Full Length Article

Sustainable aviation fuel prescreening tools and procedures

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ABSTRACT

This paper outlines the benefits and procedures for prescreening Sustainable Aviation Fuel (SAF) candidates before entering the official ASTM D4054 evaluation process. Specific properties are identified, that if not met, may result in extensive and costly efforts to correct if not recognized until later in the fuel development process. Hence, an approach with specific techniques that use low fuel volumes is suggested that enable (1) early estimates of critical properties and subsequently (2) direct measurement of these properties to guide fuel processing development prior to formally entering the ASTM evaluation process. The process is demonstrated with two exemplary candidate fuels.

1. Introduction

Anthropogenic emissions from combustion systems are one of the leading contributions to climate change globally, which have harmful effects on overall societal stability. Carbon emissions need to be zeroed or offset in the coming decades to mitigate forecasted impacts. The contribution of global aviation in 2011 was calculated to be 3.5% of the net anthropogenic effective radiative forcing [1]. These relative emissions will grow with market demands and as ground-based electrification becomes more prevalent. Sustainable Aviation Fuels (SAFs) offer advantages relative to conventional fuels as they mitigate climate change, may improve air quality, offer domestic economic opportunities (e.g., low-cost energy source), provide stable and diverse energy supply, and may ultimately improve aircraft operations with higher-performance properties.

Production rates of currently approved SAF technologies can only meet a fraction of commercial airlines's market size. Furthermore, no SAF production technology is currently approved for commercial use as a 100% synthetic drop-in, despite demonstration flights at higher concentrations [2]. (Sasol Fully Synthetic Jet Fuel is approved as a 100% synthetic drop-in by DefStan 91-091, but does not reduce carbon emissions [3].) Novel pathways and compositions are being developed to increase production potentials, leverage diverse-locally available feedstocks, and identify hydrocarbon compositions that enable increased blending limits beyond the current 50% constraint.

SAF's development and market penetration is arduous since SAFs are subject to tighter tolerances and more qualification hurdles than alternative fuels for ground transportation. SAFs need to be hydrocarbons absent of olefinic content, oxygenates, and other heteroatoms. (These materials are deleterious to aviation fuel performance and safety metrics.) Compromises of such metrics are unacceptable. SAFs need to be "drop-in fuels" that are fungible with petroleum fuels, composed solely of hydrocarbons, produced from alternative sources such as bio-derived feedstocks, and that provide at least as good as performance to that from petroleum-derived jet fuels.

SAFs are approved for usage via a Tiered Test or Fast Track Programs under ASTM D4054 [4]. The Tiered Test Program currently has seven approved fuels and six annexes [5], and currently allows approved blend ratios up to 50% with conventional fuel. With a maximum of a 10% blend limit, the Fast Track evaluation process has led to the approval of one fuel and production pathway annex in ASTM D7566 (Annex 7). Thus, SAF technologies with the most significant impact, high blend ratios, or novel compositions must undergo the Tiered Test Program. Of note with this Tiered Test Program is the path for approval. Novel SAF candidates may require tests exceeding millions of dollars in tests, tens of thousands of liters of fuel, years of testing, and sustained commitment of resources for fuel producers. Additional information on approved conversion processes can be found on the CAAFI website [6].

Prescreening tools and procedures can minimize cost, fuel volume, program risk, and time requirements. Prescreening novel SAF candidates refers to testing or predicting key fuel properties and performance metrics before entering the formal ASTM D4054 evaluation process. The

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National Jet Fuels Combustion Program (NJFCP [7]) and the JET fuel SCREENing and optimization (JETSCREEN [8]) program have identified multiple prescreening methods. These tools can collectively predict deleterious fuel effects that may not be apparent until after high volume production and high-test costs late in the ASTM evaluation process. These tools offer an opportunity to evaluate a SAF's acceptability for aviation applications before the fuel formally enters the evaluation process and enables feedback to the producer to fine-tune the formulation or workup stages and handling. This paper describes the landscape by using experiments, emerging tools, and partnerships for prescreening new aviation fuels.

2. Jet fuel requirements and alternative fuel qualification

Aviation safety is built around redundancy and verification of critical system operations, and Jet A/A-1 is the only energy source in current commercial aircraft. Jet A/A-1 not only provides the energy source to propel the aircraft, but it also performs other essential functions within the aircraft beyond chemical heat release. Fig. 1 illustrates many of the interdependencies of jet fuel as it interacts with various aircraft functions and operations. For example, approved alternative fuels need to operate sufficiently as a coolant, seamlessly with pumps and seals, stably in long-term storage, and safely under severe operability conditions.

An aviation fuel's compositional and resulting properties can have a wide range of impacts on the handling, airframe, and engine. Some critical compositional properties (off-centered blue oval) are highlighted. These compositional properties then cascade (arrows) to impact chemical and physical properties as well as broad systems and stakeholders. Three concentric circles (brown, orange and, red) illustrate this diverse cascade of impacts on the engine, airframe, and handling, making variance in the compositional variance a substantial financial and safety risk. The chemical and physical properties (boxes in the green
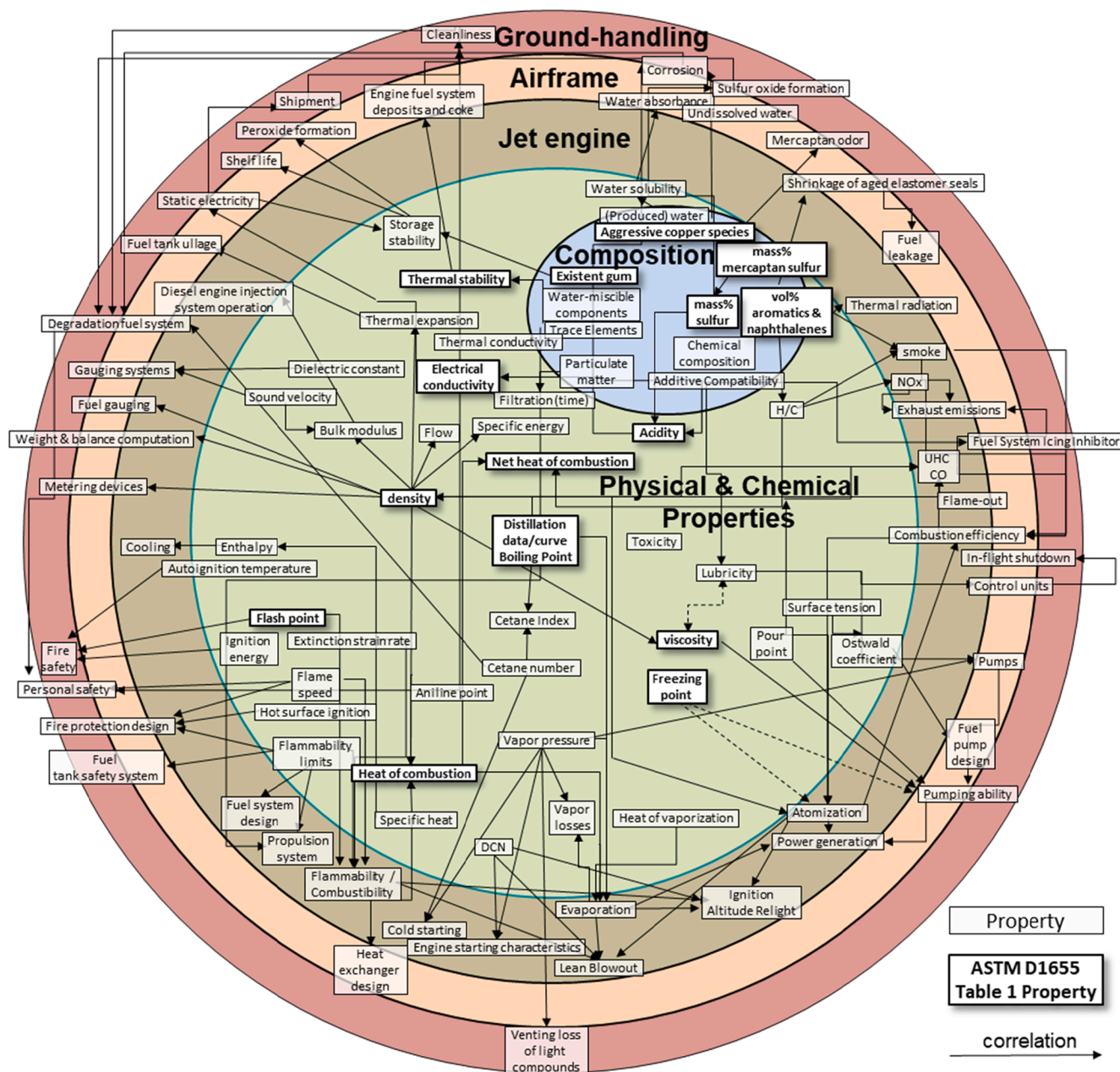

Fig. 1. Overview of interdisciplinary and interdependency of the properties [8] tested during the ASTM D4054 process. Properties (boxes) are grouped by discipline (circles); an error indicates the relationship between properties. ASTM D1655 Table 1 properties are shadowed and boxed with thicker lines.

circle) of SAFs need to be constrained to eliminate and derisk the impact on subsequent sub-processes and components (concentric circles). Density, for example, is noted to impact a diverse array of these sub-processes and sub-component performances. Variance in the density impacts heat exchangers, pumps, gauging, fueling, and balance. Early alternative fuel evaluations involved extensive testing (boxed metrics), making the process arduous. Further, the functional form of these arrows and their impact on stakeholders has been the focus of the aforementioned NJFCP and JETSCREEN programs.

Fig. 2 illustrates the Tiered Testing Program under ASTM D4054. Included in the figure are estimated costs and durations for several of the steps [9], as described previously.

The process ranges from the relatively inexpensive Tier 1 and 2 (laboratory) tests to the more expensive and time-consuming engine and flight tests [10], and final review and balloting by all ASTM committee members. It must be noted that the discussed costs do not include the expenses for fuel development and production, delivery, and personnel on behalf of the fuel producer.

3. Prescreening and pre-qualification testing

The complexity, cost, and timeliness of the traditional Tiered evaluation process warrant methods and procedures to minimize resources. Low fuel volume testing procedures could be used to identify new candidate jet fuels with a high probability for evaluation or provide feedback to identify problem areas with troublesome candidate fuels. With low cost and low fuel volume methods, limited but useful information can be extracted. The challenge is to extract as much information from as little fuel as possible and to target properties that, if not within an acceptable range, will have a high-cost impact for the fuel producer later in the evaluation process. Specifically, operability and safety issues

are key concerns that may not exhibit themselves until Tier 3 or 4 testing and after substantial costs in testing and fuel production have been expended.

The National Jet Fuels Combustion Program (NJFCP) was dedicated [5] to the understanding of combustor operability based on the Figure of Merits (FOM) at three conditions, as suggested by Original Equipment Manufacturers (OEMs) concerning the impact of fuel properties and compositions. These FOM operability points (lean blowout [LBO], cold start, and altitude relight) represent the most critical and fuel sensitive metrics for qualification. Based on years of this work with hundreds of collaborators and dozens of institutions, several predictive tools have been produced, and a shortlist of critical properties have been tabulated. These properties are summarized as [9,10]:

- viscosity at -20 and $-40\ °C$,
- density at $15\ °C$,
- surface tension at $22\ °C$,
- the Derived Cetane Number (DCN),
- the distillation curve, and
- flash point.

Combined, these properties at various temperatures were able to predict fuel effects on the Figure of Merit combustor behavior across multiple architectures for LBO [11,12] and ignition [13] for selected fuels. For ignition, physical and distillation properties dominate [13], while fuel property dependence on LBO transitions from physical property dominance to chemical property dominance with increases in temperature and decreases in spray break-up time-scales [14].

The JETSCREEN program investigated a broad range of a fuel's effect on the aircraft, not only on the combustion system but also on the fuel system, focusing on safety-, environmental-, and operation-related sub-
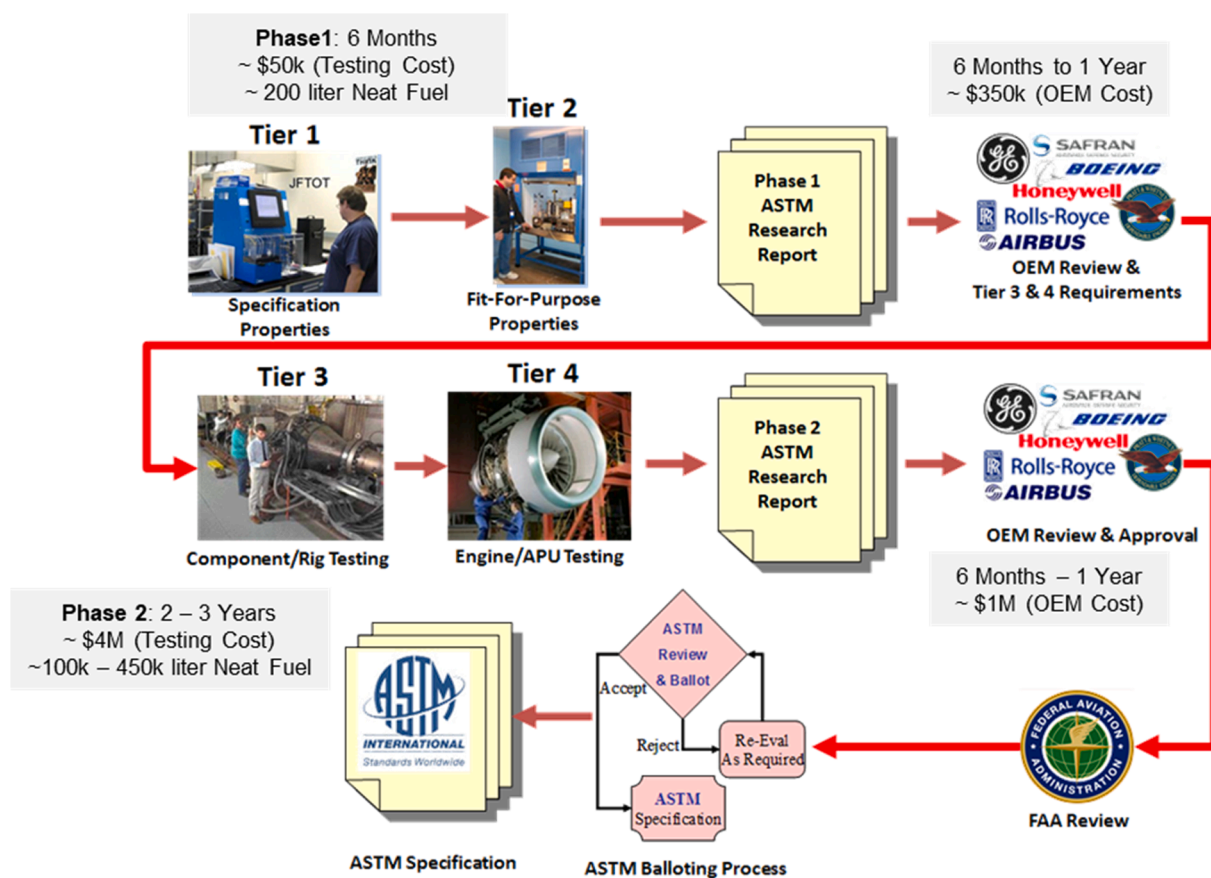

Fig. 2. A nominal ASTM D4054 evaluation process for fuels above 10%v blend limits with fuel and costs requirements. The cost of fuel production is not included [8].

processes [8]. For example, lowering the aromatic content reduces soot emissions significantly, but yields a material compatibility risk, i.e., o-ring shrinkage and fuel leakage. To provide services that derisk novel SAF production pathways, a fuel prescreening platform was developed that incorporates models and data from a network of partners from different disciplines. The screening of new fuels is performed by first analyzing the fuel composition (qualitative and quantitative GCxGC and trace components analysis) and then inferring selected fuel properties through their similarity with properties from already approved fuel pathways.

We recommend the addition of two early tiers as prescreening to collect property information upstream of the evaluation process at early stages of development to determine fuel characteristics and modify the processes quickly with low costs. Characteristics of Tier α consist of a composition-based screening from, with model-based predictions of key properties, and Tier β characteristics consist of experimental verification of Tier α key property predictions. The process is demonstrated on two exemplary candidate fuels: Candidate fuel 1 (an FT research fuel [15]) and Candidate fuel 2 (POSF 5018).

4. Tier α

The first of these two tiers, Tier α, define an experimental method that requires minimal amounts (milliliters) to characterize the fuel. Data from these low volume tests are used to glean additional information regarding a fuel's potential impact on the engine, airframe, and handling system metrics in Fig. 1. Correlations or detailed modeling take test data and predict, at minimum, the physical and chemical properties critical to the Tier 3 and 4 operability tests. For reference, ~400 L are required to initiate entry to the formal ASTM D4054 Tier 1 and 2 test process, even though test volumes for Tier 1 and Tier 2 may be as low as ~ 200 L.

As properties are a function of the composition of the fuel, one of the first steps in prescreening is to analyze the fuel composition of the candidate fuel blendstocks. However, jet fuel specifications impose only a few limits on the fuel composition and ensure operability by an empirically evolved set of fuel property limits. These constraints result in a difficult development target for new fuel producers. In recent years, comprehensive two-dimensional Gas Chromatography (2D-GC or GCxGC) has been extensively used to derive the composition of conventional jet fuels as well as synthetic fuel candidates, sometimes referred to as hydrocarbon type analysis (HTA). Furthermore, 2D-GC has become a pivotal part of the ASTM D4054 Fast Track process. Systematic compositional characterization of already approved fuels helps to elucidate the fuel composition-fuel property relation in particular when it comes to identifying potential fuel chemical families (e.g., alkenes, oxygenates) or specific molecules (e.g., hetero-atomic compounds) that will bring a fuel candidate outside (or inside) the specification requirements.

Fig. 3 depicts this by comparing fuel family mass fractions of the two candidate fuels with those of ASTM D7566 approved synthetic hydrocarbons (colored areas) and of 57 conventional fuels from the CRC World fuel survey [16] (bar and whiskers). Candidate fuel 1 is typical for a fuel in the early-stages of development, as the production process may not be well defined, and an early assessment of the fuel product can refine the product compositions. Here Candidate fuel 1 was found to contain 21% of n-/iso-alkenes and 3% of oxygenates, which would violate the compositional requirements in ASTM D1655 and D7566. Moreover, such a fuel would not eclipse the ASTM D4054 evaluation process as it would not pass the thermal stability and water solubility tests due to the high alkene and oxygen content. Candidate fuel 2, however, is more consistent with compositions within ASTM D1655 and D7566; namely, it is within the range of an approved ASTM D7566 FT-SPK fuel. At this stage of evaluation, it could also be useful to evaluate a fuels trace composition, such as nitrogen content, for Candidate fuel 2.

Beyond this initial stage, additional information concerning the physical and chemical properties of Candidate fuel 2 is required. Further evaluations of Candidate fuel 1, as reported in Fig. 3, would yield little value. The fuel first needs alkenes and oxygenates removed before revised compositions can be evaluated, and further property predictions would be useful.

The determination of fuel property values from small volumes of fuel samples is a research area that has long been investigated. In fact, many such methods have been adopted by ASTM over the years. Vozka and Kilaz [17] recently have performed a review of many older as well as some recent screening techniques for property determination that use small volumes of fuel. In fact, data derived from their summary table of
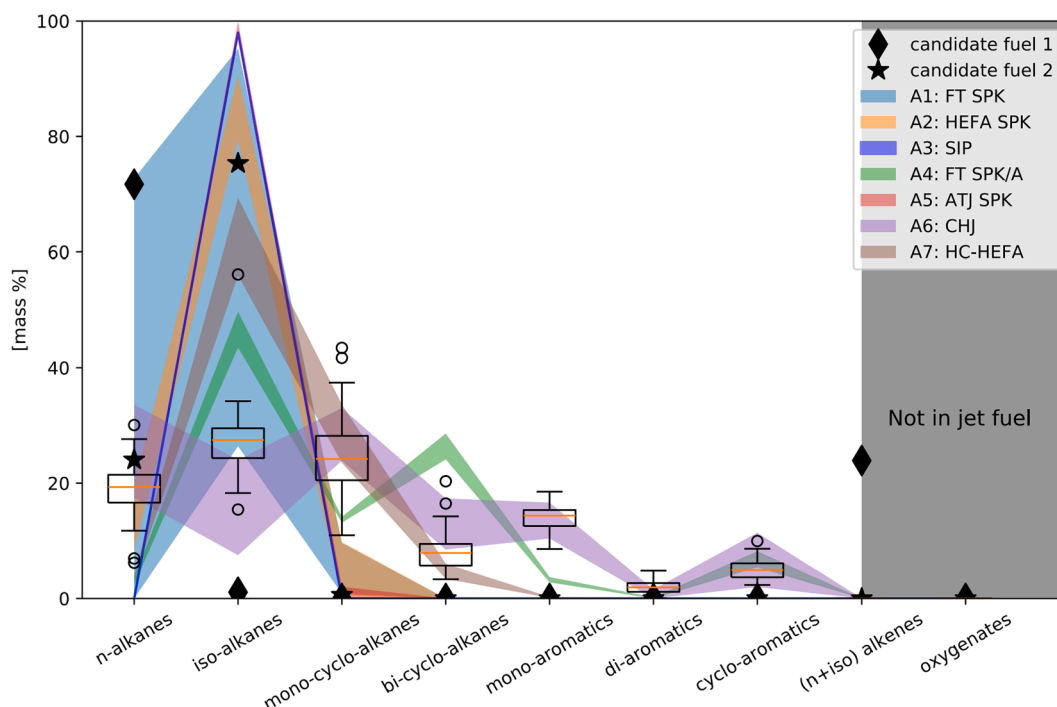

Fig. 3. Comparison of fuel composition of two research candidate fuels with already approved pathways. Data are based on GCxGC measurement results.

the lowest error experimental methods appear very promising, as shown in Table 1.

Several other properties are reported in [17], and these results seem very encouraging as the errors are small and should be acceptable for use. However, it should be noted that the uncertainties provided in the table are based on fits of existing data sets and are unlikely to be representative of their predictive capability, especially for fuel types not considered in the fitting routines. In fact, most of these methods are not direct property determinations but rather deduced using 'spectral' or species information; they have been mostly calibrated using petroleum-derived fuels. Moreover, the majority of these references are based on jet fuels or distillate fuels only. Ref. [20] includes 78 fuels, with 3 of these fuels being 'upgraded synfuels' from the direct hydroliquifaction of black and brown coal. Ref. [25] implies the inclusion of non-petroleum fuels in their correlations (of mostly diesel fuels), but no data is provided. In general, correlations based on petroleum/distillate fuels may not be applicable to synthetic aviation fuels, and significant uncertainties can exist. For example, the ASTM correlation (D4737 [26]) for Cetane Index based upon petroleum fuels works poorly for estimating the cetane number of alternative fuels [27]. Issues with other ASTM methods have been noted in detailed reports elsewhere [28,29]. While not comprehensively state here, these issues many times stem from the unique compositions and selective isomeric structures of alternative fuels.

From time to time [29] there may be problems with surface tension, freeze point, permittivity, and heat of combustion (HOC) measurements, although, in many of these cases, there are problems both with the correlation method and the experimental measurement as well. Hence, other methods for measurement and predictions are desirable. The incorporation of more diverse property-composition training sets that include more alternative fuels and fundamentals is desired.

Specifically, the variance across properties from SAF candidates can span the range of potential isomeric variances across all hydrocarbon types of the Jet A/A-1 distillation range. The reason for this is the lack of diagnostic capability in both the current GCxGC and absorption methods used. GCxGC methods cannot identify specific isomeric variances; at least one library at the University of Dayton (UD) has 1226 potential SAF molecules. As an extreme example within that database, the freeze point range amongst 73 iso-alkane isomers with 10 carbons is 158 °C. Current GCxGC methods are indiscriminate for a given peak. Although methods can be trained to be more selective, molecules for a given hydrocarbon type and carbon number are typically lumped. Separation is generally governed by distillation and polarity, and mass spectrometry (MS) identification cannot distinguish between two isomers of similar hydrocarbon group compositions. For SAF candidates with distributed isomeric variance on a given peak, the error would be minimized via the cancelation of errors. However, in the case of a single isomeric conformation, the prediction of these properties with historical methods for

conventional fuels degrade. Already, several fuels have been approved that meet these criteria, Gevo ATJ and Amyris farnesane, as they are composed of only one or two components with very selective isomeric structures.

UD and the German Aerospace Center (DLR) have applied two different modeling approaches that attempt to quantify the uncertainty and potential variation in the predictions. The DLR model [30,31] is a Gaussian Progress Regression algorithm that is trained on conventional and synthetic fuels. Uncertainties in the prediction are a result of the similarity of the fuel with the fuels used to train the model. UD predictions [32] leverage a database of 1226 molecules and their associated properties. Molecules from this database are randomly sampled and matched with the corresponding GCxGC hydrocarbon type analysis concentrations. Properties from unique molecules are blended with the hydrocarbon type concentrations resulting in a set of bulk properties. Sampling is repeated until convergence, approximately ten thousand additional times. The statistics from the sampling are then represented with an expectation value and confidence intervals. The modeling approaches are complementary in the sense that the DLR model correlates directly to the fuel composition with the bulk physical properties of the fuel, while the UD model composes the bulk-physical properties out of single molecules. By using contrasting modeling approaches, additional reliability is provided to the prediction results.

Fig. 4 illustrates the Tier α compositional and distillation property screening plot with comparisons to conventional fuels. The scope of this step in the prescreening process is to understand if the properties influencing the operability of a candidate fuel lie within fuel specification and the range of experience for conventional fuels, represented by values for the Coordinating Research Council (CRC) World Fuel Survey [16]. Fig. 4 (a) compares the hydrocarbon type distribution of a Candidate fuel 2 and the distribution of an average jet fuel, Jet A POSF 10325. The light green region illustrates the hydrocarbon distribution of Jet A fuel as a reference, with the vertical green line being the average carbon number of that fuel. This light green region and dark green vertical line calibrate the candidate SAF composition, which is plotted in the purple, magenta, and yellow bars. The composition of Candidate fuel 2 is largely n- and iso-alkanes with no aromatics and minimal mono-cycloalkanes. The average carbon number of Candidate fuel 2 is approximately 12.2 carbon numbers, which is slightly above the composition of an average Jet A. Nonetheless, the distribution of hydrocarbons is favorable.

Fig. 4(b) illustrates the distillation curve of Candidate fuel 2 via ASTM D2887. Here the data (black symbols) representing Candidate fuel 2, are compared against a range of conventional fuels, namely POSFs 10325, 10264, and 10289, which represent an average, 'best' and 'worst' case jet fuel [33]. (The authors note that other reference fuels could be used to calibrate the experience range, and in fact, the CRC World Fuel Survey fuel database would be more comprehensive.)

Table 1
Minimum Standard Error of Prediction of selected properties as reported by Vozka and Kilaz and computed relative error based on reference jet fuel.

Property	Standard Method		Screening technique		
	ASTMMethod	Reproducibility	Reproducibility standard deviation	Minimum Standard Error of Prediction	Technique*
Hydrogen Content, wt%	D7171	0.28	0.099	0.04	NIR [18]
Net Heat of Combustion, MJ/kg	D4809	0.32	0.114	0.04	NMR + LC[19]
Freezing point, °C	D5972	0.8	0.29	0.90	GC [20]
Density (15 °C), kg/m^3	D4052	0.00052	0.0002	0.0006	FTIR [21]
Initial boiling boint, °C	D86	8.75	3.12	1.70	FTIR [22]
10% Boiling point, °C	D86	3.87	1.38	2.28	FTIR [23]
20% Boiling point, °C	D86	3.83	1.37	3.30	NIR [24]
50% Boiling point, °C	D86	3.0	1.07	3.20	NIR [24]
Final boiling point, °C	D86	7.1	2.54	1.10	FTIR [22]
Flash point, °C	IP 170	3.2	1.14	0.61	FTIR [23]
Viscosity, mm^2/s	D445	0.0315	0.01	0.09	FTIR [22]
Cetane Number	D6890	2.55	0.91	0.57	NIR [18]

*NMR – Nuclear Magnetic Resonance; NIR – Near Infrared; GC – Gas Chromatography; FTIR – Fourier Transform Infrared; Raman – Raman Spectroscopy.
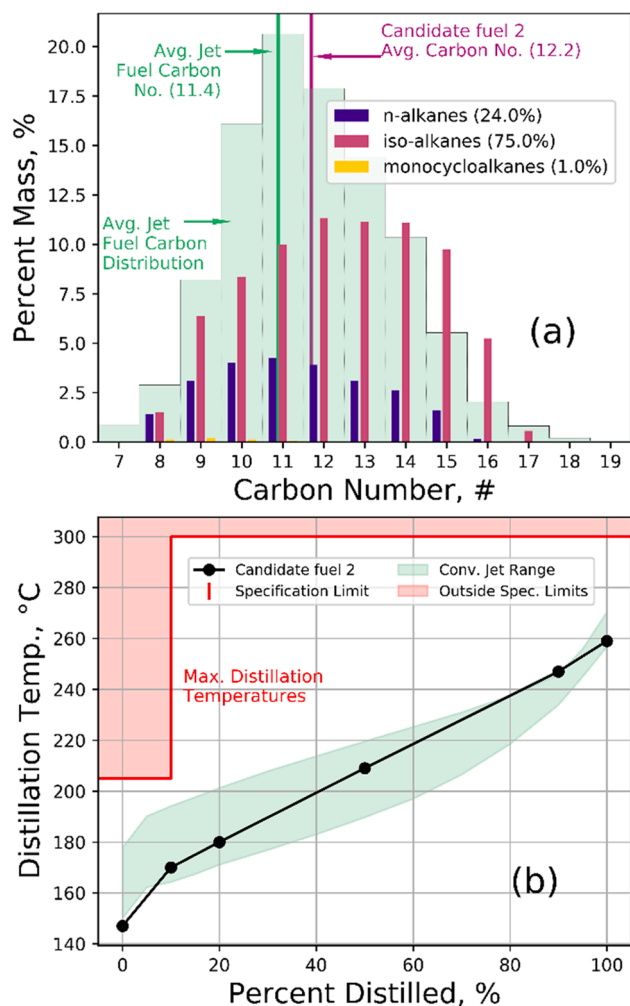
Fig. 4. Exemplar plot of Tier α prescreening for composition and distillation analysis. The green region represents the range of conventional fuels, namely POSFs 10325, 10264, and 10289 [33].

Blended fuel distillation temperatures outside this range would likely be subjected to additional scrutiny. The red line and region in Fig. 4(b) illustrate distillation temperatures and regions that are outside of ASTM D1655 specification. Candidate fuel 2 neat/unblended data are within the range of conventional fuel distillation temperatures, and therefore favorable.

Fig. 5 illustrates the predictive component of Tier α prescreening. Here data from GCxGC results are used to predict critical properties of jet fuel that influence combustor operability. At this point, depending on the availability of the fuel volume, only the property predictions would be completed. Measurements would come later in Tier β. Nominal predictions and their associated uncertainties from the UD (empty circles) and DLR (empty triangles) models are reported. The filled black circles are the measured properties via ASTM test methodologies, which are discussed in the next section. The solid and dashed lines for the predictions represent the 68.2% and 95% confidence intervals, respectively, for each model.

DLR confidence intervals are based on the similarity of the fuel with the fuels used to train the model, while UD confidence intervals are based on the statistics from random sampling from a database of more than 1200 molecules. Descriptions of these methods are detailed elsewhere [32,32]. The shaded regions represent the typical range of Jet A/A-1 properties (green) and their respective ASTM D1655 defined limits (red). Candidate fuels with properties within or near the range of Jet A/A-2 (green) could be strong candidates, with other fuels potentially
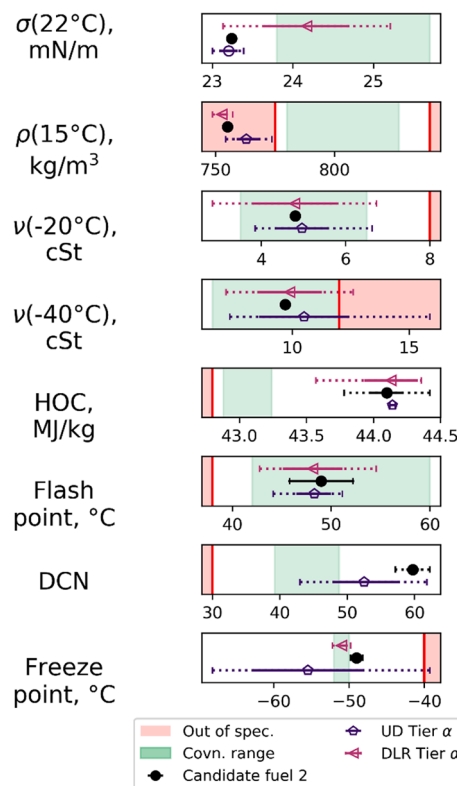

Fig. 5. Illustration of Candidate fuel 2 predicted (Tier α) and measured (Tier β) properties. (No standard uncertainties are established for the surface tension (σ), and DCN values are not available from DLR. Also, note the hydrogen content is not reported as there is a negligible difference amongst methods.)

needing augmenting. Already, experience from the authors has facilitated the development of SAF technologies more poignantly, targeting the development of SAF at this level of Tier α evaluation.

The properties predicted for neat Candidate fuel 2, here, can subsequently used to determine blend limits or if a fuel is a more likely candidate for Fast Track or the Tiered Testing Program mentioned earlier. Overall, the neat SAF Candidate fuel 2 is observed to have favorable predicted properties relative to the specification limits and conventional fuel property distributions. The only property predicted to be outside in the ASTM D1655 specification range is the density, which at a 50/50 blend with Jet A/A-1 would not be an issue. Moreover, this deviation lies within the experience range of approved SAFs, making Candidate fuel 2 still favorable.

It is important to note that the models used in this work are not described in detail (although references are provided) in recognition that there are quite a few alternative methods that can provide a similar capability if the uncertainties are well established. The article by Vozka and Kilaz [17] provides an excellent review of possibilities via NMR, IR, Raman, GC/GCxGC, and combinations of these techniques, although they did not correct the percent uncertainties reported by Johnson et al. [34] as they were incorrectly described in the tables presented by the original authors. Alternative methods for interpretation of GCxGC data have been reported by Vozka et al. [35]. A recent good alternative is provided by Wang et al. [36] for interpretation of mid-IR (FTIR) spectra, although extensions to these methods promise increased accuracies (R. Hanson, personal communication [37]).

5. Tier β

Tier β eliminates concerns on the predictive aspects of Tier α and measures properties directly. This exercise minimizes property uncertainty and derisks a fuel production pathway but requires higher

amounts of fuel (Tier α: 1–5 mL, Tier β: 150–500 mL for properties reported here), with the DCN alone requiring $\sim$ 140 mL. Tests can be prioritized (based on the volume of fuel available) using predictions gleaned in Tier α. These measured properties can then be used to predict more clearly the Figures of Merit operability limits in the Referee Rig, for example [11]. The total list of properties testing for Tier β can vary based on the concerns of producers and fuel screeners, but it nominally includes the same list of properties considered in Tier α and reported in Fig. 5.

Fig. 5 reports property measurement methods as well as their respective reproducibility (and accuracy based on CRC Report No. AV-23-15/17 [28]). The measurement accuracy is typically better than the Tier α predicted uncertainty, with one exception. The heat of combustion (HOC) prediction for UD also has lower variability than the ASTM method. This method by UD utilizes the National Institute of Standards and Technology (NIST) reference database [38] and estimated heat of vaporizations. The small variations in the predictions result from the reduced uncertainty of the NIST database ($+/-$ 0.018 MJ/kg for n-dodecane) and the associated variance across molecules in a given hydrocarbon type and carbon number pair ($2\sigma = 0.092$ MJ/kg for C12 iso-alkanes). In addition to other noted inconsistencies, this observation needs to be clarified with additional work [29,39] to take into account even more detailed and holistic uncertainty quantifications than in the current UD HOC model, such as heat of vaporization and the impact of GCxGC hydrocarbon type analysis uncertainties.

The property predictions of Tier α are nominally in good agreement with the property measurements and the associated errors. The details of these computations and uncertainties are not the focus of this paper but are discussed in other publications [30,32]. Collectively, Candidate fuel 2 has favorable neat/unblended properties consistent with other approved ASTM D7566 SAFs. The density, which, when blended, would fall in the specification range. The recommendation for the producer of candidate fuel 2 would be to start scaling up production and initiate the communications with ASTM. Upon production scale-up, an additional Tier β evaluation would be useful to confirm scale-up has not imparted deleterious effects. After this final Tier β evaluation, it would be recommended to submit a batch of 400 L for formal ASTM D4054 evaluation.

6. Conclusion

This manuscript addresses the need for a low-cost entry into the synthetic aviation fuel market. Specifically, a set of priority property determinations have been identified, that if not satisfied, may cause significant delays and costs later in the evaluation process that precedes balloting to approve new components in the ASTM D7566 specification. It is hoped that early tests can provide feedback to a producer to adjust the refinement process early enough to save resources later. For this purpose, a Tier α and Tier β set of experiments and analysis are proposed; the first is a low volume method (1–5 mL) using GCxGC traces to characterize fuel composition, along with correlative modeling to infer properties, and the second tier is a set of direct measurements of specific properties for confirmation of model predictions with industry-standard methods and requires 150–500 mL. Both tiers are outside of the ASTM evaluation process, but the results, assuming they are well documented, may be used to defer costs in Tier 1–4.

A set of techniques to characterize the fuel while requiring low fuel volumes along with correlation methods have been identified that have the potential for estimating key properties. However, it is argued that traditional techniques, for which correlations were based solely on petroleum and distillate fuels, may contain bias that is not displayed in model accuracy metrics when applied to synthetic fuels. Hence much of that work on accuracies of techniques may have to be redone for synthetic fuels.

The suggested prescreening process was applied for two candidate fuels. In the prescreening step comparing fuel composition of the candidate fuels with already approved fuels, it was shown that Candidate fuel 1 contains considerable amounts of alkenes and oxygenates that are not part of jet fuels and that would cause poor thermal stability and water solubility behavior of the fuels. Hence, it is recommended that the fuel production process be changed to remove these fuel components. In contrast, Candidate fuel 2 exhibited a composition similar to FT-SPKs and would be recommended to proceed into the next phase. Property prediction for properties critical for operability were performed by two complementary models and compared with specification limits and the range of experience when using conventional fuels. It was shown that besides density, which can be resolved by appropriate blending ratios and was in the experience range of approved fuels, all properties satisfy the requirements. This finding was confirmed by adding measurements in the Tier β step of the prescreening. Although the two models applied provided reliable property prediction with associated uncertainties, measurements with industry standards are still advised for systematic derisking. However, at least in one instance (e.g., HOC), it is argued that modeling methods may result in greater precision and potentially greater accuracies lower than presently approved experimental methods for a bulk property, and ASTM D4809 measurements of Candidate fuel 2 exceed the reported ASTM method reproducibility. As a result of this exemplary fuel screening exercise, the fuel producer of Candidate fuel 2 would be advised to scale up fuel volume production. As the production scale is known to influence properties and trace contaminants, the producer should complete another Tier β evaluation before submitting and producing the 400 L required to start the fuel evaluation process. Around this commencement of Tier β evaluations the producer would be advised to initiate a conversation with ASTM.

Future work is recommended to (1) expand the list of properties that can be predicted well in Tier α and measured with non-destructive low-volume Tier β methods, (2) increase the accuracy of predictions via spectral methods (IR/FTIR, UV, and NMR) and other analytical methods (GCxGC), (3) increase the collective accuracies and reliabilities of property estimation/determination techniques of a variety of physical and chemical properties, (4) expand existing property databases to include more diverse feedstock-pathway combinations, and (5) new research on low volume measurement methods ($<$1 mL) that enable direct property determinations are strongly encouraged.

CRediT authorship contribution statement

Joshua Heyne: Conceptualization, Methodology, Software, Formal analysis, Resources, Writing - original draft, Writing - review & editing, Visualization, Supervision, Project administration, Funding acquisition. **Bastian Rauch:** Conceptualization, Methodology, Software, Formal analysis, Resources, Writing - original draft, Writing - review & editing, Visualization, Supervision, Project administration, Funding acquisition. **Patrick Le Clercq:** Conceptualization, Methodology, Resources, Writing - original draft, Supervision, Project administration, Funding acquisition. **Meredith Colket:** Conceptualization, Resources, Writing - original draft, Supervision, Project administration, Funding acquisition.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

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