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

Modeling Sustainable Aviation Fuels via a hybrid Machine Learning - Functional Group Mechanism (FGMech) Approach

Qiren Zhu[1]*, Sirio Brunialti[1], Qi Wang[1], Xiaoyuan Zhang[2], S. Mani Sarathy[1]
*lead presenter: qiren.zhu@kaust.edu.sa
[1] Clean Energy Research Platform (CERP), Physical Science and Engineering (PSE) Division, King Abdullah University of Science and Technology (KAUST), Thuwal, 23955-6900, Saudi Arabia
[2] Department of Thermal Science and Energy Engineering, University of Science and Technology of China (USTC), Hefei, 230026, China

The aviation industry contributes significantly to climate change, not only through CO_2 emissions but also via non-CO_2 effects such as contrail formation, together accounting for approximately 3.5% of total current radiative impact on climate [1]. As pressure mounts to decarbonize the sector, sustainable aviation fuels (SAFs) have emerged as promising alternatives to conventional aviation fuels such as Jet A-1, offering substantial reductions in life-cycle carbon emissions. However, accurately predicting their combustion behavior remains challenging, particularly when integrating detailed fuel kinetics into computational fluid dynamics (CFD) models due to the complexity and size of traditional mechanisms.

This work introduces a hybrid AI-physics framework based on the Functional Group Mechanism (FGMech) approach [2,3] to develop compact lumped kinetic models for both SAFs and conventional jet fuels. FGMech describes real fuels using surrogate species that reflect the functional group distribution of the actual fuel. Oxidative pyrolysis sub-mechanisms are generated using Mamox++ [4], a tool that automates mechanism development for large hydrocarbons, and are further enriched with published data to expand a kinetic database. This database is then used to train neural networks that correlate fuel functional group profiles with pyrolysis product distributions.

The study focuses on three representative SAFs—a Fischer-Tropsch fuel, a hydrotreated esters and fatty acids (HEFA) fuel, and an alcohol-to-jet (AtJ) fuel—alongside conventional Jet A-1. The combined model is validated against ignition delay times, laminar burning velocities, and species data, shows good agreement with experiments across jet engine-relevant conditions. The resulting AI-enhanced FGMech approach improves the prediction of reaction rates, thermodynamic properties, and transport coefficients, enabling fast, scalable, and accurate simulation of SAF combustion, with minimal reliance on detailed fuel-specific characterization.

References

[1] Lee, D. S. et al. Uncertainties in mitigating aviation non-CO2 emissions for climate and air quality using hydrocarbon fuels. Environmental Science: Atmospheres 3, 1693-1740 (2023).
[2] Zhang, X., Yalamanchi, K. K. & Sarathy, S. M. A functional-group-based approach to modeling real-fuel combustion chemistry – I: Prediction of stoichiometric parameters for lumped pyrolysis reactions. Combustion and Flame 227, 497-509 (2021).
[3] Zhang, X. & Sarathy, S. M. A functional-group-based approach to modeling real-fuel combustion chemistry – II: Kinetic model construction and validation. Combustion and Flame 227, 510-525 (2021).
[4] Brunialti, S., Zhang, X., Faravelli, T., Frassoldati, A. & Sarathy, S. M. Automatically generated detailed and lumped reaction mechanisms for low- and high-temperature oxidation of alkanes. Proceedings of the Combustion Institute 39, 335-344 (2023).