Project 066 Evaluation of High-Thermal-Stability Fuels

University of Dayton and University of Dayton Research Institute

Project Lead Investigator

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University Participants

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- P.I.s:
    1. Joshua Heyne, Associate Professor
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- FAA Award Number: 13-C-AJFE-UD, Amendments 27 and 30
- Period of Performance: June 1, 2020 to September 30, 2022
- Tasks:
    1. Identify/create a jet engine model including all components necessary to evaluate the impact of fuel properties.
    2. Build and apply a heat transfer model for the fuel system.
    3. Identify engine cooling trade-offs that can be leveraged to optimize engine/aircraft system efficiency.
    4. Estimate gains in fuel efficiency.
    5. Identify critical blend components and solvents to study.
    6. Create and test blends for thermal stability in jet fuel thermal oxidation testing (JFTOT) and quartz crystal microbalance testing (QCM).

Project Funding Level

FAA provided $284,997 in funding, which is allocated between amendments 27 and 30 as follows:

- 13-C-AJFE-UD-027: $184,997
- 13-C-AJFE-UD-030: $100,000

Cost sharing is provided by DLR Germany.

Investigation Team

- Joshua Heyne (University of Dayton) is the project lead investigator, responsible for building the team and coordinating team activities, driving toward the completion of major milestones.
- Randall Boehm (University of Dayton) is a research engineer with 20 years of relevant industry experience and is responsible for leading the technical efforts on this project.
- Lily Behnke (University of Dayton) is a graduate student research assistant, responsible for integration of the engine performance models (EPMs) and fuel property models with JudO, a tool developed internally to help optimize fuel composition against user-defined objectives.
- Jeffrey Spruill (General Electric [GE]-Aviation) is a product performance engineer, responsible for applying audited EPMs as necessary to judge potential drop-in fuel effects on a variety of engines for various mission points,

environmental conditions, and engine deterioration levels. Additionally, Jeff is responsible for estimating non-drop-in fuel effects arising from conceptual design changes to engine thermal management systems that lead to increased reliance on fuel as a coolant instead of compressed air.

- Gurhan Andac (GE-Aviation) is a combustion engineer, responsible for coordinating the efforts at GE in support of this project.

Project Overview

It has long been understood that increasing the reliance on jet fuel as a primary coolant for both the engine and the aircraft has significant performance and efficiency benefits relative to the use of air as a coolant (Bruening, 1999) but fuel degradation and coking at high temperatures restrict how much heat can be put into the fuel. In some military applications, the performance benefits are sufficiently large to justify the creation of specialty fuels such as JP7 and JPTS, which can tolerate much higher temperatures than petroleum-derived Jet A or Jet A1 (JP8) (Edwards, 2007). In land-based applications of gas turbines, weight is of little consequence; thus, the operations of waste heat recovery (WHR) for plant efficiency or the reduction of combustor inlet temperature for emission reductions can be accomplished by a wide variety of techniques, all of which are impractical for flight because of their impact on the mass of the power plant. Nonetheless, these applications provide some common examples of how controlling the air temperature along its flow path through the engine can have a large impact on performance, durability, and energy efficiency (Wilfert, 2007). Numerous works relating to fuel deoxygenation (Zabarnick, 2020) and other methods for decreasing coking propensity and its impacts (Mancini, 2004) have largely been motivated at the sponsorship level by these benefits.

More recently, sustainable alternative fuels (SAFs) have received much attention because they can contribute to high-priority geopolitical goals to diversify energy supply chains and reduce greenhouse gas emissions. Most of these efforts have focused on streamlining the evaluation and approval processes to use synthetic fuels at some blend ratio with petroleum-derived jet fuel to create a so-called drop-in fuel that can be used within existing infrastructure without objection from any stakeholders (Colket, 2021). Additionally, there have been discussions regarding characteristics of synthetic blend components (such as low aromatics, high specific energy, and high thermal stability) that would make these components attractive as potential specialty fuels (such as JPTS) or high-performance fuels. Kosir et al. (2020) recently published work highlighting the efficiency gain that could be realized by using fuels with high specific energy via a lower aircraft weight at take-off, resulting in less mass that must be lifted and held against the force of gravity.

The weight of fuel uplifted to an aircraft, as necessary to complete its mission, is certainly an important component to consider in assessing the integrated engine/aircraft energy demand and efficiency. The energy efficiency of the engine is also expected to be influenced by other fuel properties, including the following:

1. **Hydrogen/carbon (H/C) ratio**. Through its impact on combustor exhaust gas composition, this ratio has a small impact on the ratio of heat capacity (gamma), combustor exit temperature, and work extracted during expansion through the turbine, even when the total enthalpy created at the combustor is unchanged.
2. **Viscosity**. Viscosity impacts the heat transfer coefficients, which ultimately determine how much waste heat is recovered by the fuel (coolant) and delivered back to the engine via the combustor.
3. **Energy density**. Energy density, measured in joules per liter (J/L), impacts volumetric flow rates, which in turn impact heat transfer coefficients.
4. **Specific heat**. The specific heat influences heat transfer coefficients but, perhaps more importantly, also has a direct impact on the temperature rise in the fuel per unit of heat energy absorbed, which in turn may impact the coking rate.
5. **Coking rate**. The coking rate drives several high-level design decisions relating to the thermal management of an engine. Coking rate is also known as fuel thermal stability.

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Task 1 - Identify/Create a Jet Engine Model Including All Components Necessary to Evaluate the Impact of Fuel Properties

University of Dayton

Objectives

This work has three primary objectives. The potential impact of fully synthetic SAFs on the specific fuel consumption (SFC) of a jet engine with no associated change in engine design or logic will be assessed in Phase 1. In Phase 2, the team will evaluate the impact of leveraging the high thermal stability of SAF candidates by increasing WHR up to a limit driven by the requirement that the fuel vapor pressure must remain below the normal working fuel pressure for all operating conditions. To achieve an increased WHR for this phase of the assessment, only straightforward, evolutionary design changes will be considered. In Phase 3, the aim is to identify and examine the coupled influence of increased WHR with optimized cooling flow schedules (Deveau, 1985).

Research Approach

At some level, one might argue that the maximum additional WHR is determined by the proposed shift in the maximum fuel temperature requirement, for instance, (160-127)*Cp, where 160 °C is the proposed temperature for high-thermal-stability fuels, 127 °C is the requirement corresponding to petroleum-derived Jet A, and Cp is the heat capacity of the proposed fuel. While this is true at some level, it provides only part of the story. For this study, a fuel system thermal model (FSTM, Figure 1) was created to simulate the heat pickup of fuel in real engines. This model allows us to quantify the influence of fuel property variations on the temperature rise and WHR within existing architectures. This model also enables evaluations of concept-level design changes that are intended to drive more heat into the fuel. A high-level EPM (Figure 2) was created to enable evaluations and comparisons of different conceptual designs that drive the same amount of total heat into the fuel (approximately 33*Cp more than baseline) but take heat from difference sources. The EPM also enables evaluations of the H/C impact on combustor exit temperature and turbine work extraction, which is usually neglected in performance models because it is thought to be a small impact and the H/C ratio of fuel onboard an aircraft is generally not known. The final component in the overall impact on system efficiency is the weight, including the difference (decrease) in fuel weight necessary to complete the same representative mission, as well as the difference (increase) in weight created by the concept-level design changes being considered.

A distribution of properties for potential SAFs is created by virtually blending individual molecules by a random association of mole fractions, whose values are also randomly determined, with specific molecules possessing known physical and chemical properties (Lemmon, 2018; Kroenlein, 2019). The fuel properties of the mixtures are derived from the mixture definition and constituent properties according to ideal mixture blending rules, which have been documented elsewhere (Flora, 2019). This trial guess at a SAF candidate is then passed through a filter to determine whether it is expected to pass ASTM D1655 and ASTM D7566 fuel specifications. If the candidate passes this filter, it is included within the distribution that is input to the FSTM and EPM as part of a simulation. See Figure 3 for a graphical representation of the fuel selection methodology. The motivation behind this approach was to maintain a physical link between different properties, as the full set of properties is derived from each fuel and the property variation is driven by fuel composition variation rather than arbitrary simulation. All liquid fuel properties include first-order temperature dependence, whereas none of the properties include pressure dependence.

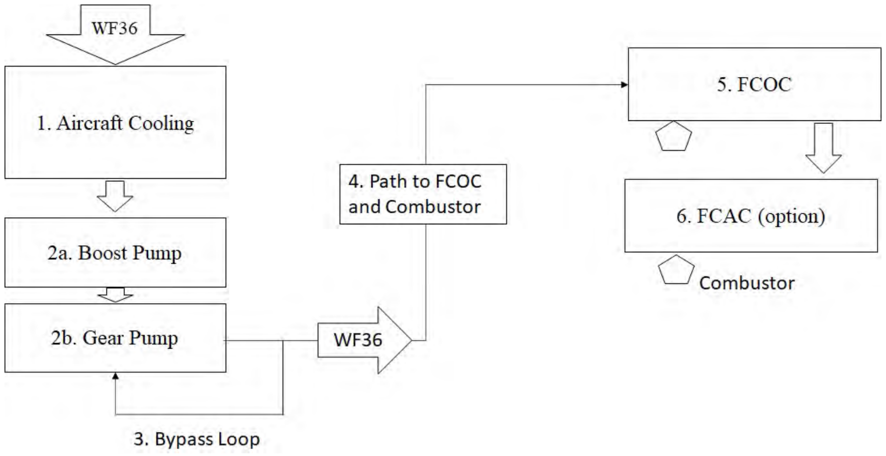

Figure 1. Block diagram of the fuel system thermal model for the pilot study (Boehm, 2021) and fuel optimization. FCAC: fuel-cooled air cooler; FCOC: fuel-cooled oil cooler; WF36: fuel flow rate to the combustor.

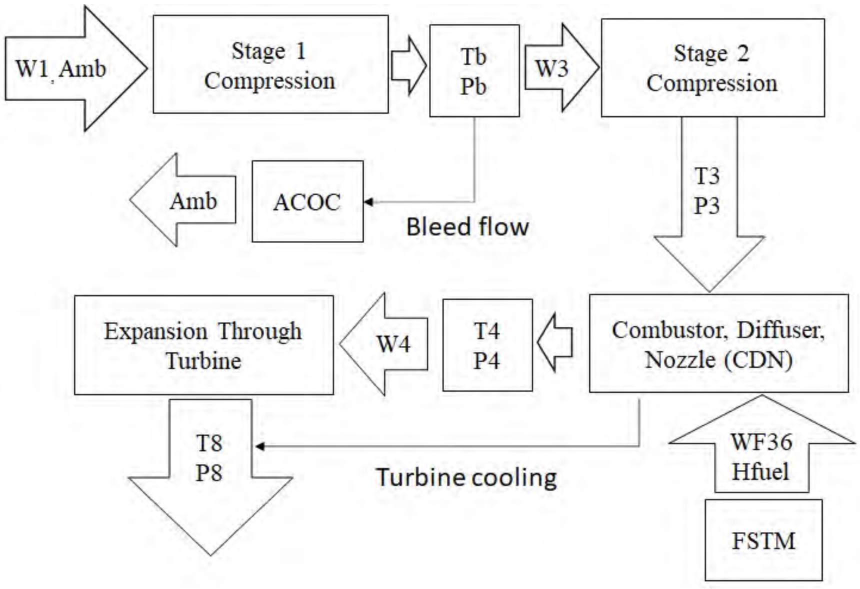

Figure 2. Block diagram of the engine performance model for the pilot study (Boehm, 2021) and fuel optimization. ACOC: air-cooled oil cooler; FSTM: fuel system thermal model; WF36: fuel flow rate to the combustor.

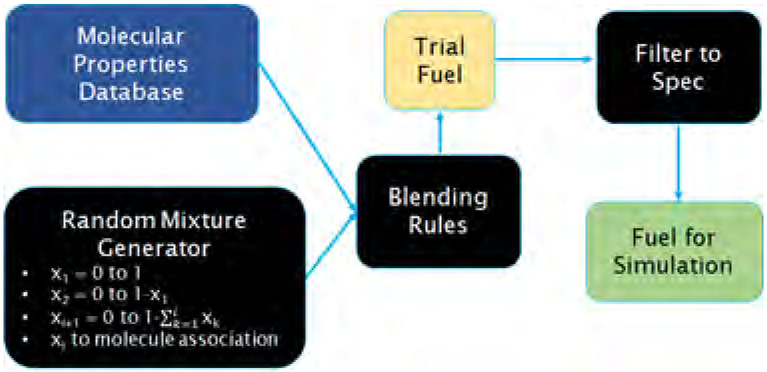

Figure 3. Fuel creation flow chart.

For bookkeeping convenience, the total enthalpy supplied to the engine per unit time (W_f * LHV) is to be conserved for all initial simulations. The net work per unit time (P_{net}) from the engine (expansion plus compression) varies in these simulations depending on fuel composition and conceptual design, in contrast to real applications, where thrust * air speed (~P_{net}) would be conserved and the fuel flow (W_f) would be changed to meet that demand. Once the initial calculation is made, the fuel flow is varied in the simulation, as it would be in a real engine, until P_{net} is equal to the value for the baseline engine model and reference fuel. The relative difference in fuel flow between the initial and final calculation represents the energy savings.

A graphical summary of the methodology is provided in Figure 4. Major inputs include the diameters and lengths of each element in the FSTM, engine operating conditions such as the pressure ratio and air flow splits at each station in the EPM, the baseline fuel-to-air ratio, and temperature boundary conditions for the FSTM. Several fuel properties are provided to the FSTM, while the EPM receives the H/C ratio and lower heating value (LHV) as input.

A validation of this model, relative to fuel property influences and cooling strategy, will be accomplished by comparison to audited performance models of jet engines produced by GE-Aviation.

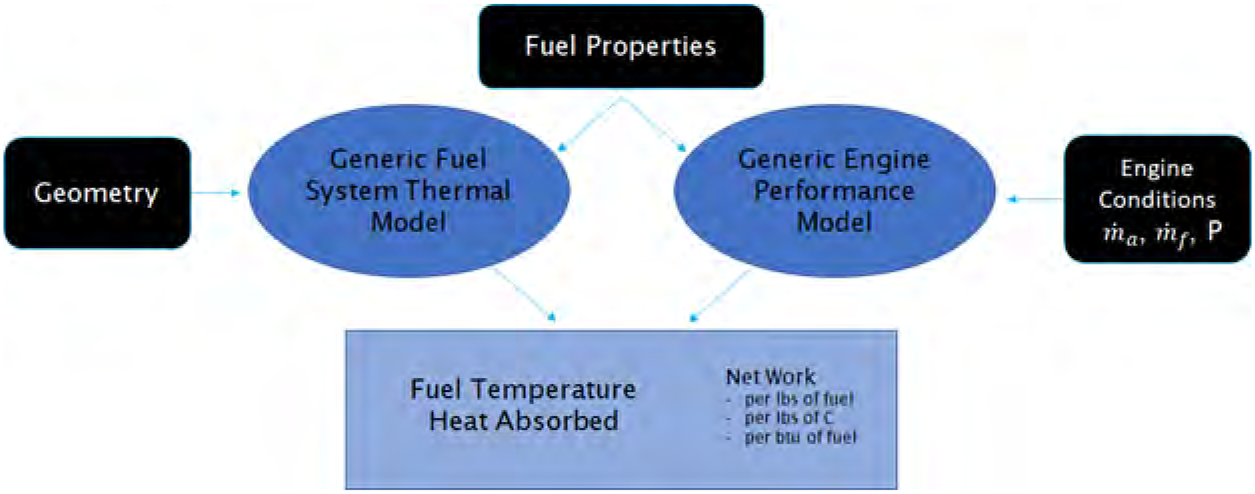

Figure 4. Flow chart of fuel effects and conceptual design evaluation.

Milestones

- The conceptual design of a model jet engine to serve as a tool for evaluating the impact of fuel property variation on jet engine fuel efficiency was completed (August 2020).

- All models used in proof-of-concept work were integrated into JudO, which has been previously used (Kosir, 2020) to optimize fuel composition against defined objectives (September 2021).
- A reference mission (December 2021) and aircraft (March 2022) were established, affording the integration of fuel effects on system-level efficiency.

Major Accomplishments

- As a major accomplishment, we constructed and verified the FSTM and EPM and their integration with Monte Carlo methods, which was necessary to complete most of the remainder of this project.
- All tools needed to assess fuel effects on SFC have been integrated into our internal code for SAF optimization (JudO).

Publications

Boehm, R. C.; Scholla, L. C.; & Heyne, J. S. (2021). Sustainable alternative fuel effects on energy consumption of jet engines. Fuel *304*, 121378. https://doi.org/10.1016/j.fuel.2021.121378

Outreach Efforts

None.

Awards

None.

Student Involvement

- Lily Behnke, M.S. student, accomplished integration/translation of the Excel-based EPM and FSTM into the Python-based JudO program and was responsible for the results shown in Figures 1–6,10, and 11.
- Jack Hoog, M.S. student, participated in the identification and selection of a reference aircraft.

Plans for Next Period

- Integrate/code the reference mission and aircraft into the optimizer to reduce the dimensionality of the optimization.

References

Boehm, R. C., Scholla, L. C., & Heyne, J. S. (2021). Sustainable alternative fuel effects on energy consumption of jet engines. *Fuel*, *304*, 121378. https://doi.org/10.1016/j.fuel.2021.121378

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Task 2 - Build and Apply a Heat Transfer Model for the Fuel System

University of Dayton

Objective

The goal of this task was to create a model that would output heat absorption, representative of real jet engine fuel systems, based on applied boundary conditions such as fuel properties, fuel velocity and momentum, and hot-side temperatures.

Research Approach

The fuel system was broken down into elements for which the author had experience-based guidance relating to fuel inlet and outlet temperatures. In concert with experience-based guidance relating to fuel momentum and system pressure losses, the fuel system geometry, including the flow diameter and length, and hot-side boundary conditions were established for a baseline fuel flow through the modeled fuel system. This model then became the basis for assessing the impact of varying fuel properties.

In the pilot study (Boehm, 2021), Monte Carlo simulations resulted in population distributions plotted against the normalized WHR, as shown in Figure 5. In this context, the recovered waste heat is defined as the total heat absorbed by the fuel in route from the fuel tank to the combustor, which is then divided by the reference enthalpy of the fuel (LHV*W_f) supplied to the combustor for the initial calculation of P_{net}. The fuel flow rate at high power is approximately ten times higher than it is at low power, and the flow within the fuel system is turbulent regardless of the fuel properties. Under these circumstances, heat transfer coefficients are not very sensitive to fuel property variations, and thus, the two curves representing high-power operation are nearly vertical. At low-power operation, the flow within the fuel system starts out as laminar and transitions to turbulent as the viscosity drops with increasing fuel temperature. Under these circumstances, heat transfer coefficients are sensitive to fuel property variations, and thus, the two curves representing low-power operation show 0.2% variation in the normalized WHR.

The WHR term is not expected to have a large impact on the overall system efficiency because relatively little fuel is used at low power (top of descent) relative to take-off, climb, or long-haul cruise and because WHR is small compared with LHV*W_f. Nonetheless, this savings is worth optimizing because it can be potentially realized without sacrificing any other measure of fuel performance and without any change to the engine. We have already begun to optimize the fuel composition to maximize the LHV and total savings resulting from WHR, which will be discussed further under Task 4. In support of this goal, we have collected the necessary property data for thousands of molecules, which have been pruned to 1,124 molecules based on volatility, expected thermal stability, data completeness, and data consistency relative to similar molecules. We have also added the capability to predict the smoke point for each random composition.

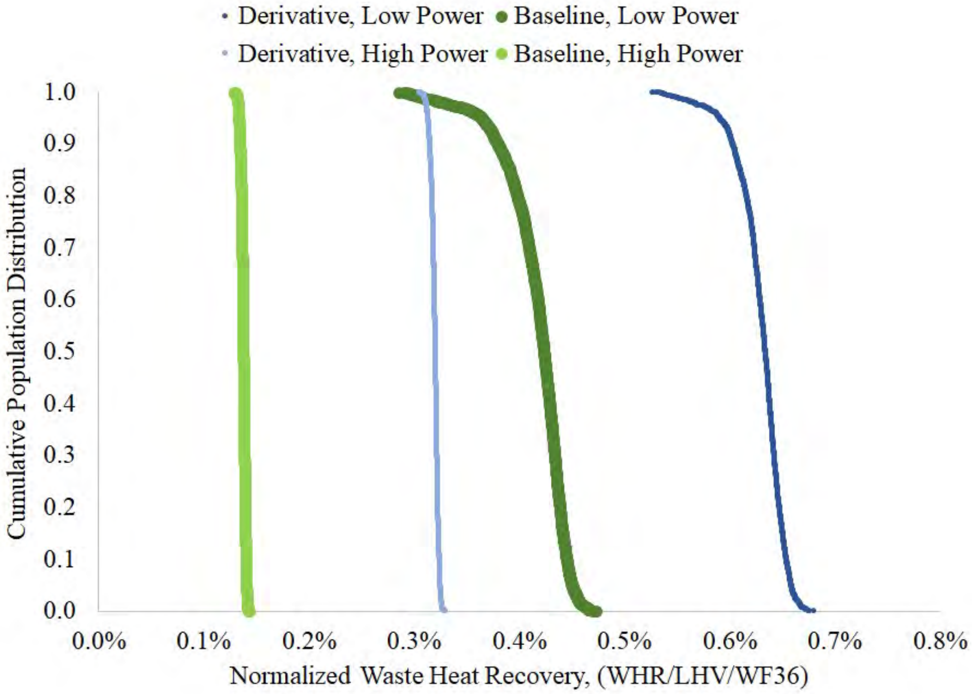

Figure 5. Impact of fuel properties on heat recovered from the engine by the fuel. LHV: lower heating value; WF36: fuel flow rate to the combustor; WHR: waste heat recovery.

Milestones

- Preliminary construction of this model, including integration with Monte Carlo methods and verification of heat transfer coefficient correlations, was completed (October 2020).
    - All models used in proof-of-concept work were integrated into JudO, which has been previously used (Kosir, 2020) to optimize fuel composition against defined objectives (September 2021).

Major Accomplishments

- As a major accomplishment, we constructed and verified the FSTM and EPM and their integration with Monte Carlo methods, which was necessary to complete most of the remainder of this project.
- All tools needed to assess fuel effects on SFC were integrated into our internal code for SAF optimization (JudO).

Publications

Boehm, R. C.; Scholla, L. C.; & Heyne, J. S. (2021). Sustainable alternative fuel effects on energy consumption of jet engines. Fuel *304*, 121378. https://doi.org/10.1016/j.fuel.2021.121378

Outreach Efforts

None.

Awards

None.

Student Involvement

- Logan Scholla, M.S. student, participated in the identification and selection of heat transfer coefficient correlations.
- Lily Behnke, M.S. student, accomplished integration/translation of the Excel-based EPM and FSTM into the Python-based JudO program and was responsible for the results shown in Figures 1–6,10, and 11.

Plans for Next Period

None.

References

Boehm, R. C., Scholla, L. C., & Heyne, J. S. (2021). Sustainable alternative fuel effects on energy consumption of jet engines. *Fuel*, *304*, 121378. https://doi.org/10.1016/j.fuel.2021.121378

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Task 3 - Identify Engine Cooling Trade-Offs That Can Be Leveraged to Optimize Engine/Aircraft System Efficiency

University of Dayton and GE-Aviation

Objective

The goal of this task was to document ideas relating to how original equipment manufacturers (OEMs) might design an engine thermal management system to minimize air pressure losses due to cooling or to reduce the overall system weight by capitalizing on the improved thermal stability of fully synthetic SAFs. This task also focused on estimating the savings afforded by each design change concept.

Research Approach

One advantage of simplified EPMs is that they facilitate conceptual design trades. For this project, we have considered four conceptional design variations to the thermal management system that increase the reliance on fuel as a coolant. The simplest concept is to add a heat exchanger anywhere in the system, sized such that the fuel temperature at the limiting design point is increased from its current limit, taken as 127 °C, to a new higher limit, taken as 160 °C. The current limit is driven by fuel thermal stability. Once this limit is elevated via high-quality synthetic fuel, the next temperature limit is driven by elastomeric material specifications or platform/fuel volatility requirements, which coincidentally are both near 160 °C for existing elastomeric seals and conventional jet fuels. Provided that the heat recovered by this new heat exchanger is truly waste heat and neglecting the impact of the exchanger's weight on aircraft fuel efficiency, the afforded energy savings of this configuration can be determined without an EPM or FSTM under the design-limiting operating condition, although the FSTM is necessary for other operating conditions. This simple configuration is labeled as "D" in Figure 6. In the next simplest concept, the fuel-cooled oil cooler is enlarged just enough to enable elimination of the air-cooled oil cooler (ACOC). Such a configuration would be lighter than the baseline engine, which would provide some fuel efficiency benefit at the system level, but this aspect is neglected in the calculations summarized in Figure 6. This configuration is labeled as "C" in Figure 6. The large difference between the savings at high power and the savings at low power for this configuration arises because the sink pressure (altitude-dependent ambient pressure) is unrelated to the pressure ratio achieved by the first stage of compression. The savings at the design point are driven by an input to the model, namely, the fraction of heat removed from the lube oil by air, with the remaining heat removed by fuel. Presently, there is significant uncertainty in the aero-savings estimate for this configuration; thus, work is underway at GE-Aviation to provide a better estimate by using a derivative of an audited performance model of a GE engine for a narrow-body airframe. This estimate will also include the influence of the weight savings. However, based on a simple model of the heat exchanger performance, GE has determined that complete elimination of the ACOC in this application would not be possible unless the maximum fuel temperature limit were raised by 107 °C instead of the 33 °C increase presumed for this analysis based on the fuel system material limits (e.g., elastomers) and fuel volatility. In the most involved concept, the cooled cooling air is coupled with active clearance control of the turbine airfoils. The configuration representing this concept is labeled as "E" in Figure 6. The turbine efficiency is an input to the EPM, and the difference between the savings of configuration E and that of configuration D is primarily driven by this input. The fuel savings is approximately double the increase in turbine efficiency because the Brayton cycle efficiency (i.e., overall engine efficiency) is approximately 50%. While this term is represented by the arbitrary choice of a 0.1% improvement in turbine efficiency for all operating conditions, a detailed design of an active clearance control concept is needed to estimate how airfoil clearances change with cooling airflow split variation. The airflow supplied to the regions that most need cooling (usually the mid span of the blades and vanes) can be reduced when the cooling air is cooled. This frees up air flow that can be used to cool the case (outer diameter) under operating conditions (usually high power) in which the clearance between the case and the blades is highest. To determine the impact on gap height, a detailed heat transfer analysis is required, and to gauge the impact of a gap height change on the aerodynamic efficiency of the engine, a detailed fluid dynamics calculation is needed. These analyses require a full definition of product geometry, which is obviously OEM-proprietary. Although we have requested that GE-Aviation include representative results of such a concept as part of their contribution to this project, they have not agreed to this request. Because turbine inefficiency is generally the largest source of engine inefficiency after accounting for the unavoidable heat engine (Brayton cycle) inefficiency, there is a strong possibility that cooled cooling air can be utilized most effectively by coupling it with active clearance control.

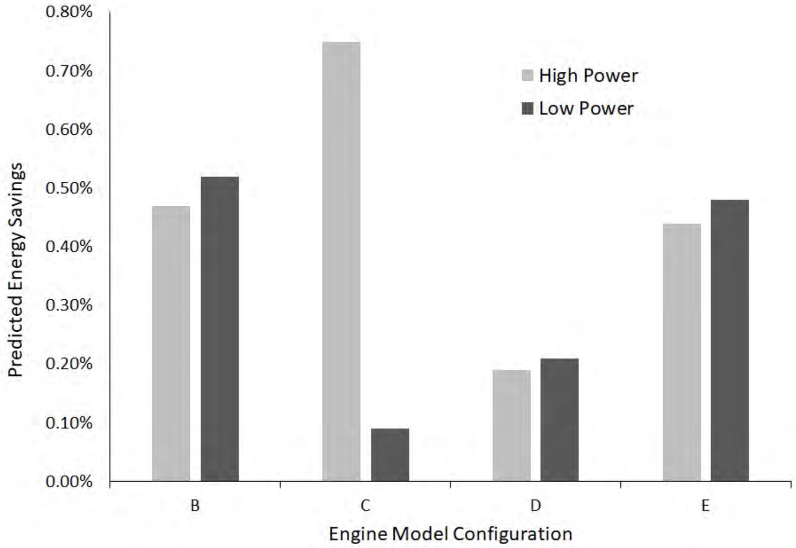

Figure 6. Summary of predicted energy savings for a variety of engine model configurations. B. Cooled cooling air with a reduced cooling flow. C. Enlarged fuel-cooled oil cooler in place of an air-cooled oil cooler. D. Cooled cooling air alone. E. Cooled cooling air and improved turbine efficiency (0.700 to 0.701).

The configuration labeled as "B" in Figure 6 is the same configuration labeled as "derivative" in Figures 5 and 7. For this configuration, the turbine cooling air flow budget is reduced such that the change in enthalpy of the cooling air is matched to that of the baseline configuration at high power. In this study, the cooling flow was reduced to 29.75% of W3, compared with 30.00% of W3 for the baseline configuration, where 30% was an input to the model. By comparing the results for configuration B with those for configuration D, we can see that the savings achieved by reducing parasitic air flows can exceed the savings obtained from improvements in WHR.

By definition, none of the thermal management system design changes considered here correspond to drop-in fuel benefits. To take advantage of the higher thermal stability of SAFs relative to conventional jet fuel and to improve SFC, some design changes are necessary. Such changes should be expected to afford an improvement of 0.5%, which compares favorably with the savings that could potentially be realized on a drop-in basis, as discussed in the next section.

As an independent effort, GE-Aviation estimated an engine efficiency benefit of 0.28% and a weight savings of 22.5 kg per engine if the ACOC is completely removed from an undisclosed engine in a narrow-body application, for each of the mission mixes shown in Table 1. These results are consistent with the earlier estimate (item C, Figure 6) made by the team at the University of Dayton.

Table 1. Time weightings of mission points used by General Electric to estimate fuel effects.

	Take-off	**Climb**	**Cruise**	**Flight Idle**	**Ground Idle**
Short Haul	5%	35%	50%	5%	5%
Long Haul	5%	30%	55%	6%	4%

Milestones

- Three potential cooling trade-offs have been identified, and the sub-models needed to execute these trade-off studies were built (November 2020).
- The simulations necessary to support the proof of concept were completed (November 2020).
- A scientific paper summarizing this progress was accepted for publication (July 2021).

Major Accomplishments

- A proof-of-concept paper was published in the journal *Fuel*.

Publications

Boehm, R. C.; Scholla, L. C.; & Heyne, J. S. (2021). Sustainable alternative fuel effects on energy consumption of jet engines. Fuel *304*, 121378. https://doi.org/10.1016/j.fuel.2021.121378

Outreach Efforts

None.

Awards

None.

Student Involvement

None.

Plans for Next Period

None.

Task 4 - Estimate Gains in Fuel Efficiency

University of Dayton and GE-Aviation

Objectives

The first goal of this task is to estimate the impact of fuel property variation on engine-level fuel consumption (SFC). The second goal is to optimize fuel composition in order to minimize the SFC while maximizing the specific energy (LHV), which could minimize aircraft fuel consumption, where the fuel LHV is factored into the mass of fuel uplifted into the aircraft.

Research Approach

To accomplish the first goal, the tools developed in Tasks 1 and 3 were used in conjunction with a Monte Carlo simulation of fuel composition derived from a database of 94 molecules, where a filter was used to eliminate random compositions that led to certain properties outside of fuel specifications or fit-for-purpose properties, as predicted via algebraic blending rules. For the second goal, we improved our approach regarding the SAF volatility requirements, added a requirement for the smoke point, and placed a limit on the number of ingredients allowed in the fuel. In addition, the database was expanded to 1,124 molecules. A small (un-converged) Monte Carlo simulation serves as a starting point for optimizing the randomly chosen mole fractions of each molecule from the master database. The engine-level fuel economy and LVH are maximized via mixed-integer distributed ant colony optimization. To arrive at a global solution set, this process is repeated multiple times until all molecules in the database have been chosen at least once by the small initializing Monte Carlo simulation.

Status

Progress toward this task was documented by a presentation given in January 2022 at the American Institute of Aeronautics and Astronautics SciTech Forum in San Diego. For convenience, this paper is included within this section of the report (see Appendix A). Another paper, sponsored in part by this project, documents the creation of a model to predict the sooting propensity of a fuel based solely on its composition. To avoid double-dipping on credit for this work, its reproduction is included with the annual report for Project 65A.

The database used to derive fuel compositions and property estimates now includes 1,124 species, and for each of these molecules, the database contains ten (meaningful) properties, of which four include their respective temperature dependence. Relative to the pilot study, the number of species was increased by a factor of 12.6, and the number of properties was increased by 30%. In addition, we now have an improved model that enables the prediction of freeze points and potentially guides us to restrict the concentration of individual species to a maximum of 10% or that enables a reasonably conservative estimation of freeze points for candidate fuels suggested by the optimizer. In the near term, we expect to add the dielectric constant and energy density to the property filter and seal swell to the list of properties to estimate for candidate fuels.

We also developed a transfer function to relate fuel weight (heating value per unit mass, LHV) to energy savings, corresponding to 0.4% savings per MJ/kg increase in LHV. This scalar is based on a rough physical model of a Boeing 737-800 aircraft and a mission consisting of climb and cruise. This scalar has been validated against an empirical model supplied by Georgia Tech, which was derived from real fuel usage and mission data for the Boeing 737-800. This transfer function will enable consolidation of the LHV and engine savings objectives into one dimension, thereby trimming the number of near-optimal compositions toward a point rather than a line. There will be fewer candidates for considering the harder-to-estimate properties such as seal swell, volatility ranges, freeze point, acquisition cost, and thermal stability.

Figures 7–10 are included in Appendix A to document the noted benefits of SAF relative to petroleum-derived fuel and the current status of progress toward composition optimization. Of note, the difference between Figure 10 in Appendix A and Figure 5 included in Task 2 is the result of several weeks of computation.

Milestones

- A database of 2,000 fully synthetic SAF candidates and a variety of reference fuels was created (November 2020).
- The number of entries in the molecular properties database was increased from 94 to over 2,000 (July 2021).
- Data consistency and completeness were verified (October 2021).
- A model was built and validated to generate smoking propensity data for all molecules in the database (October 2021).
- A peer-reviewed article covering smoking propensity models was published (January 2022).
    - All models used in proof-of-concept work were integrated into JudO, which has been previously used (Kosir, 2020) to optimize fuel composition against defined objectives (September 2021).
- A smoke point filter was added to JudO, and volatility-related predictions and filters were streamlined (August 2021).
- The first successful evolution toward optimized SAF composition was achieved (November 2021).

Major Accomplishments

- The molecular properties database was expanded ten-fold.
- A model was created to estimate the smoking propensity of potential SAF.
- We demonstrated that 100% SAF compositions meeting all considered specifications can favorably impact both fuel weight and engine efficiency.

Publications

Boehm, R. C.; Scholla, L. C.; & Heyne, J. S. (2021). Sustainable alternative fuel effects on energy consumption of jet engines. Fuel *304*, 121378. https://doi.org/10.1016/j.fuel.2021.121378

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Behnke, L. C.; Boehm, R. C.; & Heyne, J. S. (2022). *Optimization of Sustainable Alternative Fuel Composition for Improved Energy Consumption of Jet Engines*. In AIAA Scitech 2022 Forum; p 2056. https://doi.org/10.2514/6.2022-2056

Outreach Efforts

Conference Presentation: AIAA SciTech 2022, San Diego, CA. Video: **https://doi.org/10.2514/6.2022-2056.vid**

Awards

None.

Student Involvement

- Logan Scholla, M.S. student, managed the proof-of-concept, fuel properties database, and Monte Carlo composition selection.
- Lily Behnke, M.S. student, accomplished integration/translation of the Excel-based EPM and FSTM into the Python-based JudO program, was responsible for the results shown in Figures 1–6,10, and 11, and participated in many discussions and decisions regarding this program.
- Jack Hoog, M.S. student, participated in this program.

Plans for Next Period

- Complete the identification of molecules that tend to improve fuel properties toward system efficiency and publish a peer-reviewed journal article on this topic.
- Complete a producibility evaluation of the identified molecules (golden molecules).
- Revise the working-level database, exclude molecules that offer no benefit, and verify the properties of golden molecules.
- Make recommendations regarding fuel quality control specifications for non-drop-in 100% SAF.
- (Boom) Complete OEM trade studies on system-level fuel economy vs. fuel temperature and effective enthalpy.

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Tasks 5 & 6 - Identify, Create, and Test Blends for Thermal Stability in Jet Fuel Thermal Oxidation Testing (JFTOT) and Quartz Crystal Microbalance Testing (QCM)

Objective

The goal of these tasks is to evaluate the solutions identified by the second goal of Task 4 for thermal stability.

Research Approach

The solutions identified in the second goal of Task 4 will be analyzed to find common threads in terms of fuel properties and compositions. It is expected that a relatively small number of molecules with high concentration in several solutions will be identified, and we will discuss these molecules with experts regarding their potential impact on thermal stability. Any such molecule, judged by subject-matter experts to present an elevated risk of coking relative to isoparaffins, will be targeted for experimental evaluation of thermal stability at varying concentrations. Other factors to consider in these selections include availability of the molecule and its potential impact on seal swelling, freeze point, and distillation fraction temperature distribution. These tasks cannot be initiated until more progress is made on the fuel optimization. The current status of identifying golden molecules is presented in Figure 11.

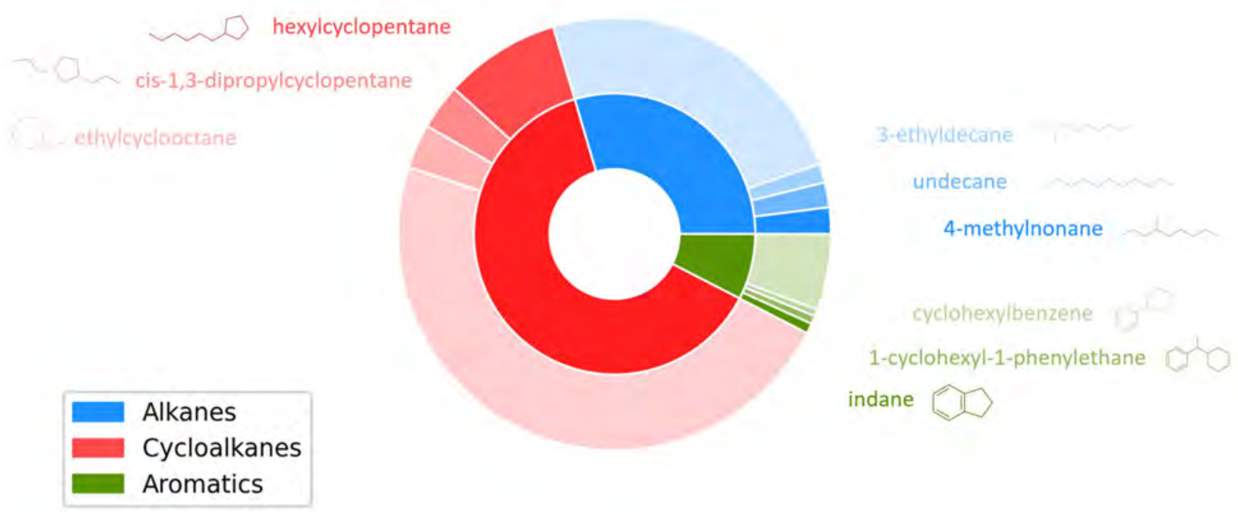

Figure 11. Average composition of 100% sustainable aviation fuel candidates (drop-in) by hydrocarbon type and most prevalent species within each type.

Student Involvement

Lily Behnke, M.S. student, participated in long-range planning for this task.

Plans for Next Period

From the pool of compositions identified in Task 4, select at least two compositions for detailed evaluation of thermal stability in blends with a variety of petroleum jet fuel samples.

Appendix A

Optimization of Sustainable Alternative Fuel Composition for Improved Energy Consumption of Jet Engines

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Abstract

As anthropometric emissions continue to rise globally, reducing emissions from combustion systems is critical to environmental preservation. It is understood that a method for decreasing emissions contributions from the aviation sector is sustainable aviation fuel (SAF). SAF adoption relies on the ability to maintain or surpass the current performance metrics of petroleum derived fuels while also complying with critical operability limitations. High thermal stability SAFs have the potential to provide value in terms of reducing maintenance cost associated with coking and the ability to drive more heat into the fuel therefore increasing energy delivered to the combustor. It was determined that SAFs composed of mostly cycloalkanes with some aromatics maximize the energy savings for both high and low power engine operating conditions. This result is likely tied to the effects of H/C ratio on turbine performance. Furthermore, this work demonstrates that at least a 0.05% savings is possible at the high power conditions from SAF mixtures that meet critical operability limits necessary for SAF approval. However, it was observed that at the low power condition identified SAF mixtures had not yet surpassed conventional petroleum fuel in terms of energy savings. This work provides preliminary results for the design of a high thermal stability SAF that will increase savings over the course of a mission requiring operation at both low and high power conditions respectively.

Nomenclature

SAF = sustainable aviation fuel
TSI = threshold sooting index
FSTM = fuel system thermal model
EPM = engine performance model
LHV = lower heating value

Introduction

As global carbon emissions continue to rise, current research shows that the levels of anthropogenic emissions generated by combustion systems are one of the leading contributions to global climate change (Lee, 2021). Failure to combat the damaging effects of climate change has the potential for devastating global impacts and overall societal instability. It is, therefore, critical that aviation technologies are developed to meet the rising demand for air travel in such a way that anthropogenic emissions do not proportionately increase. One technique that provides a near term solution to minimizing greenhouse gas emissions is sustainable aviation fuel (SAF). Figure 1 outlines the key performance and operability metrics for SAF approval and compatibility with modern day aircraft (Kosir, 2020). The yellow-red shading outlines properties influencing aircraft safety and operability that a SAF candidate needs to satisfy. Furthermore, properties associated with the potential for SAF performance improvements are shown with the green shading. It can be observed that total energy content and thermal stability metrics of a potential SAF are known to add value and performance benefits in addition to the environmental advantages (Flora, 2019). While the benefits of increased energy content have been previously investigated, the benefits of high thermal stability for SAFs remains largely unexplored (Kosir, 2019).

Figure 1. Key performance and operability metrics for jet fuel.

Increasing reliance on jet fuel rather than the use of air as a coolant for the engine and aircraft adds both performance and efficiency benefits (Bruening, 2014). Increased thermal stability of a fuel allows for better thermal management of the engine and, in turn, more energy delivered to the combustor and extracted by the turbine. Furthermore, increased thermal stability of SAFs enables decreases in specific fuel consumption and maintenance costs associated with coking. Coke deposits within fuel nozzles and other fuel system components on jet engines result from waste heat, which is absorbed from other engine and aircraft fluids, and trace amounts of contaminates like transition metals, sulfur, nitrogen, and dissolved oxygen. The presence of coke in the fuel nozzles precipitates maintenance by creating hot streaks or increased spread in exhaust gas temperature. This increased variation in temperature around the circumference of the combustor in turn causes increased combustor emissions and negatively impacts turbine efficiency, which drives up CO2 emissions and fuel cost (Mellor, 1990). Moreover, deposits can affect fuel spray quality, which also impacts operability and increases CO and NOx emissions. Therefore, the significance of increased thermal stability yields both performance and environmental benefits.

A previously conducted pilot study was carried out to observe the engine-level energy savings for SAF fuels for both a baseline engine configuration and a derivative engine configuration (Boehm, 2021). Monte Carlo simulations resulting in population distributions of 2500 SAFs were evaluated in terms of savings benefits for sustainable aviation fuels. The results of this simulation revealed the sensitivities of the model and which fuel properties had the largest effect on the final savings metric. While this work focused on the trends and general methodology for evaluating high thermal stability aviation fuels, there remains work to identify SAF species most suited for harnessing thermal stability benefits. This requires SAFs that are able to remain within important property limits such as viscosity, threshold sooting index (TSI), density, etc. while improving performance metrics as discussed in Fig. 1 (Yang, 2021).

The aim of this research is to utilize optimization techniques to identify SAF candidates yielding high savings and specific energy while complying with crucial operability constraints. It is anticipated that the results of this work will extend into experimental testing for further evaluations of the coking effects of favorable molecules. The results of this work will extend the current capabilities of SAF species from a performance standpoint while also leading to a greater understanding of effects that currently lead to maintenance and emissions issues in modern aircraft engines.

Methodology

Material

As previously outlined, the focus of this work is to identify SAF candidates for increased thermal stability benefits to add value from an efficiency and maintenance standpoint. Furthermore, understanding the effect that various molecules and functional groups have on savings metrics and properties of significance is valuable. For the scope of this work, a database of 1,124 SAF species with respective property data was compiled and utilized as constituents appropriate for optimization. The fuels in this database were composed of a variety of carbon types including aromatics, cycloaromatics, naphthalenes, cycloalkanes, alkanes, bicycloalkanes, and tricycloalkanes. Fuel property data for this work was obtained from the National Institute of Standards and Technology (NIST) fuel property database. Properties relevant to both ASTM D1655 and ASTM D7566 specifications as well as temperature dependent properties necessary for calculating saving benefits were obtained

(ASTMa, n.d.; ASTMb, n.d.). For each generated SAF mixture throughout the course of the optimization the mixture properties were calculated from known physical and chemical properties based on the mole fractions assigned to each of the constituents. For each theoretical SAF mixture the chemical and physical properties were derived from blending rules based on the mixture definition and constituent properties which are detailed elsewhere (Kosir, 2019).

FSTM and EPM

This work fundamentally relied on the ability to evaluate the potential efficiency and performance benefits of a fuel as a function of its fuel properties. A tailored version of a previously developed fuel system thermal model (FSTM) and engine performance model (EPM) were leveraged to quantify the thermal stability benefits of SAFs (Boehm, 2021). The FSTM quantifies the heat pick-up of a fuel by calculating the waste heat recovery and temperature rise as a function of the fuel properties. Furthermore, an EPM was also implemented to compare savings metrics through different conceptual engine design changes that vary the manner in which heat is driven into the fuel. The combination of these models along with fuel property inputs allowed for a final savings comparison to conventional petroleum derived aviation fuel. Additionally, each of these models allows for alterations to accommodate a potential design change that would drive more heat into the fuel and therefore decrease the losses from using air as a coolant. The scope of this work focused solely on the baseline configuration in order to evaluate SAF fuel candidates most suited for modern day aircraft combustion systems.

In addition to calculating fuel savings, several fuel properties including viscosity, heat capacity, thermal conductivity, and energy density influence the performance of heat exchangers, while H/C and molecular weight influence burnt gas composition which effect combustor exit temperature and turbine performance in the EPM model. The pilot study highlighted that low H/C ratio was favorable for turbine performance but also runs the risk of soot issues as a result of high TSI. Considering this key finding, this work combined an updated method for TSI mixture predictions (Boehm, 2022). As a result, a wide array of molecules were selected to appeal to the sensitivities of these models and further explore the impact of fuel properties on energy savings.

Optimization

While previous work demonstrated fuel savings benefits for both the baseline and derivative cases, it was observed that optimization would determine whether comparable savings could be realized without an engine design change. Including optimization methodology allowed for a greater consideration of SAF species and the identification of species with the greatest thermal stability benefits. Furthermore, a constrained optimization allows for the consideration of critical operability constraints that may be limiting factors for realistic savings benefits not filtered in the pilot study. A flowchart demonstrating the general optimization methodology is demonstrated in Fig 2.

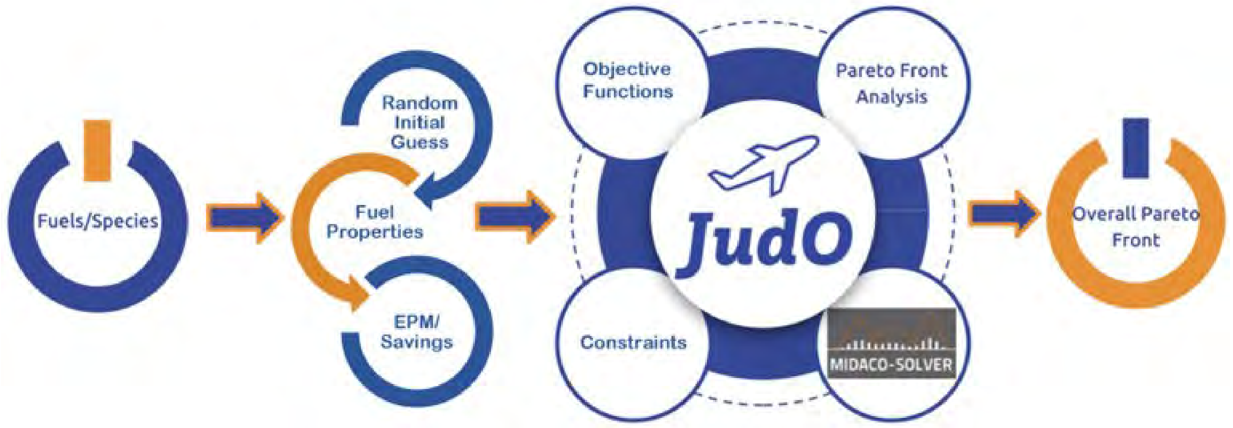

Figure 2 Optimization methodology labeled as the Jet Fuel Blend Optimizer (JudO) incorporating the FSTM and EPM.

As illustrated in Fig. 2 each optimization began with a randomly generated initial guess from the array of 1,124 SAF species which were each assigned a random mole fraction. Due to the number of species in the database, the maximum number of species for each mixture was constrained to 20 to avoid copious amounts of species being selected with nearly negligible concentrations. Then the fuel properties required for the objective functions, constraints, and temperature dependent coefficients required for the FSTM and EPM were calculated for the randomly generated SAF mixture. These properties included, lower heating value (LHV), TSI, viscosity at -20˚C, density at 20˚C, H/C ratio, molecular weight, vapor pressure at 160˚C, T10, and temperature dependent coefficients for density, viscosity, specific heat and conductivity. As previously discussed, these properties are significant specifications required for the aviation fuel approval process. Viscosity and density are known to be key combustor figure of merit operability limits (i.e. e.g. ignition probability at cold conditions) (Colket, 2017). TSI is significant from an emissions standpoint and LHV acts as an important performance metric and weight parameter. These properties were then fed into the FSTM and EPM models for the evaluation of energy savings as a single metric. JUDO then combined the objective functions, constraints, and mixed-integer ant colony optimization (MIDACO) software with pareto front analysis to identify optimal fuel compositions for the respective objective functions (Schlueter, 2013). Specific optimization settings were chosen based on recommendations outlined elsewhere (Midaco-Solver, 2018). The respective objective functions and constraints used in this work can be seen in Table 1.

Table 1. Optimization parameters used in this study for high and low power settings.

Setting	Objective Functions	Constraints
High Power	LHV, Savings	viscosity at -20˚C (<8 cSt), density at 20˚C (< 0.84 , > 0.775 kg/m^3), TSI (< 20), T10 (< 205˚C), $\sum x_i = 1$, Pvap at 160˚C < 1
Low Power		

The parameters outlined in Table 1. Show the objective functions and constraints used for both the high and low power scenarios that were run. The low power condition is meant to represent to the mission conditions from cruise to flight idle while the high power scenario represents conditions for takeoff and climb. Specifically, the two conditions are intended to capture the minimum and maximum fuel flow of the operating envelope. For each optimization, energy savings and LHV were maximized to simultaneously maximize the performance metrics of the SAF mixture. Furthermore, the operability limits as previously described acted as constraints.

Results and Discussion

The results presented in this section focus on the savings metrics and corresponding fuel compositions for both the high and low power baseline engine configurations. While previous work focused on outlining the methodology for obtaining the savings value, these results investigate the SAF species and functional groups best suited for simultaneous savings and LHV benefits. Each scenario utilizes “A2”, a specific sample representing average petroleum derived conventional jet fuel, as a point of comparison.

Fig. 3 shows the pareto front for the high power optimization demonstrating the trade-off between LHV and energy savings. The pink star represents the reference fuel A2 which has a savings value of zero since the FSTM and EPM are normalized to the fuel flow and mission demand for conventional petroleum jet fuel. The larger points with the color bar represent the identified SAF mixture solutions with the color bar representing the mole fraction of aromatic content present in each mixture. Strong consideration is placed on the limiting of aromatics from an emissions standpoint (i.e., smoke point), therefore the amount aromatics in a SAF mixture requires specific consideration. It can be observed that generally the solutions with higher savings values have a greater amount of aromatic content. While most of the SAF mixtures have savings values that are less than zero, there are some that yield positive savings benefits. Furthermore, there are a few solutions that provide marginal savings benefits as well as LHV improvements to A2. Furthermore, Fig. 3 illustrates a few points that stray from the general cluster of points. This is due to the fact that this is a highly constrained optimization with a large database to choose from. It is anticipated that with more computational time, which is not in the scope of this paper, coupled with an initial guess filter that requires the initial guess to pass ASTM specifications would lead to more solutions that could push the overall front outward towards higher LHV and savings metrics.

The high power pareto front shows the relative aromatic content for each optimal solution while Fig.4 further details the composition of each optimal solution as a function of savings. The composition is expressed from zero to one to demonstrate the breakdown of the mole fraction representation from each carbon group for the mixture. The brown area represents the

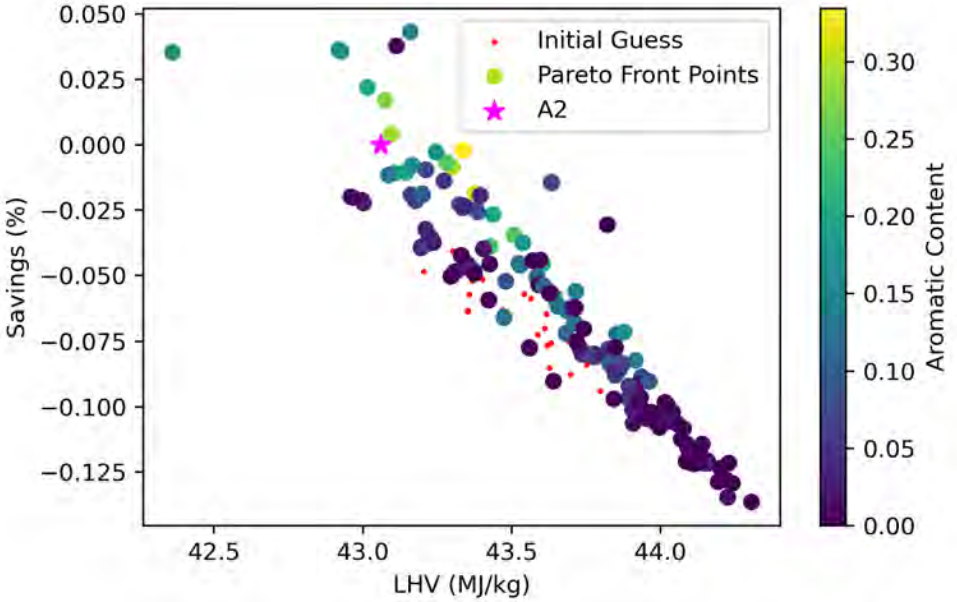

Figure 3. Pareto front solutions from the high power engine operating condition show a potential savings and LHV increase from SAF mixtures compared to standard petroleum fuel A2.

Mole fraction of the composition that is made up of alkanes while the pink represents the mole fraction of cycloalkanes in the mixture and the green represents the mole fraction of aromatics in the mixture. In this case, cycloalkanes include monocycloalkanes, bicycloalkanes, and tricycloalkanes, and aromatics include aromatics, cycloaromatics, and naphthalenes. Fig. 4 shows that generally as savings increases so does cycloalkane content and aromatic content. Conversely, as savings increases alkane content decreases. This is likely a result of the dependency of the FSTM and EPM on H/C ratio with a low H/C ratio increasing savings metrics as a result of improved turbine performance with increasing gamma (Cp/Cv). While low H/C ratio may potentially lead to sooting issues and high TSI, the incorporation of the TSI constraint within this optimization allows for solutions to be within the acceptable range. This affect also describes a potential limiting factor for mixture solutions that provide increased savings and will act as a metric for identifying favorable SAF species.

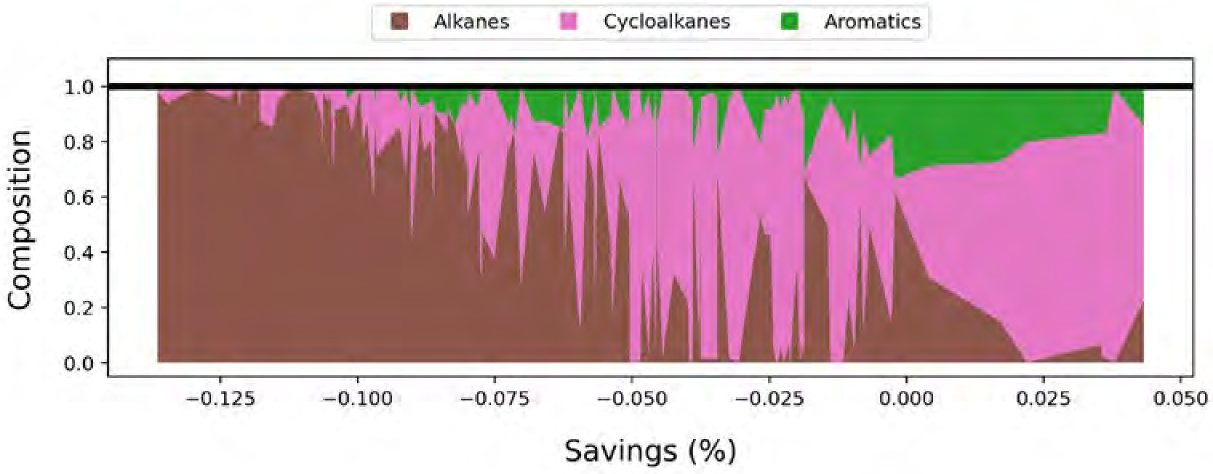

Figure 4. Graphic showing the composition of each optimal solution for high power as a function of savings. The constituents in the optimal solutions are grouped by functional group, alkanes, cycloalkanes, and aromatics.

Fig. 5 exemplifies the pareto front results for the low power setting of the EPM and FSTM. The pink star once again represents A2 while the points with the color bar are the identified pareto front points. Similar to the high power result, the color bar represents the amount of aromatic content present in each of the solution. It can be seen that generally the solutions with higher savings values contain more aromatics. Moreover, there is only one solution that offers a positive savings metric with an LHV that is slightly less than A2. This indicates that for this scenario the current pareto front has not exceeded the benefits of A2. As discussed with the high power result, it is worth noting that this is a highly constrained optimization problem. With added computational time and an initial guess filter there is room to further explore the results of this optimization.

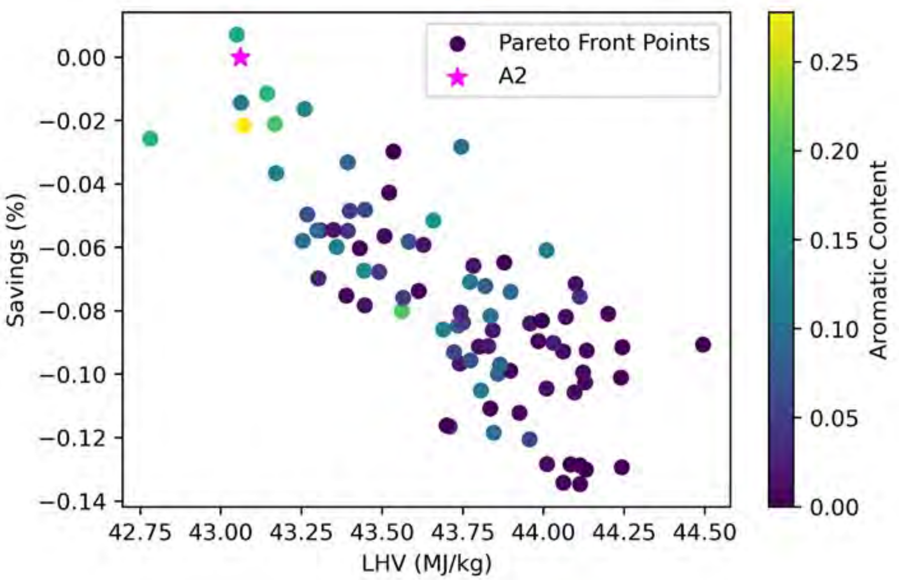

Figure 5. Pareto front solutions from the low power engine operating condition showing mostly negative savings impacts from SAF mixtures compared to standard petroleum fuel A2.

Similar to the high power result, Fig. 6 portrays the breakdown from a carbon group standpoint of the pareto front solutions for low power. Composition of the optimal solutions as a function of savings is shown with composition ranging from zero to one to show the mole fraction representation from each carbon group. At lower savings values the composition of the optimal solution is largely alkanes, while larger savings values result in higher concentrations of cycloalkanes and aromatics. Once again, cycloalkanes include monocycloalkanes, bicycloalkanes, and tricycloalkanes, and aromatics include aromatics, cycloaromatics, and naphthalenes. This result is similar to what is observed in the high-power scenario and further suggests that higher savings values could be achieved from mixtures that are higher in cycloalkanes with some aromatics.

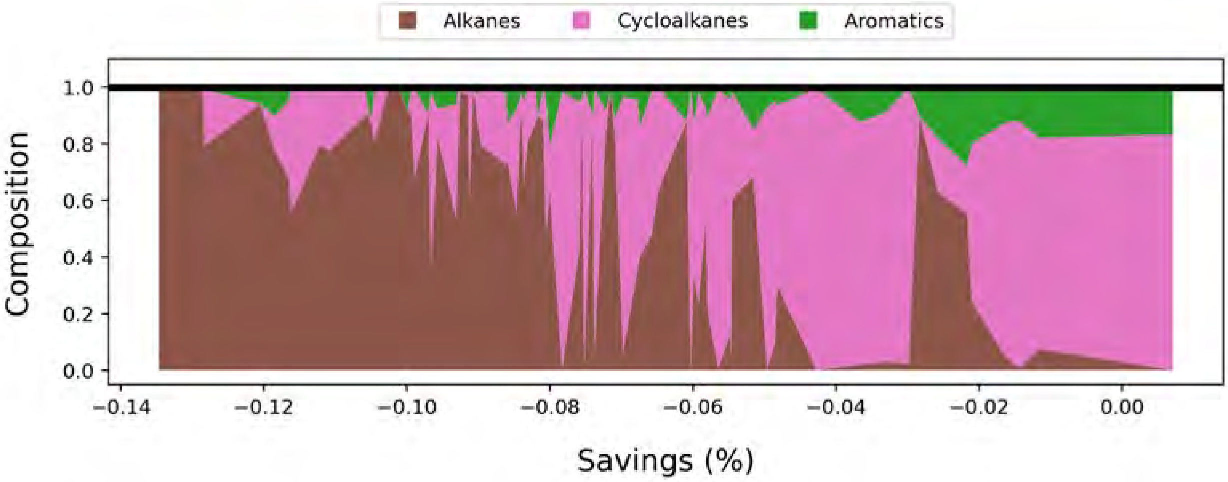

Figure 6. Graphic showing the composition of each optimal solution for low power as a function of savings. The constituents in the optimal solutions are grouped by functional group, alkanes, cycloalkanes, and aromatics.

Conclusion

This research has sought to identify SAF mixtures and carbon groups with properties providing value from an efficiency and energy content perspective. The high power model results indicate that several SAF mixtures composed of primarily cycloalkanes with a few aromatics have the potential to add energy savings from high thermal stability benefits. However, the low power result has not yet yielded a result that predicts improved savings from SAF mixtures. Despite this result, the low power results confirm the conclusion from the high power result that a greater presence of cycloalkanes with some aromatics yields higher savings metrics than mixtures of primarily alkanes. It is anticipated that with increased computational time much more of the composition space will be explored and many more solutions with both higher savings and LHV relative to A2 will be found.

In this work the low power and high power conditions were analyzed separately, however in reality each of the operating conditions would be met throughout the course of a flight. Future work will focus on combining and weighting the fuel consumed at each condition into a single savings metric. The repeating of the optimization with a combined mission savings term with added computational time allowed for exploration of optimal mixtures. Furthermore, following the combined optimization, SAF identified optimal species will be experimentally tested for thermal oxidative stability metrics.

Acknowledgments

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We would like to acknowledge Zhibin Yang, and the Heyne Energy and Appropriate Technologies lab members for their support in this research effort, of which, would not be possible without their help.

Noted Benefits of SAF

This section includes three figures (Figures 7–9) that clearly illustrate the potential benefits of 100% SAF and one figure (Figure 10) that clearly illustrates the status of the fuel optimization when work was suspended on this project. Figure 7 has been shown on multiple occasions in quarterly reports, prior annual reports, and the proof-of-concept journal article on this topic. It illustrates that fuel composition does directly impact engine efficiency at both high and low power but that increased fuel temperature (enabled via the high thermal stability of SAF) can have a much larger impact, provided that the engine design is modified to take advantage of this characteristic. Figure 8 presents the results of a commonly used test for inferring jet fuel thermal stability and the differences between petroleum jet fuel and currently approved SAF blend components. The results shown in Figure 8 justify the proposal to raise the maximum fuel temperature limit on aircraft designated for 100% SAF usage, as suggested by the results shown in Figure 7. The reduced sooting propensity of SAF relative to petroleum fuel, proven by the flame visualization shown in Figure 9, is also a direct benefit of SAF, but one that is difficult to quantify. This benefit is primarily linked to the aromatic concentration in the fuel.

The data shown In Figure 10 are sufficient to demonstrate that it is possible to simultaneously increase the specific heat (LHV) and engine operating efficiency, with the latter being primarily increased via reduced viscosity or H/C ratio. The composition of potential SAFs meeting these objective is strongly represented by cycloalkanes.

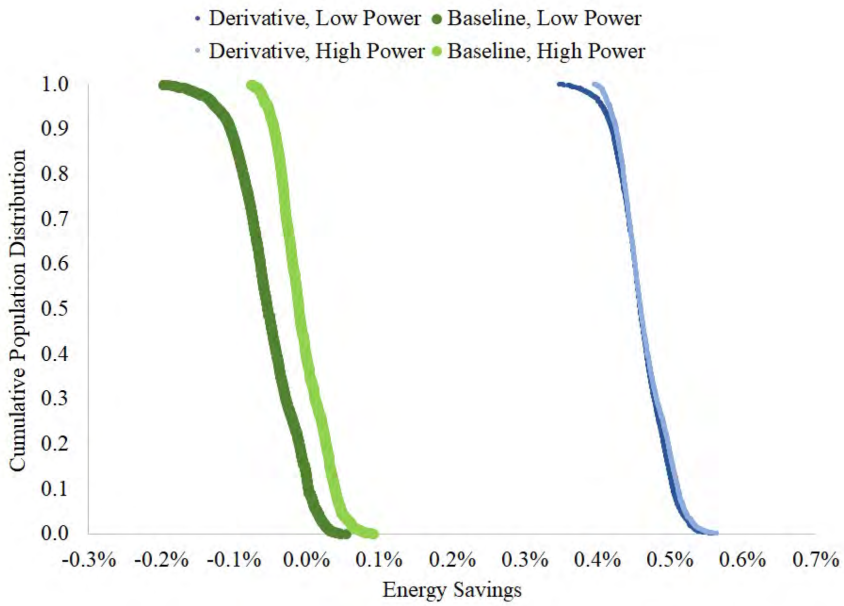
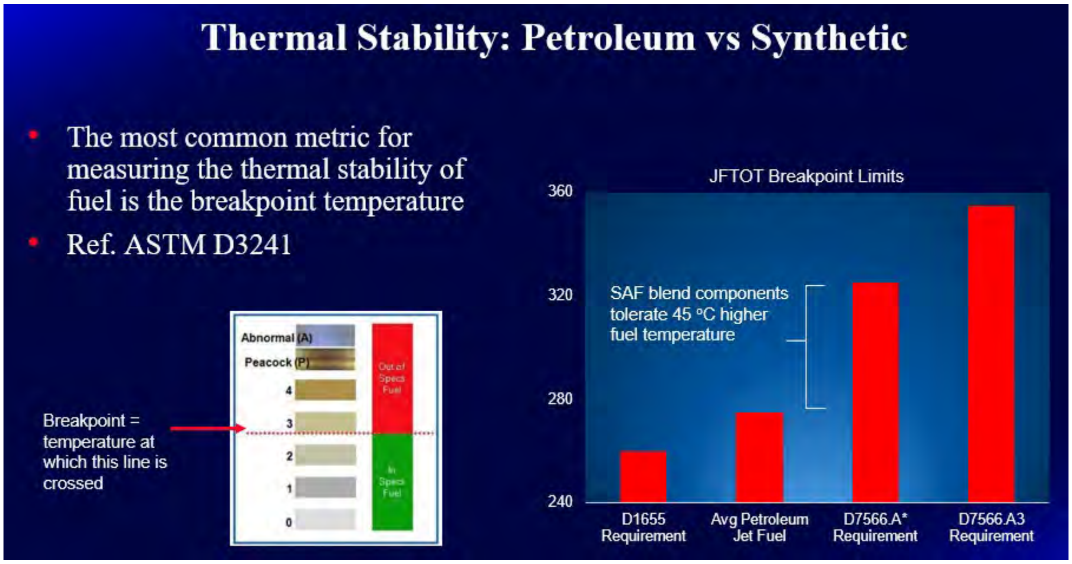


Figure 7. Impact of design and fuel property on fuel energy savings.



Thermal Stability: Petroleum vs Synthetic

- The most common metric for measuring the thermal stability of fuel is the breakpoint temperature
- Ref. ASTM D3241

Figure 8. Comparison of fuel thermal stability between sustainable aviation fuel (SAF) and petroleum-derived fuel. ASTM: American Society for Testing and Materials; JFTOT: jet fuel thermal oxidation test.

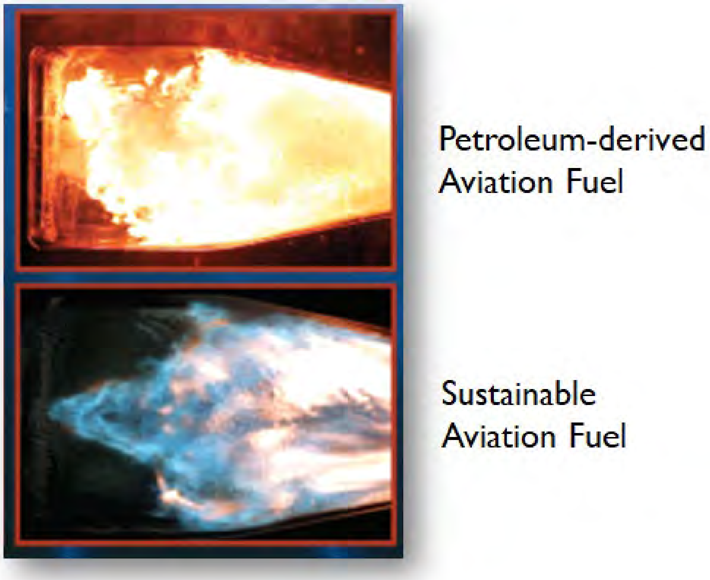


Figure 9. Comparison of flames produced by sustainable aviation fuel or petroleum-derived fuel under similar operating conditions.

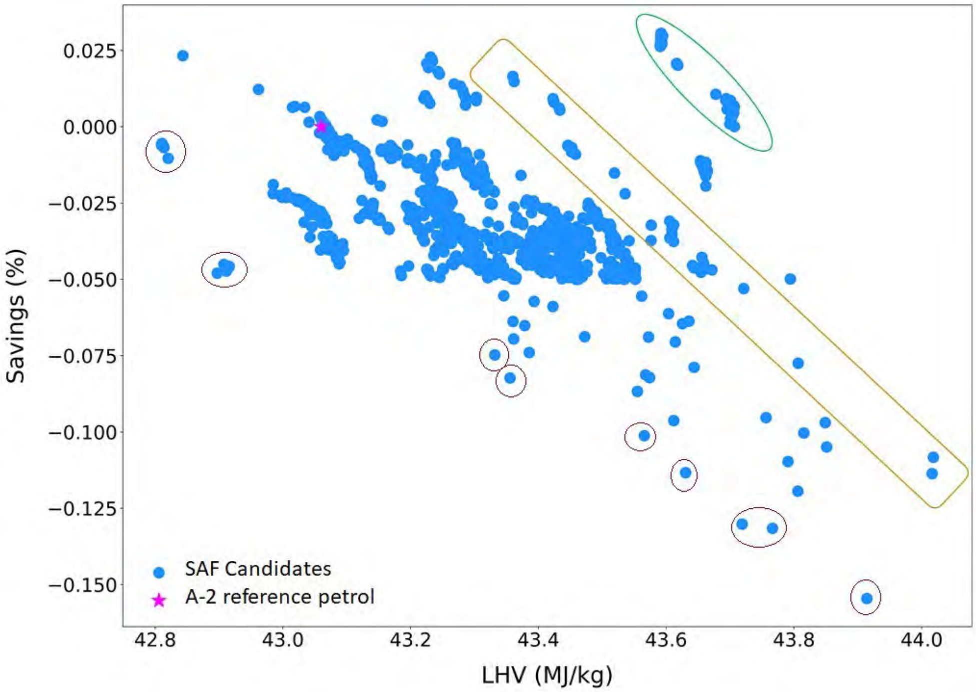


Figure 10. Lower heating value (LHV) and relative energy efficiency at low power for 100% sustainable aviation fuel (SAF) candidates (drop-in).

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