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

Artificial intelligence-driven design of sustainable aviation fuels

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The global aviation sector is under increasing pressure to reduce its carbon footprint, with sustainable aviation fuels (SAFs) emerging as a critical enabler of decarbonization. Yet, the conventional development and certification of SAFs remain constrained by protracted experimental procedures and high costs associated with ASTM D4054 and D7566 evaluations [1]. To address this challenge, we propose an artificial intelligence (AI)-based framework for the rapid design and screening of novel SAF mixtures that meet both performance and regulatory criteria. This framework integrates a graph neural network (GNN) architecture capable of predicting a comprehensive set of SAF-relevant properties—including energy density, flash point, viscosity, density, freezing point, and more—directly from molecular composition. The GNN leverages molecular graph representations to learn chemically meaningful features [2], outperforming traditional descriptor-based models in accuracy and generalizability across diverse molecular classes relevant to SAF development.

To capture the complex behavior of real-world fuel blends, the model incorporates a mixing operator [3] approach that combines learned latent representations of individual molecules according to their relative composition. This enables accurate prediction of mixture-level properties while accounting for non-linear effects such as azeotropy, intermolecular interactions, and synergistic reactivity—phenomena often overlooked by simple additive mixing rules.

Beyond forward prediction, the platform includes a latent space search algorithm for inverse design. Given a target set of properties—such as adequate cetane number, low freezing point, and optimized density—the system performs multi-objective optimization to identify novel candidate mixtures that satisfy the specified performance envelope. These formulations are scored using merit functions aligned with ASTM specifications, enabling data-driven prioritization of the most promising blends for experimental validation.

By fusing predictive modeling with generative design, this AI-powered framework enables high-throughput exploration of the SAF formulation space, reducing the dependency on exhaustive empirical testing. It represents a scalable tool for accelerating SAF discovery and supporting the aviation industry's transition toward more sustainable, certifiable fuel solutions.

References

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