Developing Open-Source Tools for Increasing the Efficiency of Synthetic Aviation Turbine Fuel Certification Process

David Montgomery, Bruce Perry, Shashank Yellapantula, Samah Mohamed, Marc Day, Gina Fioroni, and Robert McCormick

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FuelLib[1] is an open-source Python-based fuel library, developed by NREL, that leverages the group contribution method (GCM) of [1] to systematically estimate the thermodynamic and transport properties of hydrocarbon fuels. FuelLib predicts these properties based on the molecular structure of individual compounds or compound families, using weight percentages of a fuel's composition, typically measured using techniques such as gas chromatography (GC). FuelLib enables property estimation over a wide range of temperatures and pressures of multi-component fuels in the absence of detailed molecular composition data, making it particularly valuable for complex fuel mixtures where detailed experimental characterization of fuel composition is unavailable. These capabilities contribute directly to synthetic aviation turbine fuels (SATF) development, supporting the short-term American Society for Testing and Materials (ASTM) qualification of drop-in fuels while potentially expanding ASTM boundaries to certify a broader range of fuels.

Background

Aircraft engines must deliver large amounts of power with high energy density while operating in harsh conditions, yet also require extremely high system robustness, safety, and reliability. Liquid hydrocarbon fuels remain the only viable energy carrier for commercial aviation, particularly for long distances, high capacities, and higher-speed flight, and are likely to remain so for many years. However, price volatility of conventional jet fuel is a significant drag on the commercial aviation industry [2]. SATF have many potential advantages as a supplement to conventional jet fuel. These fuels enhance energy security by providing an additional domestic source of aviation fuel and could eventually help to insulate against the price volatility of conventional fuels on the global market [3]. The supply chain for production of bio-based fuels promotes economic growth and creates jobs in rural/agricultural communities [4]. SATFs also typically have lower aromatic content than conventional fuel, which reduces the formation of particulate pollutants that are harmful to human health [5]. Gaining regulatory acceptance and certification of neat SATF as a fuel is critical for the U.S. aviation industry both to meet the demand of domestic airlines that wish to use these fuels [6] and for domestic manufacturers to remain competitive on the global market where SATF use is required in many places [7]. For these reasons, scientific research to understand the impacts of synthetic fuels on aviation combustor directly aligns with the goals set out in the first Secretarial Order of the current Secretary of Energy to "unleash American energy at home and abroad to restore energy dominance" and "bolster America's manufacturing competitiveness and supply chain security".

To be certified for commercial aviation in the U.S., fuels must comply with ASTM standards: ASTM D1655 for petroleum-based fuels [8] and ASTM D7566 for SATF [9]. These standards define acceptable ranges for key physical and chemical properties, including density, viscosity, flash point, freezing point, heat of combustion, smoke point, and aromatic content. A fuel that meets all specifications may be certified for drop-in use. To date, eight SATF blends, ranging between blend limits of 5-50% with Jet-A from petroleum, have been certified, but no SATF formulation has been approved for 100% drop-in use without blending. Given the high cost of experimental testing, simulations can play a crucial role in de-risking and reducing cost of certifying SATF candidates.

[1] https://dmontgomerynrel.github.io/FuelLib/

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To support the development and certification of new SATF blends, NREL has developed and maintained multiple open-source tools including the Pele[2] suite of reacting flow simulators and analysis tools [10, 11], and our most recent addition, FuelLib.

Properties of SATFs can have a significant effect on the liquid fuel atomization and vaporization process leading to significant impact on flame stabilization and pollutant formation from aviation gas turbine combustors [12]. Therefore, to assess the potential viability of new SATF pathways through combustor simulations, it is essential to have accurate property prediction capability, despite the fuels being complex mixtures of molecules for which measurements at the relevant conditions may not be practical. FuelLib builds toward a capability based on compositional measurements coupled to the GCM that enables accurate property estimation for new SATF pathways. Figure 1 shows density and kinematic viscosity predictions from FuelLib compared against property measurements at Air Force Research Laboratories (AFRL) and NREL's Fuel characterization laboratory, of three different fuels, petroleum-based Jet-A, SATFs - hydroprocessed esters and fatty acids (HEFA) and Alcohol to Jet (ATJ).

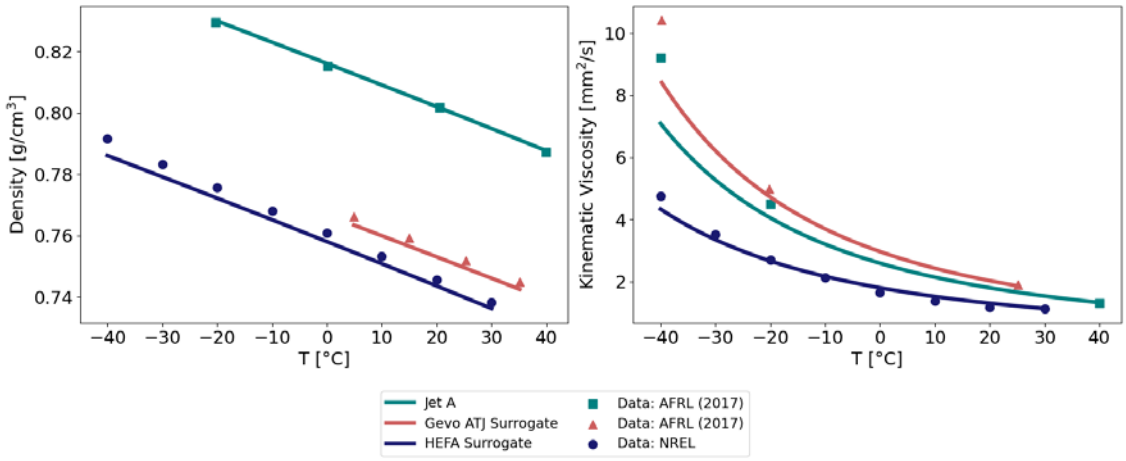

Figure 1: Comparison of property predictions from FuelLib with measurement data from the Air Force Research Lab [13] and NREL's Fuels and Combustion Science team. Plots illustrate differences in density and kinematic viscosity for conventional Jet A fuel and surrogates of ATJ [14] and HEFA-SPK. The symbols are experimentally measured data, and solid lines are FuelLib predictions.

References

1. Constantinou, L., and R. Gani. 1994. "New group contribution method for estimating properties of pure compounds" [in en]. AIChE Journal 40, no. 10 (October): 1697–1710. ISSN: 0001-1541, 1547-5905, accessed July 8, 2024. https://doi.org/10.1002/aic.690401011.

2. Wang, H., and X. Gao. 2020. "Oil price dynamics and airline earnings predictability." Journal of Air Transport Management 87:101854.

3. Shahriar, M. F., and A. Khanal. 2022. "The current techno-economic, environmental, policy status and perspectives of sustainable aviation fuel (SAF)." Fuel 325:124905.

[2] https://amrex-combustion.github.io/index.html

This report is available at no cost from the National Renewable Energy Laboratory (NREL) at www.nrel.gov/publications

4. Martinez-Valencia, L., M. Garcia-Perez, and M. P. Wolcott. 2021. “Supply chain configuration of sustainable aviation fuel: Review, challenges, and pathways for including environmental and social benefits.” Renewable and Sustainable Energy Reviews 152:111680.

5. El Helou, I., J. M. Foale, R. S. Pathania, R. Ciardiello, A. W. Skiba, and E. Mastorakos. 2023. “A comparison between fossil and synthetic kerosene flames from the perspective of soot emissions in a swirl spray RQL burner.” Fuel 331:125608

6. Smith, P., M. Gaffney, W. Shi, S. Hoard, I. I. Armendariz, and D. Mueller. 2017. “Drivers and barriers to the adoption and diffusion of Sustainable Jet Fuel (SJF) in the US Pacific Northwest.” Journal of Air Transport Management 58:113–124.

7. Panoutsou, C., S. Germer, P. Karka, S. Papadokostantakis, Y. Kroyan, M. Wojcieszyk, K. Maniatis, P. Marchand, and I. Landalv. 2021. “Advanced biofuels to decarbonise European transport by 2030: Markets, challenges, and policies that impact their successful market uptake.” Energy Strategy Reviews 34:100633.

8. ASTM International. 2024a. ASTM D1655-24: Specification for Aviation Turbine Fuels. West Conshohocken, PA. https://doi.org/10.1520/D1655-24B.

9. ASTM D7566-24: Specification for Aviation Turbine Fuel Containing Synthesized Hydrocarbons. West Conshohocken, PA. https://doi.org/10.1520/D7566-24D

10. Esclapez, L., M. Day, J. Bell, A. Felden, C. Gilet, R. Grout, M. Henry de Frahan, E. Motheau, A. Nonaka, L. Owen, et al. 2023. “PeleLMeX: An AMR low Mach number reactive flow simulation code without level sub-cycling.” Journal of Open Source Software 8 (NREL/JA-2C00-85410). https://doi.org/10.21105/joss.05450.

11. Henry de Frahan, M. T., L. Esclapez, J. Rood, N. T. Wimer, P. Mullowney, B. A. Perry, L. Owen, H. Sitaraman, S. Yellapantula, M. Hassanaly, et al. 2024. “The Pele Simulation Suite for Reacting Flows at Exascale.” In Proceedings of the 2024 SIAM Conference on Parallel Processing for Scientific Computing (PP), 13–25. SIAM. https://doi.org/10.1137/1.9781611977967.2

12. Nadakkal Appukuttan, S., B. Perry, S. Yellapantula, L. Esclapez, H. Sitaraman, and M. Day. 2023. Simulations of fuel-air mixing in a 7 element lean direct injection (LDI) aviation combustor. Technical report. National Renewable Energy Laboratory (NREL), Golden, CO (United States). https://www.osti.gov/biblio/1995457.

13. Edwards, J. T. 2017. “Reference Jet Fuels for Combustion Testing” [in en]. In 55th AIAA Aerospace Sciences Meeting. Grapevine, Texas: American Institute of Aeronautics / Astronautics, January. ISBN: 978-1-62410-447-3, accessed January 17, 2025. https://doi.org/10.2514/6.2017-0146. https://arc.aiaa.org/doi/10.2514/6.2017-0146.

14. Luning Prak, D. J., M. H. Jones, P. Trulove, A. M. McDaniel, T. Dickerson, and J. S. Cowart. 2015. “Physical and Chemical Analysis of Alcohol-to-Jet (ATJ) Fuel and Development of Surrogate Fuel Mixtures” [in en]. Energy & Fuels 29, no. 6 (June): 3760–3769. ISSN: 0887-0624, 1520-5029, accessed January 17, 2025. https://doi.org/10.1021/acs.energyfuels.5b00668.

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