International Conference on Numerical Combustion
Rome, Italy, October 14-17, 2025
www.icnc2025.com

Supporting Sustainable Aviation Fuels (SAFs) Design and Certification via the *BayeSAF*-based Multi-Fidelity Modeling Framework

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Institutions and regulatory agencies have set ambitious targets for achieving mid-century carbon neutrality. As the demand for air transport is expected to double by 2040, Sustainable Aviation Fuels (SAFs) emerge as the near-term solution for decarbonizing commercial aviation. In this context, our research group developed a numerical framework based on the MATLAB©-implemented BayeSAF algorithm [1], designed to formulate surrogate mixtures that replicate the physicochemical properties of candidate SAFs leveraging Bayesian inference and Global Sensitivity Analysis (GSA), and meant to support fuel design and pre-screening by facilitating robust numerical analyses of SAF vaporization and combustion. By way of example, the statistical description of SAF surrogates' composition might drive uncertainty quantification (UQ) in reduced-order models (ROMs) for droplet vaporization [2]. Furthermore, the formulation of ad-hoc oxidation mechanisms through our recent development of the MC-HyChem methodology [3] fosters the multi-fidelity investigation of SAF properties' effect on combustor figures of merit (FOM), from low-dimensional reactors to computational fluid dynamics (CFD).
In this contribution, we illustrate a comprehensive characterization of the alcohol-to-jet C1 POSF-11498 to demonstrate the potential of the BayeSAF-based framework. Relying on a database of 992 chemical species based on experimental measurements and descriptors-based machine learning (DB-ML), a surrogate fuel composed of two highly-branched C_{12} and C_{16} iso-paraffins is formulated via the BayeSAF algorithm. Furthermore, experimental measurements of pyrolysis product evolution and ignition delay times support the development of a 130-species MC-HyChem reaction mechanism capturing high- and low-temperature chemistry. Finally, the impact of C1's distinctive physicochemical traits — such as its bimodal distillation curve — is assessed in: (i) a 0D vaporization model accounting for surrogate composition uncertainty via deep long short-term memory (LSTM) recurrent neural networks; (ii) a lab-scale swirled spray flame combustor using a multi-mixture-fraction Flamelet-Progress Variable (FPV) approach to capture preferential vaporization effects.

References

[1] *Liberatori, J. et al.. BayeSAF: Emulation and Design of Sustainable Alternative Fuels via Bayesian Inference and Descriptors-Based Machine Learning.* Fuel (under Review).

[2] *Liberatori, J. et al.. Deep learning-based forward UQ on Bayes-informed sustainable aviation fuel surrogates: a case study on bio-jet fuel vaporization.* International Journal of Heat and Mass Transfer (under Review).

[3] *Blandino, M. et al.. Multicomponent HyChem Kinetic Mechanism Generation Using Trust-Region Bayesian Optimization.* MCS13 Corfu, Greece, June 1–5, 2025.