Commercial Aviation Alternative Fuels Initiative®

Prescreening of Candidate Synthetic Aviation Turbine Fuel (SATF)[1]

EVALUATION METRICS, METHODS, AND CRITERIA

Prepared for the CAAFI R&D Committee to Facilitate the Evaluation of Novel AJFs

Joshua Heyne
Washington State University
joshua.heyne@wsu.edu

INTRODUCTION

The ASTM International approval and evaluation process of non-fossil or synthetic jet fuels, as detailed elsewhere,[1–4] can involve four tiers of testing, two research reports, and multiple balloting junctions. This resource-intensive process ensures that any alternative fuel qualified will be safe, fungible, and otherwise compliant to stakeholders, but usually spans multiple years. The extensiveness of this process creates a need for early-stage low volume, low cost, and rapid prescreening techniques outside the formal ASTM D4054 approval and evaluation process; especially those that relate to the assessment of combustor operability, which are among the most expensive testing requirements of the ASTM process. This document recommends prescreening methods that can provide early-stage confidence to fuel developers.

These prescreening methods have been developed based on learning acquired from the National Jet Fuels Combustion Program (NJFCP),[5] JetScreen,[6] prior ASTM qualifications of synthetic blend components (SBC) or synthetic aviation turbine fuels (SATF), and other associated SBC/SATF programs. These methods do not replace the ASTM qualification process or its requirements. Results from prescreening provide an early assessment of issues that could be encountered in the formal qualification process. Two primary objectives that led to the development of the prescreening concept by the NJFCP are:

1. *Defining the properties, associated tests, and volumes needed to maximize the confidence of a fuel's behavior before entering the formal ASTM D4054 process.*[2]

[1] Sustainable aviation fuel (SAF) is an SATF that also meets additional carbon intensity and sustainability requirements.

[2] ASTM D4054 requires a producer to deliver approximately 100 gallons neat fuel to enter the process.

2. *Defining test methods that require minimum volumes of fuel and minimum cost to conduct, that will provide information on product composition, the fuel's relationship to chemical and physical properties, and its blend effects on the critical evaluation of combustor operability and approval metrics.*

To meet these objectives, the NJFCP created two low volume testing tiers, Tier and Tier , which can inform fuel producers in advance of the submission of a fuel to the ASTM D4054 process on the suitability of the candidate fuel as a jet fuel, the blend limits of the fuel, and other potential pitfalls.

ROLE OF ALTERNATIVE FUEL PRESCREENING

Prescreening is not a mandatory step in the ASTM D4054 process. Instead, it is a voluntary process designed to provide candidate fuel producers with insights into the viability of their fuel as a jet fuel blending component. Prescreening allows producers to test small volumes of fuel for select properties that serve as indicators of the candidate fuel's potential to meet the capital-intensive D4054 Tier 3 and 4 test requirements. While prescreening does not guarantee the successful completion of the ASTM D4054 process or ultimate qualification by aviation original equipment manufacturers (OEMs), it guides producers in making improvements to the candidate fuel, thereby increasing its chances of success in the formal qualification process.

It is important to note that prescreening does not need to be conducted by any one specific institution. However, some institutions have more extensive experience in handling, testing, and understanding the impact of fuel properties on combustor operability and ASTM D4054 considerations. Prescreening data are often used in product development, managing expectations (such as blend ratios, timelines for qualification, education of process, and blend ratios), and initial discussions when entering the ASTM D4054 qualification process, such as before the establishment of an ASTM task force or submission of materials to a Clearinghouse.

TARGETED METRICS FOR PRESCREENING

Novel fuels must be compliant with safety (e.g., flammability, toxicity, etc.), operability (of components such as the combustor and the engine itself), material compatibility (metallic and non-metallic components), and various other performance metrics. Importantly, these prescreening methods and predictions assume that any fuel screened is free of metals, heteroatoms, or olefins, which are unacceptable in jet fuel.

Given these requirements, the fuel must maintain acceptable properties under extreme conditions, such as remaining in a liquid state with acceptable viscosity under cold conditions and having a flash point above the specification limit. Additionally, the ability of a fuel to ignite and sustain a flame under potentially extreme conditions associated with the operating envelopes of main engines and auxiliary power units is critical from an operability perspective. Any novel fuel must exhibit acceptable performance within the same envelope as conventional jet fuels. Novel fuels that negatively impact these metrics pose a threat to safety and aircraft operations.

Combustor and engine operability tests under ASTM D4054 (Tiers 3 and 4) involve significantly higher fuel volumes and capital expenditures than the fuel property tests of D4054 Tiers 1 and 2. Many of these tests have been the focus of the NJFCP, which has measured the operability performance of multiple worst-case test fuels with fundamental experiments and tests in more than a dozen combustor rigs. The results of these tests, which include hundreds of observations on nearly 20 different fuels tested on multiple rigs, are detailed in several publications.[2] In addition, complementary and overlapping fuels are investigated in the EU program JETSCREEN. These JETSCREEN results contribute to a database on fuels that are outside of the fuel specifications box and help map fuel composition to critical properties and evaluation metrics.

The overarching results of the NJFCP work suggest that nearly all observed combustor operability variance is captured by the physical and chemical properties of the fuel, which in turn are controlled by the chemical composition of the fuel. Explicitly, unacceptable operability behavior of an alternative fuel can be avoided by ensuring that the properties of the alternative fuel fall within the typical range of conventional fuels. The most important fuel properties for combustor operability are:

- Viscosity at -20 and -40 °C
- Distillation characteristic
- Mass density
- Flash Point temperature
- Cetane Number (CN)
- Surface tension
-

Viscosity, distillation characteristics, and mass density are well-known to be critical properties for combustor performance[3] and are captured in the major jet fuel specifications. Historically, CN and surface tension have not needed specification requirements as these properties were constrained by the relatively limited compositional variation of petroleum fuels. Recently, CN has been shown to have a direct effect on combustor lean blowout performance in swirl stabilized combustion. Sensitivity to surface tension has also been identified as important, but its values may be constrained sufficiently by a fuel’s density.

Compatibility and fungibility refer to the ability of a fuel to coexist, without negative impacts, in existing hardware and infrastructure. Novel fuels, for example, must maintain the swelling character of O-rings and be non-corrosive. Furthermore, they cannot have deleterious effects for the existing fuel transport and delivery systems. Finally, the performance of jet fuels requires a minimum specific energy and maximum aromatic content. The evaluation of compatibility and fungibility is addressed in ASTM D4054, but to date, novel fuels have not encountered issues in these areas.

TIER : Hydrocarbon type analysis and property predictions

Three testing methods for chemical composition characteristics that require very low volumes of fuel have been identified to predict some of the performance properties described above:

- Two-dimensional gas chromatography (GCxGC or 2D-GC), ~1 mL and
  GC (ASTM D2887)
- Mid-Infrared (IR) absorption, <100 mL
- Nuclear Magnetic Resonance (NMR), <10mL

Volume requirements for these tests vary from lab to lab but are likely to require the minimum volume for any blend predictions. GCxGC methods have been documented that predicted, directly and indirectly, the following aspects:

[3] Examples of appropriate bounds are illustrated in Figure 1.

- operability effects[1,7–9]
- distillation curves[10]
- blend limits[10]
- vapor pressures[11]
- viscosity[12]
- distillation[13]
- swelling[14]
- freeze point[15]
- flash point[16]
- density[16,17]
- DCN[16]
- heat capacity[18]
- conductivity[18]
- dielectric constant [19–21]
- olefin sensing[22]
- sooting or the threshold sooting index (TSI)[23]
- lower heating value (LHV)[24]

Recently, a comprehensive literature review[25] on predicting properties also became available. Further, GCxGC with vacuum ultraviolet (VUV) light spectroscopy has shown the ability to identify isomeric constituents in the candidate materials, yielding higher fidelity property predictions.[18,26–28] Isomers have been identified as an important uncertainty not typically encountered with fossil fuels.[29] Moreover, GCxGC analysis is included as part of the official ASTM D4054 qualification process, including the Fast Track provision.[30]

Mid-IR spectroscopy has shown great potential in predicting a variety of critical physical and chemical properties of SAFs. These properties include: density, derived cetane number (DCN), LHV, initial boiling point (IBP), flash point, kinematic viscosity, threshold sooting index (TSI), hydrogen-to-carbon (H/C) ratio, and molecular weight (MW).[31,32,32,33] This mid-IR leverages the absorption characteristics of hydrocarbon molecules to establish correlations with these properties, making it a powerful prescreening tool in SATF development and certification processes. Mid-IR spectroscopy's ability to provide accurate property estimates with relatively low fuel volume requirements supports its integration into rapid, cost-effective fuel evaluation strategies.

NMR has been shown to predict the chemical properties of a fuel that impact the CN/ignition quality[34], density, and surface tension[35]. Additionally, there is the potential to predict additional properties with future work.

No Tier method is currently capable of capturing all ASTM required properties. Further, it must be cautioned that there is significant variance in terms of equipment and testing methods, and while there is currently work ongoing towards standardizing GCxGC methods, great care should be taken when interpreting the results from the above methods. However, these methods require the lowest volumes, predict the widest range of characteristics, and have the most promise of the prescreening approaches.

TIER : Measurement of critical properties

Entry into ASTM D4054 has historically required at least 100 gallons total of fuel from several batches to be submitted for initial evaluations. From each batch, approximately 10 gallons is consumed for the Tier 1 and 2 tests. While essential for a comprehensive evaluation process, many of these Tier 1 and 2 tests have consistently returned the 'null-hypothesis' as no "red flags" were identified. The Tier 1 and 2 tests and volumes listed in Table 1 are recommended as a Tier β prescreening simply because later Tier 3 and 4 (engine and aircraft system and component) tests are sensitive to these properties. The evaluation of the fuels with the listed methods in Table 1 facilitates the direct comparison of fuels to conventional fuel and previously approved SATFs, minimizing future uncertainties with while consuming less than 50 mL of test fuel.

Table 1: Minimally Recommended Tier properties

Property	ASTM Test Method	Approximate Volume Required
Viscosity	D7042	4 mL
Density	D4052	
Distillation	D2887	*GC/Tier*
Flash Point	D93	5 mL
Surface Tension	D1331A	10 mL
DCN	D6890	15 mL

SUMMARY AND EXAMPLE EVALUATION METRICS

While not essential for the approval of a novel fuel, early prescreening of a limited set of properties using Tier and Tier *β* methods outlined above facilitates confidence in a proposed fuel development path. Furthermore, before the start of formal ASTM D4054 process, it can illuminate pathways to refine processes and alter feedstocks to maximize the possibility that a fuel can be approved. Below is one exemplar prescreening test campaign result.Regardless of whether a sample material is tested for tier or tier and tier *β*, a GCxGC evaluation is completed on the sample material. Many properties can be inferred from GCxGC results. For example without detailed computational results outlined above, critical properties such as the viscosity, density, surface tension, and vapor pressure can all be inferred via intuition from a GCxGC hydrocarbon type analysis result. Moreover, inferences can be made from the hydrocarbon type analysis regarding the physical and chemical properties of a droplet and composition as the fuel evaporates. Chemical and physical properties can change within the constituent material as fuel evaporates, potentially impacting the operability of the fuel in an engine and aircraft.Figure 1 leverages a GCxGC hydrocarbon type analysis to compare against the carbon number distributions of a reference Jet A (POSF 10325) and a candidate SATF. The reference Jet A carbon number distribution is shown in the background as light green, with an average carbon number around 11.4 carbons per molecule. The candidate SATF carbon number distribution is displayed in the colormap in the foreground. The average carbon number for this molecule is 11.3 carbons per molecule. Additionally, the hydrocarbon type compositional distribution is communicated in the legend. While not necessary to match the carbon number distribution of Jet A, deviations from the reference Jet A carbon number distribution are often perceived as risk by the OEMs. Thus, matching the carbon number and distribution of this reference Jet A with a novel SATF composition minimizes both the perception and real risk to the operation of the engine with the novel SATF. The novel SATF carbon distribution deviates from this reference Jet A by having higher concentrations of 9, 10, and 16 carbon chain molecules. Additionally, there are carbon number fractions that are lower for the novel SATF in comparison to the reference Jet A. While not conclusive in this example, the high concentrations of 16 carbon chain molecules could be an issue, as heavier molecular weight iso-alkanes can have higher than desired low temperature viscosities. Therefore, this result highlights the need for additional information.

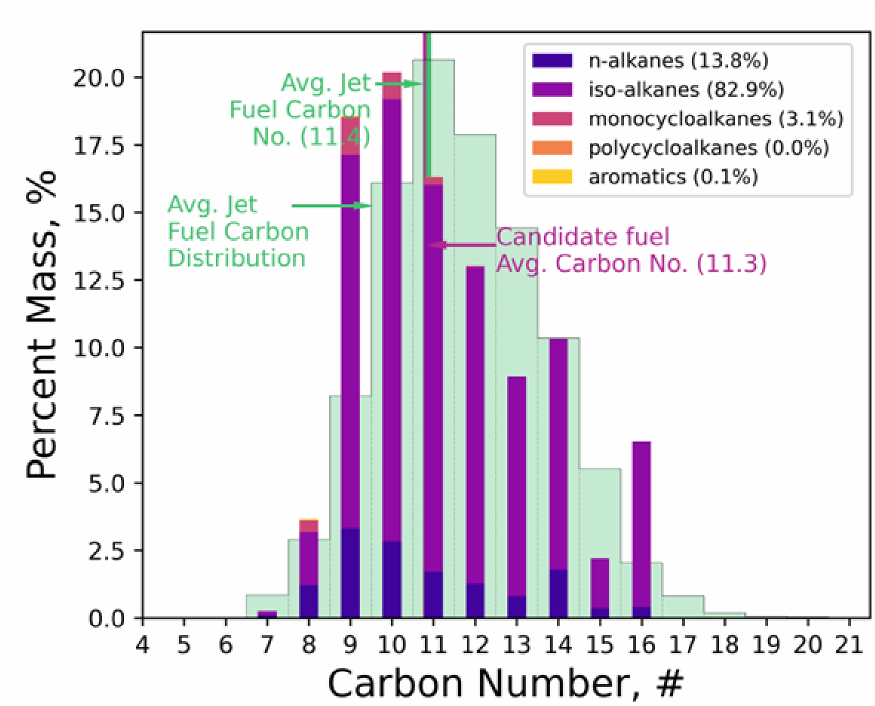

Figure 1: Carbon number distribution comparison between a reference Jet – A and a novel SAF.

The physical properties of the fuel are a more direct method of determining the impact of sustainable aviation fuel candidates on engine and aircraft operability. Under a tier prescreening protocol, properties are predicted, whereas, if there is sufficient material available for direct testing, properties are measured under the tier *β* protocol. Figure 2 illustrates property measurements, tier *β* , the candidate SATF reported in Figure 1. Figure 2 reports a range of conventional fuel properties in the background as light green. The property limits for a fully formulated jet fuel are reported in red lines, and shaded in red outside the limits. It is not necessary for a candidate SATF material to be compliant with these property limits, as most approved SATF compositions fall outside these limits and are therefore blended become fully-formulated and drop-in. However, similar to the hydrocarbon type distribution illustrated in Figure 1, deviations from conventional fuel ranges and ASTM D 1655 limits can be perceived as risk. Additionally, deviations from these limits and ranges can bound expectations for eventual blend limits. In the figure below, filled black symbols represent tier *β* property measurements, while open symbols represent tier property predictions. In the example illustrated herein, all of the requisite tier *β* properties were measured.

Surface tension () has been observed to be important for spray break up and atomization.[11] The higher the surface tension the more difficult it is to break up the spray and combust. While surface tension is not a specification property in ASTM D1655, it is important for characterizing novel SATF. Here the novel SATF has a lower surface tension than the conventional fuel range, which is acceptable. The density () here was measured to be lower than the ASTM D1655 value but is well within the experience range of other approved sustainable aviation fuels, e.g., ASTM D7566 Annex A1. The kinematic viscosities for the candidate SATF were measured at -20 and -40° C, and with both of these temperatures the candidate material is within the experience range of conventional fuel and below the specification limits typically imposed. The candidate materials composed of almost entirely saturated, or paraffinic, materials increasing the lower heating value (LHV) of the fuel, similar to other approved ASTM D7566 annexes. The derived cetane number (DCN) is not a prescribed property in ASTM D1655, however, it has been observed to be important for the lean blowout limit of jet fuels in several architectures. Here the derived cetane number of the candidate SATF is outside the conventional fuel range, but within desired limits. Finally, freeze point is lower than the required limit for conventional fuel.

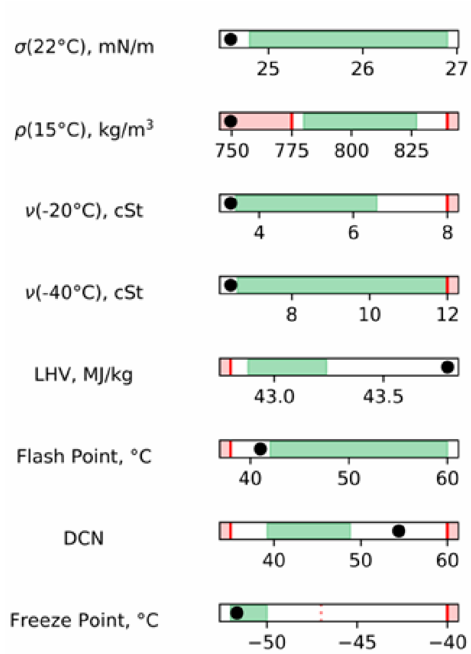

Figure 2: Property comparison of candidate SATF to conventional fuel ranges (light green) and fully formulated property limits (red lines and shaded regions).

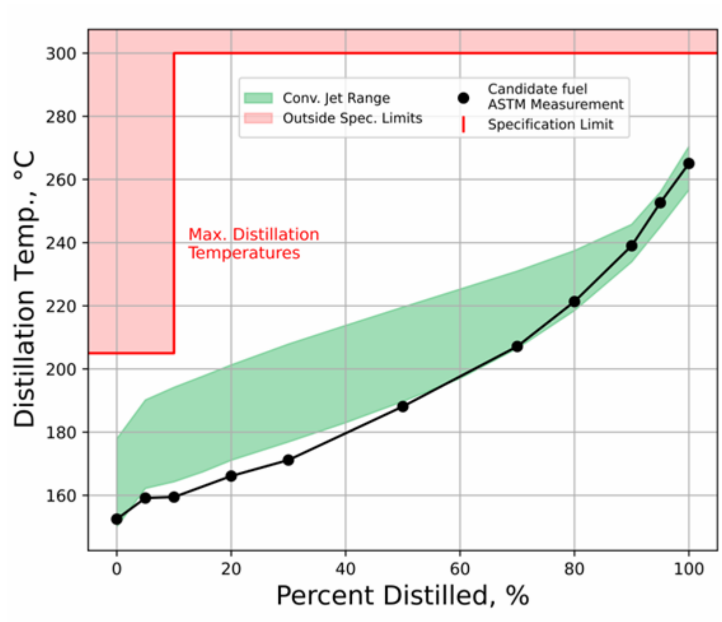

Figure 3: Several key jet fuel metrics, the typical experience range, and specification limits plotted. The property range of conventional fuels with extreme properties is plotted in the contour filled regions. (left) The range of distillation temperatures for a range of extreme jet fuels with the specification limits plotted in red. (right) The properties of several aviation-focused metrics with extreme jet fuels. The experience range of conventional fuels, where applicable, is illustrated with yellow and red regions. In the case of density and viscosity, the red dashed lines represent the spec limits of Jet A.

DISCLAIMER:
This document is not meant to suggest that an alternative fuel process and fuel can avoid the ASTM D4054 process by applying the tests and methods described here. Rather, this document is only a resource for summarizing current state-of-the-art evaluation and prescreening methods to facilitate the development of alternative jet fuels.

ACKNOWLEDGMENTS

The author thanks the many readers, editors, and contributors to this document including the CAAFI R&D Team (more specifically Mark Rumizen, Stephen Kramer, Gurhan Andac), Med Colket, Mohan Gupta, and JETSCREEN collaborators (Bastian Rauch and Patrick LeClercq).

REFERENCES

(1) Colket, M.; Heyne, J. Fuel Effects on Operability of Aircraft Gas Turbine Combustors. August. *Prog. Astronaut. Aeronaut.* **2021**.

(2) Rumizen, M. A. Qualification of Alternative Jet Fuels. *Front Energy Res* **2021**, *9* (November), 676. https://doi.org/10.3389/fenrg.2021.760713.

(3) Heyne, J.; Rauch, B.; Le Clercq, P.; Colket, M. Sustainable Aviation Fuel Prescreening Tools and Procedures. *Fuel* **2021**, *290*, 120004. https://doi.org/https://doi.org/10.1016/j.fuel.2020.120004.
(4) Rumizen, M. Alternative Jet Fuel (AJF) Certification; CAAFI: ICAO Headquarters, Montreal, CA.
(5) Colket, M. B.; Heyne, J. S.; Rumizen, M.; Edwards, J. T.; Gupta, M.; Roquemore, W. M.; Moder, J. P.; Tishkoff, J. M.; Li, C. An Overview of the National Jet Fuels Combustion Program. *AIAA Journal* **2017**. https://doi.org/doi:10.2514/6.2016-0177.
(6) Rauch, B. *JetScreen*. https://www.jetscreen-h2020.eu/.
(7) Yang, Z.; Stachler, R.; Heyne, J. S. Orthogonal Reference Surrogate Fuels for Operability Testing. *Energies (Basel)* **2020**, *13* (8), 1–13. https://doi.org/10.3390/en13081948.
(8) Boehm, R. C.; Colborn, J. G.; Heyne, J. S. Comparing Alternative Jet Fuel Dependencies Between Combustors of Different Size and Mixing Approaches. *Front Energy Res* **2021**, *0*, 440. https://doi.org/10.3389/FENRG.2021.701901.
(9) Colborn, J.; Heyne, J.; Stouffer, S.; Henderschott, T.; Corporan, E. Chemical and Physical Effects on Lean Blowout in a Swirl-Stabilized Single-Cup Combustor. *38th International Symposium on Combustion* **2020**.
(10) Yang, Z.; Boehm, R. C.; Bell, D. C.; Heyne, J. S. Maximizing Sustainable Aviation Fuel Usage through Optimization of Distillation Cut Points and Blending. *Fuel* **2023**, *353*, 129136.
(11) Opacich, K. C.; Heyne, J. S.; Peiffer, E.; Stouffer, S. D. Analyzing the Relative Impact of Spray and Volatile Fuel Properties on Gas Turbine Combustor Ignition in Multiple Rig Geometries. In *AIAA Scitech 2019 Forum*; American Institute of Aeronautics and Astronautics: Reston, Virginia. https://doi.org/10.2514/6.2019-1434.
(12) Boehm, R. C.; Hauck, F.; Yang, Z.; Wanstall, C. T.; Heyne, J. S. Error Quantification of the Arrhenius Blending Rule for Viscosity of Hydrocarbon Mixtures. *Front Energy Res* **2022**, *10*.
(13) Yang, Z.; Bell, D. C.; Cronin, D. J.; Boehm, R.; Heyne, J.; Ramasamy, K. K. Volatility Measurements of Sustainable Aviation Fuels: A Comparative Study of D86 and D2887 Methods. *ACS Sustain Chem Eng* **2024**, *12* (19), 7414–7420. https://doi.org/10.1021/acssuschemeng.4c00678.
(14) Faulhaber, C.; Borland, C.; Boehm, R.; Heyne, J. Measurements of Nitrile Rubber Absorption of Hydrocarbons: Trends for Sustainable Aviation Fuel Compatibility. *Energy & Fuels* **2023**, *37* (13), 9207–9219. https://doi.org/10.1021/acs.energyfuels.3c00781.
(15) Boehm, R. C.; Coburn, A. A.; Yang, Z.; Wanstall, C. T.; Heyne, J. S. Blend Prediction Model for the Freeze Point of Jet Fuel Range Hydrocarbons. *Energy and Fuels* **2022**, *36* (19), 12046–12053. https://doi.org/10.1021/acs.energyfuels.2c02063.
(16) Yang, Z.; Kosir, S.; Stachler, R.; Shafer, L.; Anderson, C.; Heyne, J. S. A GC × GC Tier α Combustor Operability Prescreening Method for Sustainable Aviation Fuel Candidates. *Fuel* **2021**, *292*, 120345. https://doi.org/https://doi.org/10.1016/j.fuel.2021.120345.
(17) Hall, C.; Rauch, B.; Bauder, U.; Le Clercq, P.; Aigner, M. Predictive Capability Assessment of Probabilistic Machine Learning Models for Density Prediction of Conventional and Synthetic Jet Fuels. *Energy & Fuels* **2021**, *35* (3), 2520–2530. https://doi.org/10.1021/acs.energyfuels.0c03779.
(18) Heyne, J.; Bell, D.; Feldhausen, J.; Yang, Z.; Boehm, R. Towards Fuel Composition and Properties from Two-Dimensional Gas Chromatography with Flame Ionization and Vacuum Ultraviolet Spectroscopy. *Fuel* **2022**, *312*, 122709. https://doi.org/https://doi.org/10.1016/j.fuel.2021.122709.
(19) Yang, Z.; Bell, D. C.; Boehm, R. C.; Fischer Marques, P.; Boze, J. A.; Kosilkin, I. V.; Heyne, J. S. Assessing the Effect of Composition on Dielectric Constant of Sustainable Aviation Fuel. *Fuel* **2025**, *380*, 133230. https://doi.org/10.1016/j.fuel.2024.133230.

(20) Faulhaber, C.; Bell, D. C.; Boehm, R.; Heyne, J. Dielectric Constant Predictions for Jet-Range Hydrocarbons: Evaluating the Clausius–Mossotti Relation and Correcting for Molecular Dipole Moments. *Energies (Basel)* **2024**, *17* (18). https://doi.org/10.3390/en17184700.

(21) Kosir, S.; Landsaw, A.; Steinecker, W. H.; West, Z. J.; Zabarnick, S. Synthetic Blend Component Study: The Effects of Hydrocarbon Composition on Aviation Fuel Dielectric Constant. *Energy and Fuels* **2024**, *38* (17), 16451–16457. https://doi.org/10.1021/acs.energyfuels.4c02342.

(22) Kosir, S.; Feldhausen, J.; Bell, D.; Cronin, D.; Boehm, R.; Heyne, J. Quantitation of Olefins in Sustainable Aviation Fuel Intermediates Using Principal Component Analysis Coupled with Vacuum Ultraviolet Spectroscopy. *Frontiers in Fuels* **2023**, *1*. https://doi.org/10.3389/ffuel.2023.1246950.

(23) Boehm, R. C.; Yang, Z.; Heyne, J. S. Threshold Sooting Index of Sustainable Aviation Fuel Candidates from Composition Input Alone: Progress toward Uncertainty Quantification. *Energy & Fuels* **2022**. https://doi.org/10.1021/acs.energyfuels.1c03794.

(24) Boehm, R. C. R.; Yang, Z.; Bell, D. C.; Feldhausen, J.; Heyne, J. S. Lower Heating Value of Jet Fuel from Hydrocarbon Class Concentration Data and Thermo-Chemical Reference Data: An Uncertainty Quantification. *FUEL* **2022**, *311*, 122542. https://doi.org/https://doi.org/10.1016/j.fuel.2021.122542.

(25) Boehm, R. C.; Yang, Z.; Bell, D. C.; Faulhaber, C.; Mayhew, E.; Bauder, U.; Eckel, G.; Heyne, J. S. Perspective on Fuel Property Blending Rules for Design and Qualification of Aviation Fuels: A Review. *Energy & Fuels* **2024**. https://doi.org/10.1021/acs.energyfuels.4c02457.

(26) Feldhausen, J.; Bell, D. C.; Yang, Z.; Faulhaber, C.; Boehm, R.; Heyne, J. Synthetic Aromatic Kerosene Property Prediction Improvements with Isomer Specific Characterization via GCxGC and Vacuum Ultraviolet Spectroscopy. *Fuel* **2022**, *326*, 125002. https://doi.org/https://doi.org/10.1016/j.fuel.2022.125002.

(27) Bell, D. C.; Boehm, R. C.; Feldhausen, J.; Heyne, J. S. A Data Set Comparison Method Using Noise Statistics Applied to VUV Spectrum Match Determinations. *Anal Chem* **2022**. https://doi.org/10.1021/acs.analchem.2c01931.

(28) Bell, D. C.; Feldhausen, J.; Spieles, A. J.; Boehm, R. C.; Heyne, J. S. Limits of Identification Using VUV Spectroscopy Applied to C8H18 Isomers Isolated by GC×GC. *Talanta* **2023**, *258*, 124451. https://doi.org/https://doi.org/10.1016/j.talanta.2023.124451.

(29) Hall, C.; Bell, D. C.; Feldhausen, J.; Rauch, B.; Heyne, J. Quantifying Isomeric Effects: A Key Factor in Aviation Fuel Assessment and Design. *Fuel* **2024**, *357*, 129912. https://doi.org/https://doi.org/10.1016/j.fuel.2023.129912.

(30) Striebich, R.; Shafer, L.; West, Z.; Zabarnick, S. *Flow Modulation GCxGC for Hydrocarbon Type Analysis of Conventional and Alternative Aviation Fuels (UDRI Method FC-M-101)*; Dayton, OH.

(31) Boddapati, V.; Ferris, A. M.; Hanson, R. K. Predicting the Physical and Chemical Properties of Sustainable Aviation Fuels Using Elastic-Net-Regularized Linear Models Based on Extended-Wavelength FTIR Spectra. *Fuel* **2024**, *356*. https://doi.org/10.1016/j.fuel.2023.129557.

(32) Boddapati, V.; Ferris, A. M.; Hanson, R. K.; Siheung, S. *Unclassified Unclassified Prediction of the Derived Cetane Number of Hydrocarbon Fuels Using Extended-Wavelength FTIR Spectra and Support Vector Regression July 2023 Prediction of the Derived Cetane Number of Hydrocarbon Fuels Using Extended-Wavelength FTIR Spectra and Support Vector Regression*; 2023; Vol. 7. http://www.icders.org/ICDERS2023/abstracts/ICDERS2023-131.

(33) Wang, Y.; Cao, Y.; Wei, W.; Davidson, D. F.; Hanson, R. K. A New Method of Estimating Derived Cetane Number for Hydrocarbon Fuels. *Fuel* **2019**, *241*, 319–326. https://doi.org/10.1016/j.fuel.2018.12.027.

(34) Won, S. H.; Haas, F. M.; Dooley, S.; Edwards, T.; Dryer, F. L. Reconstruction of Chemical Structure of Real Fuel by Surrogate Formulation Based upon Combustion Property Targets. *Combust Flame* **2017**, *183*, 39–49. https://doi.org/10.1016/j.combustflame.2017.04.032.

(35) Parker, R.; Kelly, M.; Watson-Murphy, T.; Ghaani, M. R.; Dooley, S. Prescreening of Liquid Density and Surface Tension for Synthetic Aviation Turbine Fuels by Nuclear Magnetic Resonance Atom Types. *ChemRxiv* **2024**. https://doi.org/10.26434/chemrxiv-2024-v3m2s.