Project 065(A) Fuel Testing Approaches for Rapid Jet Fuel Prescreening

University of Dayton

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- PI: Joshua Heyne
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- Tasks:
    1. Prescreening of sustainable aviation fuels (SAF).
    2. Develop novel testing methods for the evaluation of SAF candidates.

Project Funding Level

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Investigation Team

- Joshua Heyne (University of Dayton) is the Project Lead Investigator for coordinating all team member (both ASCENT and non-ASCENT efforts), communicating prescreening results with SAF producers.
- Linda Shafer (University of Dayton Research Institute) is a senior research engineer responsible for two-dimensional gas chromatography (GCxGC) measurement of SAFs.
- Zhibin (Harrison) Yang (University of Dayton) is a Ph.D. student conducting Tier Alpha prediction and Tier Beta measurement.
- Shane Kosir (University of Dayton) is a graduate student research assistant working on hydrocarbon properties prediction.
- Allison Coburn (University of Dayton) is an undergraduate student research assistant working on freeze point blending rule.

Project Overview

This project will focus on further developing Tier Alpha and Beta test methods which can help minimize the fuel volume needed for testing and improve a fuels potential for meeting ASTM approval criteria. Tier Alpha refers to low-volume analytical testing approaches (i.e., GCxGC, nuclear magnetic resonance (NMR), and IR analytical testing). Tier Beta tests focus on testing the physical and chemical properties rather than predicting those key properties from GCxGC methods.

Task 1 – Prescreening of Sustainable Aviation Fuels

University of Dayton

Objective

A tiered prescreening process for new alternative jet fuels using low fuel volumes that will improve the potential for meeting ASTM approval criteria. This work lowers the technology readiness level (TRL) at which meaningful information can be provided to fuel producers, while simultaneously strengthening their readiness for the approval process.

Research Approach

1. Introduction

The aviation industry is facing mounting pressure to address current and growing anthropogenic emissions [1]. In response to the growing threat, the International Civil Aviation Organization (ICAO) has instituted emission reduction targets through the Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA) [2]. Sustainable aviation fuels (SAFs) are identified as the only medium-term solution to the growing relative impact of aviation emissions on the environment. Recent life-cycle analysis (LCA) has shown that SAFs can reduce well-to-wake greenhouse gas (GHG) emissions by 60% to 104% relative to petroleum-based jet fuel [3]. To date, seven alternative fuels have been approved through the industry's standard approval and evaluation process (ASTM D4054 [4], D7566 [5]). The evaluation of alternative fuels through this process requires that novel fuels be compliant with safety, engine operability, compatibility, and minimal performance metrics. Safety, in the context of jet fuel, refers to the ability of a fuel to maintain acceptable properties under extreme conditions, such as maintaining a liquid state with acceptable viscosity under cold conditions, having a flash point above a determined limit, and others. A proposed prescreening test sequence requires that candidate fuels maintain these properties at a 50% blend ratio with Jet A.

Engine operability, in this context, refers to the ability of a fuel to ignite and hold a flame under potentially extreme conditions associated with the operating envelopes of main engines and auxiliary power units. Any novel fuel must exhibit acceptable performance within the same operating envelope as conventional jet fuels. Novel fuels that illustrate deleterious operability 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. Moreover, many of these operability tests have been the focus of the National Jet Fuels Combustion Program (NJFCP), which has measured the operability performance of multiple novel fuels with fundamental experiments and testing in more than a dozen combustor rigs. The results of these tests, hundreds of observations, nearly 20 different fuels, and numerous rigs are detailed in several publications [6–10].

The overarching results of the NJFCP work implies that nearly all observed combustor operability variance is captured by the physical and chemical properties, which in turn are controlled by the chemical composition of a fuel. Explicitly, deleterious operability behavior can be captured by bounding properties of a jet fuel within the typical experience of conventional fuels. The most important properties for combustor operability are viscosity at -20˚C and -40˚C, density, derived cetane number (DCN), distillation curve, flash point, and surface tension. DCN and surface tension have not historically needed independent specification requirements because they were constrained by other property limits of petroleum fuels. Recently, DCN has been shown to have a direct effect on lean blowout (LBO) performance in swirl-stabilized combustion [11,12]. Sensitivity to surface tension has also been identified [9], 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 deleterious effects, 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 stakeholders responsible for parts of the existing fuel transport and delivery systems. The performance of jet fuels requires a minimum heat of combustion (HOC) and aromatic content within a range. Historically, novel fuels have not encountered issues with these two properties, but prescreening could cover these performance metrics if they did exist. SAFs that exhibit high HOC and density values also have the potential to be high-performance jet fuels (HPFs), which can confer benefits to end-users via increased aircraft payload, increased aircraft range, or reduced fuel volume required for a flight [13,14]. The use of gas chromatography (GC) to estimate specification tests properties for conventional jet fuel has been explored by Striebich el al. [15]. Striebich et al. were able to predict the distillation curve, freezing point, flash point, and sulfur content with a correlation for *n*-alkanes in conventional jet fuel. However, with the diverse profile of SAFs, they may deviate from this correlation or they might not contain *n*-alkanes. Here, a Tier Alpha testing procedure was developed to predict the above-mentioned important properties for combustor operability with only one mL of the candidate

fuel. This tool is intended to precede Tier 1 testing and provide fuel producers with information about the potential of a candidate fuel to pass subsequent tiered testing.

2. Material and methods

2.1 Material

A total of six SAFs were screened in this work, with their relevant information displayed in Table 1. The fuels encompassed three of the seven currently approved SAF conversion pathways [5]. All the fuels had high concentrations of *iso*-alkanes with smaller amounts of *n*- and cycloalkanes. Because of the high *iso*-alkane concentration of these fuels, it is expected that O-ring swelling, density, and DCN will represent the key limiting operability properties that necessitate blending with Jet A [16]. Properties for these SAFs were measured to validate Tier Alpha predictions, with testing methods and reproducibility errors detailed in the Supplementary Material.

Table 1. Information for SAFs screened in this work. Composition is in terms of *n*-alkanes, *iso*-alkanes, cycloalkanes, aromatics, and alkenes respectively.

Fuel	POSF	Average Formula	ASTM D7566 Annex	Composition, vol% (*n*/*iso*/cyclo/aro/alkene)
Syntroleum FT-SPK	5018	$C_{11.8}H_{25.6}$	A1	24.2/75.2/0.6/<0.1/ND
Dynamic Fuels HEFA-SPK	7272	$C_{12.4}H_{26.7}$	A2	9.7/88.4/1.9/<0.1/ND
Sasol FT-SPK	7629	$C_{10.8}H_{23.4}$	A1	0.3/92.4/4.8/0.5/2.0
UOP HEFA-SPK	10301	$C_{12.0}H_{25.9}$	A2	10.2/86.2/3.5/0.1/ND
Gevo ATJ	11498	$C_{12.6}H_{27.2}$	A5	0/99.6/0.1/<0.1/0.3
Lanzatech ETJ	12756	$C_{11.7}H_{25.4}$	A5	0.8/96.5/2.6/<0.1/ND

2.2 Methods

The methodology for this study involved five components: (1) development of a hydrocarbon property database, (2) prediction of properties not available in the literature, (3) two-dimensional gas chromatography (GCxGC) measurements for SAFs, (4) random sampling using the hydrocarbon database and GCxGC data, and (5) SAF bulk property predictions using blending rules. These components are depicted relative to one another in Figure 1 and described in detail in the subsequent sections.

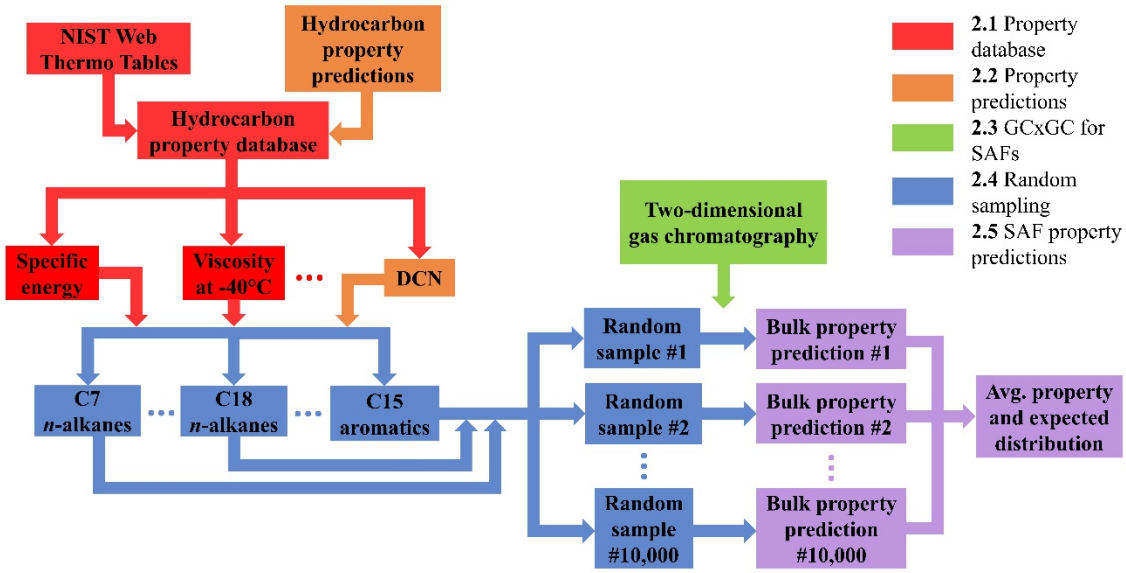

Figure 1. Flow chart of the methodology used for this study.

2.2.1 Hydrocarbon property database

Hydrocarbon property data used for this study consisted of 1,226 unique hydrocarbon compounds from nine molecular groups (i.e., *n*-alkanes, *iso*-alkanes, monocycloalkanes, dicycloalkanes, tricycloalkanes, alkylbenzenes, diaromatics, cycloaromatics, and dienes) ranging from C7 to C20. All the molecules were taken from the National Institute of Standards and Technology (NIST) Web Thermo Tables [17]. Each molecule had both temperature-dependent and temperature-independent properties. Surface tension at 22˚C, density at 15˚C, kinematic viscosity at -20˚C, and kinematic viscosity at -40˚C were temperature-dependent properties used in this study. Temperature-independent properties were boiling point, flash point, and HOC. Figure 2a shows the four most common molecular groups contained in SAFs that are in the hydrocarbon database plotted against a green histogram representing the composition of Jet A. The hydrocarbon database follows a quasi-normal distribution, indicating that it is a reasonable approximation of the composition and properties of Jet A. Because Jet A has a balanced distribution of all the major molecular groups, this means that the hydrocarbon database is representative of most fuels that can be expected for screening. Figure 2b illustrates property variance for 73 molecules that classify as C10 *iso*-alkanes. Blue circles are properties that were predicted for this work, and green squares represent properties taken from the literature. The large span for these properties indicates that the fidelity of predictions will be limited without further quantifying isomeric variance.

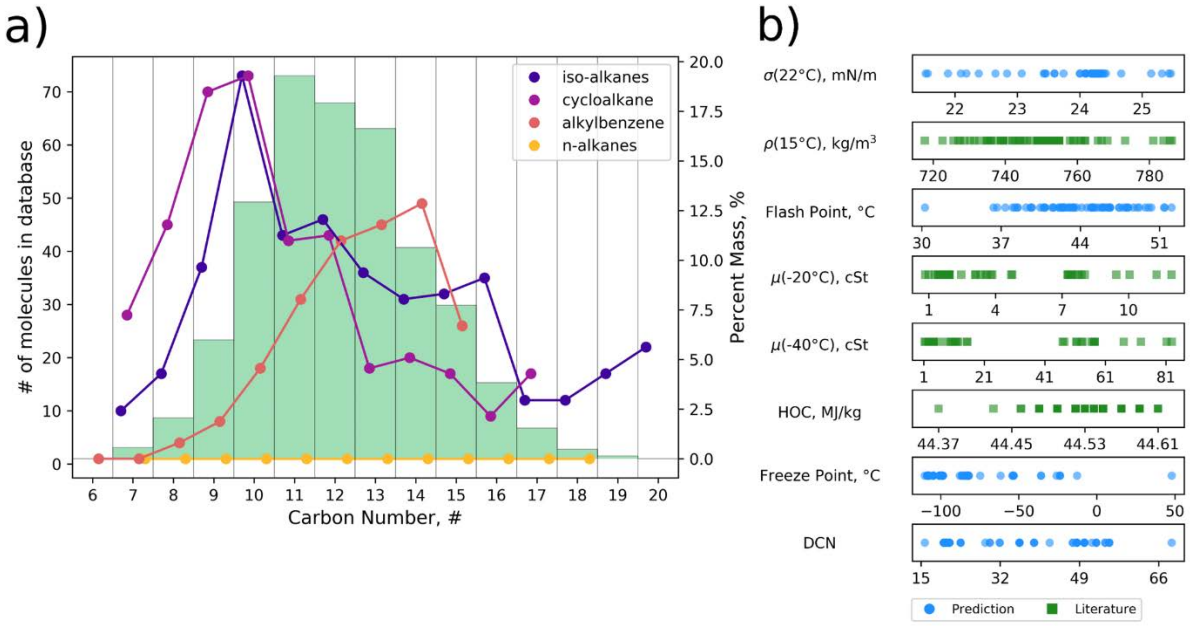

Figure 2. a) A frequency plot of the four most common molecular groups in the hydrocarbon database -*iso*-alkanes, cycloalkanes, alkylbenzenes, and *n*-alkanes- with green bars representing the composition by mass of Jet A and circles representing the number of molecules for each carbon number in the hydrocarbon database. b) A scatter plot of properties for 73 molecules that classify as C10 *iso*-alkanes. Green squares represent literature values and blue circles represent properties predicted in this paper.

2.2.2 Hydrocarbon property predictions

Properties not available on NIST were predicted with various methods. Flash point values for all molecules were predicted using Hshieh's work [18] on the relationship between boiling point and flash point. Hshieh developed a linear correlation of closed-cup flash points with normal boiling points with R-squared value of 0.966.

DCN values for molecules in the hydrocarbon database were predicted using a deep learning neural network trained using H_2O Flow [19], with a five K-fold cross-validated mean absolute error (MAE) of 4.6 and an autocorrelation (R-squared) value of 0.94. 63 DCN observations for saturated hydrocarbons without heteroatoms were taken from the literature [20]. Only observations with DCN tested via ASTM D613 [21] and ASTM D6890 [22] were used for uniformity. Structural descriptors were generated from canonical smiles using the open-source cheminformatics software RDKIT [23]. An overview of the training data can be seen in the Supplementary Material. H_2O's automated machine learning (AutoML) feature was used to optimize weights and biases, with the final parameters displayed in the Supplementary Material. Feature importances from the neural network were subsequently used to screen observations from the hydrocarbon database with a threshold of 90% of the cumulative feature importance, similar to previous efforts in the literature [24]. This resulted in the removal of 161 molecules from the hydrocarbon database that did not fall within the range of structural variance encompassed by the training data.

A similar approach was taken to predict freezing point and surface tension for molecules in the hydrocarbon property database. 287 freezing point observations were taken from the literature [25] and used to train a neural network. A cross-validated MAE of 24.5˚C and an R-squared value of 0.82 was achieved. The large MAE and modest R-squared value can be attributed to the fact that freezing point is widely regarded as a difficult property to predict because it is influenced by both crystal packing and neat molecule properties [26]. The surface tension model was trained using 260 observations from the literature [25]. The result was a cross-validated MAE of 0.83 mN/m and an R-squared value of 0.98. The low error achieved for surface tension is because it scales closely with density, which was used as a training feature.

2.2.3 Two-dimensional gas chromatography

GCxGC was used in this study to determine the hydrocarbon group-type composition of the SAFs using minimal volumes (i.e. one mL per SAF) [15]. The GCxGC analysis relies on the fact that hydrocarbon groups elute in certain regions of the GCxGC chromatogram based on both their volatility and polarity. All the compounds within a region have the same molecular formula and are identified and quantified as a group. Individual compounds are not identified except in the case of single-compound regions (e.g. n-alkanes, naphthalene). For instance, GCxGC results for Sasol SPK (POSF 7629) indicate that this fuel contains 31% C11 *iso*-alkanes, but 43 compounds can meet this classification. 2,2,3,4,5-pentamethylhexane and 3-ethylnonane are both C11 *iso*-alkanes; however, they have drastically different physical and chemical properties.

2.2.4 Random sampling of database properties

In the absence of any further information regarding the specific isomers contained within an eluted fraction (carbon number and molecular group), the best guess estimated properties corresponded to utilizing the hydrocarbon property database and GCxGC data to concurrently generate random samples of a given candidate fuel. From the respective GCxGC data, the corresponding weight or volume percent of the various hydrocarbon species can be identified for each molecular group and carbon number. Each relevant hydrocarbon grouping (via carbon number and molecular group) is paired with a random hydrocarbon with the same criteria in the hydrocarbon property database. This randomization of species primarily affected *iso*-alkanes and cycloalkanes as there are various isomerization and substitution patterns that affect their properties. Each of the randomly sampled species properties was extracted from the hydrocarbon property database and used for the bulk fuel property predictions. This randomization process occurred 10,000 times, creating 10,000 random candidate fuels to investigate variance and establish confidence in the given predictions. See Section 3 for discussion on random sampling convergence.

2.2.5 SAF property predictions

After random sampling of the molecules, appropriate blending rules were used to predict the proprieties of the bulk fuel being screened. For the average molecular weight, DCN, density, kinematic viscosity, and distillation curve, blending rules were taken from the work of Bell et al. [27]. Freezing point, flash point, and HOC blending rules were taken from the work of Flora et al. [28]. The surface tension blending rule used was the Macleod-Sugden correlation [29]. After 10,000 rounds of random sampling followed by bulk properties predictions, the average of each property was taken. The determined average of each property represented the most likely value for each property, and standard deviation was calculated to establish the confidence intervals.

3. Calculation

Random sampling, also known as Monte Carlo sampling, is used in this paper to predict the operability and safety properties of SAFs. Numerous examples of Monte Carlo sampling exist in the fuel literate, including for particulate matter segregation [30], combustion simulation [31], and separation modeling [32]. An important consideration for Monte Carlo sampling is to ensure that the samples have converged. In this study, convergence refers to the stability of the random sampling in terms of both the predicted average values and confidence intervals. If a property is converged, its fidelity can be considered as good as computationally possible without improving the accuracy of the hydrocarbon database or the capabilities of the GCxGC measurement.

As previously stated, 10,000 random samples were taken for each property considered in this study. Figure 3a depicts the running average property values plotted against the number of random samples and Figure 3b depicts the 95% confidence intervals plotted against the number of random samples. It can be seen that all properties have converged before reaching 10,000 random samples, justifying this threshold. The sporadic nature of the average values and the confidence intervals at low numbers of random samples can be attributed to the higher influence of outliers when the total number of samples is small. After about 2,000 random samples, density had few variations in its average value, indicating that the variance in each molecular group/carbon number bin was small. Properties like freezing point and DCN maintained larger variations in their average values, meaning that variance in each molecular group/carbon number bin was larger. This variation represents an inherent limitation for this approach unless molecules in SAFs can be identified with more exactness to inform the random sampling beyond molecular groups and carbon numbers.

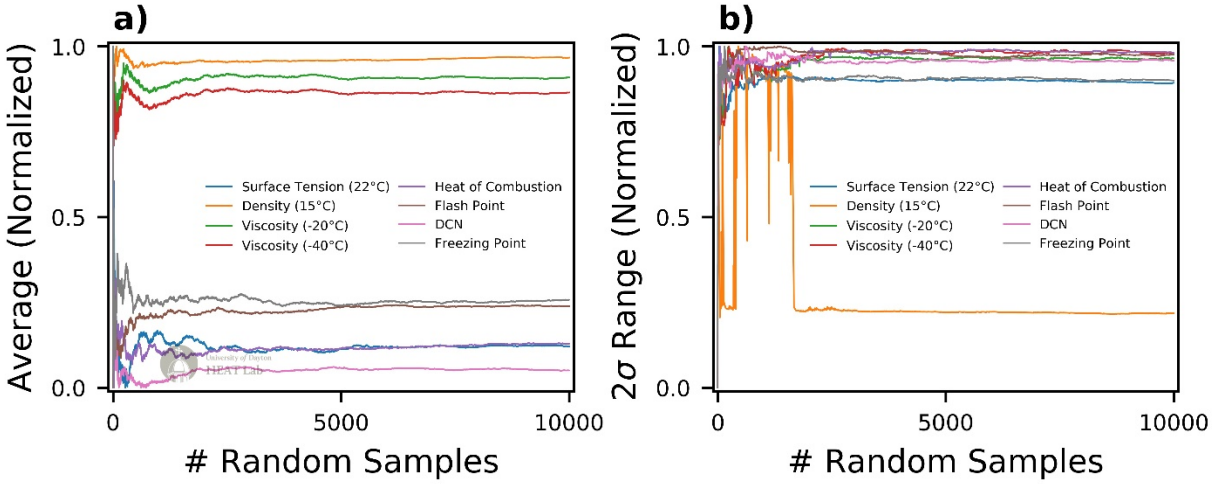

Figure 3. a) Average values and b) (95%) confidence intervals plotted against the number of random samples. Straight lines indicate that the predicted values have converged.

4. Results and discussion

The measured properties for the six SAFs listed in Table 1 (black solid markers) and the Tier Alpha property predictions (colored open markers) of each SAF are plotted in Figure 4, with green shaded regions representing the conventional jet fuel range and red shaded regions representing violations of the specification limits. One sigma (solid colored lines) and two sigma (dashed colored lines) are plotted to show the confidence intervals of property predictions. Due to the known high uncertainty of the HOC and DCN measurements, the ASTM reproducibility (black solid line) is also reported for these properties. Relevant symbols include: surface tension (σ), density (ρ), and kinematic viscosity (υ).

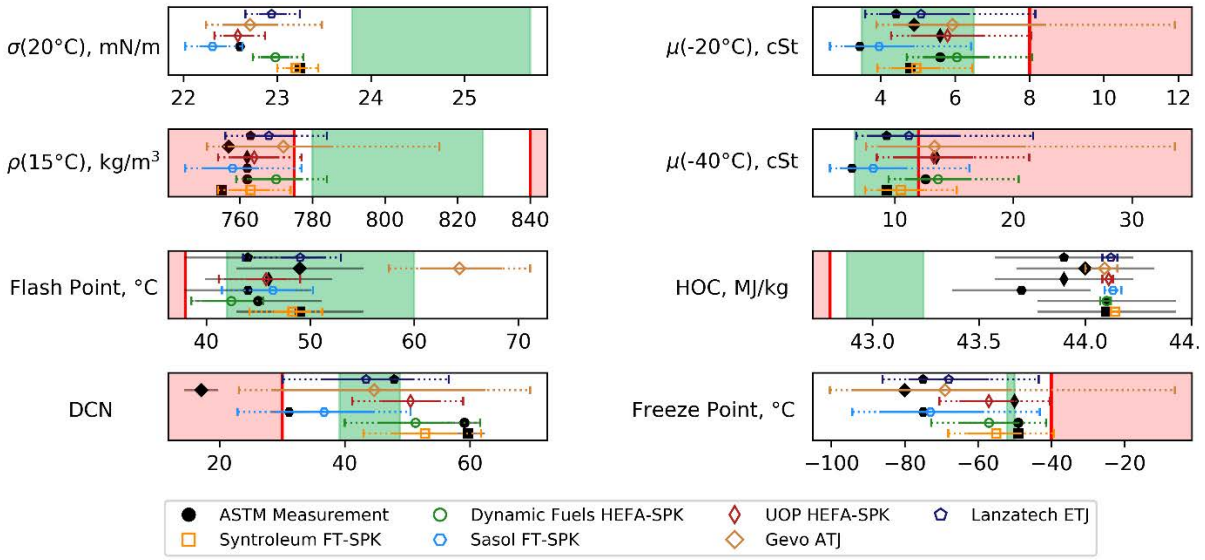

Figure 4. Tier Alpha property predictions and experimental measurements for SAFs. The open markers represent Tier Alpha predictions and solid markers are property measurements. The solid and dashed non-black lines represent one sigma and two sigma for the Tier Alpha predictions. The reproducibility of the ASTM measurements for HOC and DCN are reported as solid black lines.

The measured surface tension values for FT-SPK-Syntroleum and FT-SPK-Sasol are within the one sigma and two sigma range respectfully. There are only two surface tension measurements because surface tension has only recently been discovered as a key property to determine FOM. As Figure 4 shows, surface tension has a tight confidence range, which is because the majority of surface tension values for neat molecules have a positive linear correlation with density.

All SAF density measurements fall within the two sigma range and five are within the one sigma range. Dynamic Fuel HEFA SPK (POSF 7272) falls outside the one sigma range, largely because the range is very tight due to the low variance of density within the molecular group/carbon number bins.

Flash point had confidence intervals with medium magnitudes relative to the other properties. All flash point predictions except Gevo ATJ are within the two sigma range. Gevo ATJ likely fell outside the two sigma range because it contains 98% C12 *iso*-alkanes. Because of the specificity of C12 *iso*-alkanes, it is likely that they were not properly represented by the normal distribution generated during random sampling.

DCN and freezing point have some of the largest confidence intervals of any property. This is in part due to the uncertainty for neat molecule predictions, and also the result of factors influencing DCN and freezing point beyond molecular group and carbon number. Four out of five DCN measurements are within the two sigma range. Again, the outlier is Gevo ATJ, which could be due to the high concentration of a single carbon number molecule. All six measured freezing points are within the two sigma range and four of them are in the one sigma range. Dynamic Fuel HEFA SPK and UOP HEFA SPK fell slightly outside the one sigma range.

Viscosity experienced larger one sigma and two sigma ranges than the previously described properties because it is influenced by factors such as intermolecular attraction and bond rigidity in addition to molecule size. All viscosity measurements were inside the one sigma ranges.

There are only two measurements of HOC that fell outside the two sigma range. HOC also has the smallest confidence range of all the properties. There are four ways to test HOC (i.e., ASTM D1405, D3338, D4529, and D4909), and each one has different reported reproducibility errors. Because the HOC is directly linked to the hydrogen/carbon (H/C) ratio, and therefore easily predicted, it is preferred to use Tier Alpha rather than the ASTM methods to reduce uncertainty associated with the reproducibility errors.

The large uncertainty of Tier Alpha predictions came from property variance within a given molecular group and carbon number as shown in Figure 2b. Because the GCxGC data considered in this work only indicate molecular group and carbon number, the property variance associated with isomeric variance was propagated through to the final prediction. For instance, 2,2,3,3-tetramethylpentane and 2,2,3,4-tetramethylpentane are both classified as C9 *iso*-alkanes. However, the literature freezing points for these two molecules are -9.9˚C and -121.1˚C respectively [25]. That is a 111.2 ˚C difference from a single branch variance. Another example of significant property variance caused by a relatively small stereochemical difference is the experimentally determined DCN for *trans*-decalin and *cis*-decalin at 32.0 and 41.6 respectively [33]. With the vast range of properties for each carbon number and molecular group, it is inevitable to have a large uncertainty unless more information is provided by the fuel producer or the fidelity of the analytical technique is improved.

Figure 5 is a panel plot intended to show fuel producers SAF composition, Tier Alpha property predictions, and distillation properties. The left plot in Figure 5 shows GCxGC results for the SAF, with the green shaded region and the green line representing the carbon distribution and average carbon number for an average Jet A (POSF 10325). The carbon distribution of the SAF for various molecular groups is displayed on top of the green shaded region, and the vertical magenta line is the average carbon number of the sample. The middle plot in Figure 5 shows the Tier Alpha predictions (blue markers) with green shaded regions representing the conventional jet fuel range and red shaded regions representing violations of the specification limits. One sigma (solid blue lines) and two sigma (dashed blue lines) are plotted in these figures to show the confidence intervals of property predictions. The right plot in Figure 5 shows the distillation curve plotted to show the ASTM D2887 results as determined from the GCxGC data. The green shaded region is the conventional jet fuel range and the red shaded region is outside the ASTM D1655 specification limit.

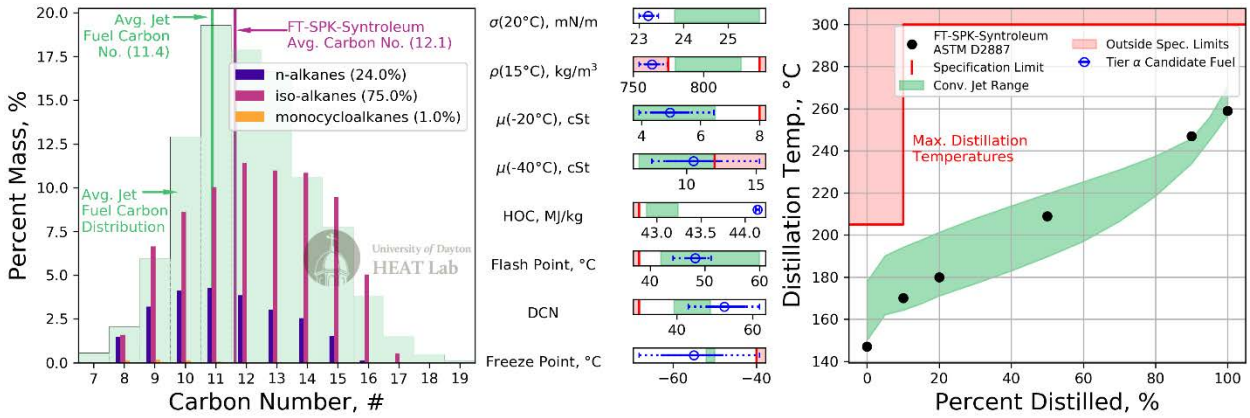

Figure 5. Panel plot for FT-SPK-Syntroleum (POSF 5018).

It is desirable for the fuel producer to match the general trend with the average conventional jet fuel on the left hand side of Figure 5 to reduce the risk of falling outside property specification limits. The risk of deleterious effects increases as the average carbon number of the SAF moves away from the average carbon number of Jet A. As the average carbon number of the SAF moves to the right, the SAF is expected to have higher density, surface tension, viscosity, flash point, and distillation curve. Having a high flash point is beneficial, but it could also push the viscosity outside the specification limit. Conversely, as the SAF becomes lighter, it is expected to have a lower density, surface tension, viscosity, flash point, and distillation curve.

4. Conclusion

A Tier Alpha prescreening tool has been developed and validated to screen candidate alternative fuels at the earliest stage and to give the fuel producer early feedback regarding what is likely to occur during later tiered testing. Tier Alpha is capable of predicting eight properties that are the most important for combustor operability variance during Tier 3 and Tier 4 testing. Tier Alpha prescreening can be used as a proof of concept, as GCxGC requires less than one mL to run. In this way, the fuel producer only has to produce a small amount of fuel to test the concept instead of the 10 gallons required for Tier 1 testing [34]. If the producer has more available volume (i.e., ~150 mL), Tier Beta testing can be done at the University of Dayton to experimentally determine the properties that are important for combustor operability. As more volume is available, more tiered testing becomes possible and the uncertainty of the candidate fuels goes down. However, the required volume increases significantly relative to the uncertainty decrease as a candidate fuel passes through each technology tollgate as aligned with each tier of testing.

As previously stated, the GCxGC data considered in this work does not distinguish between molecules for each carbon number and molecular group. Instead, the GCxGC results show the fraction of each carbon number in each molecular group. Within each specific molecular group and carbon number, numerous isomers exist. Therefore, Tier Alpha does not predict the absolute value of each property, but rather it provides a range of possible values and the most likely value. If additional information is given by the fuel producer (i.e., molecules or functional groups that are expected to be in the SAF), then the confidence range can be significantly reduced. To date, Tier Alpha testing has been performed on 22 SAF samples from numerous national labs and industrial companies. The knowledge gained from Tier Alpha has helped fuel producers to adjust feedstock processing and conversion methods to achieve improved SAFs.

Tier alpha represents a work in progress, with significant reductions in the confidence intervals still possible. Future work should focus on the resolution of GCxGC or other analytical techniques to determine the composition of SAFs with greater fidelity. Neat molecule predictions for DCN and freezing point should be improved and the freezing point blending rule should be experimentally validated to narrow the confidence range of DCN and freezing point predictions. Filling gaps in the hydrocarbon database per Figure 2a would facilitate more accurate Tier Alpha predictions. Screened SAFs can also be optimized using the Jet Fuel Blend Optimizer (JudO) [35] to determine potential HPF blends that can provide performance benefits for aircraft and help eclipse the cost-benefit threshold of SAFs.

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Milestones

- Tier Alpha performed 12 times.
- Tier Beta performed 15 times.
- Maximum blending ratio determined for three SAFs.

Major Accomplishments

Reporting key combustor operability properties prediction for 12 SAFs, key combustor operability properties measurement of 15 SAFs, and maximum blending ratio for 3 SAFs.

Publications

Peer-reviewed Publications

Yang, Z., Kosir, S., Stachler, R., Heyne, J., Shafer, L., and Anderson, C., "A GCxGC Tier Alpha Combustor Operability Prescreening Method for Sustainable Aviation Fuel," pp. 1–18. Fuel. (In review)

Outreach Efforts

Conference presentation

ACS Fall 2020 National Meeting & Exposition in San Francisco, CA.

Awards

None

Student Involvement

Zhibin (Harrison) Yang, Ph.D. student, leads this effort.

Plans for Next Period

Finalize the publication in progress, improve Tier Alpha prediction accuracy, and reduce volume required for Tier Beta measurement.