Research & Development Team
Technical Guidance Document[a]

Prescreening of synthesized hydrocarbons intended for candidates as blending components for aviation turbine fuels (a.k.a. alternative jet fuels or AJF)[b]

INTRODUCTION

The aviation industry's evaluation and qualification process for synthesized jet fuel components, as detailed in ASTM D4054[c] and elsewhere,[1] can involve four tiers of testing, two research reports, and three balloting junctions. This process can be resource-intensive but ensures that any alternative fuel specification approved by the industry outlines the production of safe, fungible Alternative Jet Fuel (AJF) that is compliant with stakeholder demands arising from their insights into the need for such physical and fit-for-use properties. However, this process can span multiple years at significant cost to all parties involved, making mid-course fuel qualification corrections painful to prospective AJF developers. The extensiveness of this process has highlighted 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 jet engine combustor operability, which are among the most expensive testing requirements of the evaluation process. This document identifies prescreening methods that can provide early-stage confidence to fuel developers on whether AJF formulations might encounter downstream challenges with the completion of the ASTM D4054 evaluation process.

These prescreening methods have been developed from learning acquired from the National Jet Fuels Combustion Program (NJFCP),[2] JETSCREEN,[3] prior industry approvals of AJF, and other associated AJF programs. These methods do not replace the ASTM D4054 evaluation process and its requirements. However, results from this prescreening should provide an early assessment of whether serious combustion issues could be encountered in the formal approval process. This could help AJF developers make early decisions on AJF composition or production processes that could help facilitate later approval, either for Fast-Track or Standard approvals (see ASTM D4054 Standard Practice).

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[a] Prepared by members of the National Jet Fuel Combustion Program (NJFCP) and other CAAFI constituents to facilitate the early evaluation of new jet fuel component candidates in conjunction with a potential producers' engagement with the aviation community via CAAFI through their R&D Team. Special thanks to Dr. Joshua Heyne of the University of Dayton for his expertise and commitment to identify and formulate this pre-screening protocol enabling the early assessment of candidate AJF viability.

[b] After completion of the blending requirements of ASTM D7566, and meeting various sustainability criteria, these AJF may also be referred to as drop-in Sustainable Aviation Fuels (SAF), the aviation industry's current consensus naming convention.

[c] ASTM International publication, Standard Practice for Qualification and Approval of New Aviation Turbine Fuels and Fuel Additives.

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 in an AJF's behavior before entering the formal ASTM D4054 process.*[d]
2. *Defining test methods that require minimum volumes of AJF 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 jet engine combustor operability and approval metrics.*

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

ROLE OF AJF PRESCREENING

Prescreening is not a required step in the ASTM D4054 process. Rather, prescreening is a process intended to provide insight to the candidate AJF developer regarding the viability of their proposed AJF as a jet fuel blending component. Prescreening allows the candidate fuel producer to voluntarily test small volumes of fuel for select properties which will provide indicators of the candidate AJF's potential to meet capital intensive D4054 Tier 3 & 4 test requirements. Prescreening does not guarantee the successful completion of the ASTM D4054 process nor ultimate approval by the aviation OEMs and broader jet fuel community. Prescreening may, however, guide a producer towards making improvements to the candidate fuel, thus improving its chances of success in the formal approval process. Results from prescreening may also assist the aviation OEMs in thinking about needs or extensiveness for subsequent Tier 3 & 4 tests.

TARGETED METRICS FOR PRESCREENING

The evaluation of AJF requires that proposed candidate fuel components 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 AJF screened is absent of metals, heteroatoms, or olefins, which are unacceptable in jet fuel.

Given these requirements, the AJF must maintain acceptable properties under extreme conditions, such as maintaining a liquid state with acceptable viscosity under cold conditions and a flash point above the specification limit, up to a proposed blend limit. Additionally, 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 is important from an operability perspective. Any AJF must exhibit acceptable performance within the same envelope as conventional jet fuels. Novel AJF that negatively impact these metrics pose a concern to OEMs for maintaining the certification basis of the engine and aircraft (for operability and performance) as well as safe and efficient aircraft operations, and as such, their desirability

[d] ASTM D4054 requires a producer to deliver approximately 100 gallons neat fuel to enter the Tier 1 and Tier 2 evaluation process.

as a blending component would be either reduced (assuming they will still meet ASTM D7566 and D1655 specification limits following blending), or eliminated from consideration.

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 test fuels evaluated on multiple rigs, are detailed in several publications.[2] In addition, complementary and overlapping AJF are investigated in the EU program JETSCREEN. These JETSCREEN results add to a database on hydrocarbons which are outside of the jet fuel specifications box and contribute to the mapping of jet fuel composition to critical properties and evaluation metrics.

The overarching results of the NJFCP work imply 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 AJF can be avoided by bounding the properties of the AJF within the typical experience of conventional jet fuel. The most important fuel properties for combustor operability are

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

Viscosity, distillation curve, and mass density are well known to be critical properties for combustor performance[e] and are captured in the major jet fuel specifications. Historically, DCN and surface tension have not needed specification requirements as these properties were constrained by the relatively limited compositional variation of jet fuels refined from petroleum. Recently, DCN 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, 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 aviation equipment and infrastructure. AJF formulations, 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. 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 AJF have not encountered issues in these areas.

NEW SCREENING TIERS AS DEFINED FOR EARLY ENGAGEMENT BY FUEL DEVELOPERS WITH CAAFI R&D TEAM

Tier α (Alpha)

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

- GCxGC and GC (ASTM D2887) (~1 mL);

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

- Mid-IR absorption (<100 mL), and;
- NMR (<10mL).

Volume requirements for these tests vary lab to lab but are likely to offer the minimum AJF volume needed of any predictive property testing methodology. GCxGC methods have been documented that have predicted (directly and indirectly) distillation curves, blend limits, operability effects, and vapor pressures of novel AJF. Additional documentation for predictions of viscosity, swelling, freeze point, flash point, density, DCN, and heat of combustion is also available.[4] Moreover, GCxGC analysis is included as part of the official ASTM D4054 evaluation process, including the Fast Track provision (ASTM D4054, Annex A4). Mid-IR methods have been developed to predict 15 different physical and chemical properties, including density, initial boiling point, surface tension, viscosity, and DCN for 64 hydrocarbon fuels.[5] NMR has been shown to predict the chemical properties of a fuel that impact the DCN/ignition quality[6] and has shown the potential to predict the physical properties of a fuel. No Tier α method is currently capable of validating 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. Hence the CAAFI R&D Team proposes that NJFCP and other industry practitioners (e.g. the University of Dayton Research Institute) be involved with such testing and interpretation. At present, these methods enable the lowest AJF volume demands, predict the widest range of characteristics, and have the most promise of the prescreening approaches.

Tier β (Beta)[f]

Entry into the ASTM D4054 process has historically required at least 100 gallons of fuel to be submitted for initial evaluations, of which at least 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 exclusionary attributes were identified. The Tier 1 and 2 property test types listed in Table 1 are recommended as a Tier β prescreening simply because later Tier 3 and 4 tests are sensitive to these properties. The evaluation of the fuels with the listed methods and screening volumes in Table 1 facilitates the direct comparison of candidate AJFs to conventional fuel and previously approved AJFs, minimizing future uncertainties of requisite property compliance, while only consuming less than 500 mL of test AJF.

Table 1: Minimally Recommended Tier β properties

Property	ASTM Test Method*	Approximate Volume Required
Viscosity	D445	20 mL
Distillation	D2887	*GC/Tier α*
Density	D4052	5 mL
Flash Point	D93	50 mL
Surface Tension	D1331A	100 mL
DCN	D6890	250 mL
Swelling**		50 mL

**In an effort to continue lowering volumes required, other methods may be considered, assuming technical validation of efficacy and equivalency – more guidance to follow.*
***Optional test dependent on fuel developer's objectives.*

ENGAGEMENT GUIDELINES: METHODOLGY AND COST

The combined fuel evaluation community (e.g. CAAFI, NJFCP, ASTM D02.J) expects that AJF developers can and should bear the cost of prescreening. It is estimated that these Tier α and β tests as

[f] Although NJFCP initially identified this as Tier Zero, initially thinking this could be a normal step that would occur prior to ASTM D4054 Tier 1, CAAFI will modify the name to Tier β for expediency of combining the concepts of Tier α and Tier β as stand-alone efforts, separate from the D4054 process, primarily used as engagement tools and processes associated with CAAFI R&D work.

well as associated NJFCP-informed implications can be accomplished with less than 500 ml of proposed blending component, and for approximately $10,000. Members of the screening community hope to continue lowering cost and volume as methods are still in development. As has happened in other cases affiliated with AJF development, there may be opportunities where funding can be supported by other entities and other mechanisms (domestic and international),[g] but such has not yet been put into place.

At present, the University of Dayton has graciously agreed to serve as an initial laboratory where this prescreening testing can be accomplished, under the oversight of Dr. Joshua Heyne. The screening community will strive to continue expanding the number of entities who can execute these tests, with the prerequisite that these entities have been able to assimilate the body of knowledge developed within NJFCP that allows for appropriate inferences to be drawn between screening test results and implications for the blending agent of interest. It is likely that this will initially be other institutions who have been affiliated with the work of NJFCP, but the testing can be expanded to other qualified institutions. The NJFCP team will be providing additional guidance on this topic in the coming year, via academic papers, a reference book (currently in development), and subsequent NJFCP reports.

AJF developers can contact the following individuals to initiate discussions on screening, or to initiate testing, including:

CAAFI R&D Team Co-Chairs (via email at R&D@caafi.org):

- Gurhan Andac, GE Aviation
- Joshua Heyne, University of Dayton
- Stephen Kramer, Pratt & Whitney
- Michael Lakeman, Boeing

CAAFI Administrative Leadership Team (via email at info@caafi.org):

- Steve Csonka, CAAFI Executive Director (steve.csonka@caafi.org)
- Peter Herzig, Volpe, CAAFI Program Specialist, R&D Team Liaison
- Kristin Lewis, Volpe, CAAFI Head Research and Technical Advisor, R&D Team Liaison

SUMMARY

While not essential for the approval of a proposed AJF specification, early prescreening of a limited set of properties using the Tier α and Tier β methods outlined herein facilitates confidence in a proposed AJF development path. Furthermore, before the start of formal ASTM D4054 process engagement, it can illuminate approaches for a fuel developer to refine production processes and/or alter feedstocks to maximize the likelihood that an AJF can be qualified by the industry in a timely fashion, and at a reasonable max blend level. Prescreening can also be accomplished with very modest levels of fuel, and at modest cost. These prescreening methods and low volume testing concepts will be periodically updated at https://sites.udayton.edu/alternative-jet-fuel/. Updates could include the adoption of additional screening concepts and methodologies whose development and consideration continues to occur via the work of the NJFCP, JETSCREEN, and others. At appropriate intervals, CAAFI will update this guidance to reflect thinking and recommendations for state-of-the-art screening.

[g] Parties interested in supporting this work with funding should contact CAAFI or the FAA for further discussion of the topic.

ADDENDUM: EXAMPLES OF EVALUATION CRITERIA

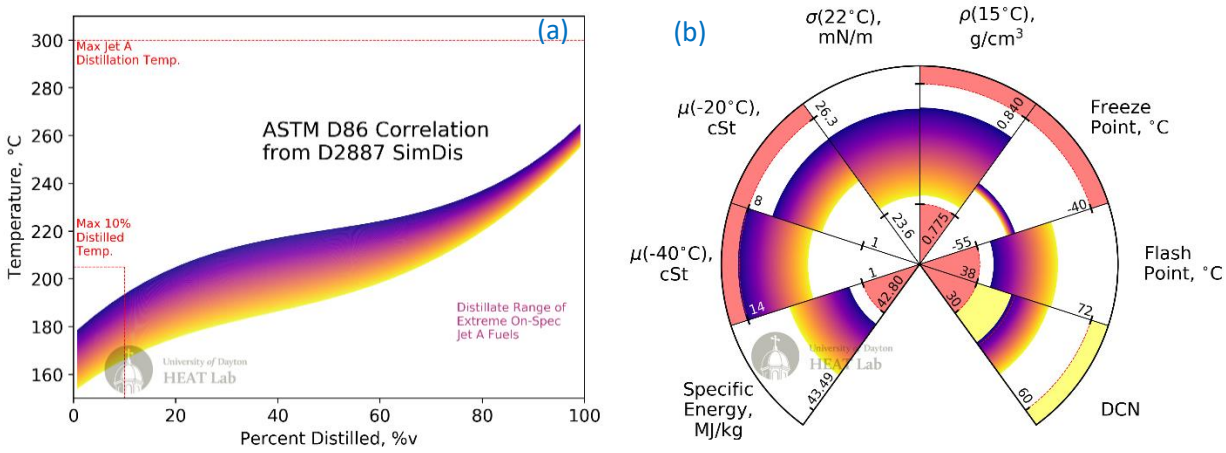

Figure 1: Several key jet fuel metrics, the typical experience range, and specification limits plotted. The experience range of conventional fuels with extreme properties is plotted in the contour filled regions, with purple/yellow illustrating a 'worst'/'best' case limit. In the case of specific specification limits, the red dashed lines represent these hard limits. (a) The range of distillation temperatures for a range of extreme jet fuels with the specification limits plotted in red. (b) The properties of several aviation-focused metrics with extreme AJF candidates.

DISCLAIMER:
This document is not meant to suggest that an AJF developer 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 help facilitate the development of commercially and technically viable AJF.

ACKNOWLEDGMENTS

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