Bayesian Inference for the Development of Conventional and Alternative Jet Fuel Surrogates

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Abstract
The endorsement of mid- and long-term climate neutrality policies by governments and other institutions in the last decade strengthens the ambition to identify sustainable alternatives to fossil fuels for any category of transportation systems. In this context, the aviation industry is one of the most impacted sectors, with precise climate neutrality targets to be achieved by mid-century. One potential solution for transitioning towards a low-carbon future is blending conventional and alternative jet fuels. Among the latter sustainable aviation fuels (SAFs) constitute the most practical way forward, given their "drop-in" nature, with their use being expected to increase in the coming years. However, the impact of unusual physical and chemical properties of SAFs may deeply impact the performance and operability of engines, e.g., in terms of altitude relight, lean blow-out, and cold start. In this respect, adequate characterization of alternative jet fuels is a necessary step toward the application of large-scale computational fluid dynamics (CFD) aimed at assessing the performance of SAF-fueled combustion devices. Thus, several approaches have been proposed to formulate surrogate fuels that emulate the physicochemical properties of real hydrocarbon mixtures. These strategies typically hinge on genetic optimization algorithms, which address objective functions combining specific fuel properties, e.g., the liquid-phase viscosity and the cetane number, and provide a single optimal surrogate composition. In the present work, we illustrate a novel strategy that resorts to the Bayesian inference framework to statistically characterize the possible surrogate fuel composition based on available experimental data, the intrinsic uncertainty of which is naturally considered. Moreover, the Bayesian framework fosters employing polynomial chaos expansion (PCE) representations of the major chemical observables, e.g., the ignition delay time, characterizing the real fuel, which could not be easily incorporated into standard optimization algorithms. This way, a comprehensive probability description of the surrogate composition is returned instead of a single set of optimal components' proportions and paves the way toward the cost-effective use of ad-hoc surrogate mixtures in CFD codes.