Project 034 National Jet Fuels Combustion Program – Area #7: Overall Program Integration and Analysis

University of Dayton

Project Lead Investigator

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- P.I.: Joshua Heyne
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- Task:
    1. Overall integration and coordination of the National Jet Fuels Combustion Program (NJFCP)
    2. Investigation of alternative jet fuel dependencies between combustors of different sizes and mixing approaches

Project Funding Level

Amendment No. 9: $134,999.00 (September 18, 2015, to February 28, 2017)
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Cost share is from the University of Dayton, DLR Germany, Raytheon Technologies Research Center (RTRC), and the National Research Council (NRC) Canada.

Investigation Team

- Joshua Heyne (University of Dayton) is the project's lead investigator and is responsible for coordinating all NJFCP teams (both ASCENT and non-ASCENT efforts).
- Randall Boehm (University of Dayton) is a research engineer combining the results from various combustor observations.
- Jen Colborn (University of Dayton) is a graduate student research assistant helping with fuel testing on the Referee Rig.
- Zhibin Yang (University of Dayton) is a graduate student research assistant working on Tier Alpha and Tier Beta.

Project Overview

The NJFCP is composed of over two dozen member institutions that contribute information and data, including expert advice from gas turbine original equipment manufacturers (OEMs), federal agencies, and other ASCENT universities as well as corroborating experiments at the German Aerospace Center (DLR Germany), National Research Council Canada, and other international partners. This project involves coordinating and integrating research among these diverse program stakeholders and academic PIs; cross-analyzing results from other NJFCP areas; collecting data from a well-stirred reactor for modeling and fuel comparison purposes; conducting large eddy simulations of sprays for the Area 3 high-shear rig; and procuring additional swirler geometries for the NJFCP areas and allied partners while developing an interface for NJFCP modeling capabilities and OEM requirements. Work under this program consists of, but is not limited to:

- conducting meetings with member institutions to facilitate the consistency of testing and modeling,
- coordinating timely completion of program milestones,
- documenting results and procedures,
- creating documents critical for program processes (e.g., fuel down selection criteria),
- soliciting and incorporating program feedback from OEMs,
- reporting and presenting on behalf of the NJFCP at meetings and technical conferences,
- integrating state-of-the-art combustion and spray models into user-defined-functions (UDFs), and
- advising the program steering committee.

Task 1 - Integration and Coordination of NJFCP Teams

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Objective(s)

The objective of this task is to integrate and coordinate all ASCENT and non-ASCENT team efforts by facilitating meetings, summarizing results, presenting results external to the NJFCP, communicating regularly with the steering committee, and performing other related activities.

Research Approach

The NJFCP is integrated and coordinated via two main techniques: (1) the structural combining of various teams into six topic areas; and (2) routine meetings and discussions both internal and external to individual topic areas. The topic areas are distinguished by the dominant physics associated with them (topics I and IV), the culmination of all relevant combustion physics (topics II, III, V), and the wrapping of all work into a single OEM graphical user interface package (topic VI). These six topic areas are as follows:

Topic I. Chemical kinetics: A chemical kinetic model, with the validation data to anchor modeling predictions, is foundational to any combustion model.

Topic II. Lean blowout (LBO): This topic covers data, screening, and validation, under relevant conditions, to statistically and theoretically anticipate the effects of fuel properties on this figure of merit (FOM).

Topic III. Ignition: Similar to Topic II, the focus of this topic is obtaining experimental screening and validation data for statistical and theoretical predictions.

Topic IV. Sprays: Historically, the dominant effect of fuel FOM behavior has been the spray character of the fuel relative to others. Experiments in this topic area focus on measuring the effects of fuel properties on spray behavior. Like Topic I, spray behavior is not a FOM (like Topics II and III), but it is critical to bounding the effects of physical properties on combustion behavior relative to other processes (i.e., chemical kinetics).

Topic V. Computational fluid dynamics (CFD) modeling. Complementary to the empirical Topics II, III, and IV, CFD modeling focuses on the theoretical prediction of measured data and facilitates the development of theoretical modeling approaches.

Topic VI. User-defined function development: Once the theoretical modeling approaches established in Topic V are validated, user-defined functions are developed for OEM evaluation of fuel performance in proprietary rigs.

The topic area teams meet and coordinate regularly. At minimum, NJFCP-wide meetings are held monthly, and topic area meetings typically occur every 2 to 3 weeks.

Milestone(s)

- NJFCP American Institute of Aeronautics and Astronautics (AIAA) Book was published.
- Developed Tier Alpha prescreening tool for novel sustainable aviation fuel (SAF) prescreening.

Major Accomplishments

- Edited, coordinated, and published a NJFCP AIAA book.

- Developed and published a Civil Aviation Alternative Fuels Initiative (CAAFI) R&D prescreening document to aid novel companies and producers in the refinement and development of fuels that can most easily eclipse the Tier 3 and 4 testing.
- Reported the alternative jet fuel dependencies between combustors of different sizes and mixing approaches.

Publications

Peer-reviewed journal publications

Boehm, R. C., Colborn, J. G., & Heyne, J. S. (2021). Comparing alternative jet fuel dependencies between combustors of different size and mixing approaches. Frontiers in Energy Research, *9*. https://doi.org/10.3389/FENRG.2021.701901

Book publication

Colket, M., & Heyne, J. (2021). *Fuel effects on operability of aircraft gas turbine combustors*. American Institute of Aeronautics and Astronautics. https://doi.org/10.2514/4.106040

Book chapters

Colket, M., Heyne, J., Andac, G., Rumizen, M. (2021). Chapter I. Introduction. In T. C. Lieuwen (Ed.), *Fuel effects on operability of aircraft gas turbine combustors* (pp. 1-20). American Institute of Aeronautics and Astronautics.

Rock, N., Stouffer, S., Hendershott, T., Heyne, J., Blunck, D., Lukai, Z., Khandelwal, B., Emerson, B., Mastorakos, E., Colket, M. (2021). Chapter V. Lean blowout studies., In T. C. Lieuwen (Ed.), *Fuel effects on operability of aircraft gas turbine combustors* (pp. 143–196). American Institute of Aeronautics and Astronautics.

Heyne, J., Rauch, B., Hanson, R., Dooley, S., Blakey, S., Yang, Z., Ferris, A., Ure, A., Le Clercq, P., Boehm, R., Lewis, C., & Colket, M. Chapter XII. Prescreening of Sustainable Aviation Jet Fuels. In T. C. Lieuwen (Ed.), *Fuel effects on operability of aircraft gas turbine combustors* (pp. 487–523). American Institute of Aeronautics and Astronautics.

Heyne, J., Colket, M., Edwards, T., Moder, J., Rumizen, M., & Oldani, A. (2021). Chapter XIII. Summary. In T. C. Lieuwen (Ed.), *Fuel effects on operability of aircraft gas turbine combustors* (pp. 525–534). American Institute of Aeronautics and Astronautics.

Outreach Efforts

Invited talks

- Heyne, J. (2020, November). High value drop-in aviation fuels: From molecule selection to mission benefits [Panel presentation]. Fuel Quality Matters, DOE BETO/PNNL HTL Workshop, Virtual meeting.
- Heyne, J. (2020, November). Prescreening of HTL SAFs: Rapid low-volume, low-cost testing. Sustainable Aviation Fuel Certification, DOE BETO/PNNL HTL Workshop, Virtual meeting.
- Heyne J. (2021, May). Summative results of the national jet fuels combustion program [Panel presentation]. Properties and Emissions, CRC Aviation Fuels Meeting, Virtual meeting.
- Heyne, J. (2021, June). Prescreening of sustainable aviation fuels [Panel presentation]. CAAFI Virtual Mini-Symposium.
- Heyne, J. (2021, June 2). Sustainable aviation fuel prescreening, benefits, and a proposed streamlined evaluation process [Panel presentation]. National Academies, Transportation Research Board (AV030), Sustainable Aviation Fuels subcommittee midyear meeting.
- Heyne, J. (2021, August 17). Sustainable aviation fuel: Properties, compositions, and qualification requirements [Sponsored seminar]. Sandia National Laboratory.
- Heyne, J., (2021, August 17). Sustainable aviation fuel property needs and some solid waste candidates [Panel presentation]. Seminar on Hydrothermal Liquefaction: biocrudes and advances towards drop-in fuel potential, Aalborg University, Denmark.
- Heyne, J. (2021, November). Sustainable aviation fuel: Properties, compositions, and qualification requirements [Sponsored travel]. Center for Multiphase Flow Research and Education, Iowa State University.

Conference presentations

None.

Awards

Joshua Heyne

- 2021 Net Good Summit on sustainable travel, honored guest
- 2021 US Frontiers of Engineering Symposium, National Academies of Engineering, selected participant

- 2021 Vision Award for Excellence in Scholarship, School of Eng., University of Dayton

Student Involvement

Jen Colborn, graduate research assistant, leads this effort.
Zhibin (Harrison) Yang, Ph.D. student (October 2020 to September 2021), is working on developing the Tier Alpha prescreening tool.

Plans for Next Period

Continue to coordinate across various federal agencies and research institutions for SAF testing.

Task 2 – Investigation of Alternative Jet Fuel Dependencies Between Combustors of Different Size and Mixing Approaches

University of Dayton

Objective

The objective of this task is to investigate alternative jet fuel dependencies between combustors of different sizes and mixing approaches.

Research Approach

1. Introduction

As global fuel demand increases, various environmental, economic, and security interests have led to the investigation of SAFs for broader use. Due to differences in composition between SAFs and petroleum-derived fuels, SAFs must undergo a certification and qualification process before being deployed. The process for SAF qualification, known as ASTM D4054, focuses on developing "drop-in" hydrocarbon fuels, meaning that no changes need to be made to engine, aircraft, or airport infrastructure for a fuel to be compatible. Unless a candidate fuel qualifies for fast-track approval, this evaluation is an extensive process that takes years to complete, millions of dollars, and thousands of gallons of fuel (Oldani [1]). As shown in Figure 1, the approval process for non-fast-track jet fuel qualification involves four levels of testing as well as two stages of research reports with comprehensive stakeholder review. Fuel is first tested for general specifications and fit-for-purpose properties before the Phase 1 report is released to the stakeholders, who then complete a technical review of the data before the fuel can proceed to Tier 3 and Tier 4 testing. Both rig and engine testing are then conducted in Tiers 3 and 4. The amount of fuel required for testing increases about 10-fold with every tier in the qualification process.

A renewable jet fuel called RediJet, which was produced through catalytic hydrothermolysis, was recently submitted to ASTM subcommittee J for aviation fuels for approval. According to Coppola [2] , approximately 72,000 gallons of RediJet was required to complete the test plan. Component and rig tests were performed by three different engine manufacturers across nine different test conditions. Engine testing was completed by two engine manufacturers and included a flight test with a twin-engine Falcon 20. Three fuel mixtures were used for each test condition: neat Jet A as a baseline, neat RediJet, and a 50:50 blend. Overall, 144,000 gallons of jet fuel were used for full qualification of the new "drop-in" SAF. Reducing the volume of fuel required for the qualification process would be advantageous for both fuel manufacturers and the sponsors who have a vested interest in SAF.

The aim of the NJFCP was to shorten and redirect the process for jet fuel qualification (Colket et al. [3]). By developing predictive models for fuel behavior and adding some tailored, low-volume testing prior to the phase I research report, additional feedback would be provided to the ASTM evaluation committee and fuel manufacturers to guide early fuel development. The scope of tier 3 and tier 4 testing could then be directed toward a narrower range of potential concerns, thereby reducing the total amount of fuel required. Alternatively, the candidate fuel could be reformulated into a product that has a higher probability of achieving qualification. Importantly, there is a need to understand how fuel effects in small-scale rigs compare with engine observations. Validating small-scale rigs against full-scale engines is also essential for developing predictive models and testing methodology.

At the program level, we identified a range of operating conditions where lean blowout (LBO) or ignition is most likely to be impacted by differences in fuel composition and properties (Colket & Heyne [4]). The most sensitive LBO conditions involve

(i) a throttle-chop from cruise to flight idle and (ii) a start transient where the increase in fuel flow rate may not sufficiently keep up with the increase in airflow rate if the control schedule is improperly set for the fuel being used. Fuel impacts on ignition are most important at cold conditions such as a cold-soaked auxiliary power unit (APU) at altitude or a cold-soaked main engine on the ground. Figure 2 shows operating conditions for the typical temperatures (T_{cmb}) and pressures (P_{cmb}) in the combustion chamber. In this figure, "altitude relight" and "cold start" both refer to ignition cases. These conditions were selected because they are some of the most extreme conditions that can exist within an engine and are consistent with the tests required by ASTM D4054 (Coppola [2]; Colket et al. [3]). Similar fuel dependencies have been noted for cold ground start and altitude relight (Hendershot et al. [5]; Stouffer et al. [6]).

Nine experimental rigs within the NJFCP, featuring a wide range of geometries and time scales, were used to observe fuel effects (Colket & Heyne, 2021). As shown in Figure 3, eight of the nine rigs showed a correlation between the derived cetane number (DCN) and the relative equivalence ratio at LBO (Φ_i). The parameter Φ_i is defined as the LBO performance of fuel (i) relative to the LBO performance of the reference fuel (A2) and is expressed as a percentage (see Equation 1).

$$\Phi_{\mathrm{i}} = \frac{\phi_i - \phi_{A2}}{\phi_{A2}} \quad (1)$$

The only rig that did not show a correlation between DCN and Φ_i was the Honeywell 131-9 APU combustor rig (APU-CR), one of the two industry combustors used in the program. This result appears to be incongruent with the goal of the NJFCP; namely, to reduce tier 3 or tier 4 testing. However, closer examination of results from both the Referee Rig (RR) and a GE9X full annular combustor rig (GE9X-FAR) showed that fuel dependencies vary with operating conditions.

Colborn et al. [7] showed that the relative LBO in the RR at an air temperature and pressure of 65 °C and 107 kPa, respectively, is dominated by the Ohnesorge number (Oh) at 2% DP/P. In contrast, the DCN dominates at 6% DP/P, with a smooth transition from one extreme to the other. At 3.5% DP/P and 107 kPa, the fuel with the lowest DCN and most favorable atomization properties (hereafter labeled as C1) showed no sensitivity to air temperature between 65 °C and 83 °C. Boehm et al. [8] found this same fuel (C1) had measurably worse LBO performance in a GE9X combustor than the other three fuels tested at three of their four test conditions. At a lower air temperature, C1 showed the same LBO performance as the reference petroleum-derived fuel when the two fuels were heated to 60 °C, which was the reference fuel temperature for this set of tests. These results are summarized in Figure 4. Overall, the data suggest that the physical and chemical properties of the fuel are both important near the low-temperature boundary of the GE9X engine operating range at conditions important to the aircraft engine LBO margin, whereas only chemical properties are important at higher air temperatures and loadings.

In this report, we show that the results introduced above are consistent with LBO theory (Plee & Mellor [9]; Mellor [10]) and that the RR, in concert with a well-thought-out test plan, can show the same fuel dependencies as the APU-CR and the GE9X-FAR. The timescales of evaporation and chemical reactions are impacted significantly by fuel and air temperature, suggesting that the range of operating conditions being tested is critical to a thorough investigation of fuel dependencies. We assert that commercial combustor geometry does not need to be matched with specific operating conditions if the test combustor is tested over a sufficiently wide range of operating conditions to sweep through the range of timescale ratios that are relevant to commercial combustor operability.

2. Background

2.1 Previous work

Several investigations of how fuel affects LBO have already been completed. For example, Rock et al. [11] measured the LBO threshold in an un-cooled flame tube using 18 different fuels and three different inlet air temperatures. They noted a correlation to DCN, T10, T90, or surface tension, dependent depending on the inlet air temperature. Using the same set of 18 fuels, Casselberry et al. [12] demonstrated a correlation between pyrolysis products at 625 °C and the LBO threshold in the RR when the RR was operated at chop-like (warm) conditions. Won et al. [13] investigated the role of preferential vaporization and suggested that the DCN of the front end of the distillation may be a better indicator of LBO than the DCN of the fully vaporized fuel. They also observed that LBO is more strongly correlated with fuel physical properties than with fuel chemistry at low temperature operation. Grohmann et al. [14] similarly observed that both physical and chemical properties of a fuel influence combustor LBO. In a study of the effects of atomization, Muthuselvan et al. [15] related atomization quality with timescales relevant to LBO.

Many experiments and analyses of the ignition characteristics of hydrocarbon fuels have focused on either pre-vaporized and premixed fuel or other fuels and conditions that depart significantly from the most extreme start-up requirements for gas turbines used in aviation. Excellent reviews on these topics have been published by Aggarwal [16] and, more recently, by Colket and Heyne [4]. Mayhew [17] observed correlation between ignition probabilities at cold altitude relight conditions in a derivative of the RR and each of four fuel properties: viscosity, surface tension, 20% recovered temperature (T_{20}), and flash point. Opacich et al. [18] observed similar correlations within datasets derived from both the RR and the APU-CR, although they represented volatile properties using vapor pressure and heat capacity instead of T_{20} and flash point. Part of this work directly follows up on the work introduced by Opacich et al. [18].

2.2 LBO Theory

A common theme in several of the works cited above is that LBO performance can be evaluated by considering three timescales that impact LBO limits, as shown in Equation 2: chemical, mixing and evaporative timescales (Plee & Mellor, 1979; Mellor, 1980). This theory is further illustrated in Figure 5.

$$\frac{1}{\phi_{LBO}} \sim \left(\frac{1}{\tau_{chem}} + \frac{1}{\tau_{mix}} + \frac{1}{\tau_{evap}}\right)^{-1} \qquad (2)$$

Fuel physical properties, along with aerodynamic shear forces, flow field, fuel nozzle design, and fuel pressure all affect fuel spray atomization, including droplet size distribution and spray distribution. While combustor design and operating conditions are important to atomization, fuel properties are also an important factor for some commercial combustors at relevant, in-service operating conditions.

Fuel vapor pressure (and/or thermal conductivity), spray characteristics, and combustor aerodynamics all influence the evaporation timescale. From the perspective of fuel dependencies on LBO, it is important to note that the evaporation timescale of some commercial combustors will be impacted significantly by vapor pressure, which varies not only with droplet surface temperature but also with the time-varying composition of the liquid fuel throughout the evaporation process. In systems that are evaporation-limited, fuels with a higher vapor pressure at a given temperature are expected to ignite more readily than fuels with a lower vapor pressure.

The mixing of fuel vapor with air depends on the flow field, turbulence intensity, and the spatial relationship between the fuel spray, the eddies within the flow field, and the flame. Because turbulence is overwhelmingly more important than laminar diffusion in most commercial combustors, there is ample technical justification for neglecting this term when considering fuel effects. Moreover, the characteristic mixing time of a given commercial combustor at any well-defined operating condition is likely to be kept proprietary by the engine companies.

The specifics of fuel-air mixing also influence the gaseous mixture residence time and reactant concentration. These two variables, along with species reactivity, determine the fuel chemistry of combustion and blowout. The chemical timescale is relevant to the physics and may be comprised of different pieces, such as autoignition and extinction.

2.3 Cold Ignition

At extremely low fuel temperatures, the fuel vapor pressure is low. When the inlet air temperature is equally low, fuel droplets are not heated until they reach a heat source, which could be either a plasma discharge or the kernel of a previously ignited fuel/air mixture. The size and spatial distribution of liquid fuel droplets within the combustor flow field at extremely cold conditions is expected to be critical for most, if not all, combustors in aviation service. Very little evaporation occurs outside of the domain of the plasma discharge (spark), and it must therefore supply enough energy to both evaporate the fuel and overcome the critical kernel radius (Kim et al., 2013). Each kernel must release enough heat to both sustain the flame and sufficiently evaporate enough surrounding liquid fuel droplets to replenish the fuel consumed by combustion within the kernel. Only under these conditions can the flame kernel grow, propagate upstream to an anchor point, and transition to a self-sustaining flame. This process can be influenced significantly by fuel volatility, thermal properties, and the physical properties that influence atomization.

2.4 Atomization

Atomization is affected by the viscosity, density, and surface tension of the fuel [(Guildenbecher et al., 2019; Lefebvre & McDonnell, 2017). Increased surface tension inhibits fuel breakup, increased viscosity dampens the instabilities that allow for breakup, and increased density drives lower flow rates in engines that are controlled to deliver a scheduled enthalpy flux or equivalence ratio. This in turn reduces the gage pressure, which supplies the energy that drives atomization.

3. Experiments, Data and Methods

3.1 Referee Rig Experiments

Experiments performed in the RR were completed at the Air Force Research Laboratory (AFRL) located at Wright-Patterson Air Force Base and have previously been published (Henderschott et al., 2018; Colborn et al., 2020). The RR is a non-proprietarty, single-cup, swirl-stabilized combustor designed by GE (this article's corresponding author) with input from four other leading engine manufacturers. The rig simulates representative aerodynamic characteristics of both legacy and emerging swirl-stabilized combustors (Colket & Heyne, 2021). It is a classic rich-quench-lean combustor with effusion-cooled liners, a flat dome protected by an impingement-cooled heat shield, primary dilution holes located at ½ the dome height downstream from the dome, and seconday dilution holes located just aft of the primary reaction zone. The rig features a modular construction to facilitate swapping of fuel injectors and swirlers, which allows researchers to evaluate different swirler effective areas, swirl numbers, spray angles and flow numbers. However, most of the data collected from the RR to date has come from just one design configuration. The AFRL modified the rig's original four-cup design to a single-cup design, and the University of Dayton Research Institute (UDRI) custom-buillt a thryatron-based exciter to achieve better control over spark energy and frequency relative to jet engine exciters. Readers interested in fabricating a copy of this combustor should contact the authors for information on where to find a copy of the drawings.

In this study, we analyzed four operating conditions of the RR (Table 1). Fuel and air temperature were matched in each condition, and LBO was determined after each successful ignition. For all test conditions, the normalization described by Equation 1 was reset so that its value, corresponding to the fuel sample designated as A2, was always zero. This normalization reduces the dependencies on operating conditions and highlights fuel dependencies.

3.2 APU-CR Experiments

The APU-CR experiments were performed in the combustor component test facility at Honeywell Aerospace. For all experiments, the APU-CR was operated at simulated engine conditions (Culbertson & Williams [22]). APUs are small gas turbine engines used to provide power to spool-up the main engine during starter-assisted air starts. APUs are particularly sensitive to the physical properties that influence atomization and vaporization (Pfeiffer et al. [23]) because of their small volume and correspondingly low combustor residence time ($t_{cmb}= r_{air}V_{cmb}/W_{air}$). The 131-9 combustor is swirl-stabilized and relies on a rich-quench-lean combustion process, like many of the much larger, main engine combustors. A standard 131-9 ignition system was used with the igniter located at approximately the eight o'clock position of the combustor (Culbertson & Williams [22]). Readers who wish to reproduce any of the data presented in the noted publications should contact Honeywell Aerospace.

The warm ignition (T_{fuel} = 15 °C) light-off boundary was determined at a baseline air temperature (-35 °C) and pressure (1.05 atm) along with single-point derivatives to higher temperature or lower pressure, as listed in Table 1. The cold ignition (T_{fuel} = -37 °C) light-off boundary was determined at each of the conditions used for warm ignition, plus two additional points at a colder air temperature and low pressure (also listed in Table 1). The LBO data set included six operating conditions. As with the RR data, the equivalence ratios for all test conditions were normalized using Equation 1.

3.3 GE9X-FAR Experiments

The GE9X-FAR experiments were performed in the GE's combustor component test facility. The combustor was operated at simulated engine conditions; although these conditions are proprietary information, sanitized data are publicly available through reference (Boehm et al., 2020), and readers who wish to reproduce this data may contact GE. Unlike the RR and the APU-CR, the GE9X is a large combustor that achieves lean combustion for low NOx emissions using a twin annular premixing swirler. Limited details about this combustor design have been published by Dhanuka et al. [24]. The understandable restrictions around sharing proprietary test data, procedures, and combustor designs from fuel evaluation tests such as these remain one of the prime motivators behind the development of the RR.

The GE data was not available in a format appropriate for the statistical analyses used in this study. The LBO data shown in Figure 4 was normalized at the baseline operating condition using an equation like Equation 1, but it was not reset at each operating condition because dependence on operating condition was part of the story GE communicated. The un-disclosed constant denoted by 'Δ' in the axis label of Figure 4 represents the difference between the actual and displayed equivalence ratio at the reference condition, which disguises proprietary engine LBO performance. However, the original source indicates that the tested points track along a reference velocity, which scales with the log of air flow multiplied by the square of air temperature and occurs in the same order presented in Figure 4 with roughly equal spacing.

3.4 Fuel Property Data

The RR and APU-CR experiments were directly or indirectly part of the NJFCP, and the fuels used in this study were distributed to affiliated labs by a control center led by Tim Edwards at the AFRL. Dr. Edwards was also responsible for acquiring and publishing fuel property data (Edwards, [25]), which is available through the National Alternative Jet Fuels Test Database ([26]. The fuel samples designated as A1, A2, A3, C1, C2, and C5 were tested in both the RR and APU-CR, whereas the fuel samples designated as C3, C4, and C7 were only tested in the RR. The GE9X experiments were part of a different program but included one fuel (C1) provided by the AFRL. Various properties of the fuels used by GE are provided in Table 2.

The fuel densities used in the analyses of the LBO datasets were as measured at 15 °C. For analyses of the ignition datasets, all fuel properties were transformed into their respective values at the tested fuel temperature following the approach described by Opacich et al. (Opacich et al . [18). Fuel properties that were measured over a range of temperatures that bounded the tested fuel temperature (e.g., density) were interpolated to the test temperature. Temperature-dependent fuel properties that were not measured over a sufficient temperature range to warrant interpolation (e.g., vapor pressure) were determined as outlined here. First, we derived a surrogate fuel composition by matching measured fuel property data and GCxGC-determined hydrocarbon class concentration data, using published blending rules (Flora et al. [27]) to relate molecular properties and compositions to mixture properties. Next the molecular properties over a range of temperatures were calculated based on using the models provided in the molecular properties database published by the National Institute of Standards and Technology (Kroenlein et al. [28]), and the blending rules were applied at each modeled temperature. The resulting temperature-dependent mixture properties were then curve-fitted, and those models were used to estimate the fuel properties at each tested fuel temperature.

3.5 Analysis

The previously described random forest statistical analysis (Colborn et al. [7]; Pfeiffer et al. [23]) was used for this investigation. In summary, the method uses random sampling and replacement to decrease overfitting and allows for one dependent variable (e.g. LBO or ignition performance) to be evaluated against multiple independent variables (e.g. fuel properties) (Hastie et al. [29]). Standard Monte Carlo methods were used to simulate uncertainties in each independent variable based on measurement reproducibility, as quoted in the relevant ASTM standard with an assumed Gaussian distribution. These distributions represent the uncertainty domain within the random forest method. We used the same regression approach as Peiffer et al. [18] and Opacich et al. [23]. The simulation included numerous trials to capture the full distribution of possible values within the reproducibility domain of each measured value. The relative importance values of each independent variable were recorded during each trial. Using this approach, we estimated confidence bands around each relative importance value.

One set of random forest analyses was used to assess the relative importance of atomization, evaporation rate, autoignition and extinction in each of two LBO datasets. Because none of these fundamental processes were clearly known or regress-able for all the fuels used in both test articles, it was necessary to choose a set of four independent, orthogonal properties that are known to strongly correlate with each of these four fundamental processes. Primary and secondary droplet breakup at incipient LBO conditions were represented by fuel density at 15 °C. T_{20} was selected to represent the evaporation rate. Extinction was represented by the radical index (RI), and autoignition was represented by the DCN. The idea here was to compare these two analyses and assess how well one dataset (i.e., LBO in the RR at cold conditions) represents the other (i.e., LBO in the APU-CR at normal operating conditions).

A second set of random forest analyses was used to assess the relative importance of five independent variables in each of three cold ignition datasets. We represented atomization dependencies using the Ohnesorge Number, which combines dynamic viscosity (μ), density, surface tension (σ), and the nozzle diameter, *D*, into a single dimensionless parameter (Equation 3):

$$Oh = \frac{\mu(T)}{[\rho(T)\sigma(T)D]^{0.5}} \quad (3)$$

Fuel dependency on the evaporation rate was represented by vapor pressure, and fuel dependency on droplet heating was represented by specific heat. The definition of the dependent variable, representing ignition performance, was somewhat different between the RR dataset and the APU-CR datasets. In the APU-CR datasets, the ignition variable was defined by the minimum equivalence ratio required to achieve ignition within a Honeywell-standard duration of time, during which the ignitor is firing periodically as it would in a commercial APU. In the RR dataset, the ignition variable was defined by the equivalence ratio corresponding to a 10% ignition probability per spark along a binomial regression fitted curve to the equivalence ratio and light/no-light data corresponding to each spark. Details of this binomial regression have been published by Hendershot et al. (2018).

4. Results

4.1 LBO Results

Although several laboratory rigs showed a strong correlation between LBO and the DCN (Figure 3), the APU-CR did not. Instead, it showed a strong correlation to physical and volatility properties such as viscosity (ν), and 20% recovered temperature (T_{20}) as shown in Figure 6. At cold conditions, in contrast to the results at warm conditions, the RR also showed a correlation to physical and volatility properties, but not the DCN. Due to the relatively low fuel temperatures at cold start, temperature-dependent physical properties such as density, viscosity, and surface tension trend higher, which is detrimental to fuel atomization. In addition, vapor pressure trends lower, which is detrimental to evaporation. It is therefore not surprising that the effects of such properties would be more observable at these conditions. In essence, the cold temperature in the cold LBO experiments with the RR serves to prolong the time scale of the physical processes necessary for combustion (namely, evaporation) and drive this time scale closer to the combustor residence time.

Main effects plots of Φ versus fuel properties, shown in Figure 6, suggest that both the RR and the APU-CR show a correlation between Φ and fuel physical properties when the time scale of evaporation is on the same order as the combustor residence time. To further analyze this fuel property dependency, we repeated a random forest statistical analysis 100 times. The results of the random forest analyses are summarized in Figure 7.

Overall, three important results were observed from the random forest analysis. First, each rig showed nearly the same relative importance of T_{20} (representing evaporation rate) and density (representing atomization) on LBO, which suggests that the RR, when operated at cold conditions, adequately represents the relevant physics that largely determine LBO performance in the APU-CR operated at representative engine conditions. Second, the fuel properties that influence evaporation rate are clearly more important than those that correlate strongly with chemical reactivity. This result suggests that the LBO performance of the RR and APU-CR, as operated in these tests, is affected by evaporation more than chemical reactivity. Data collected in this way should therefore be used to evaluate the impact of variation in fuel physical properties, not fuel chemistry, on LBO. Third, the relative importance of the DCN and RI at these conditions was not equal between the RR and the APU-CR, which suggests that the RR is not a good surrogate for the APU-CR in this context. However, that is not a requirement because the LBO performance in the APU-CR is not determined by the DCN or RI. In contrast, the LBO performance of the GE9X-FAR was more strongly determined by the fuel chemical properties. A useful surrogate laboratory combustor for the GE9X-FAR should therefore produce similar relative importance values for influential fuel chemical properties.

With respect to the data from the GE9X-FAR, Table 2 documents the notable differences between the petroleum-derived reference fuel and the SAF blend component (designated as C1). Sample C1 is 6.3% lighter, has 1.7% higher specific energy, and has a much lower DCN than the reference fuel. The lower density and higher specific energy of C1 are expected to push LBO toward a lower (and more favorable) Φ_{C1}. The lower density leads to a higher volumetric flow rate, which leads to higher fuel pressure and, consequently, finer atomization, whereas the higher LHV leads to a higher flame temperature for a given equivalence ratio. Conversely, the lower DCN of C1 is expected to lead to a higher (i.e., less favorable) Φ_{C1} based on the empirical trends shown in Figure 3. The data shows higher Φ_{C1} at three of the four test conditions, which is consistent with the much lower DCN of C1 relative to the reference fuel. However, at the lowest air temperatures that were tested, Φ_{C1} and Φ_{Ref} were essentially the same, presumably because the favorable density and specific energy of C1 compensate for its unfavorable DCN.

GE also provided LBO data for Jet A fuel at two different temperatures. Although these two tests did not employ fuel from a quarantined tank dedicated for such tests, the commercial jet fuel was acquired from the same supplier, and we therefore assumed that the properties of the two fuels are comparable. The colder fuel had higher density, viscosity, and surface tension and lower initial vapor pressure, but the chemical properties of the fuel vapor were the same. These differences in physical properties were reflected in the data: at the lowest air temperatures, $\Phi_{Ref,32C}$ was higher than $\Phi_{Ref,60C}$. At the three conditions where C1 showed measurably worse LBO performance than the reference fuel, the colder reference fuel performed as well as the warmer reference fuel. Together, these trends suggest that the LBO phenomenon in the GE9X-FAR is governed by fuel chemistry at three of the four test conditions, but evaporation becomes important when the air temperature is reduced. The two SAF fuels that were partially derived from hydrogenated esters and fatty acids (HEFA) showed similar results to each other at all conditions and outperformed the reference fuel at the lowest-temperature test condition, as expected based on their lower viscosity and density relative to the reference fuel.

4.2 Ignition Results

Main effects plots of Φ versus fuel properties, shown in Figure 8, suggest that both the RR and APU-CR showed a correlation between Φ and both fuel physical properties (viscosity) and volatile properties (T_{20}). To further analyze this property dependency, we performed a random forest statistical analysis with 2,000 iterations. Figure 9 provides a summary of the random forest results. As noted in section 3.1, $Oh(T_{fuel})$, $C_p(T_{fuel})$ and $P_{vap}(T_{fuel})$ were used to represent atomization, droplet heating, and droplet evaporation rate, respectively, for the random forest analyses.

The three fuel properties we selected were of similar importance in the RR at cold conditions and in the APU-CR at both cold and warm conditions. Each property accounted for about 27% of the observed variation in ignition performance. The random forest analysis suggested that 4-5% of the observed variation in ignition performance within each of the three datasets could be attributed to variation in combustor air temperature and pressure, and the remaining ten percent of the variation could not be accounted for.

Ideally, the ignition performance data would be normalized, and the datasets would be selected in such a way as to remove all dependencies on combustor operating conditions. However, data are collected prior to the analysis, and pre-test predictions are not yet capable of informing the researchers with enough information to make this possible. Moreover, the highly non-linear dependencies of ignition performance on operating conditions are difficult to completely obscure using any straightforward normalization. Although the unexplained variation in our results (~10% for each dataset) is not as low as some may like it to be, it is nevertheless excellent for a one-dimensional ignition model that does not resort to overfitting. Machine learning analyses, such as the random forest regressions used here, could be integrated with a physical two- or three-dimensional model, but further development of such an approach is still needed.

Overall, the main result of our ignition analysis is that the fuel property dependencies within each of the three datasets are nearly the same, which suggests that a small, standardized set of test articles can be used to characterize fuel dependencies on ignition within the industry-wide fleet of combustors. This result has important practical implications for the evaluation of potential SAFs. From a more fundamental perspective, our observation that two fuel properties were required to account for the evaporation timescale suggests a need for more detailed data relating to fundamental heat and mass transfer processes within the intersecting region of cold fuel droplets and plasmas or pre-existing flame kernels. Such data could lead to an even better understanding of the fundamental processes that govern fuel property dependencies on kernel initiation and growth.

5. Conclusion

In this study, we suggested that combustor operating conditions can be used to vary the relative importance of the evaporation, chemical, and mixing timescales that are characteristics of combustion phenomena. By adjusting the operating conditions of the LBO experiments the ratio of the evaporation time to residence time can be matched. For example, we demonstrated that the RR, when operated at cold fuel and air conditions, exhibits the same fuel property dependencies on LBO (i.e., density and the 20% recovered temperature) as the APU-CR at normal operating conditions in spite of large difference in residence time between these two combustors. Furthermore, when operated at representative flight idle conditions, the RR exhibits the same LBO dependencies on fuel properties (i.e., DCN) as the GE9X-FAR at similar operating conditions. We additionally observed that when the GE9X-FAR is operated at lower temperatures, the LBO phenomenon is governed by a combination of chemical and physical fuel properties rather than by the DCN. This result is consistent with previous work in the RR [7] exploring the transition in operating condition space between evaporation- and chemistry-governed LBO.

Analysis of data from cold ignition in the RR and both standard-day and cold ignition in the APU-CR, shows that the Ohnesorge number (which represents atomization), specific heat (which represents heat absorption from a nearby plasma or flame kernel into a fuel droplet), and vapor pressure (which represents evaporation from the surface of a droplet that has been transported into the path of the plasma or flame kernel) were all equally important to the ignition phenomenon. This was true, independent of the large differences in combustor cup volume between the RR and APU-CR and in the operating conditions being tested.

Collectively, our data indicate that results from the RR are strongly correlated to those from real engines in tests designed to gage the fuel dependencies of combustor operability. The RR therefore shows potential as a standard, laboratory-scale test article for representing swirl-stabilized combustors in the ASTM fuel evaluation process for SAFs.

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Figures and Tables

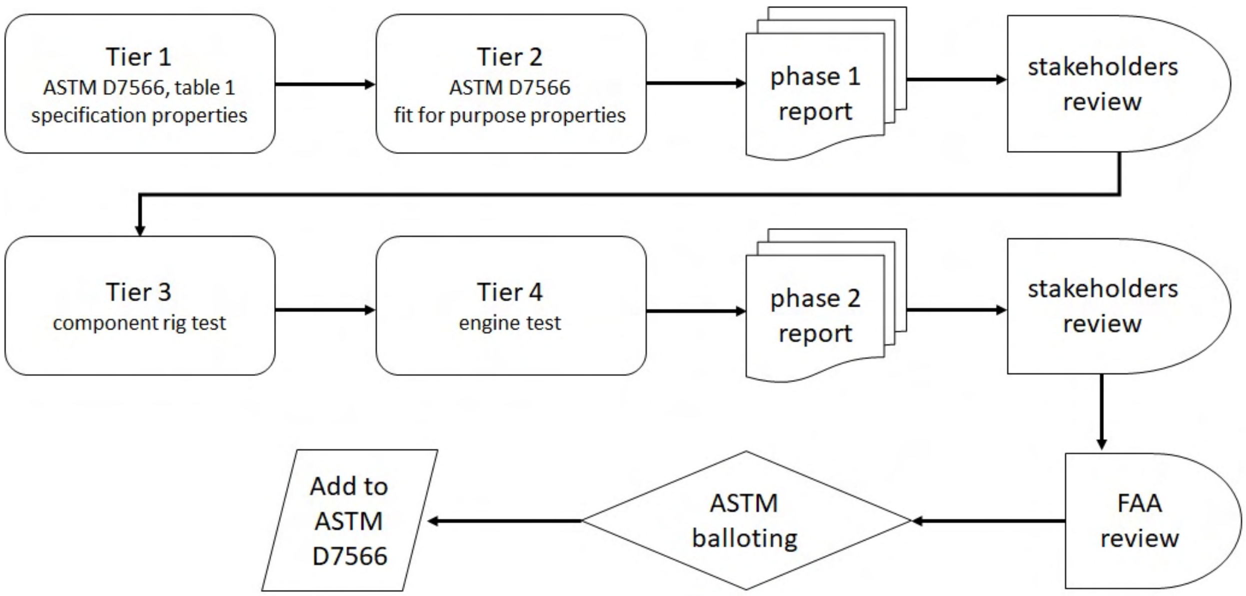

Figure 1. ASTM D4054 fuel evaluation process.

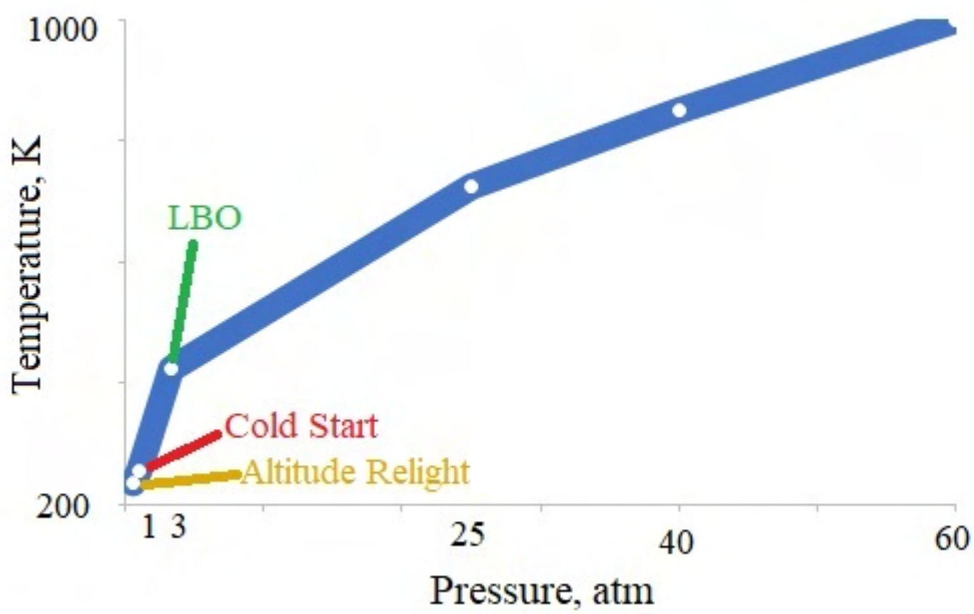

Figure 2. Visual representation of operating conditions relevant to combustion figures of merit.

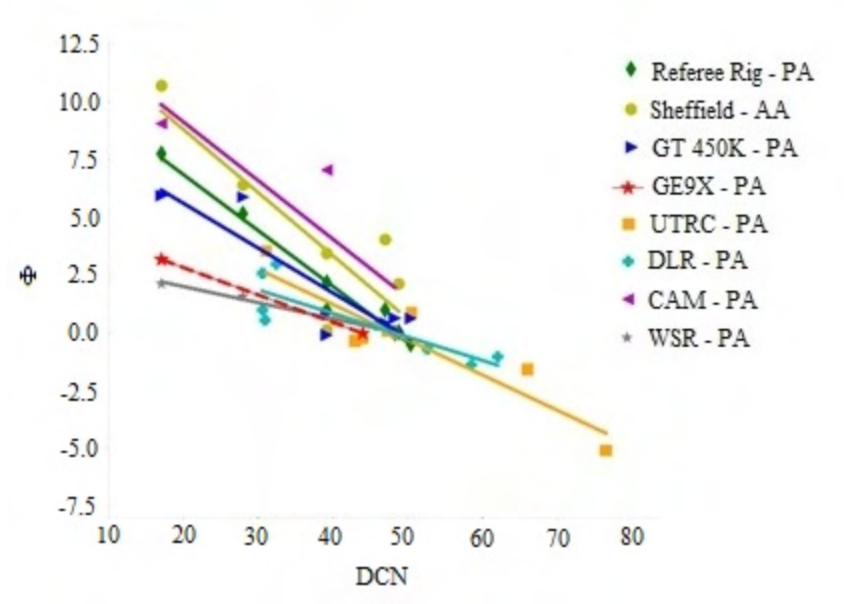

Figure 3. Lean blowout limit as a function of derived cetane number (DCN) for eight different rigs used within the National Jet Fuels Combustion Program.

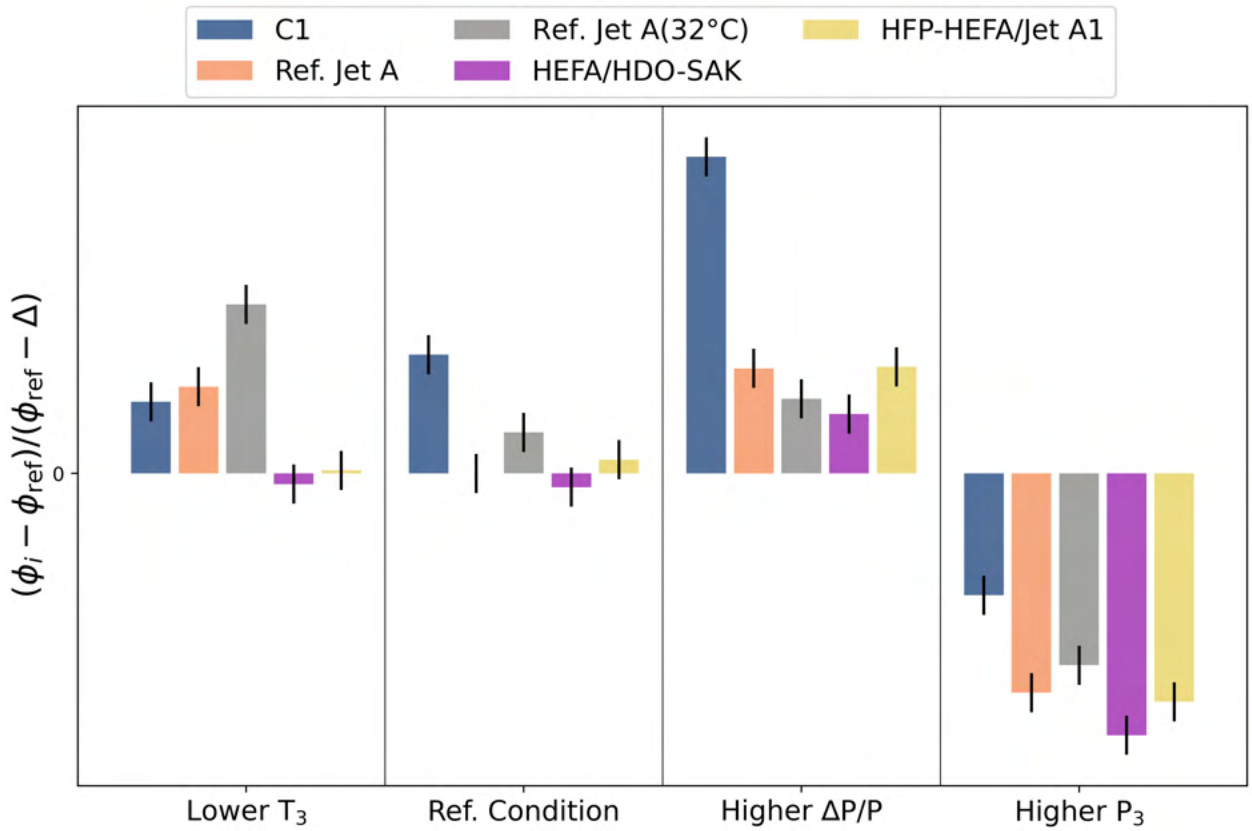

Figure 4. Relative lean blowout at four operating conditions in the GE9X full annular combustor rig. This figure was redrawn using data that was digitally extracted from the GE report to the FAA, which was part of the CLEEN II Consortium Program Update Public Plenary.

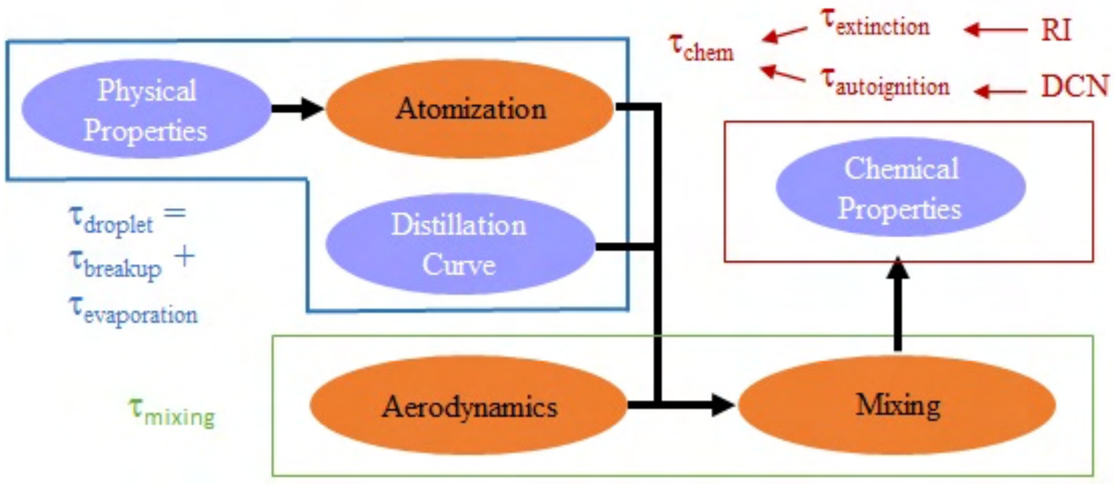

Figure 5. Available lean blowout pathways. Orange ovals represent combustor-specific characteristics and purple ovals show any fuel-dependent properties that can impact lean blowout limits.

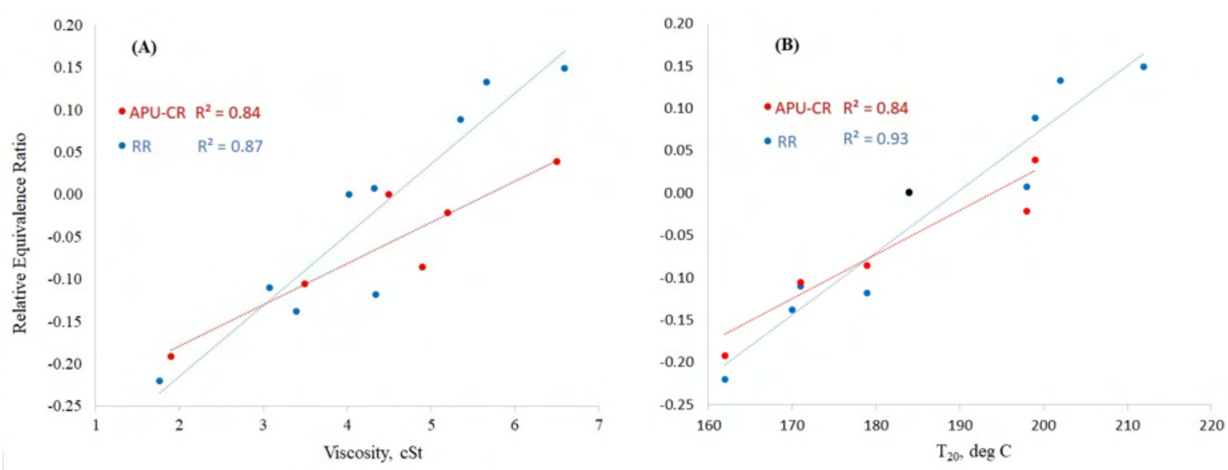

Figure 6. APU combustor rig (APU-CR) and Referee Rig (RR) LBO performance correlation with (a) viscosity (ν) and (b) 20% recovered temperature (T_{20}). Data is from Colborn et al. ⍰.

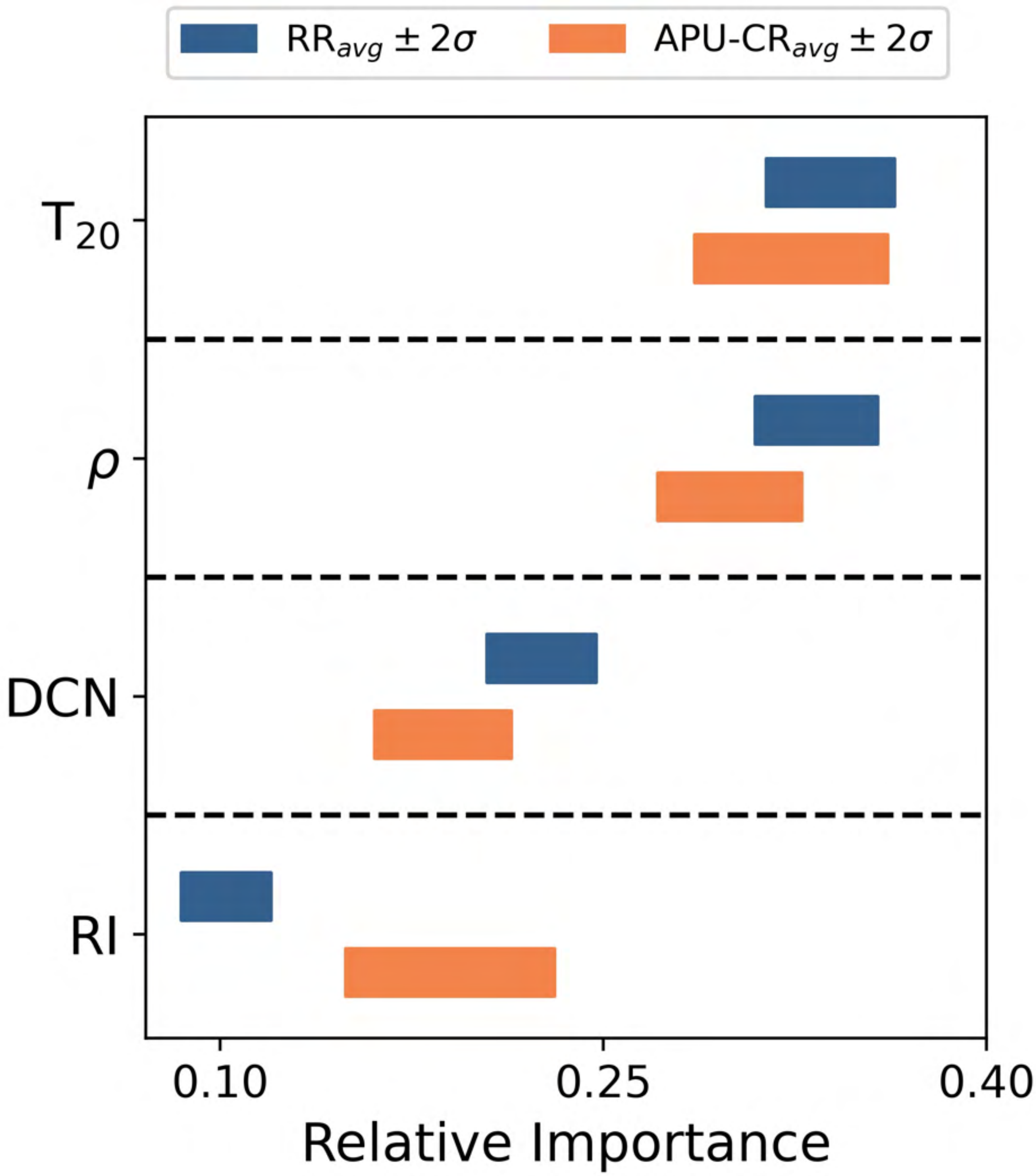

Figure 7. LBO determinants importance values for the RR at cold conditions and the APU-CR at normal operating conditions. On average, 98.6% of the LBO performance variance in the RR is explained by the chosen independent variables, while 91.8% of the LBO performance variance in the APU-CR is explained. Abbreviations: T20, 20% recovered temperature; ρ, density; DCN, derived cetane number; RI, radical index.

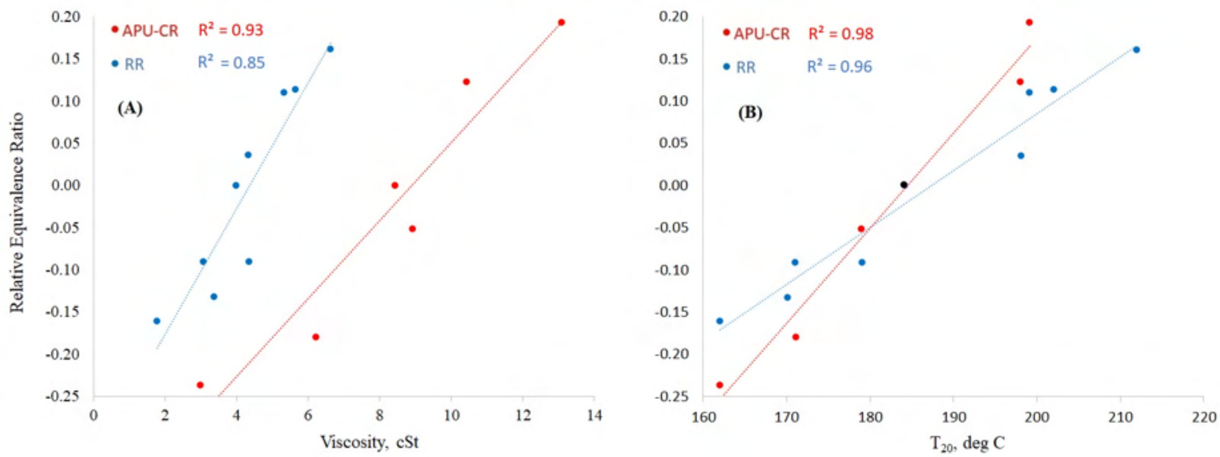

Figure 8. RR and APU-CR ignition equivalence ratio as a function of (a) Viscosity and (b) 20% recovered temperature (T_{20}). Data is from Hendershot et al. [5].

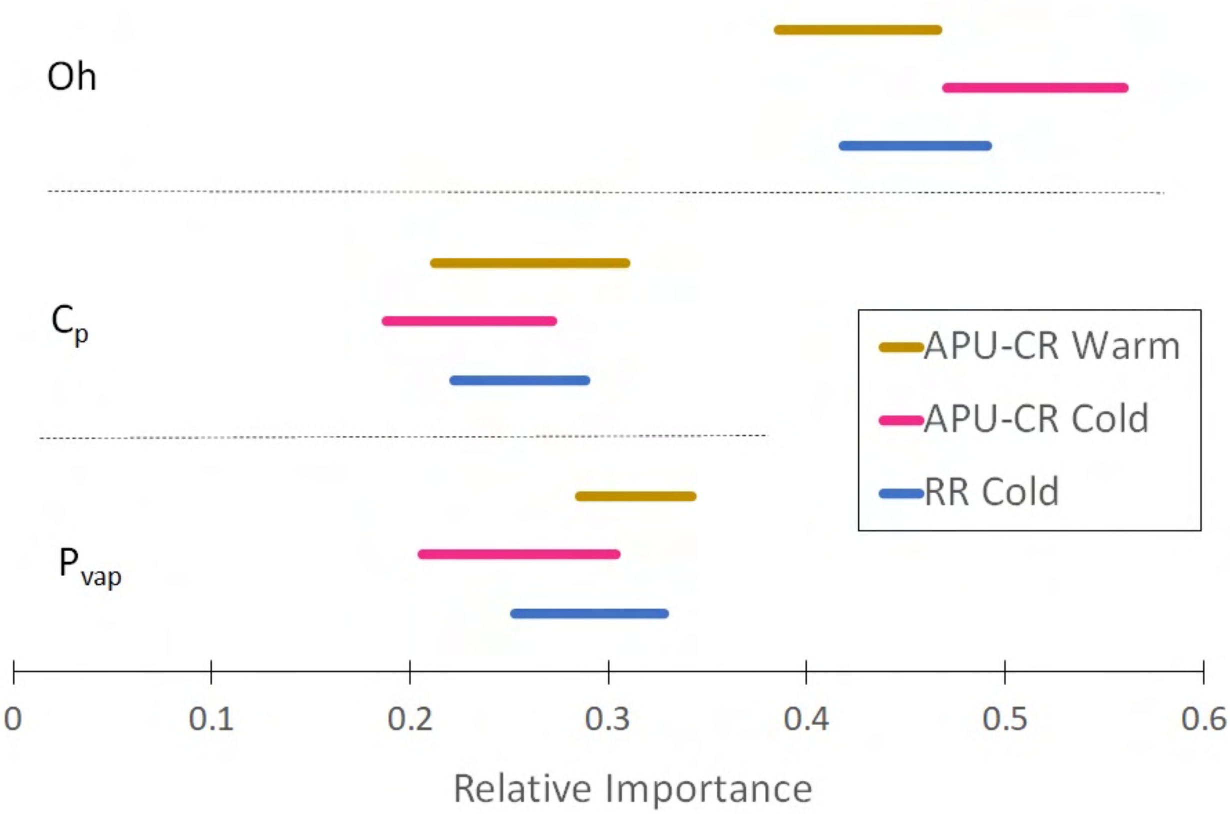

Figure 9. Ignition equivalence ratio determinants importance values for the RR at cold conditions and the APU-CR at both cold and warm conditions. On average, 89% of the ignition performance variance in the RR is explained by the chosen independent variables, 91% of the ignition performance variance in the APU-CR at cold conditions is explained, and 87% of the ignition performance variance in the APU-CR at warm conditions is explained.

Table 1. Operating conditions for the APU combustor rig (APU-CR) and Referee Rig (RR).

Rig	Operating Condition	Fuel Temperature [°C]	Air Temperature [°C]	Pressure [atm]	$\Delta P/P_{cmb}$ [%]
RR	Cold Lean Blowout [7]	-34, -15	-34, -15	1.02	2%
	Cold Start [5]	-34, -15	-34, -15	1.02	2%, 3.5%
APU-CR	Lean Blowout [22]	15	51 to 314	1.0, to 5.7	
	Cold Ignition [22]	-37	-44, -35, 15	1.05, 0.2, 0.3	
	Warm Ignition [22]	15	-38, 15	1.05, 0.2	

Table 2. Properties of fuels used in GE9X-FAR testing

Property	Jet A	C1	HFP-HEFA / Jet A1	HEFA / HDO-SAK
Density@15.6C (g/ml)	0.809	0.758	0.786	0.789
LHV (MJ/kg)	43.3	44.0	43.4	43.2
Hydrogen (wt%)	13.91	15.25	14.23	13.90
Viscosity@37.8C (cSt)	1.49	1.53	1.16	1.21
Viscosity@-20C (cSt)	5.02	4.99	3.15	
Viscosity@15.6C (cSt)		2.41 (curve fit)		1.66
DCN	~48	17.1		

Milestone(s)

- Determined alternative jet fuel dependencies between combustors of different sizes and mixing approaches.

Major Accomplishments

- Reported the alternative jet fuel dependencies between combustors of different sizes and mixing approaches.
- Published the NJFCP book.

Publications

Peer-reviewed journal publications

Boehm, R.C., Colborn, J. G., & Heyne, J. S. (2021). Comparing alternative jet fuel dependencies between combustors of different size and mixing approaches. Frontiers in Energy Research,*440*. https://doi.org/10.3389/FENRG.2021.701901.

Book publication

Colket, M., & Heyne, J. (2021). *Fuel effects on operability of aircraft gas turbine combustors*. American Institute of Aeronautics and Astronautics. https://doi.org/10.2514/4.106040

Book chapters

Colket, M., Heyne, J., Andac, G., Rumizen, M. (2021). Chapter I. Introduction. In T. C. Lieuwen (Ed.), *Fuel effects on operability of aircraft gas turbine combustors* (pp. 1-20). American Institute of Aeronautics and Astronautics.

Rock, N., Stouffer, S., Hendershott, T., Heyne, J., Blunck, D., Lukai, Z., Khandelwal, B., Emerson, B., Mastorakos, E., Colket, M. (2021). Chapter V. Lean blowout studies., In T. C. Lieuwen (Ed.), *Fuel effects on operability of aircraft gas turbine combustors* (pp. 143–196). American Institute of Aeronautics and Astronautics.

Heyne, J., Rauch, B., Hanson, R., Dooley, S., Blakey, S., Yang, Z., Ferris, A., Ure, A., Le Clercq, P., Boehm, R., Lewis, C., &Colket, M. Chapter XII. Prescreening of Sustainable Aviation Jet Fuels. In T. C. Lieuwen (Ed.), *Fuel effects on operability of aircraft gas turbine combustors* (pp. 487–523). American Institute of Aeronautics and Astronautics.

Heyne, J., Colket, M., Edwards, T., Moder, J., Rumizen, M., & Oldani, A. (2021). Chapter XIII. Summary. In T. C. Lieuwen (Ed.), *Fuel effects on operability of aircraft gas turbine combustors* (pp. 525–534). American Institute of Aeronautics and Astronautics.

Outreach Efforts

Invited talks

Heyne, J. (2020, November). High value drop-in aviation fuels: From molecule selection to mission benefits [Panel presentation]. Fuel Quality Matters, DOE BETO/PNNL HTL Workshop, Virtual meeting.

Heyne, J. (2020, November). Prescreening of HTL SAFs: Rapid low-volume, low-cost testing. Sustainable Aviation Fuel Certification, DOE BETO/PNNL HTL Workshop, Virtual meeting.

Heyne J. (2021, May). Summative results of the national jet fuels combustion program [Panel presentation]. Properties and Emissions, CRC Aviation Fuels Meeting, Virtual meeting.

Heyne, J. (2021, June). Prescreening of sustainable aviation fuels [Panel presentation]. CAAFI Virtual Mini-Symposium.

Heyne, J. (2021, June 2). Sustainable aviation fuel prescreening, benefits, and a proposed streamlined evaluation process [Panel presentation]. National Academies, Transportation Research Board (AV030), Sustainable Aviation Fuels subcommittee midyear meeting.

Heyne, J. (2021, August 17). Sustainable aviation fuel: Properties, compositions, and qualification requirements [Sponsored seminar]. Sandia National Laboratory.

Heyne, J., (2021, August 17). Sustainable aviation fuel property needs and some solid waste candidates [Panel presentation]. Seminar on Hydrothermal Liquefaction: biocrudes and advances towards drop-in fuel potential, Aalborg University, Denmark.

Heyne, J. (2021, November). Sustainable aviation fuel: Properties, compositions, and qualification requirements [Sponsored seminar]. Center for Multiphase Flow Research and Education, Iowa State University.

Conference presentations

None.

Awards

Joshua Heyne:

- 2021 Net Good Summit on sustainable travel, honored guest
- 2021 US Frontiers of Engineering Symposium, National Academies of Engineering, selected participant
- 2021 Vision Award for Excellence in Scholarship, School of Eng., University of Dayton

Student Involvement

Jen Colborn, graduate research assistant, leads this effort.

Plans for Next Period

Continue to coordinate across various federal agencies and research institutions regarding SAF testing.