flights that are limited in range by a maximum weight, high specific energy might enable carrying an additional payload and thus become more profitable. Flights that are range-limited by fuel capacity, less common for commercial aircraft but more common for business jets, can benefit directly from a fuel that has higher energy densities. The Bioenergy Technologies Office (BETO) is sponsoring studies to bound the potential benefits of increasing the range or payload.⁸

Higher thermal stability benefits may be achieved by using redesigned or adjusted hardware to achieve higher efficiency. Thermal stability benefits may result in decreased engine maintenance. These benefits, however, will remain unknown and unquantified until a substantial level of experience is accrued with the use of SAFs that have high thermal stability and until OEM concurrence of the benefits is obtained.

To reiterate, while what an airline *may* be willing to pay can be modeled by others, keep in mind that there is low accuracy in such a number. Further, airlines will not pay more for a fuel based on model output and will require in-depth flight testing for anything other than modest adjustments to price based on energy content (J. Holladay, personal discussions with Alaska Airlines and Airlines for America, October 2018).

Finally, fuel storage and delivery infrastructure must also be accounted for when considering the full cost of the fuel. SAFs today are approved in blends of 10% up to 50% and when blended are fully fungible drop-in fuels. Fuels are stored at airports and delivered through a hydrant system. For example, at Los Angeles International Airport, SAF blended 30:70 with petroleum is purchased by United Airlines. The fuel is mixed with all other jet fuel at the airport and delivered through the hydrant system to all planes. Through an accounting system, United Airlines is charged a premium for the fuel and receives “credit” for its use. Similarly, any fuel will: (1) need to be a fully fungible and drop-in compatible and (2) be delivered most cost-effectively through the hydrant system, hence it must be diluted. While the fuel could be stored separately and delivered by a fueling truck, this would add cost and time and must be taken into account when considering what an airline would be willing to pay for the fuel. Having a fueling truck and a hydrant cart at the same gate in a major airport may not be practical because of limitations on fueling time and space.

2.4 Review of Chapter 2

Fuel properties needed in SAF must meet three general requirements: (1) performance, (2) operability, and (3) drop-in compatibility. These requirements are essential for safety, general usage, and execution of commercial and military missions.

The bulk properties of jet fuel are derived from the hydrocarbon classes that make up the fuel, which include *n*-alkanes, iso-alkanes, cycloalkanes, and aromatics. Aromatics have lower heats of combustion, do not burn cleanly—particularly in older hardware—and are responsible for up to 90% of particulate emissions, which in turn contribute to wear on combustor liners.

⁸ Preliminary model output based on a theoretical fuel and for a sample flight route suggests a potential benefit of up to 54 cents per gallon for what could be a theoretical maximum of unblended high-energy fuel (44.9 MJ/kg, 37.7 MJ/L) by improving the range of the aircraft. A fuel composed of only conventional fuel molecules could be reconfigured to garner an 18-cent-per-gallon benefit (43.6 MJ/kg, 36.1 MJ/L) or, in the case of a fuel partially composed of known strained molecules, a 30-cent-per-gallon benefit (44.0 MJ/kg, 36.8 MJ/L).

Trace properties derived from impurities and minor components are also critical for fuel performance, operability, and drop-in compatibility, and affect the relative cost of jet fuel versus fuels that do not have the same criteria. An understanding of trace properties is vital for researchers to consider at the bench scale.

Rather than mimic petroleum-derived jet fuel, there is an opportunity to produce jet fuel of higher quality through focusing chemistry and biology on producing the hydrocarbon classes most desirable for bulk properties. An SAF that has a lower aromatic content and higher energy and specific density is one example. Current fuel specs allow migration in this direction while maintaining drop-in compatibility.

Jet fuels are primarily delivered to aircraft through hydrant systems. Hence, SAF fractions today are highly diluted with the conventional petroleum fuel and aromatic concentrations in the composite fuel, providing adequate swelling character. This means there is little reason for renewable fuels to contain aromatics to ensure seal swelling.

Finally, cost cannot be understated in importance. SAFs with low (or no) aromatics offer greater performance attributes in many ways. However, current projected performance increases do not eclipse the increase in costs. High-quality SAFs must be near price parity to sell and scale in volume.

3 Jet Fuel Certification

Jet engines and airplanes are certified by the Federal Aviation Administration (FAA) to operate on a fuel that is specified by ASTM. Any new fuel, therefore, must meet conventional fuel ASTM specifications and be approved through the ASTM D4054 process, or it cannot be used in commercial flight. This chapter provides details on the ASTM fuel approval process, currently approved pathways, and pathways in the ASTM approval pipeline.

3.1 Getting a Fuel Approved

ASTM D4054, *Standard Practice for Evaluation of New Aviation Turbine Fuels and Fuel Additives*, was developed to ensure safe and reliable operation of aircraft on alternative aviation fuels (Radich 2015). This standard practice comprises a four-tiered process for testing new aviation fuels and fuel additives (Figure 8) (Rumizen 2017), with two reports submitted for OEM review and approval:

- Specify the new fuel (Tier 1)
- Establish the “fitness for purpose” (Tier 2)
- Test the components and rig operability limits (Tier 3)
- Test the aircraft, engine, and associated durability (Tier 4).

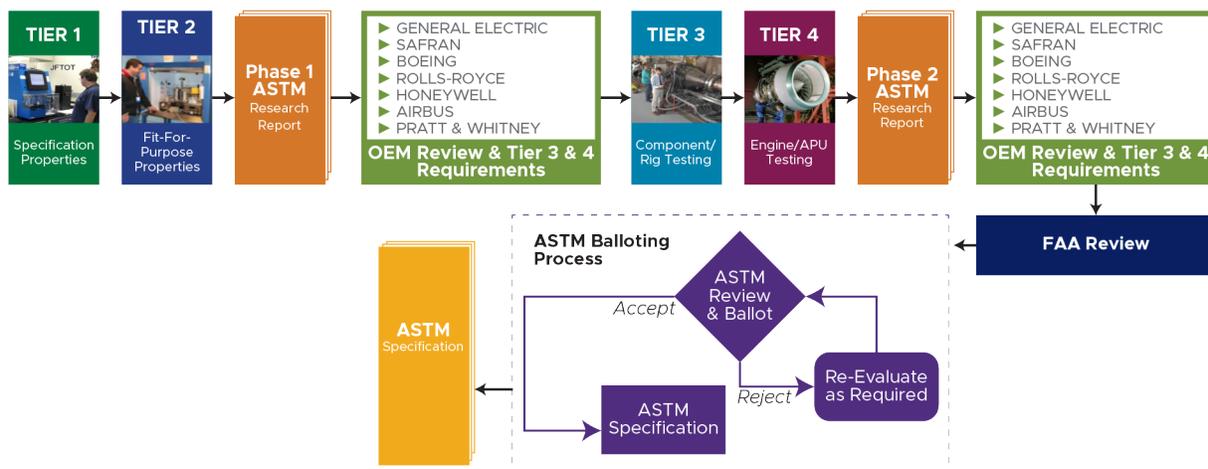


Figure 8. Four-tiered process for testing new aviation fuels and fuel additives, per the ASTM D4054, *Standard Practice for Evaluation of New Aviation Turbine Fuels and Fuel Additives*

Upon completion of the D4054 tests, the approval process for D7566, *Standard Specification for Aviation Turbine Fuel Containing Synthesized Hydrocarbons*, begins. For this approval process, data developed under the D4054 testing protocols enable the ASTM subcommittee to compare SAF properties and characteristics relative to conventional fossil-derived fuels. If the SAF is deemed equivalent to conventional jet fuel, then it is referred to as a drop-in fuel and the pathway used to develop the fuel can be included under ASTM D7566. A provision under D7566 allows any fuel meeting the specifications to be reidentified as a conventional fuel. With this inclusion, any SAF can be seamlessly integrated into the fuel delivery infrastructure without the need for separate tracking or regulatory approval; in other words, the fuel is fully fungible. The overall process for D7566 approval includes the following steps:

1. Fuel producers draft a Phase 1 research report based on Tier 1 and Tier 2 outcomes
2. Aircraft engine manufacturers review the draft research report with requirements needed for Tier 3 and 4 tests
3. Fuel producers draft a revised Phase 2 research report following Tier 3 and Tier 4 tests
4. Aircraft engine manufacturers review the draft research report
5. Fuel producers prepare the final research report incorporating manufacturers' feedback
6. The ASTM subcommittee votes on the final Phase 2 research report
7. The ASTM full committee votes on specification(s) to be added to ASTM D7566.

The D4054 process is an iterative and rigorous evaluation process that requires candidate fuel producers to generate a range of fuel volumes so that their properties, compositions, and performance can be tested. Volumes of fuel for the D4054 tests (listed in Table 6) are significant and are required early in the technology development stages.

Table 6. Approximate Fuel Volumes, Time, and Cost for D4054 Testing (CAAFI 2019)

Tier	Approximate Fuel Volume in Gallons (Liters)	Approximate Time in Months	Approximate Cost in U.S. Dollars
Tier 1 – Fuel specification properties	10 (40)	6 months	\$50,000 (testing cost)
Tier 2 – Fit-for-purpose properties	10–100 (40–400)		
OEM Review		6–12 months	\$350,000 (OEM cost)
Tier 3 – Component and rig testing	250–10,000 (950–40,000)	24–36 months	~\$4 million (testing cost)
Tier 4 – Aircraft and engine testing	Up to 225,000 (850,000)		
OEM Review and Approval		6–12 months	~\$1 million (OEM cost)

While both testing fuel specification properties and fit-for-purpose properties may be provided at no cost to the fuel producers, scaling up new technologies for producing the required volumes for Tier 3 and Tier 4 testing is a challenge. Moreover, scaling capacity is seen as a requirement for formally entering the process by many involved in the approval process.

Component and rig tests can represent significant costs to the fuel producers dependent on the level of testing, but fortunately some of the cost has been borne by the FAA and OEMs. Engine tests that can require even larger volumes may be required for the most innovative cases, but the very large fuel volumes have not been approached in practice for SAFs. The extent of required testing varies. As OEMs become more comfortable with SAF, they have the option to relax the Tier 3 and Tier 4 testing requirements.

Typically, the certification process takes from 3 to 5 years and costs in excess of \$5 million and has been as high as \$10 to \$15 million (Colket et al. 2017). There is a clear need to drive down the certification and production costs and reduce the time required for certification. As a multiagency-led program, the NJFCP aims to streamline these costs and the fuel and resource requirements to secure ASTM approval of SAFs for commercial uses (Colket et al. 2017).

While there is room to adjust the ASTM specification process, the opportunity to change the fuel specification is limited and more about tightening the specification rather than expanding it. Finally, note that no fuels that are oxygenated or have heteroatoms, olefins, or metals will be approved, as they have deleterious properties associated with jet fuel.

3.2 A Fast Track to ASTM Approval

In January 2020, ASTM approved a Fast Track Annex to D4054 (Figure 9) that meets the strict compositional and performance requirements of conventional jet fuel and which limits the blend level to a maximum of 10% with Jet A or Jet A-1.

Composition requirements include limits on the types of hydrocarbons in the blend. The cycloparaffin concentration must be less than 30 wt%, and the aromatic composition less than 20 wt%. Furthermore, tetralins and indans must have a composition less than 6 wt% (or less than 30 wt% of the aromatics). Metals and organic heteroatoms (S, N, and O) must be limited to trace amounts. The blend must have a well-distributed carbon range with a distillation point distribution having the slope of typical jet fuel. The blend must meet strict thermal stability standards.

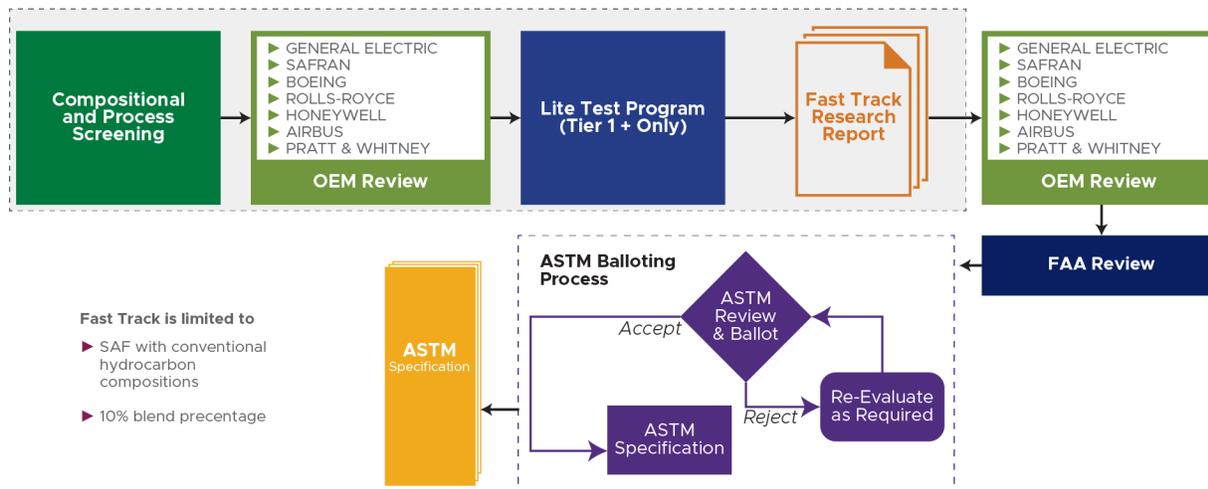


Figure 9. ASTM-D4054 Fast Track Annex for qualification and approval of new aviation fuels that meet the compositional and performance standards with a limit of 10% blend (highlighted portion differs compared to Figure 8)

3.3 Currently Approved and Emerging Fuels

Synthetic paraffinic kerosene (SPK) consisting of *n*- and iso-alkanes constituted the first alternative fuels approved and they came from four sources: synthesis gas (syngas), lipids (fats, oils, greases), sugars, and alcohols. While there are differences in the carbon chain length and level of branching, OEMs have become comfortable with SPK in jet fuel. More recently, SAF fuels are expanding beyond *n*- and iso-alkanes. Annexes with the addition of aromatics and cycloalkanes have been approved. Nevertheless, to date, no alternative fuel is approved at larger than 50% blending with conventional fuel.

As of January 2019, six fuels are approved as annexes to ASTM D7566 (Figure 10):

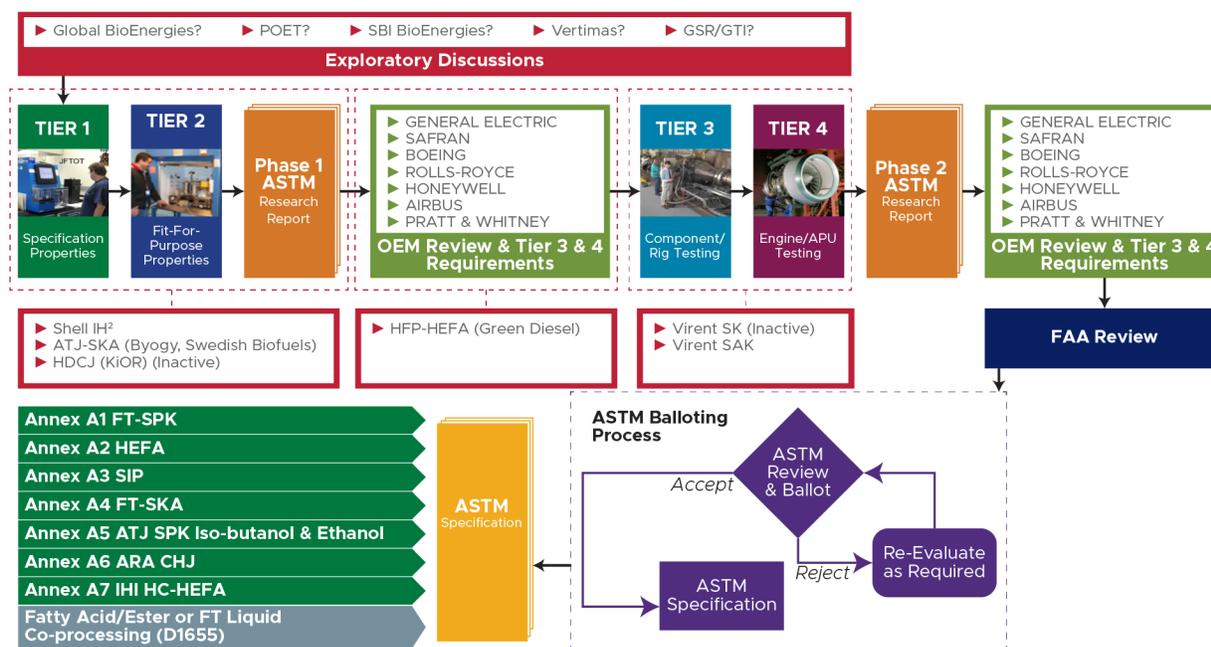
- Annex A1 (Fischer-Tropsch [FT]-SPK) was approved in June 2009 for up to a 50% blend with petroleum-derived jet fuel. FT-SPK is a mixture of iso- and *n*-alkanes derived from synthesis gas using the FT process. Syngas can be produced from reforming natural gas or from gasifying coal or biomass.
- Annex A2 (HEFA-SPK) was approved in July 2011 for up to a 50% blend with petroleum-derived jet fuel. The molecular composition of HEFA-SPK is similar to FT-SPK, consisting of iso- and *n*-alkanes. The alkanes are the product of hydrotreating esters and fatty acids from fats, oils, and greases and from oilseed crops or algae.
- Annex A3 (SIP, hydroprocessed fermented sugar-synthetic iso-paraffins) was approved in June 2014 for up to a 10% blend with petroleum-derived jet fuel. Unlike SPK from HEFA or FT, this is a single molecule, a 15-carbon hydrotreated sesquiterpene called farnesane, produced from fermentation of sugars. Today, the fermentation is done commercially from sugar cane juice and is used in higher-value applications, most commonly in personal care.
- Annex A5 (alcohol-to-jet [ATJ]-SPK) was approved in April 2016 for SPK from iso-butanol (30% blend with petroleum) and expanded in April 2018 for SPK from ethanol and for fuel blends up to 50% with petroleum. ATJ-SPK consists of iso-alkanes of 8, 12, or 16 carbons when starting from iso-butanol. The iso-alkanes are highly branched and have lower DCNs than FT or HEFA, based on data from Gevo, Inc.

The carbon number is broadened and the branching level can be significantly reduced, leading to a DCN similar to FT and HEFA when starting from ethanol.⁹

- Annex A6 (Applied Research Associates Catalytic Hydrothermolysis Jet, or ARA CHJ) was approved in January 2020 as a 50% blend. The fuel is produced from lipids using a supercritical hydrothermal process, creating a blendstock that contains all four hydrocarbon families: *n*-, iso-, and cyclo-alkanes and aromatics.
- Annex A7 (HC-HEFA) synthesized paraffinic kerosene from hydroprocessed hydrocarbons, esters, and fatty acids was approved in 2020 as a 10% blend. This is specifically for lipids from an *B. braunii* algae that have been hydrocracking/hydroisomerization to remove all oxygen and saturate double bonds. The product is rich in iso-alkanes. This is the first approval through the fast track process.
- ASTM D1655-20b allows coprocessing of up to 5% mono-, di-, and triglycerides, free fatty acids, and fatty acid esters or up to 5% of FT hydrocarbons. Hydrocracking/hydrotreating and fractionation are required. No other coprocessing in refineries is allowed for jet fuel.

Several fuels are somewhere in the D4054 approval pipeline (Figure 10). These fuels include SPK (*n*- and iso-alkanes), cycloalkanes, aromatics, and mixtures of the four hydrocarbon families. Figure 10 shows the state as of July 2020, with some companies in exploratory discussions (Global BioEnergies, POET, SBI BioEnergies, Vertimas and GSR/GTI); some companies in Phase 1 (Shell, Byogy, Swedish Biofuels), Phase 1 review (Neste, for green diesel), or Phase 2 (Virent, for aromatics).

Figure 10. SAF pathways approved under ASTM D7566 and emerging fuel pathways in the ASTM D4054 approval process



3.4 Summary of Current SAFs

Figure 11 provides a graphical illustration of the four families of hydrocarbons in jet fuel and a summary of the properties imparted by each hydrocarbon class.

⁹ Pacific Northwest National Laboratory internal data; see also alcohol-to-jet ASTM report, <https://www.astm.org/Standards/D7566.htm>.

Since the first alternative jet fuel was approved in 2009, five additional fuels have been approved. The initial fuels were SPK blends. Later approvals included SPK in which aromatics and cycloalkanes were added or present. The starting feedstocks are synthesis gas; fats, oils, and greases; sugar; and alcohols. The carbon chain length and level of branching can vary dramatically, and hence the amount of the SAF fuel allowed in the blend with petroleum-derived jet fuel varies from 10% (farnesane) to 50%. Fuels that will be approved under Fast-Track will be limited to a maximum of 10% blends.

An SAF consisting primarily of cycloalkanes (Shell's IH²) without substantial amounts of acyclic alkanes or aromatics is now in the system at Tier 1.

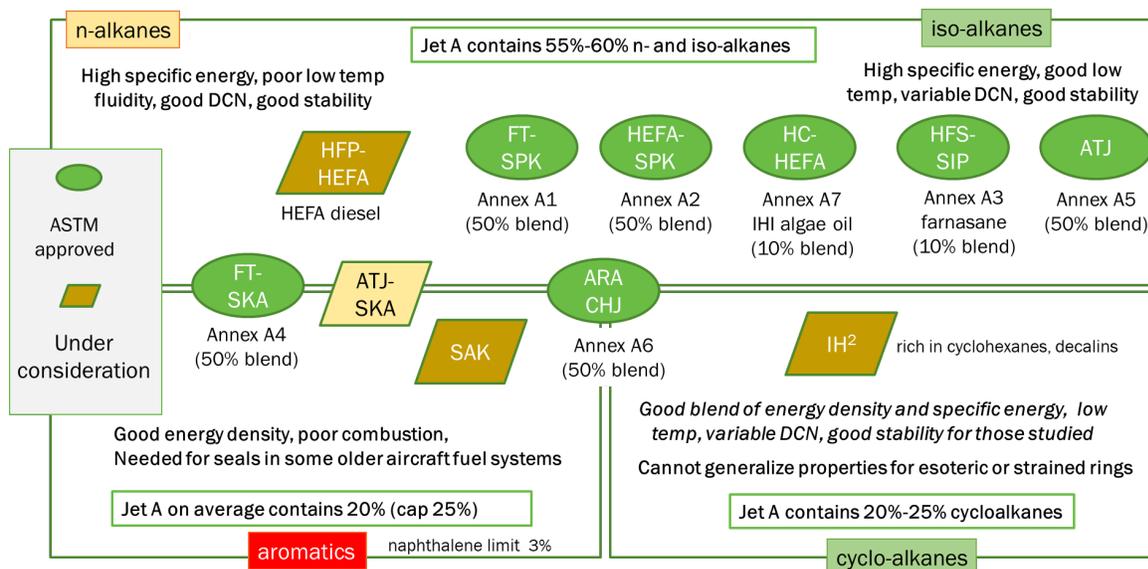


Figure 11. Summary of four classes of hydrocarbons

There is not a physics-based limitation to the 50% blend requirement of broad boiling range fuels and the restrictions on blend level could be increased in the future, even for SPK fuels. With the low amount of SAF produced today there is not a driving force to increase fuel blend levels at this time.

When blended with petroleum, the SAF-approved fuels are considered fully fungible (up to the 50% limit) as a D1655-approved fuel. Hence, approved fuels with SAF are not treated differently than current fuels from petroleum and can use airport fuel storage and hydrant systems, saving money on infrastructure costs.

4 Workshop Learnings

To move the nascent jet fuel industry from 25 million gallons to 2.5 billion gallons, and ultimately to 25 billion gallons, BETO has sponsored or cosponsored three workshops. This chapter distills the key learnings from each workshop, and more detailed summaries of the workshops are provided in Appendix 3.

Participants along the entire value chain were invited to the workshops. These included:

- Airframe manufacturers

- Engine manufacturers
- Feedstock producers
- Biorefiners
- Petroleum refiners
- Aviation fuel distributors
- Airports
- Fuel certifiers quality assurance/quality control
- Airlines
- Regulatory agencies (FAA, Environmental Protection Agency)
- Nongovernmental organizations.

This broad spectrum of participants was invited because innovators require broad stakeholder buy-in, viable technology solutions, and consistent government support in order to move forward. A fuel change in a complex market such as commercial aviation fuels must have each sector represented and ideally have each sector see new opportunities, receive financial benefit, or at least mitigate loss. Further analysis identifying the value proposition and needs of each stakeholder is warranted and outside the scope of this report.

4.1 Alternative Aviation Fuel Workshop

BETO's Advanced Development and Optimization Program held the Alternative Aviation Fuel Workshop on September 14–15, 2016. The purpose of the workshop was to engage stakeholders to gain additional knowledge related to aviation biofuels production. Input was sought specifically for the effort needed to: (1) develop technology for scalable production, (2) achieve economic competitiveness, (3) achieve environmental benefits, and (4) develop feedstock and supply chains for biojet fuel deployment. Key takeaways are listed below:

Timeline

- For 0–5 years, the near-term research and development (R&D) investment needs to reduce the cost in pathways already approved or near certification.

Markets

- Jet fuel properties fall within the light end of the diesel envelope and hence biofuels companies could sell to either market.
- Diesel fuel (ground transportation) is a significant competitor for lipids, including fats, oils, and greases. Light ends could offer a blending opportunity to meet bulk properties.
- Lipid routes are not likely to meet the SAF volume demand.
- Policy and offtake agreements are necessary but are not sufficient criteria; biofuel costs must come down. Today, several offtake agreements are in place but are not being met.

Research Opportunities

- The low sulfur and low aromatic content in approved SPK SAFs should be considered when calculating additional benefits for SAFs.
- New low-cost sources of feedstocks are needed to increase scale, including lignocellulosics.
- Techno-economic analysis (TEA) and GHG results need improved consistency and need to cover pioneer plants. Additionally, TEA should focus on identifying where cost reduction is most significant.

4.2 JET Workshop

The JET Workshop, held at the National Aeronautics and Space Administration (NASA) Glenn Research Center in Cleveland, Ohio, on September 21 and 22, 2017, was a perspective-gathering brainstorming event organized around four themes:

Theme 1: High-Performance Fuel Options

Theme 2: Engine and Combustor Options

Theme 3: Aircraft On-Board High-Performance Fuel Considerations

Theme 4: High-Performance Fuel Development to Deployment Considerations.

DOE's Office of Energy Efficiency and Renewable Energy (EERE), the U.S. Department of Defense, and NASA organized the event. In-person attendance was 75, with another 25 participating by webinar.

High-performance SAF offers tremendous opportunity, but it will take time and money and can only be accomplished by understanding the critical fuel properties required and their impact. Notionally, fuels can make air transportation safer and more efficient, produce fewer emissions—of importance to both human health and global climate change—and increase aircraft performance.

The matriculation of quantifying these benefits via research will take investment and time, with many federal agency strengths leveraged to fully capture these potential benefits. The optimum realization of these benefits will take time, money, and, perhaps most importantly, coordination.

It was noted from an OEM that it takes 14–19 years for technology development for planes, engines, and fuels to progress through product introduction phases; hence, it is necessary to identify how these can work together. General Electric spent over \$500 million to get GENx-09 from development into production (an expensive and resource-intensive process); fuel production facilities have a similar price tag. The risk of developing a new engine on a fuel that is not commercial is too high.

While there is little expectation for engine design to change radically, there is an expectation for reduced emissions. Therefore, the biofuel community can focus on improving fuel properties on engines used today and on providing fuels that have lower emissions. Opportunities exist to improve specific fuel consumption (increase payload, increase range, or reduce takeoff weight) using high-energy-content fuels with existing engines.

4.3 Trilateral Canada–Mexico–U.S. Biojet Workshop

The Trilateral Biojet Workshop, held in Richland, Washington, in May 2018 brought together researchers from Canada, Mexico, and the United States. The workshop was organized by EnerCan, SENER, and DOE, and was funded by DOE and Pacific Northwest National Laboratory (PNNL). The workshop covered the value chain, feedstock from each country in North America, research directions in each country, and how they can work together to accelerate SAF growth.

Key takeaway messages included:

- The time and cost of bringing a new fuel to market must account for the fuel certification time (4 years) and cost through piloting to pioneer plants.
- The airlines cannot meet their self-imposed targets for reducing GHG emissions based on engine and flight improvements alone; they need SAFs. Fuel cost is a significant fraction of operating cost.
- Some airports are looking at opportunities to help make up the difference between the cost to make the fuel and the price of the fuel. One option for airports is to become fuel integrators by combining more substantial long-term purchase agreements (from the airport level) and by providing land for producing biofuels. Europe has similar models that could be followed (e.g., the Oslo model, which creates a central fund to bridge the delta on the cost of production and market value).
- Fuels are delivered in hydrant systems in which life cycle analysis (LCA) accounting is attributed to those who pay for them. Refineries ask if similar accounting could be done for coprocessing even if jet fuel is not a product. (How does one draw the box around the LCA?)
- Feedstock cost must be reduced.
- Producers need to maximize value of each process stream, which includes producing higher-value coproducts that match the scale of the process stream.
- Markets span international boundaries and coordination needs to span countries.

Note that fuel prices paid by the airlines versus corporate and other “small” customers may be substantially different. Jet A may sell from between \$3.37 and \$5.05 per gallon (AirNav 2018). Prices at some major airports are even higher. The corporate jet fuel market is substantial in size and is a focus of early adoption for some SAF producers.

Part II – Analysis and Insights



5 R&D – Fuel Molecules

This chapter provides a high-level analysis of research opportunities. The purpose of the analysis is to identify research efforts that would accelerate SAF development and to note ties between programs supported by DOE, FAA, the U.S. Department of Defense, and the U.S. Department of Agriculture (USDA).

5.1 Vision: Reduce Aromatic Content and Increase iso-Alkanes and Cycloalkanes

Jet fuel consists of four hydrocarbon families: *n*-alkanes, iso-alkanes, cycloalkanes, and aromatics. The presence of other molecular families, including olefins and heteroatoms, are limited to trace quantities.

High energy content is valued in jet fuel, just as octane is for gasoline and cetane is for diesel. Blending cycloalkanes and iso-alkanes can give fuel higher energy content than Jet A fuel while meeting the density specification required by ASTM (Kosir et al. 2019).

Figure 12 shows the relationship of each hydrocarbon class to energy content, including energy density (MJ/L) and specific energy (MJ/kg). The average composition of Jet A contains aromatics, shown in yellow; cycloalkanes, shown in brown (monocyclic) and pink (bicyclic); *n*-alkanes, shown in orange; and iso-alkanes, shown in green. As a mixture, the resultant energy density and specific energy is shown in red (the red hexagon is the average energy density and specific energy for Jet A). As a note, there are small amounts of multicyclic aromatics in a jet fuel composition, which are not illustrated here.

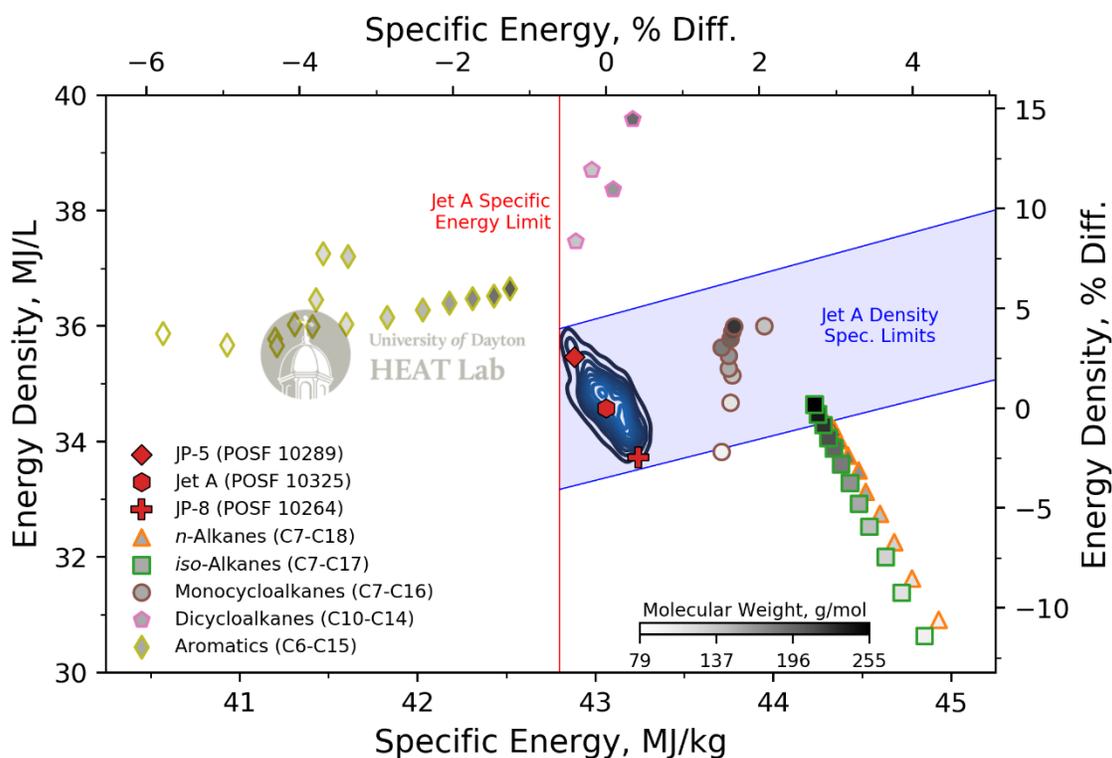


Figure 12. Energy density and specific energy of various hydrocarbons

Aromatics are more difficult to burn cleanly and the soot produced has implications for the environment, human health, and combustor life. Because fuels are delivered in hydrant systems, there is little reason to have a strategic focus on producing aromatics at a time when SAF is made in low amounts. Further, our long-term goal is to reduce and perhaps rid jet fuel of aromatics. Boeing has tested aromatic-free HEFA fuels in modern

planes without issue. Moreover, the lower specific energy of aromatics makes them disadvantageous for mission performance. Hence, there are many reasons to avoid aromatic production.¹⁰

n-Alkanes have poor jet fuel characteristics. No *n*-alkane meets all D1655 specifications—larger *n*-alkanes have high freeze points and smaller *n*-alkanes do not meet the flash point. While they are an acceptable blending source as they are readily available in fatty acids and esters, as a class they do not offer a unique performance proposition and are not required in SAF. SAF and renewable diesel produced today are rich in *n*-alkanes, as they are sourced from lipids.

From a bulk-property perspective, jet fuel only requires iso-alkanes and cycloalkanes to meet ASTM D1655 specifications. A jet fuel containing cycloalkanes (mono- and dicyclic) and iso-alkanes could increase energy density and specific energy; meet freeze point, flash point, and O-ring swelling demands; and burn much cleaner (Kosir 2019). Improvements to the specific energy result in a weight reduction for a flight, which for long ranges enables more passengers and cargo. Ninety-eight percent of flights do not operate with a payload range restriction; hence the weight savings would correlate to a modest fuel weight reduction. BETO has current work that seeks to understand the possible impact of fuel weight savings.

Keeping a strategic focus on these iso-alkanes and cycloalkanes will help define research. While aromatics or *n*-alkanes as parts of a complex mix are acceptable, the authors would like researchers to understand the issues with aromatic production.¹¹

Finally, jet fuel specifications restrict trace components—including ash, metals, and other inorganic and organic impurities—to very low levels. Understanding the cleanliness specification for jet fuel is essential in considering separation requirements coupled to conversion processes.

The possible reduction in aromatic content and increased iso-alkanes and cycloalkanes is shown graphically in Figure 13. iso-Alkanes are desirable, though they are still too expensive, and R&D focus needs to be on continuing to reduce their cost of production. Note that light branching provides a DCN that is in line with jet fuel today and volatility properties desirable for engine relight. Further, the higher DCN allows the iso-alkanes to be sold into diesel markets, which allows flexibility to biorefineries. Heavily branched mixtures have a low DCN, although DCN is not part of the ASTM specification. The low-temperature fluidity of *n*-alkanes is illustrated. Note the difference that a single methyl substitution makes on improving freezing point: for C10, the single methyl branching reduces freezing point by 42°C, and for C14, the freezing point reduction is 21°C. Jet fuel today contains alkyl cyclohexane molecules, which have excellent properties. There are many additional cycloalkane molecules that could be used in jet fuel; however, more research is required as some cycloalkanes may have flaws related to freeze point or cost of production. Research goals include both deriving more information on combustion and molecular properties and reducing cost. Aromatics have the least desirable combustion character and hence are capped at 25% in jet fuel. Multi-ring aromatics are capped at 3%. Research is needed to determine the minimum aromatic content required for backward compatibility with older fuel systems regarding seal swelling. Early data suggest that if jet fuel contains aromatics, small, lightly substituted C8–C9 aromatics will have the least impact on soot formation while providing the seal swelling for backward compatibility. Fused-ring cycloalkanes may offer similar seal swelling, offer even higher energy density, and burn cleaner than aromatics. The question of aromatics versus cycloalkanes becomes one of cost, compatibility, and combustion character.

¹⁰ The authors are not suggesting ceasing research on renewable aromatics altogether, as not all aromatics have the same soot-forming propensity, nor is there a clear understanding of the minimum aromatic content required for seal swelling in older aircraft. Nevertheless, aromatics are easy to produce due to their thermodynamic stability and are a common product in thermochemical streams, including those from lignin. A question remains on the cost–benefit analysis of converting aromatics to cycloalkanes. We are stating that separate R&D on producing aromatics for SAF does not require funding by DOE, as technology is sufficiently available and practiced, whereas producing cycloalkanes with low hydrogen demand remains a challenge.

¹¹ Further things for researchers to understand on aromatic production include: (1) aromatics are readily produced, requiring only temperature and an acid catalyst from any number of feedstocks, (2) there is sufficient aromatic content in petroleum jet fuel, and (3) seal-swelling properties may be derived from cycloparaffins, which offer better combustion behavior.

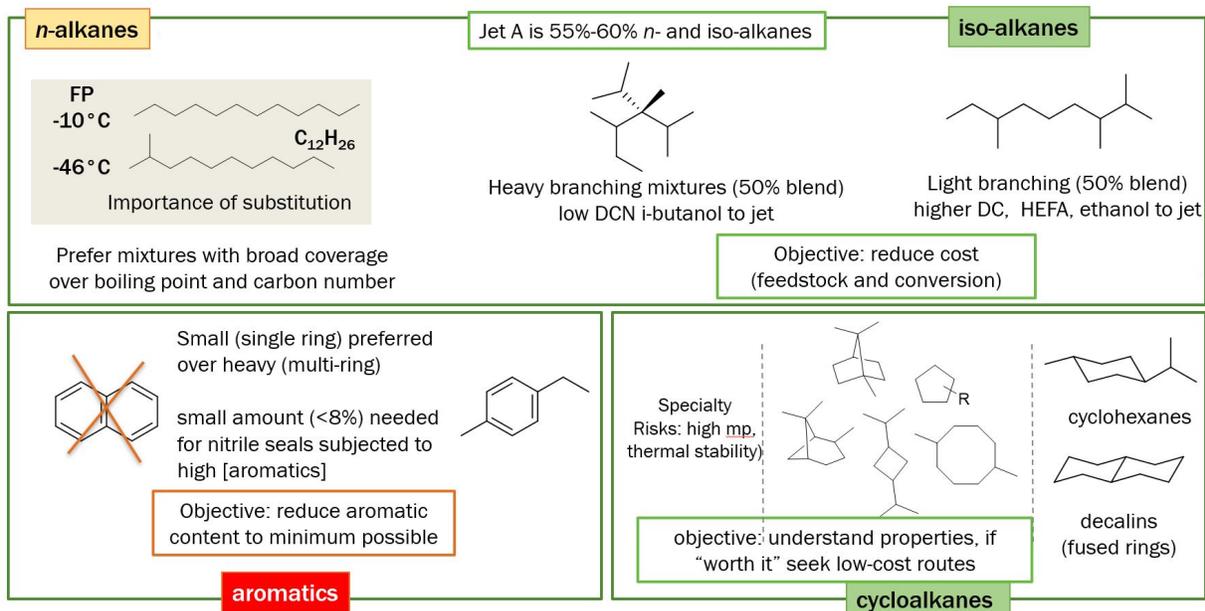


Figure 13. Strategic focus on iso-alkanes and cycloalkanes

Based on the previous analysis, the following conclusions are offered:

- Reducing aromatic content (by adding high-quality iso-alkanes) – near-term benefit
- Replacing aromatics with cycloalkanes – medium-term benefit
- Increasing specific energy by blending new fuel molecules – long-term benefit.

In the near term, SAF will be a small component of Jet A. The addition of high-quality iso-alkanes improves the quality of the fuel. Little value is provided by increasing the aromatic content over what is in jet fuel today. Over time, as SAF volume grows in the market, the aromatic content can be reduced by increasing the cycloalkane content. In the long term, as SAF dominates the market, fuels with higher energy content than is available today can be produced and, to meet Carbon Offsetting and Reduction Scheme for International Aviation (CORSA) targets, there may be blending of SAF blending components. The D7566 is written to allow blending of different SAFs to meet fuel specifications, which could entail mixing SPK with aromatics. The caveats to this strategy are stated previously, requiring further understanding of cost, compatibility, and combustion behavior of cyclic hydrocarbons versus aromatics in SAF fuels.

5.2 High-Quality iso-Alkanes

Today there are four ASTM-approved SAFs based on iso-alkanes (Figure 14). The fuels are prepared by (1) cracking and isomerizing larger alkanes derived from lipids or FT liquids, (2) building up small molecules (alkenes) to the jet range, or (3) fermenting sugar into molecules that are in (or near) the jet range. Each method is presented in more detail in Figure 14.

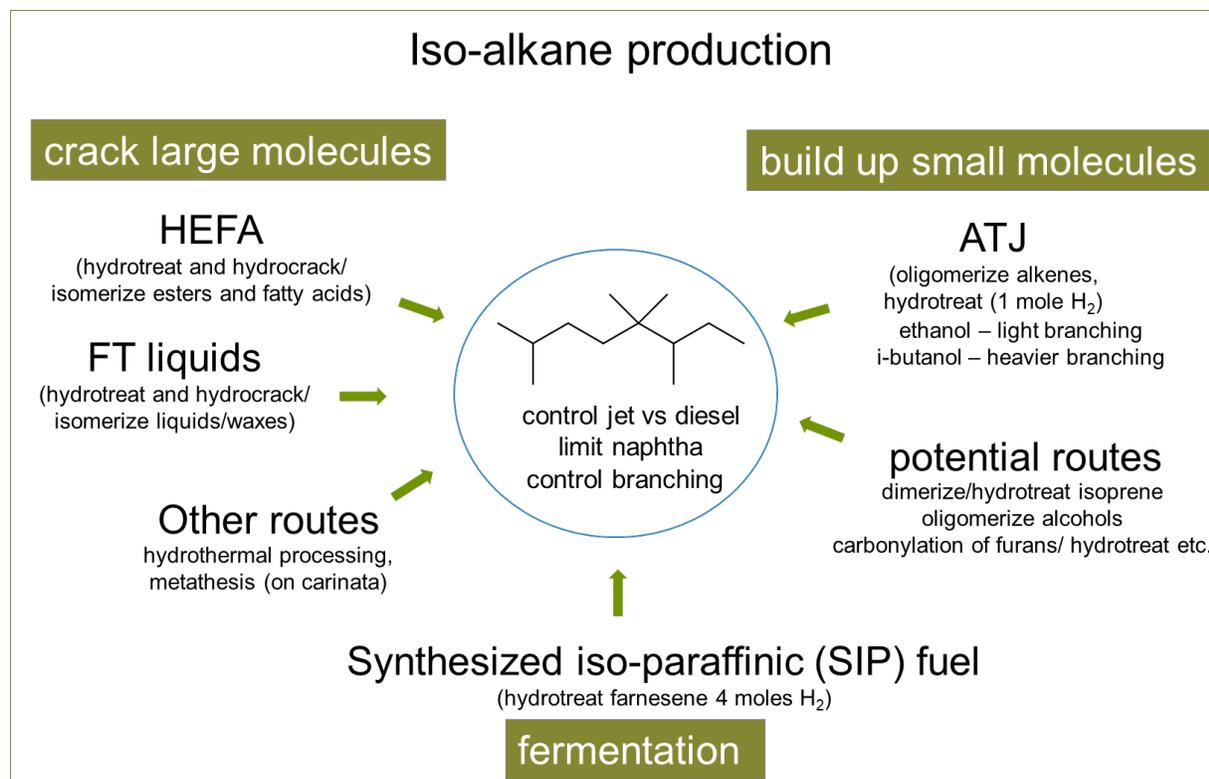


Figure 14. iso-Alkane production by cracking and isomerizing large molecules, building up small molecules, or fermentation

5.2.1 Crack Large Molecules

Cleaving larger molecules into smaller molecules is required with lipids and FT liquids, and for converting diesel or heavies into jet-range molecules. Most processes that “crack” have low specificity; hence diesel-range molecules and heavy oils are converted into both jet fuel and light naphtha. The naphtha is a lower value than the diesel or jet fraction. Hydrocracking is commonly used to crack and is part of HEFA and FT processes. HEFA employs hydrogen to remove oxygen and to crack and isomerize the *n*-alkanes into jet-range iso-alkanes.

Today, lipids are the primary source for biodiesel, renewable diesel, and renewable jet fuel, accounting for 2.2 billion gallons of U.S. renewable fuel production and 2.6 billion gallons of U.S. renewable fuel use (U.S. EPA 2019). Lipid sources are shown in Figure 15. Lipids are coproduced in protein crops, and as the demand for plant protein increases, the lipids will need to be utilized. No one source of feedstock will be sufficient to satisfy SAF demand.

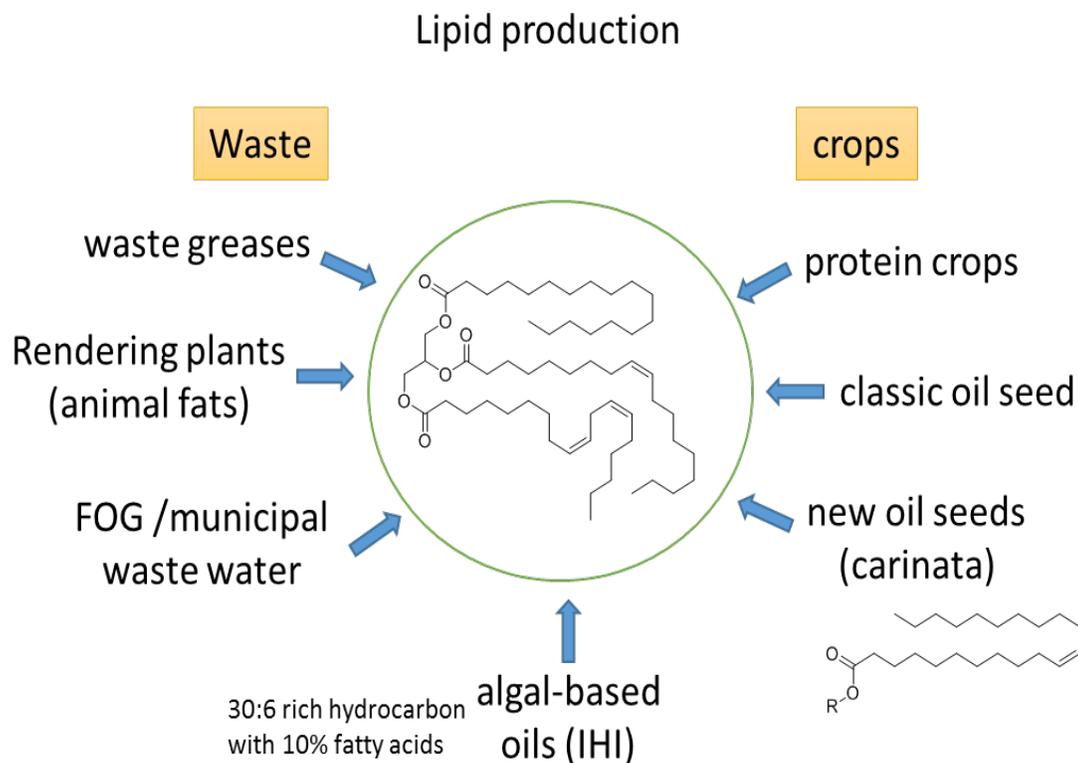


Figure 15. Lipid sources for HEFA, including waste sources and crops

FOG = fats, oils, greases

Increasing the availability of low-cost oilseed crops will be required for lipid-sourced SAF. USDA is supporting new crops, including carinata, which is rich in C22:1 fatty acids. Companies are working on commercial production of carinata. Further out, BETO is supporting research to decrease the cost of algae, which today is too expensive for fuels. In Japan, the IHI Corporation recently entered its algae oil into the ASTM approval process. IHI produces an algal oil rich in C30 that has six unsaturation units.

Conversion technologies for lipids include:

- HEFA, hydrotreating to remove oxygen in carboxylic acid moieties, saturating double bonds, and hydrocracking/isomerization of the resultant *n*-alkanes. HEFA is commercially practiced, providing both renewable diesel and renewable jet fuel today. HEFA produces *n*- and iso-alkanes.
- Hydrothermolysis, a form of hydrothermal liquefaction (HTL) using supercritical water followed by hydrotreating to produce *n*- and iso-alkanes as well as aromatics and cycloalkanes. Plans for the first facility have been announced.

Potential new conversion technologies include:

- HTL followed by hydrotreating of various lipid-containing feedstocks, including wastewater sludge and manures, which produce *n*-alkanes and cyclics.¹²

¹² Hydrothermal liquefaction in which the jet and diesel fractions have been characterized and the diesel fraction tested in engines is performed at PNNL and supported by BETO funding.

- Metathesis, a process that exchanges two double bonds through scission and recombination, is a means of reacting unsaturated esters with ethylene and hence of controlling the scission. Applying the ethylene metathesis to carinata oil, which is rich in C22:1 fatty acids, would produce two C11 compounds: an 11-carbon fatty acid triglyceride and an 11-carbon alkene. The alkene could be distilled and saturated for jet fuel blending and the fatty acid could be esterified (or transesterified) for diesel markets. This would reduce the hydrogen demand of HEFA.
- Catalytic, thermocatalytic, and thermal deoxygenation processes of Shell/SBI, Aduro, and Forge, respectively.

In summary, today large molecules are cracked to smaller molecules via hydrocracking to make fuels. The hydrogen gas demand is significant and is based on the number of ester/acid, olefin, and alcohol functional groups, as well as the amount of cracking required. The chemistry is used in HEFA and FT processes. Supercritical water hydrothermolysis provides another means of breaking down larger molecules to produce a broad range of hydrocarbons after hydrotreating. The hydrogen demand is still substantial. Other chemistries also could be applied. A challenge associated with cracking larger molecules is the loss of carbon to low-value naphtha.

5.2.2 Build Up Small Molecules

Nature excels at producing small alcohols. Through fermentation and hydrodeoxygenation, other small molecules—including olefins, carboxylic acids, and mixtures of oxygenates—are possible. Catalysis can be used to build up small molecules to the jet range with good selectivity. In the ATJ process, alkenes are oligomerized from C8 to C16 molecules. The key is controlling the growth regarding carbon length and carbon backbone (i.e., carbon length, branching level, and degree of cyclization/aromatization).

Cost Drivers

The cost of the alcohol feedstock is a critical driver. Sourcing the alcohol from high-cost sugars (e.g., biomass) is not feasible. Reports suggest that a \$0.01 increase in sugar cost results in a \$0.20 increase in fuel cost (Gruber 2018). Sourcing the alcohols from waste streams can drive down cost. Inexpensive sugars are likewise needed for other small molecules.

Sourcing carbon from low-cost waste gases can change the paradigm. There are enough waste gases (carbon monoxide [CO]-rich streams) to produce 32 billion gallons of SAF globally from steel mills and refineries, and another 18 billion gallons from unsorted municipal solid waste (MSW) gasification. When added to the 360 billion gallons of SAF available from agriculture residues via gasification, the amount exceeds global jet fuel demand (Holmgren 2019).

Chemistry

Several chemistries for building up small molecules to jet-range mixtures are supported by BETO, the Office of Basic Energy Sciences, and USDA:

- Alkene oligomerization (the underlying chemistry for ATJ)
- Prins condensation (reaction of alkene and aldehyde)
- Aldol condensation (reaction of two aldehydes)
- Ketonization (reaction of two carboxylic acids)
- Guebert chemistry (reaction of two alcohols).

From these five reaction families, all the various functional groups obtained from renewable sources can be oligomerized to larger compounds. Precursors include carboxylic acids from mixed anaerobes, furfural and other aldehydes, and olefins from dehydration of alcohols or isoprene. There are important research opportunities to reduce cost. At the same time, support for moving the current ASTM-approved processes through pilot and demonstration is critical. The value proposition for converting low-cost small molecules is high and can meet fuel demands in jet markets with feedstocks available today.

5.2.3 Direct Fermentation

Farnesane is approved for 10% blend in SAF. Many other compounds—*isoprenoids*, fatty acids, and polyketides—can also be sourced from sugars via fermentation.

In 2015, Amyris stated the production cost of farnesene is \$1.75 per liter (from cane sugar), not a price that supports fuel production, and this is before hydrotreating (Amyris 2015). While there are opportunities to increase value propositions of biorefineries with coproducts, research that focuses on reducing cost remains critical.

Additional challenges include:

- High hydrogen demand of farnesene, which requires four moles of hydrogen to saturate the molecule, nearly the hydrogen demand for HEFA. Other *isoprenoids*, fatty acids, and polyketides likewise require hydrogen.
- Single molecules will have limits on how much they can be blended, mainly when they are on the extreme of carbon number distribution, as *sesquiterpenes* are (C15).
- Hydrolysates (sugars) will need to be clarified because lignin can act like active carbon, resulting in the product agglomerating onto the lignin.

The upshot is that available fermentation routes produce large molecules. Theoretical fermentation yields of large molecules are about half the efficiency of the theoretical yield of ethanol. Weight loss of oxygen from ethanol is offset by fermentation efficiency. The challenges then are addressing the competition for the product in high-value applications versus additional processing to make fuels and achieving titer, yields, and rates needed that can match the rates of ethanol.

There may be new ways to approach large molecules by combining biotechnology with thermochemistry that can reduce separations and increase the diversity of fuel products and total yield. A recent publication explores the concept of producing lipids via fermentation (Collett et al. 2019). In one example supported by BETO, a fermentation broth containing a fatty acid is partially concentrated to approximately 20% solids and hydrothermally converted to biocrude oil. In such an approach, separations are reduced, the need to reach a high titer is relaxed, and biomass growth is acceptable because it is converted to biocrude oil, as are all the other residues. The biocrude oil is washed and converted to jet and diesel fuel (Collett et al. 2019).

5.2.4 Summary

There are opportunities to reduce costs in iso-alkane production. Low-cost lipid availability will need to be addressed and USDA has current programs doing so. Diesel is the primary competitor in lipid routes; policy drivers that do not favor one fuel over another are essential. It is critical to control the jet/diesel mix while minimizing the production of lower-value naphtha. Controlling the level of branching is also important.

Cracking large molecules is one general route. HEFA (e.g., hydrotreating) is done commercially; however, there may be some other chemistries, such as metathesis, that may be useful for large olefinic molecules, mainly C22:11-rich lipids such as are prevalent in *carinata* oil.

Five chemistries have been identified to oligomerize small molecules with common functional groups from biomass to larger molecules. Low-cost, sustainable sugar sources are needed. There are also opportunities to source the carbon from non-sugar sources, and efficient technologies that can use waste streams with minimal cleanup provide a means to reduce feedstock cost.

There are business reasons to convert alcohols to jet fuel (Brooks et al. 2016). Fermentation routes can directly produce larger molecules and the theoretical efficiency is offset by the weight loss of oxygen in dehydration. Hence, the choice is dictated by the lowest-cost fermentation.

Hydrogen demand is required for all routes (hydrocracking large molecules, building up small molecules, or saturating direct fermentation molecules). The lowest hydrogen demand is for ATJ (one mole), which is four times less than the demand to saturate farnesene and significantly lower than the demand to hydrotreat and hydrocrack lipids.

5.3 Alkylcycloalkanes, Six-Carbon Rings

Alkyl-substituted cyclohexanes can be produced through multiple pathways and from various biomass-derived materials. Such cyclohexane derivatives are within the specification range of conventional fuels, already present in Jet A fuel in large concentrations by as much as 30% by weight, and many of the molecules in the cyclohexane family can be blended at high concentrations with conventional Jet A fuel without sacrificing energy density (Kosir et al. 2019).

The combustion properties of cyclohexane and decalin (two fused cyclohexane rings) are not as good as iso-alkanes in terms of soot formation, but are much better than aromatics (Table 7). Jet A fuel contains approximately 20% alkyl cyclohexane derivatives.

Table 7. The Sooting Propensity of Various Hydrocarbons (Yang, Boehman, and Santoro 2017; Olson, Pickens, and Gill 1985)

Compound	Formula	Molecular Weight (g/mol)	Boiling Point (°C)	ρ (g/cm ³)	Threshold Sooting Index
<i>n</i> -Dodecane	C ₁₂ H ₂₆	170	216.3	0.7487	5.1
Cyclohexane	C ₆ H ₁₂	84	81	0.779	3.5
Decalin	C ₁₀ H ₁₈	138	155.5	0.8965	15
<i>n</i> -Butylbenzene	C ₁₀ H ₁₄	134	183.3	0.8601	62
Naphthalene	C ₁₀ H ₈	128	217.9	1.0253	100

Alkylcyclohexanes are a natural class of cycloalkanes to consider from biomass. They can be accessed through hydrotreating aromatic and phenolic compounds (Figure 16). Lignin provides a rich source of phenolics, as do bio-oils and biocrudes. Aromatics can be produced from catalytic processing of pyrolysis vapors, mixtures of oxygenated compounds, or simple alcohols.

Cyclohexanes

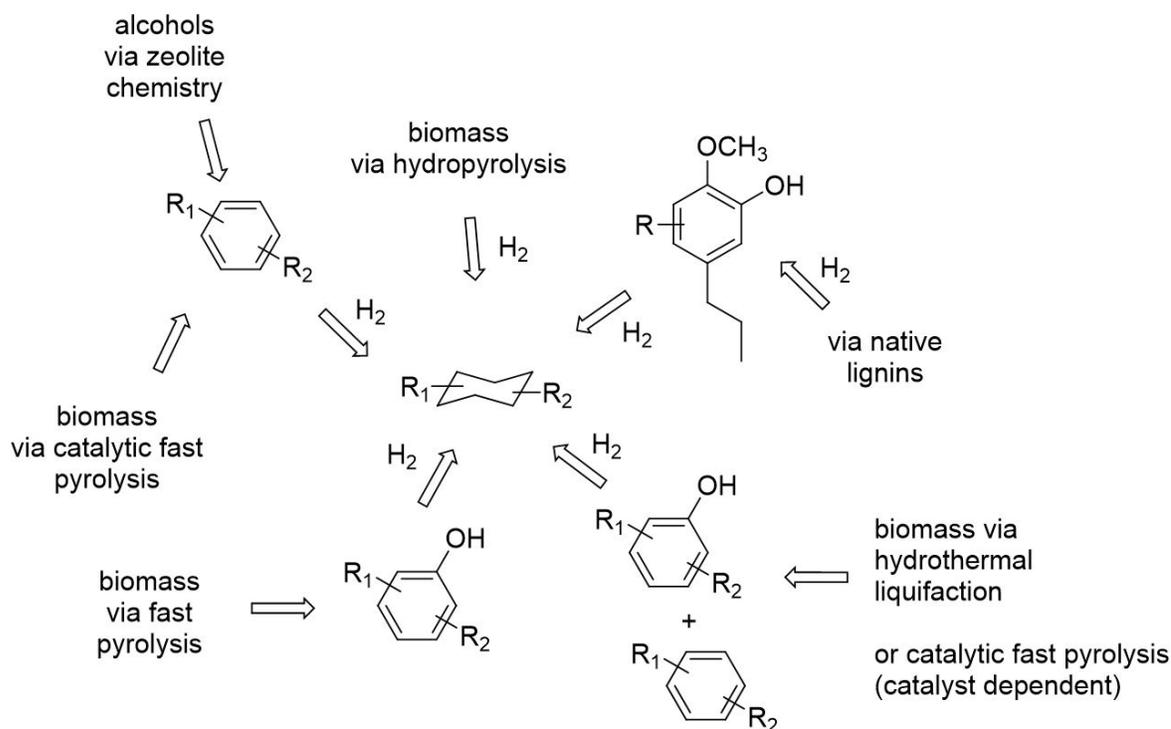


Figure 16. Routes to cyclohexanes that can be synthesized in the jet-fuel range

5.3.1 Zeolite-Catalyzed Aromatization Followed by Hydrotreating

Oxygenated compounds can be deoxygenated and aromatized using zeolite-type catalysts. The oxygenates can be simple, such as methanol or ethanol, or complex, such as mixtures of alcohols, carbonyls, and carboxylic acids. Two example sources of complex oxygenate streams are the hydrodeoxygenation of sugars (as developed by Virent) and pyrolysis vapors. Industrially, zeolite aromatization of oxygenates is established, as the chemistries are all variations of methanol-to-gasoline chemistry. There is a third example in the ASTM approval queue being piloted by Shell (IH²): hydropyrolysis, which is a catalytic pyrolysis process incorporating hydrogen gas. The product mixture from the hydropyrolysis reactor is fractionated (distillation) and the aromatics are hydrotreated.

For purposes of simplicity, three challenges in zeolite-based chemistries are highlighted:

- **Loss of carbon to coke:** Coking occurs in all zeolite reactions; the challenge appears to be greater as the oxygenate mixture becomes more complicated from simple alcohols to mixtures that have diols, carbonyls, and carboxylic acids.
- **Catalyst stability:** Steam formed during the reaction can damage the structure of the zeolite, an aluminosilicate. Research is ongoing in industry and the Office of Basic Energy Sciences in stabilizing zeolites to hydrothermal conditions.
- **Gasoline versus jet range:** Aromatization chemistry often favors gasoline range. Alkylation chemistry (reactions of aromatics and alcohols) can increase the content in the jet-fuel range.

In general, converting aromatics to cyclohexanes will require three moles of hydrogen gas. While the product mixture will vary, an example from a patented ethanol-to-cyclic process at PNNL has a composition of *n*-alkanes (0.3%), iso-alkanes (6%), monocycloalkanes (75%–85%), dicycloalkanes (6%–16%), and alkyl aromatics (2%–3%).¹³

5.3.2 Phenol Hydrogenation

Phenols are the building blocks of lignin and hence are produced by deconstructing lignin. Native lignin, after separation from carbohydrates, can be cleaved through hydrocracking and similar means to make complex phenol mixtures. Various pyrolysis techniques also produce phenol-rich streams. Examples include fast pyrolysis; catalytic pyrolysis, which depending on the catalyst and conditions may produce mixtures of aromatics and phenols; and liquefaction, which produces mixtures of phenol and aromatics. Phenols can also be produced by fermentation.

Hydrotreating is well-established chemistry; however, not all phenol mixtures are thermally stable. Fast pyrolysis oil, for example, has low stability, whereas bio-oils from a catalytic process using inexpensive (throwaway) catalysts such as “red mud” and other bifunctional catalysts engineered for robustness¹⁴ and product streams from HTL are more stable.

Challenges to phenol hydrogenation include:

- Excess hydrogen use: In the complex streams that contain small oxygenated species, hydrogen is consumed, thereby removing oxygen from molecules that form water and light gases of little value. This significantly increases cost. Removing light oxygenates before hydrotreating improves hydrogen utilization. This is done naturally in some liquefaction processes; the hydrogen demand for HTL biocrude is half that of bio-oil from fast pyrolysis, and hydrogen demand for upgrading some catalytic pyrolysis oils is also much lower, and the small organics can be treated in subsequent operations.
- Pyrolytic techniques favor products in the gasoline range: Dearomatizing gasoline is a worthy goal, but the gasoline-range cyclohexanes do not meet the necessary octane requirement. Hence, fractionation of gasoline- and jet-range material is needed. Shell fractionates IH² liquids before hydrotreating, thereby only hydrotreating fractions that require low aromaticity. Low-cost fractionations are a potential area of research. A second area of research is an alkylation step that reacts low-molecular-weight oxygenates with phenols to increase both carbon yield and extend more of the mixture into the jet- and diesel-fuel ranges.
- Lignin will need to be non-recalcitrant if it is to be a feedstock for jet fuel: Pretreatment technologies will need to leave lignin in the most native form but also provide sugars in a highly usable form.

Phenols require four moles of hydrogen to produce cycloalkanes, one mole to remove oxygen, and three moles to saturate the ring. Lignin species that have more than one oxygen on either the ring or the chain will require additional hydrogen.

One example of possible fuel composition comes from work between PNNL and CanMET energy—part of the Canadian government’s Green Aviation Research and Development Network project—showing jet-range hydrocarbon of alkanes (6%), iso-alkanes (5%), monocycloalkanes (40%), dicycloalkanes (20%), polycycloalkanes (4%), alkylbenzenes (7%), tetralins/indanes (12%), and phenols (6%). Additional hydrotreating would be required to reduce the phenols to zero and would also reduce the aromatics to meager

¹³ Data from PNNL, from an analysis by Jim Edwards on one-step ethanol to jet fuel.

¹⁴ National Renewable Energy Laboratory’s (NREL’s) platinum-on-titania catalyst is an example of a thermally stable, fast-pyrolysis catalyst demonstrated at bench scale. There are other examples from industry.

amounts, thereby increasing the mono- and bicycloalkanes and perhaps also the iso-alkanes (from ring opening). Such a mixture would be an intriguing jet fuel.¹⁵

5.4 Cycloalkanes, Other Ring Sizes, and Fused Rings

While much is known about the fuel properties of alkylated cyclohexanes, less is known about other ring structures that are available from biomass sources through catalysis and fermentation.

5.4.1 Ring Contraction

Five-member rings can be produced from cyclohexanes using a catalytic route that causes a ring contraction, and such research has been sponsored by BETO (PNNL unpublished research). This chemistry is used in petroleum refining and has been applied to pyrolysis oils to improve gasoline fuel properties at PNNL (McVicker et al. 2005; McVicker et al. 2002).

5.4.2 Ring-Forming Reactions

Larger and smaller rings sizes are possible to produce from renewables (Figure 17). BETO announced a recent award to fund work that converts isoprene to cyclobutane and cyclooctane. Three-member rings are produced for specialty chemicals and can be made from olefins using carbene chemistry.

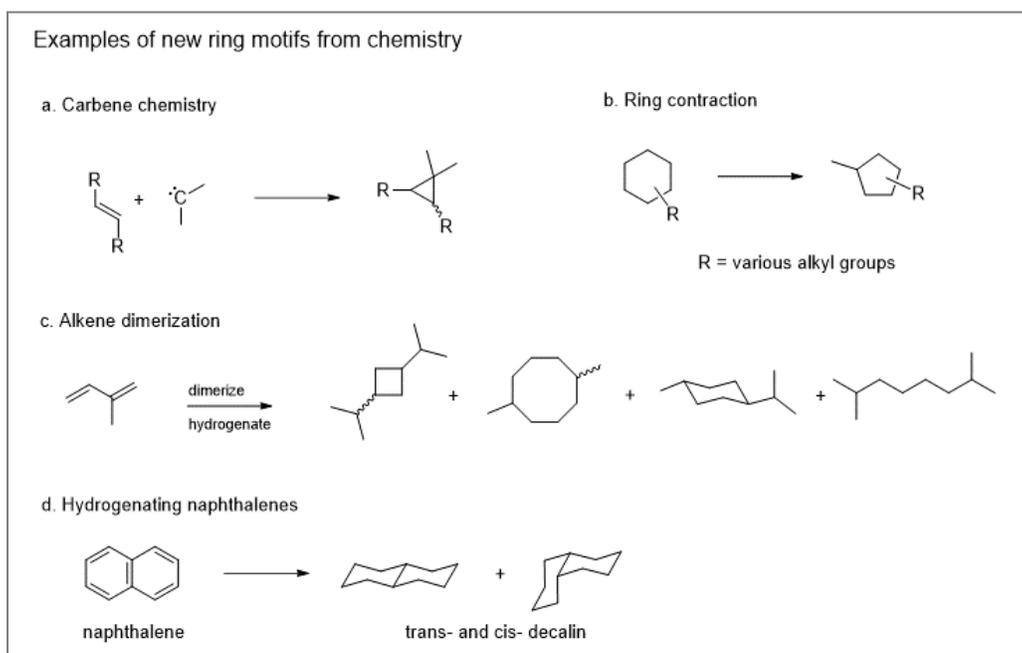


Figure 17. Smaller and larger rings from 3 to 8 carbons

Less is known about properties of larger and smaller ring sizes because they are not common in fuels. Because various ring structures are available from biomass, this as a knowledge gap that needs to be addressed. However, the cost of the compounds will have to be competitive and the value of the molecules high if this approach is to be used.

5.4.3 Ring Motifs in Wood Extractives and Fermentation

Biotechnology presents new possibilities for providing interesting possible ring structures (Figure 18). Natural product extractives such as turpentine are one source of new cyclic compounds. However, to achieve the

¹⁵ Olarte, M. V., A. Padmaperuma, E. Christensen, J. Ferrell, G. G. Neuenschwander, L. J. Rotness, A. H. Zacher, R. Gieleciak, A. Alvarez-Majmutov, and J. Chen, PNNL project document, unpublished.

amount required for fuel markets, fermentation of sugars may be required. The cost will need to be reduced if these products are to be industry-relevant.

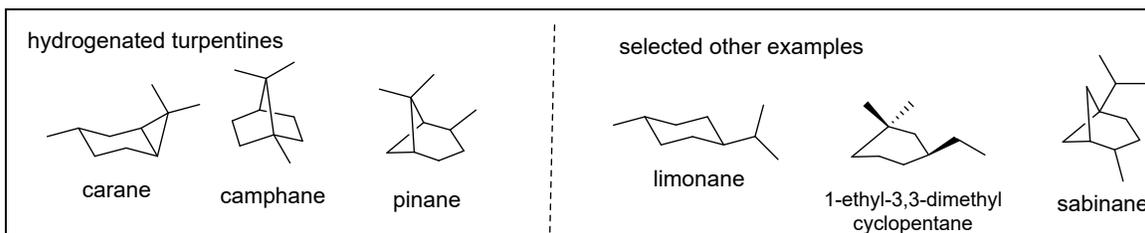


Figure 18. New ring structures, fused rings, and different ring sizes from nature

5.4.4 Esoteric Cycloalkanes

There are many esoteric cycloalkanes—from adamantane to cubane—and various molecules from sesquiterpenes to ladderanes are under study within BETO. Interest in the highly strained compounds arises from the desire to increase energy density and specific energy. Simply having a strain in a molecule is not enough to improve energy content, as many strained molecules have poor specific energy. Furthermore, alkyl substitution on esoteric rings often results in moderating the fuel property of interest. For example, alkyl-adamantane has properties more akin to common ring motifs (Harvey et al. 2016). Esoteric compounds that offer high energy density and specific energy may have flaws in other fuel properties that will strictly limit their blending levels. Such flaws include high melting points (e.g., cubane, one molecule of interest, melts above 100°C).

BETO is currently examining several molecular structure motifs for fuel properties. Those shown in Figure 19 were presented at the Advanced Bioenergy Leadership Conference and contained four- to nine-member fused-ring systems (George et al. 2018). Many of the parent compounds are sesquiterpenes containing 15 carbons with unsaturation and are of interest for their pharmacological properties; examples of terpenes containing 10 carbons may be a better fit for SAFs if they can be prepared at a sufficiently low cost.

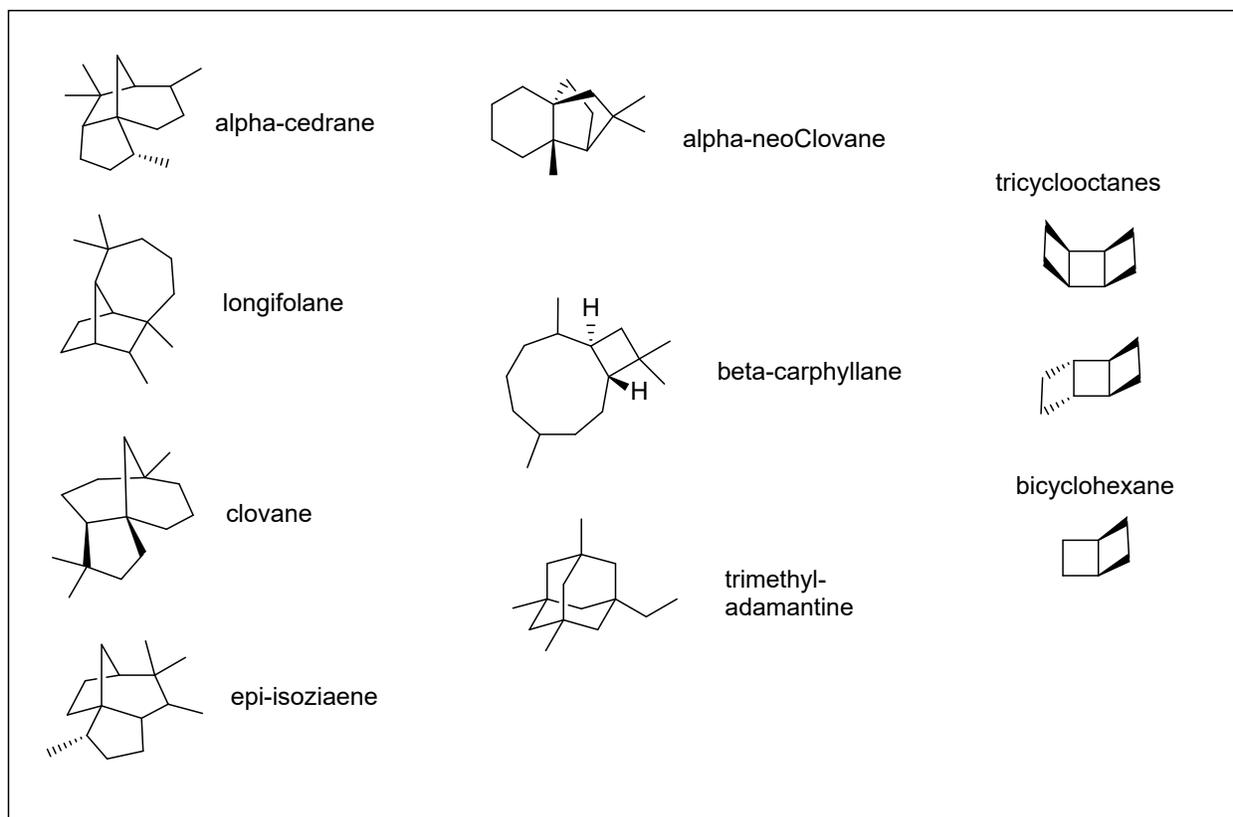


Figure 19. Esoteric molecules under examination for fuel properties

5.5 Low-Aromatic, High-Energy-Content Fuel Properties

Research co-supported by the Vehicle Technologies Office and BETO in the Co-Optima initiative, designed to look at light-duty vehicles, is not addressing underlying gaps in understanding fuel properties, and hence structure–function relationships, required for aviation. Further, the types of hydrocarbons desired for aviation vary dramatically relative to the needs of ground transportation. Combustion R&D and analysis beyond what is done in Co-Optima is an opportunity for new work within this program. Energy content is only one of many properties a jet fuel must meet. There is a rich variety of ring structures, from substituted cyclohexanes to esoteric molecules that offer a variety of ring sizes and fused rings. Further, the potential cost–value relationship should be understood regarding blend limitations.

5.5.1 Gaps in Understanding Cycloalkane Properties

The energy density of many cycloalkanes is higher than that of iso-alkanes, while the sooting behavior is less than that of aromatics. Therefore, these molecules can potentially have compelling advantages as integral blending components in a jet fuel that has low aromatic content. Today, there are no general rules to predict the behavior of fuels composed of various cycloalkanes of various ring sizes, conformers, fused rings, and level of branching. Research opportunities related to cycloalkanes include:

- Cycloalkane molecules from biomass will likely be blended with Jet A fuel for the foreseeable future. Understanding the bulk properties of blends and blending behavior is needed.
- Understanding the fundamental properties of mono-cycloalkanes and how these properties vary with the number of carbon atoms in the ring during spray atomization and combustion.

- Cycloalkanes, including those derived from lignin, will almost always have alkyl chains. An understanding of the impact of the length of the alkyl chain and isomerization on molecular properties is also necessary.
- Many biomass-based cycloalkanes can have multiple rings in many configurations. An example may be bicycloalkane, where two independent rings are tethered through an alkyl chain. Another example may be two rings that are “fused” together by sharing two carbon atoms, such as decalin. The carbon numbers of molecules in both examples can be the same, but their properties may be very different. Esoteric examples include additional fused ring structures.
- Some results show favorable swelling characteristics when using fused bicyclic alkanes. These characteristics are a mechanism for the complete removal of aromatics from jet fuel, such as decalin. The removal of required aromatics will lead to reduced aircraft particulate matter and higher specific energies. Additional work on the swelling characteristics of fused bicyclic alkanes and other material compatibility is needed.
- Safety is critical in civil aviation and more work is needed to understand the viability of strained compounds for meeting civil aviation needs.

5.5.2 Quantifying the Value of SAF

SAFs that have higher energy content, high thermal stability, and low aromatic content used at large scale can benefit the practical needs of a mission and perhaps other functions such as maintenance. Such benefits need to be quantified and understood within the larger feedstock–production–mission system. Technology opportunities and optimizations exist in this space that may further refine goals and collaborations across the fields of science, agriculture, and engineering.

Nominally, performance benefits can be attributed directly to the specific energy and energy density improvements via payload–range curve studies.¹⁶ A conceptual analysis of the thermal stability benefits of an energy-rich fuel suggests that a >3% decrease in specific fuel consumption may be possible in newer engine designs, combined with an approximately 5% drop in airline expenses associated with maintenance. Anecdotally, one engine company at the JET Workshop suggested that increases in thermal stability could revolutionize the engine market, driving down multiple costs. The required market penetration of SAFs to have this effect remains highly uncertain.

Near-term impacts: Increases in specific energy and energy density can be more rigorously quantified and bounded. Current projections of the benefits of higher-energy fuels are limited in their applicability across airlines operations and aircraft that could see the most significant benefit. Discussions and collaborations with airlines and engine OEMs are still in their infancy.

Work needs to be done on quantifying the opportunities for benefits of high-energy SAF under the three scenarios outlined throughout this report—minimization of aromatics, replacement of aromatics, and addition of novel molecules. Having a sense of the magnitude of these benefits is essential. Savings would need to be demonstrated in real-world scenarios before airlines would pay more.

Mid-term impacts: Reduced maintenance requirements from increased thermal stability, while not currently quantified, would not require hardware augmentation. As one participant noted at the Cleveland meeting, a fuel with high thermal stability has the potential to disrupt industries within the aero-engine space, although challenges would need to be overcome to gain benefits from higher-thermal-stability fuels. Investments here could be low-hanging fruit in the quantification of benefits.

¹⁶ Modeling supported by BETO at Georgia Tech is suggesting as much as a \$0.54-per-gallon value added for a hypothetical high-energy-content SAF. Modeling SAFs that are attainable is needed. Lowering the cost of SAF remains a paramount need.

Long-term impacts: The conceptual benefits of SAF with higher energy and thermal stability need to be more thoroughly and broadly explored. Increases in thermal stability are already aligned with the OEM research trajectories of increasing compression ratios and commensurate thermodynamic efficiency. Studies referenced above on thermal stability suggest a 14% potential improvement in specific fuel consumption. This result needs to be further vetted and stress-tested. The propagation of this to real benefits will require new OEM hardware that can use the fuel improvements. However, investigations in this realm require buy-in from multiple agencies at a minimum, with OEMs and fuel producers further enabling the rate and depth of progress in a co-optimization methodology. Undoubtedly, this path offers the most general benefit to all fuel, engine, and airline stakeholders.

5.6 Quantifying the Value Added with SAFs

Several performance, value-added fuel properties have been listed here. These properties are listed because industrial stakeholders have identified them as properties for which they would be willing to pay. However, the quantification of the additional value remains uncertain, although modeling can provide potential opportunity. Questions regarding these cost–benefit thresholds need to be answered to give pointed and clear requirements for successful deployment. Nominally, the benefits from properties listed in Chapter 2.1.1 need better quantification. Initial work has notionally quantified benefits from increases in specific energy and energy density. However, the monetization of thermal stability and sooting/particulate emissions is not as clear. For this work, it is important to understand and establish theoretical limits. Further study could then refine potential value with industry engagement.

5.7 Summary of Fuel Molecules

There is an R&D opportunity to further reduce cost of iso-alkanes and cycloalkanes. These two families of molecules provide all the properties needed in jet fuel. Aromatics and *n*-alkanes will often be coproduced; however, it is important for researchers to understand that their primary production is not an optimal research area.

Larger molecules can be cracked to produce jet-range molecules. One challenge is the low specificity of the chemistry, where low-value naphtha is coproduced. Chemistries are available that could have higher specificity, but require strategically placed double bonds, as is the case for carinata oil. Thermal chemistry, such as supercritical liquefaction, is being pursued as an alternate way to process lipids, and the fuel is at the balloting stage for ASTM approval.

Small molecules can be built up into jet-range molecules. Five chemistries—olefin oligomerization, aldol condensation, Prins condensations, ketonization, and Guebert chemistry—cover the functional groups common in bio-derived species, including olefins, carbonyls, and carboxylic acids. Building small molecules up provides the potential for better control of carbon chain length. BETO is currently supporting oligomerization chemistry.

Cycloalkanes offer densities and swelling capacities that complement the high specific energy of iso-alkanes. Cyclohexanes are easily assessable from aromatics using thermal catalytic processing of total biomass and from depolymerization of lignin. A significant question is defining the cost–value proposition of the added hydrogen to reduce aromatics to cyclohexanes. One industrial process is being tested by industry, the Shell IH² process, which fully hydrogenates the jet fraction to produce aromatic-free, cyclohexane-rich jet fuel.

Smaller and larger rings are also possible, including those with three, four, seven, and eight carbons. Fused rings with a variety of ring structures from four to nine carbons are available from fermentation pathways. Many compounds in this class are 15-carbon sesquiterpenes. Ten-carbon terpenes will likely be more applicable for SAF. Understanding the cost drivers and reducing cost will be necessary for these to be used in fuel applications. A hydrogenated sesquiterpene, farnesane, is approved for use today. It is produced commercially but not used in fuel application; industry analysis points to the cost of production as a

hinderance. Before pursuing other terpenoids for fuel applications, an understanding of how to reduce the cost of production is needed.

Modeling potential value can be done at a relatively low cost and provide information to the community. The value proposition of these fuels could be done with combustion modeling, small-quantity testing, structure–activity determinations on performance properties, and a study on the benefit of thermal stability on coking and engine design with strong engine company support. It is important to understand fuel properties before proceeding with development of producing the various possible compounds.

6 R&D – Cost Reduction

Generally, TEA results for most pathways show that the two most significant contributors to cost are the feedstock costs and capital cost. These are considered in this chapter.

6.1 Feedstock-Related Research

In our analysis, feedstocks ranging from lipids (fats, oils, and greases), sugars, lignin, and whole biomass (cellulosics) were considered. Feedstocks are the primary cost contributor to biofuels. Rethinking feedstock sourcing and the means of reducing costs while doing less harm to watersheds and land is a critical activity.

6.1.1 “Solve Another Problem”

Raw materials are grown or derived to provide value to the producer. Farmers are seeking the highest value for their lands. At the same time, environmental services are needed to improve soil and water quality. Solving another problem, such as providing an environmental service, provides new raw material options for biofuels, particularly materials already collected.

- Farmers grow biomass on land between crops for other purposes, such as soil preservation, nutrient recovery, and erosion control. All are examples of biomass used for an environmental service. Because this biomass is grown not as feedstock, but for another purpose, there may be opportunities to obtain it at a lower cost compared to purpose-grown crops. Often, the new crop can be mustards and other crops rich in oilseeds ideal for distillate and mid-distillate fuels. In the arid western United States, fields can lay fallow for multiple years and still require care to break down vessels to preserve water retention. Growing a crop designed to improve soil and water retention for the fallow years provides a different value proposition. While crop research is mainly conducted by USDA and the Office of Science, understanding the crops grown and how they can best be converted belongs to EERE. Further, by working together, crops can be chosen that can more easily be converted to jet fuel.
- Waste feedstock such as manures are an environmental challenge. Their use in anaerobic digestion to produce biogas has low commercial value but is considered because the environmental service provides value. The return on investment can be improved by making a product of higher value than a medium-Btu gas. One method of improving the return may be to arrest anaerobic digestion midway, produce volatile fatty acids, and then catalytically upgrade them to hydrocarbon fuels. Approximately 2,200 anaerobic digestion systems are in operation in the United States at present, and many of them are close to major airports where there is a demand for SAF. Anaerobic digestion biogas capacity in the United States is estimated to be approximately 431 trillion Btu (NREL 2013), equivalent to over 3 billion gallons of jet fuel per year. Waste gases that are rich in CO could have an enormous global impact, exceeding 32 billion gallons without including syngas.
- Similarly, environmental and other services can be addressed and wet, dry, or gaseous carbon feedstocks can be available at low cost. Other examples besides manures are landfill gas, landfill solids (sorted and unsorted MSW), and sludges from wastewater treatment plants. These require simple technologies to produce intermediates that can be cleaned and further processed to fuels. Such technologies can include liquefaction and gasification, as well as anaerobic digestion.

- Woody biomass residuals from forest production, wildfire mitigation, and forest health operations are available in many regions of the United States. Where TEA shows these residuals to be available in quantity and at reasonable cost, there are opportunities for SAF to be part of value propositions that may include products like biochar (pyrolysis) and lignosulfonates (from sulfite pretreatment pulping). Emerging processing technologies could create lower-capital options for the production of sugars and clean lignin and could be paired with ATJ SAF processing.

6.1.2 Collected Carbon from Existing or Developing Processes

Firms that produce tires are developing technology to extract rubber resin from guayule biomass using solvent extraction processes, and therefore have already factored in biomass costs and the capital infrastructure to grow, harvest, and grind the biomass to extract the rubber resin. The residual biomass after resin extraction has a low value and must be disposed. While collected residues present an opportunity for low-cost raw materials, there may be higher-value uses of the residue than fuels. Nevertheless, SAF can be developed for residue biomass for which capital, harvesting, and preprocessing costs have already been paid.¹⁷

Anaerobic digestion firms have already made investments in collecting and processing low-value waste to produce low-value biogas. These investments can potentially be repurposed to make volatile fatty acids, which then can be upgraded to SAF via ATJ or aldol condensation pathways, resulting in additional value from these investments. As discussed previously, there is more than enough capacity to supply a significant part of the jet fuel market. Anaerobic digestion systems are well-suited for this opportunity because they are located close to large cities where the waste feedstock is created and where large airports have a demand for SAF. These systems would be relatively small and thus capital requirements would be low. Benefits would be derived from process intensification to improve capital effectiveness.

6.1.3 Waste Gases

An increased emphasis on collected underused renewable carbon and other carbon in waste streams that otherwise has a liability can change the cost paradigm. Industrial waste gases, rich in CO, can produce 32 billion gallons of aviation fuel globally.

Likewise, MSW is an increasing problem. Gasification of unsorted MSW is done today in Japan. Using the synthesis gas to make fuels rather than power is a tremendous opportunity. There is an opportunity for waste-gas research to entail more than FT; waste-gas fermentation is commercially practiced today.¹⁸

Anaerobic digesters are becoming more prevalent. While anaerobic digestion does not use waste gases, it does produce methane-rich gases diluted in CO₂. Other methane-rich gas sources are not being utilized and provide R&D opportunities between EERE and the Office of Fossil Energy.

Arrested methanogenesis, a form of anaerobic digestion, offers options for producing volatile fatty acids that could be upgraded via various chemistries, such as hydrogenation (greatly increasing hydrogen demand) or ketonization (reducing carbon yield by loss of CO₂), followed by further upgrading to obtain the required carbon numbers. The feedstock–reactor interface could be expanded with new thinking about how to reduce cost in distributed processing applications that arise from anaerobic digestion and waste-gas sources.

6.1.4 CO₂ as a Carbon Source

The interest in reducing atmospheric CO₂ is prevalent among U.S. companies that compete in the global markets, as well as some state governments.

¹⁷ Guayule is a perennial desert shrub and USDA is investing in its cultivation for use in natural rubber with the residual to be converted to jet fuel. The project is led by the Center for Sustainable Bioeconomy for Arid Regions, PI Kim Ogden.

¹⁸ The first steel mill waste-gas-to-ethanol facility is now operating in China (LanzaTech 2018). Municipal solid waste has also been demonstrated in Japan (LanzaTech 2017a).

Unlike the waste gases discussed previously (CO and CH₄), CO₂ does not contain usable energy. Hence, CO₂ is merely a source of carbon in which all the energy of the fuel would need to come from an external source: hydrogen or electrons.

As an example, a Canadian company has initiated contact with the Commercial Aviation Alternative Fuels Initiative (CAAFI) about a CO₂-based FT fuel. Hydrogen gas combined with water–gas shift chemistry provides the syngas for FT (Csonka 2018).

A second example where hydrogen is used to provide energy involves fermentation of a refinery waste gas stream containing CO, CO₂, and H₂. In this case, the organism facilitates the biological equivalent of water–gas shift chemistry. The stoichiometry of the reaction is five equivalents of H₂, one equivalent of CO, and one equivalent of CO₂.¹⁹

Research based on the use of electrons to reduce and convert CO₂ is popular today and the focus of many research groups. A clean source of CO₂ is from fuel ethanol production, in which a small 40-million-gallon-per-year facility produces 114,000 metric tons of CO₂ during the fermentation process. The total domestic production of CO₂ from ethanol is 42 million metric tons. The energy required to convert the CO₂ to carbon monoxide is 12.6 MJ/kg and converting water to hydrogen is 176 MJ/kg based on Gibbs free energy. With a synthesis gas at a ratio of 1:2 CO to H₂, either FT or ATJ could be used to produce jet fuel. The electrical power requirement to convert the CO₂ and water to synthesis gas is 90 MW for a single ethanol facility and in excess of 30 GW for current U.S. ethanol facilities (Figure 20). To put this in perspective, the largest dam in the United States, Grand Coulee, produces 6.8 GW of power. The second-largest wind farm in the United States is 845 MW and exceeds 300 turbines at the cost of \$2 billion to build. The electrical power demand to add energy back to CO₂ to be used as a fuel or fuel precursor is high.

While the use of CO₂ “solves another problem,” and when sourced from ethanol plants is clean and accessible, its use for fuel applications is less straightforward as the cost and environmental stress will need to be assessed. There are cases where CO₂ conversion may make sense, such as when H₂ is also part of the waste gas.

¹⁹ A demonstration facility is being built at IndianOil’s Panipat Refinery in Hayrana, India, employing LanzaTech technology. The estimated cost of the demonstration facility is \$55 million (LanzaTech 2017b). The stoichiometry is from LanzaTech.

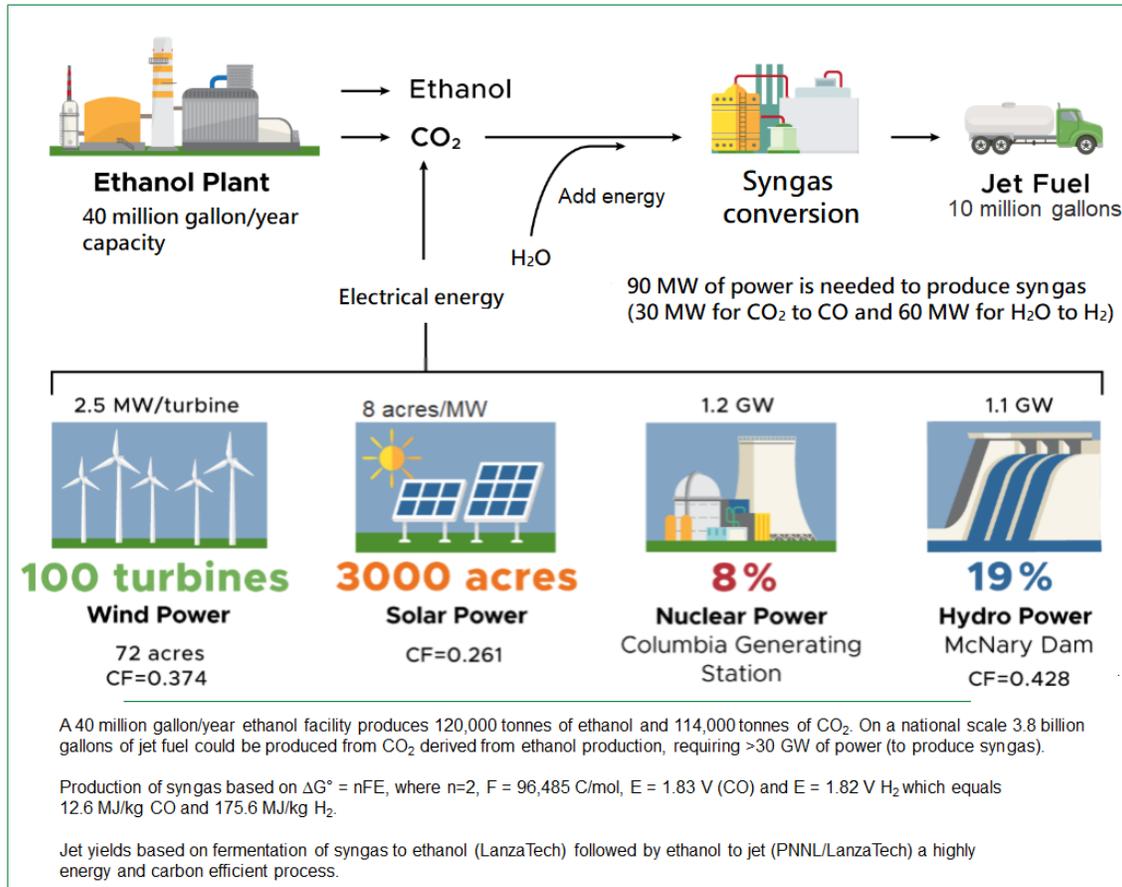


Figure 20. CO₂ from ethanol production conversion to jet fuel via synthesis gas

CF = capacity factor

While all carbon sources should be considered, electrons to convert CO₂ at a meaningful scale are not going to be free. Even at a low cost, \$0.02–\$0.04 per kWh, it is challenging to achieve the economics required to produce fuels from CO₂ and water (Weber 2019; Jouny, Luc, and Jiao 2018).

6.2 Reducing Capital Cost

The simplest level of process intensification either reduces the number of unit operations that are required to be built or reconfigures unit operations to reduce cost. This can be done by reducing or combining unit operations, minimizing the number of separations required in a process, or using infrastructure that is already in place. Process intensification can also refer to using new chemistry designed for the scale of biomass rather than petroleum.

6.2.1 Use Current and Distressed Infrastructure

Use of existing depreciated equipment and infrastructure or coprocessing with other streams can potentially be a powerful approach to reducing capital costs. Conversely, not using infrastructure in place incurs costs.²⁰ Following are examples of using existing infrastructure:

²⁰ Researchers have suggested using a second delivery system for SAF to airplanes but have not accounted for the costs incurred of not using the infrastructure in place. SAF will need to be delivered in the current hydrant systems.

- Refinery infrastructure: Hydrogenation using imported pressurized hydrogen gas is best done at a larger scale at a central refinery—the “hub” of a hub-and-spoke model. When using the infrastructure of a petroleum refinery, even a separate reactor built within the boundary of the refinery reduces cost.
- Send other streams to a refinery: Nearly all processes that produce SAF blendstocks in amounts that can be blended above 10%–15% also produce lights and heavies. Achieving the highest value from each stream is critical. Petroleum refineries provide one means of using the other streams or blending the streams in a way that is cost-effective and leverages depreciated capital.
- World Energy-Paramount located its 45-million-gallon-per-year SAF/renewable diesel facility on a former asphalt refinery that had existing fuel storage, a truck rack, rail storage, and a pipeline connecting to southern California distribution hubs. Hydrogen is trucked in, and the light fraction (naphtha) is sold into the gasoline market.
- Other infrastructure: Facilities, including paper mills and anaerobic digestion systems, are underutilized. Analysis to understand location and opportunities provide a means to reduce cost. Additional examples include Gevo, which uses dry-mill infrastructure to produce iso-butanol, and Poet, which has built a cellulosic ethanol plant next to a dry mill to share auxiliary units. A final example is corn ethanol plants, which are adding new unit operations to convert carbohydrates in distillers’ dried grains with solubles to ethanol, providing a cellulosic renewable identification number and building on existing infrastructure.

6.2.2 Petroleum Refinery Integration

Biomass being coprocessed in petroleum refineries is now occurring. The first materials to be coprocessed are lipids (fats, oils, and greases). These feedstocks go into hydrotreating units that primarily feed distillate streams. BETO is funding R&D studying coprocessing of other biocrude oils. An evaluation of the fractions—jet in addition to gasoline and diesel—could be added to such a study.

Pyrolysis oil co-refining is perhaps near commercial and can be licensed from UOP/Envergent to produce fuels with 2%–5% biofuel content. BETO is presently conducting bio-oil coprocessing trials at the Andeavor Martinez Refinery and already has capabilities to conduct coprocessing at its National Labs. One challenge to investigate is if the technology can be extended to SAF, and if the co-processed fuels could meet the tight specification. The technology would require hydrogen transfer catalysts, or more likely fractionation of the jet-range hydrocarbons. This research could include an evaluation of additional hydrotreating to produce cycloalkanes. Note that today, the only renewables that can be coprocessed in a refinery are fats, oils, and greases. Any other coprocessing will require ASTM approval.

6.2.3 Separations

Separations and purifications are a significant cost driver. While not reviewed in this report, it is important for researchers to understand the value of separation needs and increasing the focus on reactive separations.

Separations involve two opportunities:

- Reduction of the number of separations: A process may be less expensive if a separation step can be eliminated, even if the conversion is less elegant. For example, while there are catalytic forms of HTL, the cleanup requirement to protect the catalyst may make the overall process less optimal than using thermal HTL, eliminating a cleanup step up front.
- Reactive separations: A combination of reactive steps with separations step. Examples include reactive distillations in which a catalyst is combined as part of the distillation and continuous membrane separation or liquid–liquid extraction with fermentation.

6.2.4 R&D Needs for Small-Scale Distributed Refineries

The total capital cost and scale of a project, such as for FT processing, is often a deployment hurdle. This capital cost can be exacerbated for biomass because the local supply curve for feedstock is generally inelastic,

resulting in significant increases in price with increases in volume. Because feedstock cost was identified as a critical component of SAF production cost at all three workshops, biomass-based processes need to be developed at a small scale to reduce biomass demand (and therefore feedstock cost) at a location.

Small-scale plants must be designed to change the process throughput rate-limiting step paradigm so that the process economics are described by a different production curve that allows higher capital efficiency at lower throughput. Examples of the change of rate-limiting step paradigms can include a change from batch to continuous operations and the use of membrane and microchannel reactors, which scale based on area rather than volume. Labor costs generally become prohibitive for small-scale production facilities, so a high degree of automation is also required.

Small-scale plants can be mass-produced at a significantly lower cost, and manufacturing can enable economies of scale. While the engineering and production of reactors is closely aligned to the mission of the Advanced Manufacturing Office, the chemistry and chemical engineering required to change rate-limiting phenomena in a process require essential science elements that are within BETO's mission.

6.3 Rethinking Biorefineries

6.3.1 Sugars to Products, Lignin to Fuels

Presently, the biological conversion pathway for lignocellulosic biomass has been to convert the sugars to fuels and the lignin to either power or products. The aromatic nature of lignin may make it particularly suitable as a feedstock for lower-cost production of cyclohexane derivatives with desirable properties as a higher-performance SAF. Sugar from cellulose may also be a more natural feedstock for biological conversion to chemicals and products rather than lignin.

An alternate paradigm would use lignin and residues as feedstock for fuels and sugars as a feedstock for bioproducts and biochemicals, both sourced from lignocellulosic biomass. The caveat in this approach is that the lignin to be used for SAF must be processable, which often requires it be as close as possible to its native form. BETO already has programs that remove significant lignin through solvent extraction or dual-mixed refrigerant types of mild processes. Lignin from these processes may be suitable to produce SAF. The sugars must not be harmed in such a process. Finally, in some manifestations, only easily removed sugars need to go into biochemicals, with residues added to lignin for production of fuels.

There are various ways that new paradigms could be executed. BETO is funding work in which the six-carbon sugars from hydrolysate are converted to a higher-value product but without the constraints on high sugar utilization or low biomass growth. Preferably all the residuals (e.g., lignin and cell bodies, unconverted sugar) are converted to biocrude oil using liquefaction. Internal data have shown a high fraction of upgraded biocrude oil is in the jet-fuel range. Understanding the fuel properties, particularly with enough hydrotreating to produce high cycloalkane content, is in order.

6.3.2 Focus R&D on Conversion Platforms That Provide Product Flexibility

Supporting R&D that provides biorefineries with fuel and product options is critical for viability; however, chemical coproducts do not decrease the cost of fuel production and fuels cannot be sustainably sold as a loss leader. Hence, R&D will need to continue its focus on decreasing cost of the fuel pathway, and TEAs supporting R&D are best used to identify where cost can be removed from the system. The trend to have TEAs show lower selling price by invoking value in other streams can be misused, although it is wise to seek the highest value from each process stream.

Consider how petroleum refineries maximize value. Petroleum refineries do not produce high-value products. Instead, refineries extract as much value as possible from each process stream using minimal added infrastructure and wasting little carbon. Petroleum refineries ship super-commodity chemicals, such as ethylene or benzene-toluene-xylene, to standalone chemical plants, specialty chemical plants, and pharmaceutical plants. These plants produce the many products such as petrochemicals (plastics, solvents,

monomers), personal care products, and others that demand higher value. R&D needs for producing a fuel differ from those for producing a monomer or a personal-care product. Hence, producing a high-value chemical product first is not going to support the R&D to bring down the cost of the fuel. Furthermore, a biorefinery, which is much smaller in scale, cannot support the capital to produce a myriad of fuels and chemicals and instead focuses on extracting the highest value from each stream.

There is an R&D opportunity that focuses on platforms in which a common intermediate, using standard or similar processing steps, can produce fuels or commodities based on market conditions, as this would reduce risk and add value. While there are examples of this in BETO's portfolio,²¹ a greater focus on the opportunities for platforms that support SAF and products using similar infrastructure could be a higher target.

6.3.3 Feedstock Flexibility to Use Full Capacity

Today, SAF is produced from lipids that can use low-cost feedstock such as fats, oils, and greases. However, lipid routes cannot meet the SAF volume demand alone with the current feedstock supply. New low-cost feedstocks are needed. Carinata research, funded by USDA, is a potential new source of lipids.

A low-cost source of lipids that are not currently utilized are fats, oils, and greases in wastewater sludge. Algae is another source of lipids on a longer-term horizon. However, algae production rates vary dramatically from summer to winter, even in places like Florida. The variance is easily 50%. While modeling average yields is appropriate, the capital to build a plant that is only intended for full operation part of the year is a problem. If such lipids were coprocessed with more abundant lignocellulosic biomass, the biorefineries could run at full capacity year-round, yield higher output, and optimize capital.

Feedstock–conversion interface research is needed for wet feedstocks that cannot be stored and for which coprocessing other biomass sources may be necessary. The interface includes reducing the cost of lipid extraction/purification and considering coprocessing lipid streams with other streams.

Research can build on what has already been learned from other programs, such as optimization of lipid yield during combined extraction and conversion processes, with liquefaction utilizing both storage lipids (free fatty acids and glycerides) and cell wall lipids (often phospholipids). Study of coprocessing lipid-rich streams with more prevalent biomass streams is in its infancy. Further, there is an opportunity to apply the concept of mixed biomass–lipid streams to both algae and wastewater sludge.²²

While HEFA is commercial, the lipid feedstock is purified extensively before processing, which adds cost. Biocrude oils will also need to be purified for long catalyst life. More R&D on purifications is warranted.

Fats, oils, and greases prevalent in wastewater sludge present an opportunity. Coprocessing using liquefaction technologies could improve the product profile of thermal processing of lignocellulose, providing higher impact (fuel produced). Liquefaction research can be done under wet conditions, either subcritical or supercritical, in water or with other solvents. Also, dry feedstocks could be considered using more standard pyrolysis techniques.

Regardless, R&D along the feedstock–conversion interface of a broader range of liquefaction conditions and mixed lipid–biomass feedstocks will bring value to the research and biofuel communities and produce a higher volume of fuel possible from lipids alone, and of higher quality than is possible from biomass alone regarding distillate fuel requirements.

²¹ As one example of multiple products in a biorefinery-scale facility, BETO and the Advanced Manufacturing Office are supporting research at PNNL for several fuel and higher-value products using alcohol as a platform. The chemistries and infrastructure required are similar for the various products and may be assessable without added capital.

²² Initial study of wastewater sludge indicates a fuel production potential in the United States of six billion liters per year.

6.4 Sourcing Hydrogen

Hydrogen demand is high for all biofuels and unusually high for SAF, where olefins and heteroatoms such as oxygen are not allowed for operational and safety reasons. In North America, the cheapest source of hydrogen gas is from steam methane reforming. This is not true globally; exceptions include areas where natural gas is expensive or not prevalent, including remote locations such as Hawaii and much of Europe, Africa, and Asia. Furthermore, at small distributed scales, use of pressurized hydrogen gas is cost-prohibitive.

A steam methane reforming facility produces 10 tons of CO₂ for each ton of hydrogen gas (Collodi 2010). Finding new low-cost sources of hydrogen gas can lead to reduced GHG emissions for petroleum refineries and biorefineries.

Renewable electrons can provide the reducing equivalents needed to remove oxygen or saturation of biomass-sourced molecules. Advances in electrocatalysis open distributed processing opportunities that allow use of dispersed carbon sources that are underutilized.

The use of electrons as a replacement of hydrogen gas in this application differs from the use of electrons to convert CO₂ to fuels in two aspects. First, the feedstock under consideration has available energy content. Second, there are examples where the reducing equivalents can be produced from oxidation of carbon that would be lost otherwise to the aqueous phase. This could theoretically be accomplished without bringing in outside renewable electrons. An example would be upgrading HTL biocrude oil. Oxidation of the wastewater has enough energy content to provide the reducing equivalents required to upgrade the biocrude oil.

Regardless of the source of electrons, whether from nuclear energy, renewable energy, or oxidation of carbon in wastewater, both high-resolution consideration of cost–benefit and high-fidelity supply-chain analysis are needed to determine the best use of electrons. Both catalyst research and analysis are areas that fit the BETO mission.

6.5 Analysis of Cost Reduction

DOE, FAA, and USDA have developed a suite of analysis tools that could be helpful for defining research questions that can bring down the cost of SAF. These have not been sufficiently coupled to supply-chain analysis tools or to analysis tools examining the potential value of jet fuel supporting different missions. Further, TEA and GHG results are inconsistent across the industry and do not address the economics associated with pioneer plants.

TEA provides essential information about where research could be prioritized to bring down costs. Used in this manner, TEA of various systems will be invaluable. TEA can also be used to rule out some processes, such as where the costs of inputs are higher than the value of the products. High-fidelity TEA is not needed for such “back-of-the-envelope” analysis. Using TEA to choose between two paths that are plausible can be problematic, as the uncertainty in the model output commonly exceeds the difference of cost between two routes. The use of TEA without understanding uncertainty is exacerbated by assumptions (positive or negative) on chemistry and for technologies at early technology readiness levels. Simply adding consistency to models is valuable but does not address the underlying issue of uncertainty, which requires uncertainty analysis.

The LCA of pathways that are not fully developed also have a high level of uncertainty that is not expressed in the model output. However, if LCA was done to inform research, it would be a valuable addition.

Supply-chain analysis tools developed by USDA’s Northwest Advanced Renewables Alliance and used in FAA activities can offer a new look at high resolution and a regional analysis that incorporates feedstocks, products, infrastructure, and other required aspects. Supply-chain analysis is valuable in research to define conversion requirements (size of plants and the location of facilities, utilities, and water) that offer valuable insights into the required technology, which informs science questions. While a supply-chain analysis has been

done on MSW (Englund et al. 2016), it has not been done on other feedstocks or for a broad number of potential routes.

6.6 Summary of Cost Reduction

Research provides an opportunity to reduce production cost. The opportunities extend to lowering the feedstock cost and increasing availability of feedstocks. Waste feedstocks that are already collected are “low-hanging fruit.” Feedstocks need not only include lipids and sugars; waste-gas streams, rich in CO, could have a significant impact on the global markets. Synthesis gas increases the impact even more. Finally, R&D needs for mixed feedstocks that include lipids and biomass present new opportunities.

Separations are a large cost driver and there are research opportunities on process intensification—reducing and eliminating, where possible, process and clean-up steps. Reactive separations reduce unit operations and cost. There is an opportunity for separations to be considered early in process-flow planning and not wait until the later part of process development.

Analysis can continue to be used to identify cost drivers and targets. The uncertainty in model output is high and discarding routes may be done more effectively using other criteria. Supply-chain analysis, in high resolution, can help identify new opportunities and research areas to drive down cost.

It is important to “start with the end in mind,” because the fuel property requirements for gasoline, jet, and diesel fuels dramatically diverge.

7 Summary and Insights

While Chapter 6 provides a summary of important areas where R&D could reduce cost and/or increase value proposition for producing SAF, this chapter outlines research opportunities to achieve the goals set forth by the commercial aviation industry. Reducing capital, production, and feedstock costs for SAF are the key requirements for its widescale deployment. In the longer term, providing a fuel that has improved properties, within the bounds of ASTM specifications, further improves the possibility for market pull. In the near term, however, expanding production capacity of existing approved fuels is critical.

7.1 An R&D Strategy for SAF

The commercial aviation industry must significantly reduce its GHG impacts to continue to grow and support global mobility and commerce. Through the ICAO, the industry has established CORSIA, which sets voluntary carbon-reduction standards during Phase 1 (through 2026) and mandatory standards during Phase 2 (2027 and beyond). SAF use will need to rise to greater than 30% of total jet fuel consumption by 2040 to meet ICAO commitments; on a global basis, this is greater than the total jet fuel currently consumed in the United States.

Because civil aviation cannot meet CORSIA targets by efficiency gains and improving engines and flight operations alone, SAF is required. Today, there are five approved SAFs, but their use is limited. SAF fuel price, including subsidies, must be competitive with petroleum-based fuels (Jet A) because the cost of fuel is up to 30% of the operating cost of an airline.

Airports also realize that the GHG impacts of their operations will eventually have a negative impact on their ability to serve their communities. Therefore, they are supportive in helping airlines with innovative models to serve as a fuel aggregator, reduce cost, and accelerate deployment.

Jet A pricing to corporate and other private users is considerably higher than prices that airlines pay. For example, Jet A fuel is sold to corporate and noncommercial airlines at prices ranging from \$3.37 to \$5.05 per gallon for airports in a 50-mile radius of Seattle-Tacoma International Airport. Reaching this market may be a strategy for early market penetration.

The ASTM D4054 approval and evaluation process for new fuels for jet engines is expensive and time-intensive, requiring up to 100 gallons for Tier 2 testing and up to 225,000 gallons if Tier 4 engine testing is required (Table 6). The evolution of jet engine design takes 14 to 19 years and is significantly more expensive, costing several hundreds of millions of dollars, when compared to fuel certification. Therefore, the same engines that are in service at present are likely to be in use for a long time in the future. Existing engines can, however, use fuel that is up to 15% more energy dense than the average energy density of Jet A fuel, and higher energy density correlates with improved performance such as longer useful range or increased payload for select missions.

Fuels are delivered in hydrant systems in which cost and LCA accounting is attributed to those who “pay for it.” A separate delivery system is expensive and takes up valuable space. Hence, SAF will be diluted with petroleum-based fuels to a significant degree beyond the 50% blend required by ASTM, as the fuel is stored and delivered in a single system to all planes serviced at an airport. This points to the primary need to reduce cost with a longer-term goal of improving performance.

Even within the constraints on SAF based on fuel certification and fuel/engine infrastructure, there is an opportunity to make renewable fuels that offer better combustion properties than fuels derived from petroleum.

In closing, the United States currently has a strategic advantage over other countries in terms of SAF, hosting the single most extensive collection of companies, approval experts, and researchers. Continuing the momentum in SAF R&D offers the opportunity for domestic companies to expand internationally, where experience currently lags behind the United States.

7.2 Insights on R&D

Bringing down cost and improving value must be properly balanced. The following sections summarize five prioritized opportunities for research to achieve these objectives.

7.2.1 Focus R&D on Low-Cost iso- and Cycloalkane Production

Conventional Jet A fuel contains *n*-alkanes, iso-alkanes, cycloalkanes, and aromatics. Of these four hydrocarbon classes, it is important for researchers to understand the importance of only two: iso-alkanes for specific energy, and cycloalkanes for energy density. iso-Alkanes and cycloalkanes offer desired jet fuel characteristics and require R&D, whereas *n*-alkanes and aromatics, while compliant with ASTM specifications, are limited due to poor low-temperature properties (*n*-alkanes) and poor combustion properties (aromatics).²³ Chapter 6 provides suggestions in detail as to R&D on the two classes that are complementary to current pathways and potentially new pathways. Examples of coprocessing with petroleum refineries are provided and allied R&D suggested.

The focus on iso-alkane is to provide new routes to build up small molecules, with a focus on five chemical reactions that span alcohols, carbonyls, carboxylic acids, and olefins. Additional work on parallel pathways for breaking down large molecules is also presented.

Cycloalkanes provide an area in which R&D could expand the understanding of structure–activity relationships with a balanced approach of cyclohexane derivatives that could be produced at relatively low cost with other ring structures. This study facilitates front-end combustion approval needs with back-end feedstock processing approaches.

²³ In addition to offering poor combustion (and thus being a primary source of sooting), aromatic production is relatively simple owing to its thermodynamic stability, and nearly any oxygenated source when passed over a zeolite-type catalyst produces aromatics. Targeted iso-alkanes and cycloalkanes are not as simple, and R&D is warranted.

7.2.2 Focus on Low-Cost Feedstocks

Chapter 6 provides more detail on concepts that can assist in reducing the cost of SAF. R&D is required on the fundamentals of conversion processes and engineering for pioneer (first-generation) biorefineries. Two priority areas include:

- Feedstocks that are already collected and extend an environmental service (e.g., those that “solve another problem” and thus change the cost structure). These can include manures, waste gases, and other municipal waste such as plastics that, under biological and/or thermal processing, can produce high-quality intermediates that can be hydrotreated using existing capabilities.
- Mixed feedstocks that include lipids and lignocellulosic biomass. This is complementary to commercial processes that use low-cost lipids and extend the raw material to include storage lipids (fats, oils, and greases) and cell-wall lipids (phospholipids) that are available in quantities that vary seasonally or need to be augmented. Mixtures of lipids with high-volume lignocellulosics provide new opportunities to increase production, including stable, year-round processing of wet feeds otherwise difficult to store.

7.2.3 Focus R&D on Conversion Platforms that Provide Product Flexibility

For biorefineries to be viable, they must be simple (e.g., low capital cost) and extract maximum value from each product stream. Focusing R&D on platforms in which multiple products can be produced from a common intermediate using common equipment is a means to reduce risk for biorefinery operators. This differs from concepts in which small biorefineries are expected to produce several different products requiring high capital (e.g., such as seen with a wet mill versus a dry mill) or in which a biorefinery is really a biochemical facility. Ethanol is an example platform and is affordable when sourced from a low-cost gas. Another example is a carboxylic acid platform, perhaps from arrested methanogenesis, using anaerobic digestion infrastructure. A platform based on a single molecule is likely easier than one based on a complex mixture. The key is that the molecule must be inexpensive.

7.2.4 Provide Replacement for Hydrogen Gas in Distributed Processing

Hydrogenation is ubiquitous in bioprocessing and particularly important for aviation fuels that cannot contain heteroatoms or olefins. There may be opportunities to replace natural-gas-derived hydrogen with renewable electrons that provide reducing equivalents needed to remove oxygen or saturation (e.g., hydrogenation of double bonds). Advances in electrocatalysis open distributed processing opportunities would allow use of dispersed carbon sources that are underutilized. Consideration of CO₂ as a new carbon source is highly popular. CO₂ contains no energy and all the energy in the fuel would have to come from an external source such as hydrogen or electrons. Electrons may be better used for carbon still containing energy. While all carbon sources should be evaluated, higher-resolution consideration of cost–benefit and high-fidelity supply-chain analyses are needed to determine the best use of renewable electrons in upgrading raw materials at the distributed level.

7.2.5 Refine and Expand Analysis

TEA and GHG results are inconsistent across the industry and do not address the economics associated with pioneer plants. Generally, TEA results for most pathways show that the two most significant contributors to cost are the plant capital and feedstock costs. One of the approved routes for producing SAF is the lipid pathway, which can use low-cost feedstock such as fats, oils, and greases. However, lipid routes cannot meet the SAF volume demand with the current feedstock supply. New low-cost feedstocks are needed.

Additional high-fidelity modeling beyond TEA and LCA that examines the resource supply chain at high resolution will be valuable to new fuel industry and help set research directions. Note that the model output can be quite different as the granularity of the model moves from the national scale to regional and farm scales. It is important that the models use the highest resolution (smallest scale) and aggregate up.

Finally, connecting the previously described models with key R&D funded in BETO and elsewhere will help define cost–value propositions.

7.2.6 Sequencing R&D to Achieve Impact in the Short, Medium, and Long Term

Desired short-, medium-, and long-term outcomes of R&D are described in this section.

Short-term outcomes include reducing the cost of and improving value propositions for fuels already approved or far along the ASTM process, or poised to enter the ASTM Fast Track process. These are the only short-term options given the length of time to complete the D4054 approval process.

Medium-term outcomes include expanding opportunities in additional pathways, such as pathways that result in cycloalkanes. These will require that candidate molecules be screened and that more information on the performance of various classes of cyclic hydrocarbons of various ring size and substitution be collected. In this timeframe, there will be more opportunities for feedstocks and better use of all product streams in the jet-fuel-oriented biorefinery.

Long-term outcomes include targeted fuel molecules that offer even better fuel properties and higher energy. Such molecules may be produced by biological conversion of biomass-based sugars through engineered microorganisms, catalytic pathways from sugars and lignin, or a combination of biotechnology and catalysis.

7.3 Cooperative Opportunities for R&D

7.3.1 Collaboration Between the National Laboratories

In the near term, it may be most effective for BETO to start a biojet effort under the existing programs at the National Laboratories, including consortia. This will enable a cost-effective leveraging of existing investments in terrestrial biofuels and accelerate research progress for SAFs. For example:

- Catalysis work to reduce net naphtha loss, improve building up small molecules, and for chemical production of cycloalkanes from sugars, lignin, alcohols, and diols can be incorporated into the Chemical Catalysis for Bioenergy Consortium.
- Biological routes for producing cycloalkane molecules, including terpenoids, sesquiterpenes, or ketonides can be incorporated into the Agile BioFoundry. In such an approach, R&D will be necessary to reduce cost of production organisms relevant for industrial use and also reduce fermentation and separation costs.
- The separations consortium can contribute to process intensification to reduce net capital costs, including reactive separations and lowering the cost of removing heteroatoms that will impact catalyst life.
- The Feedstock–Conversion Interface Consortium can support new pretreatments for providing lignin for cyclohexanes; a complementary focus on processing mixed wastes that are often wet is also important.
- Developing structure–activity relationships and retro-synthetic analysis can be helpful.

7.3.2 Intersection with FAA Center of Excellence and USDA

USDA has several exciting feedstock programs that intersect with fuel production, including jet fuel. Forming formal relationships with USDA or large projects can reduce redundancy. Likewise, activities in FAA’s Center of Excellence, ASCENT (Aviation Sustainability Center), and other programs are important.

An example of work that could build bridges is related to the ASTM D4054 procedure, which is onerous in terms of time and money. There would be great value to the research community if new fuels could be prescreened before they are submitted to ASTM for approval at volumes well below the ASTM 100-gallon requirement. Further development of Tier α and Tier β tests to achieve more effective prescreening will be helpful. Some enhancements to Tier α and Tier β tests could be the use of statistical predictive models to

account for uncertainty in the predictions. These prescreening activities could be evaluated at some level with the CAAFI R&D committee, both in the development of comprehensive and robust prescreening activities and the evaluation of candidate fuels.

7.3.3 Intersection with North American Partners

Several synergies and opportunities exist to collaborate in partnerships across North American. Canada, which has a high percentage of the worlds certified sustainable forests, and Mexico, which has a warm climate year-round, both offer unique opportunities for collaboration.

7.3.4 SAF Working Group

Finally, there is value creating an SAF joint working group that could include researchers and experts on aviation fuels that represent BETO, USDA, CAAFI, FAA, the National Labs, a fuel provider, a biorefinery, representatives from an engine OEM, universities, and representatives from Canada and Mexico. The working group would have an express charter that could include identifying the R&D needs appropriate for each partner and cross-fertilization programs across the agencies. Alternatively, additional focused SAF discussions with various stakeholder interests represented that further explore strategies for advancing R&D may add value.

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Appendix 1. Bioenergy Technologies Office Mission

The BETO mission is to develop industrially relevant, transformative, and revolutionary bioenergy technologies to enable sustainable, domestically produced biofuels, bioproducts, and biopower for a prosperous nation.

BETO's strategic goal is to enable use of America's abundant biomass and waste resources for advanced biofuels, biopower, and bioproducts by:

- Identifying and developing biofuel pathways and innovative end uses
- Lowering the cost of production through increased efficiency, productivity, and yields
- Completing applied R&D on complex, real-world systems and integrating engineering process for promising new advanced bioenergy technologies
- All while maintaining or enhancing economic, environmental, and social sustainability.

BETO's performance goals are as follows:

- By 2022, verify integrated systems research at the engineering scale for hydrocarbon biofuel technologies that achieve a minimum 50% reduction in emissions relative to petroleum-derived fuels at a mature modeled minimum fuel selling price (MFSP) of \$3.00/gasoline gallon equivalent.
- By 2030, verify integrated systems research at the engineering scale for hydrocarbon biofuel technologies that achieve a minimum 50% reduction in emissions relative to petroleum-derived fuels at mature modeled MFSP of \$2.50/gasoline gallon equivalent.

Appendix 2. ASTM Fuel Approval Prescreening Tests

To evaluate the fuel candidates early to facilitate and reduce risk moving through the ASTM process, one could adopt the following:

- Tier α testing: Complete a quick preliminary assessment of the opportunity on general properties of molecule and class (bulk property composition, modeling, small-scale tests, and contaminants). This level of testing will rule out blendstocks prior to ASTM testing and answer questions as simple as “Can the proposed blendstock be used at any level?” ahead of platform scaling required for entering the formal approval and evaluation process.
- Tier β testing: Validate Tier α , measuring density, viscosity, and other properties detailed in a CAAFI R&D document of fuels at minimal volumes.

Appendix 3. Workshop Learnings

A brief synopsis of the workshop learnings is provided in this chapter. A higher level of detail is provided for the Cleveland workshop, as neither a workshop report nor detailed workshop minutes are available to the public.

A3.1 Macon Workshop

BETO's Advanced Development and Optimization Program held the Alternative Aviation Fuel Workshop on September 14–15, 2016, in Macon, Georgia. The purpose of the workshop was to engage stakeholders to gain additional knowledge related to aviation biofuels production. Input was sought specifically for effort needed to: (1) develop technology for scalable production, (2) achieve economic competitiveness, (3) achieve environmental benefits, and (4) develop feedstock and supply chains for biojet fuel deployment.

Key findings from the plenary presentations noted common characteristics of successful biojet pathways. These include the need to make fuel in sufficient quantity to study blending impacts and to develop strategies for scaling up. Forward-looking TEA methodology to understand profitability competitiveness drivers and stable government policies were also identified as essential capabilities required for the success of any pathway.

The breakout session on economic and technical competitiveness identified the need to develop consistent TEA methodology (in partnership with CAAFI, FAA, and other stakeholders) that considered both nth-plant and near-term, early-adopter economics. The TEA can inform the highest scale-up risks and barriers and point to further R&D needs.

The session on fuel conversion and scale-up identified technical barriers ranging from a lack of availability of data on pathways; lack of access to equipment, low-cost feedstocks, capital, and expertise; and lack of time and investment required for ASTM certification. More than 20 pathways were identified as having a need for DOE support for preliminary evaluation. Nontechnical needs were also identified, such as public education on the benefits of SAFs, consistent policies, and regulations.

The session on environmental sustainability and life cycle benefits provided insights for a consistent approach to sustainability analysis and LCA, as well as metrics for these analyses. Participants wanted researchers to understand that transparency be achieved by publication of these tools and assessments for use by stakeholders.

The session on feedstock and product supply chains identified a lack of sufficient feedstock availability and limited scaling as barriers, as well as the need for a better understanding of best practices, particularly for new and emerging feedstocks. Attendees provided insights into the importance of DOE collaboration with USDA and other stakeholders to further enhance feedstock development and explore opportunities such as double cropping to increase efficient use of land and nutrients. Other insights included BETO playing a strong role in feedstock interface opportunities to help reduce the risks related to feed and handling at the biorefinery and improve the performance of the conversion process through integration of feedstock and fuels production.

Key takeaways from the Macon workshop related to the timeline, markets, and research needs were as follows:

Timeline

- For 0–5 years, near-term R&D investment needs to reduce the cost in pathways already approved or near certification.

Markets

- Jet fuel properties fall within the light end of the diesel envelope; therefore, biofuels companies could sell into either market.
- Diesel fuel (ground transportation) is major competition for fats, oils, and greases. Light ends could offer blending opportunity to meet bulk properties.
- Lipid routes (fats, oils, and greases) are not likely to meet the SAF volume demand.
- Policies that allow a level playing field will be helpful.
- Offtake agreements are necessary but not sufficient; the cost must come down, as offtake agreements kick in only when production is established.

Research Opportunities

- Additional benefits for SAFs may be related to the low sulfur and low aromatics in SPK.
- New low-cost sources of feedstocks, including lignocellulosics, are needed to increase scale.
- TEA and GHG results are inconsistent; there is a need to improve consistency and cover pioneer plants. Additionally, TEA can identify the greatest cost-reduction opportunities.

A3.2 Cleveland Workshop

The JET workshop was held in Cleveland, Ohio, from September 21–22, 2017. The workshop was a perspective-gathering and brainstorming event organized around four themes: (1) high-performance fuel options, (2) engine and combustor options, (3) aircraft on-board considerations, and (4) fuel development to deployment considerations. The event was organized by EERE, the U.S. Department of Defense, and NASA. In attendance were 75 people and another 25 people participated by webinar.

A3.2.1 Two Schools of Thought

Two divergent schools of thought were discussed during the workshop. One was to work within current standards (drop-in fuels) but bring the cost down. This approach avoids the expense of changing the infrastructure for distribution, fueling, and use, and the exorbitant cost of FAA engine (re)certification. The challenge for large-scale adoption is the high cost of SAF versus petroleum-derived jet fuel and not inferred impediments, low blending limits, limited pathways, or low-volume production capability.

The second, alternative school of thought was to imagine what a fuel–engine combination could look like if all constraints were removed (non-drop-in fuel/engine combination). Those proposing the non-drop-in fuels discussed value propositions rather than cost.

In the middle of these two schools of thought are considerations of how engines are evolving and what fuel properties are important. In this scenario, a fuel could still meet current (or perhaps lightly modified) ASTM specifications.

Drop-in fuels are needed for near- and mid-term opportunities. There may be opportunities for commercial aviation for non-drop-in fuels in the long term, but even they will likely be bounded by high-energy-content hydrocarbons rather than single-molecule-based fuels, two-fuel concepts, metals, or gaseous-based fuels.

Drop-in fuels allow uncoordinated growth of SAFs and are forwards–backwards compatible. Non-drop-in fuels would require a system-level coordination and it is unclear how deployment could or would proceed.

A3.2.2 High-Performance Fuel Options

High-performance fuel evaluation can revolve around emissions and operability (lean blowout, cold ignition, altitude relight). This can be done by removing some components from the fuel and biasing critical fuel

properties. ASTM D1655 already enables improvements in jet fuel, such as higher energy content (optimizing specific energy and energy density without driving either to nonviability), higher heat capacity/thermal stability, lower sulfur and lower aromatics, lower freeze point, and others. The cost–benefit tradeoff must be significant if the fuel is more expensive. The question becomes whether or not there is a path for relaxing (or refining) the current fuel specification without engine recertification.

Suggestions from the workshop include that fuels must be single-phase hydrocarbons; multiphase fuels are not allowed in civil aviation, oxygen is unwanted, and metal-based fuels are not acceptable. While a specific single molecule may exist that meets ASTM specifications, it is unlikely such a fuel would have the required performance to ensure safe operation over the wide range of conditions during flight. Moving to a narrower suite of molecules will need to be understood in terms of combustion characteristics and may require engine–fuel co-optimization.

In the near term, the low-hanging fruit is producing fuels with higher thermal stability, improved lubricity, high density, and improved specific energy (higher H:C ratio) while retaining acceptable energy density and higher thermal capacity (enabling thermodynamic efficiency, higher vapor pressure, lower viscosity, and lower surface tension, and bounding the cetane number [30–55]). Lowering aromatics and eliminating heavy-end, multi-ring aromatics is critical for reducing emissions, lowering infrared thermal load (hot spots), and improving specific energy. Use of certain cycloalkanes, such as decalins, could be a route to removal of aromatics while maintaining O-ring swelling. Alternatively, small olefins, such as ethyl benzene, have good swelling properties and lower sooting than heavier aromatics.

In the medium term, options can be considered to blend noncompliant blendstocks from multiple feedstocks and pathways to achieve a renewable blend that is both compliant and meets performance targets.

Developing new fuels, perhaps with the help of additives, could drive down soot, make fuel easier to ignite, reduce surface tension, and inhibit Zeldovich NO_x (by facilitating better premixing, and in turn lower combustion temperatures). Other desired properties include lower viscosity and surface tension, higher thermal stability, and no aromatics, nitrogen, sulfur, olefins, or oxygen compounds.

Discussion of flexible-fuel and dual-fuel engines was prevalent. Flexible fuels will require material compatibility; dual fuels will require additional tanks, lines, and fuel pumps on aircraft. In addition, on-board fuel reforming was heavily discussed. Fuels that are not fully backward compatible will require a separate fueling (hydrant) infrastructure. Additives could assist in allowing backward–forward compatibility.

In closing, optimizing jet fuel is a multivariate, multi-stakeholder activity. Altering one property can affect others, at times negatively. Next steps would be to determine optimization metrics and a holistic set of operability and safety constraints.

A3.2.3 Engine and Combustor Options

Engines are certified to run on a fuel, showing a critical tie between engines and fuels. The clarion call of fuel producers and engine/airframe manufacturers to work together is exemplified in the following quotations from the JET workshop:

It is clear that there still remains a lack of understanding of the link between fuel physical and chemical properties and combustion performance. While some correlations do exist, a more complete, physics-based description is lacking. Furthermore, without having appropriate models to accurately predict combustion processes as a function of variation in combustor geometry or fuel properties, the probability of co-optimizing fuel formulations and combustor designs synchronously is low.

[There is a] tremendous potential and opportunity if a will exists to pursue it.

To achieve higher efficiency and lower emissions in the Brayton cycle, engines are moving to higher compression ratios and more premixing. Lower fuel burn is achieved by improving thermodynamic cycle efficiency.

Engines will continue to evolve, including higher pressure ratios, higher temperature and pressure at the inlet, lower parasitic (cooling) air flow, advanced materials/coatings, higher heat rejection to the fuel system, and advanced seals and avionics. These changes require improved thermal stability and low contaminants in the fuels. Reducing emissions requires reduced variation in temperature and could change fuel/air mixing, coupling heat release to pressure, the position of the flame front, and links of chemicals to emitted species.

It takes 15 years to develop an engine from scratch, and 15 years to develop a new airplane. It also takes about 15 years to move a new fuel market from discovery to pilot to production. All of these activities must be done in parallel. Hence, three questions arise: What enabling technologies are needed to begin developing now? How early in the engine/aircraft development cycle is fuel mandated? What aircraft in development could benefit from new fuel specification?

Table A.1 illustrates the relationships of select fuel properties and engine performance parameters. Linkages of fuel properties with engine operability and performance metrics are clarified where known. Because many of the fuel relationships are unknown, the table points out areas of potential future engine-fuel research. The dominant properties for which research is necessary are vapor pressure, viscosity, thermal stability, and aromatic content.

Reduction of fuel viscosity at low temperatures as well as increased thermal stability of the fuel may require improved nozzle designs in terms of uniform and finer spray performance, broader operating space, and cheaper/simpler designs.

Autoignition under high compression ratios with well-mixed fuels needs to be addressed. Nozzle design is one tool to address the challenge. Nozzle geometry changes under varying conditions experienced during takeoff and flight. The active geometries of flexible-fuel airplanes could account for the variation. Injector design needs to be investigated, as well as on-board, real-time fuel sensors for measuring critical property deviations.

Table A.1. Fuel Properties from the OEMs at the JET Workshop

	Vapor Pressure (Evap. Rate)	Viscosity	Density (mass)	Density (volume)	Ignition Time	Heat of Combustion	Thermal Stability (Coking)	Aromatics	Extinction or High Temp. Chem. (kinematic rates)	H:C Ratio
Durability: Low soot (combustor and turbine)	(soot) +	(soot) -	Wash	Wash	(Auto-ignition) -	Wash	+	(soot/radiation) -	Wash	Wash
Dynamics	Non-monatomic behavior									
Coking (injector) - low O₂	Wash	Wash	Wash	(drives velocity of fuel up) -	Wash	Wash	+	-	Wash	Wash
Coking (combustor)	* +	* (not universal)	Wash	Wash	Wash	Wash	Wash	Wash	Wash	Wash
Forced ignition	+	-	Wash	Wash	Wash	Wash	Wash	?	Wash	Wash
Lean blow out (LBO)	Depends	Depends	Wash	Wash	?	Wash	Wash	Wash	(fast) +	Wash

	Vapor Pressure (Evap. Rate)	Viscosity	Density (mass)	Density (volume)	Ignition Time	Heat of Combustion	Thermal Stability (Coking)	Aromatics	Extinction or High Temp. Chem. (kinematic rates)	H:C Ratio	
NO _x	+	-	Wash	Wash	Wash	Wash	Wash	Wash	Wash	Wash	
CO/unburned hydrocarbon (UHC)	+	-	Wash	Wash	?	Wash	Wash	Wash	(fast) +	+	
Soot/smoke/particulate matter (PM)	+	-	Wash	Wash	Wash	Wash	Wash	-	?	+	
Temp. profile/pattern	Flat +	Flat -	Wash	Flat +	Wash	Wash	Wash	Wash	Wash	Wash	
Key											
-	Down for improvement					Depends		Depends on design			
+	Plus for improvement					P		Peak			
*	Additional debate							Big effects			
?	Do not know							Smaller effects			

Variable geometric features with two or more mixer inlets allow active control of near-dome flow characteristics to meet the required performance, emissions, operability, and durability objectives. Fuel that does not coke allows for smaller injector nozzle orifices and thus finer spray. Less coking also allows staging of other functions. Lower coking fuels require very low olefins and heteroatoms. Aromatics have second-order coking effects.

R&D topics may include real-time fuel sensors, analysis (understanding of sprays, computational fluid dynamics, acoustical instabilities, etc.), development of single-cup rigs requiring very small fuel quantities (initial screening), and identification of highly targeted additives that improve fuel properties. Alternative fuel producers can collaborate with OEMs to understand the unique engine types/cycles that could be optimized with a new fuel.

A3.2.4 Aircraft On-Board Considerations

Airplanes integrate all subsystems, including engines, auxiliary power units, tanks, and fuel delivery systems. At the airframe level, critical fuel properties include material compatibility for pumps (lubricity, viscosity), tanks (flash point, vapor pressure), fuel quantity indicating system (dielectric, speed of sound, density), and energy capacity/energy density. All the auxiliary aircraft systems that touch the fuel will need to be evaluated in the presence of the new fuel. Fuel system considerations include water solubility; a small level is needed to prevent ice-crystal formation during flight and low-aromatic fuels may require additives. For airports, airlines, and the military, fire suppression for unintended ignition and water in the fuel lines is a major issue.

SAFs that are not drop-in would require that legacy engines and aircraft be recertified. For a new engine and a new plane, this may be less of a problem if the new fuel properties are understood prior to ASTM certification of the engine and plane, and if a duplicate fueling system is available at every intended destination.

As stated in Chapter 3.2 of this report, drop-in fuels encourage supply growth. Non-drop-in fuels might feature potentially better performance and operability but will require system-level coordination along the entire value

chain to ensure their compatibility with all parts that the fuel touches, and with how engines and planes are certified by the FAA.

In the near term, SAF fuels that include additives, such as ethyl benzene for ring swelling, offer advantages. Material compatibility is going to be crucial for both the near and longer term. Many remaining unknowns about new fuels will need to be addressed. Chapter 2 offers an extensive list of important fuel properties.

In the medium and longer term, swelling remains a concern for blend limits of SAF fuels that have minimal aromatic content, and lubricity is a concern with ultra-low-sulfur fuels. Identifying additives or blendstocks that assist with these properties is a research need. For example, certain cycloparaffins, such as decalin, may offer swelling properties. Trace levels of organic acids may increase the lubricity. An understanding of trace components in fuel today that lead to lubricity would be valuable. An understanding of the effect on engine components is also needed.

Considerations for different phases of flight and specific energy/fuel requirements led to many discussions of the dual-fuel option under consideration. In such scenarios, landing and takeoff (drop-in) have different requirements than cruising (non-drop-in). While a dual-fuel option could improve aircraft performance (weight, cost, etc.), its performance benefits are offset by the complexity of the additional fuel system requirements (multiple tanks, lines, pumps, control, etc.). Further, use of a dual-fuel option requires the system and logic to switch between fuels versus mission segments. Concern about producing fuel flow spikes in switching will need to be addressed. Plumbing and pumping compatibility issues for each fuel will need to be understood, as will the risk profiles, which depend on the diversity of fuel types, logistics of fuel densities such as fuel gage issues and weight distribution, misfuelling, and complexity and redundancy of units. Therefore, when considering dual-fuel options, a thorough risk-benefit analysis must be done before investing public research dollars.

In the extended long term, NASA is looking at partial to full electrification for mission-specific aircraft. This extends to considerations in commercial and cargo settings in which electricity is generated in flight and used in a hybrid concept. Which fuels could help enable hybrid engines is uncertain at this point.

A3.2.5 High-Performance Fuel Development to Deployment

Value chain buy-in: Scale-up and deployment of a new fuel, even a drop-in fuel, requires the participation of many entities along the value chain—from the feedstock providers (farmers, waste owners, foresters), fuel blenders, fuel distributors and suppliers, airports and airlines, financiers, communities (where fuels is produced and used), and, finally, consumers. Each stakeholder group needs to see a financial benefit or at least a perceived societal or other long-term benefit. This was discussed in more detail during the Richland workshop; scaling up deployment often cannot withstand antagonists, who can kill the venture.

Financing: Scaling up a new fuel facility requires extensive capital. The ability to acquire funding becomes increasingly challenging because the scale increases until risk has been mitigated, which may be after the pioneer plant or even subsequent plants have been established. Development of a new fuel without a clear line of sight for its use expressed through long-term purchase agreements is exceedingly challenging. For non-drop-in fuels, a full set of partners will need to buy in. The value added (for both drop-in and non-drop-in) will have to be unambiguous and sufficient to overcome the risk. This message was made even stronger at the Richland workshop.

Regulatory framework: Regardless of SAF sourcing, there is a need to work within a technology-neutral regulatory framework that can encompass new fuels and additives without legislative change. Few new clean-energy ventures can move to market without a favorable regulatory framework. Three elements must come together: stable policy environment, de-risked technology, and acceptable economics.

For near- and mid-term opportunities, infrastructure compatibility is important (i.e., the same pipelines, fuel delivery, tanks, and engines). Fuels streams can be differentiated to provide benefits, and the net benefit must

offset costs throughout the value chain. A system-level approach is essential to understanding tradeoffs and upstream and downstream impacts. The regulatory framework must also be technology-neutral while incorporating market-based solutions that address society's needs (e.g., California Low Carbon Fuel Standard versus the Renewable Fuel Standard of the Energy Independence and Security Act). Regulatory frameworks that incorporate market-based solutions that also address society's needs will be helpful.

There are two issues to consider in meeting the fuel specifications of ASTM D1655 (current specification). First, engine manufacturers do not have significant incentives to assume additional risks associated with certification outside of ASTM D1655. Barriers and limitations for deployment are determined by the need for the fuel to be drop-in. The fuel must comply with ASTM D1655. Second, the fuel must be within spec when it arrives at the airport (via pipeline, rail, truck, or barge). Blending offers opportunities to improve properties or to bring an out-of-spec fuel into spec. While blending is not the inhibitory challenge for large-scale production today, at large-scale production, who is responsible for quality assurance and how and where that is done will need to be addressed. Consumer infrastructure and maintenance need to be developed (developing proper metering blending infrastructure and seals).

Timing: At the workshop, it was suggested that the timing of scaling up jet fuel pathways may be as follows:

- Short term: HEFA, fat, and greases are commercially available today but limited in feedstock quantity (e.g., commercial today, but need cost reduction)
- Medium term: Waste gases, MSW, and agricultural waste can be used as feedstock (e.g., pathways that are in piloting or demonstration today)
- Long term: Algae, hybrid technology, thermo-catalytic, and direct CO₂ utilization (e.g., technologies at bench scale today).

Future fuels could be built if existing knowledge and experience are used.

A3.2.6 Key Takeaways

There may be tremendous opportunity for high-performance SAF, but it will take time and money and can only be done with the integration of engine and fuel research.

- Time: It takes 14–19 years from technology development through product introduction phases (for planes, engines, and fuels); hence, collaboration and how to work together is key.
- Money: General Electric spent over \$500 million to get GENx-09 into production from development (an expensive and resource-intensive process); fuels have a similar price tag, so there is need to focus on lowering costs of existing fuels in the near term.
- Expect engine design not to change significantly; plan for staged combustion to meet varying loads and reduce emissions.
- Opportunities exist to improve specific fuel consumption (increase payload or range or reduce takeoff weight) using high-energy-content fuels with existing engines (existing engines can use up to 15% higher energy-dense fuels).

A3.3 Richland Workshop

The Trilateral Biojet Workshop brought together researchers from Canada, Mexico, and the United States. Held in Richland, Washington, in May 2018, the workshop was organized by EnerCan, SENER, and DOE, and was funded by DOE and PNNL. The workshop covered the value chain, feedstock from each country in North America, research directions in each country, and how collaboration can be used to accelerate ATJ growth.

The workshop report covers six areas: (1) what makes a great jet fuel, (2) ecosystem and the current state, (3) capabilities and programs in each country, (4) needs and research opportunities in the near term (0–5 years), (5) needs and research opportunities in the longer term (beyond 5 years), and (6) Canada, Mexico, and the United States working together.

A3.3.1 Synopsis of the Workshop Report

The workshop covered what is in current jet fuel, jet fuel markets in each country, and the ASTM process, as well as the FAA engine–airplane certification process. Many of the learnings have been covered previously in Chapter 1 of this report and are not repeated here. FAA does not certify fuels, but rather engines and airplanes that operate using a specified fuel. In the United States and throughout North America, the specified fuel is defined by ASTM. Testing has shown that blending reduces emissions and contrail size because of the reduction of aromatic content, hence there is no reason for SAF to mimic Jet A. Starting with renewable carbon, one can target the hydrocarbon families of highest value.

The relatively low amount of SAF produced today in comparison to biodiesel and renewable diesel is sobering and indicative of challenges that producers face in the competition of the two markets. While airlines are seeking sustainable alternatives to petroleum-derived fuels, the cost of the fuel remains a critical driver. The cost of fuel between 2011 and 2019 range from 19% to 32% of the expenditures for airlines (Statista 2019). The Bureau of Transportation Statistics reported fuel costs being nearly 20% of the operating cost of U.S. airlines in 2019. (BTS 2019). At the workshop, one representative of a major airline noted that a single dollar-per-barrel increase in jet fuel price equates to a \$50-million increase in operating cost. Airlines are sensitive to the price of fuel.

A3.3.2 Key Takeaway Messages

- The time and cost of bringing a new fuel to market must account for the time and cost of fuel certification (4 years) and the time and cost through piloting to pioneer plants.
- SAF must be cost-competitive. The airlines cannot meet their self-imposed targets for reducing GHG emissions based on engine and flight improvements alone; they need biojet fuel, yet fuels are up to 30% of the operating cost.
- Some airports are looking to help meet the difference on cost by being fuel integrators, combining larger, long-term purchase agreements (from the airport level, not the airline level) and providing land to produce biofuels. Europe has similar models that could be followed (the Oslo model is creating a central fund to bridge the difference between the cost of production and market value).
- Fuels are delivered in hydrant systems in which LCA accounting is attributed to those who pay for it. Refineries ask if a similar accounting could be done for coprocessing even if jet fuel is not a product. (How does one draw the box around the LCA?)
- Feedstock cost must be reduced.
- Producers need to make coproducts; however, fuel cannot be a loss leader in the long term.
- Markets span international boundaries and coordination needs to cross countries.

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