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Manifold-based modeling of Sustainable Aviation Fuel combustion: An inherently multi-phase, multi-component model

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Advancing state-of-the-art, computationally efficient modeling is absolutely critical in accelerating the development, certification, and implementation of Sustainable Aviation Fuels (SAFs). Particularly critical will be modeling approaches that make minimal assumptions about how the fuel burns in order to understand how even small differences in composition between SAF and petroleum-derived fuels could influence engine performance, stability, and emissions.

In addition to the broader challenges of modeling turbulent reacting turbulent flows, SAFs present the additional complexities of multi-phase, multi-component fuels. Efficient modeling of single-phase combustion can be achieved through utilization of manifold-based models, in which the thermochemical state is mapped onto a reduced number of manifold variables, with state-of-the-art approaches now able to accommodate complex, multi-modal combustion processes [1]. With manifold-based models, the flow solver transports far fewer variables, and the thermochemical information is computed, stored, and referenced externally, effectively decoupling the computations of flow and chemistry. This approach has been proven successful for single-phase applications, but attempts to extend it to multi-phase combustion make oversimplified assumptions that neglect critical multi-phase phenomena. The classical approach to computing the thermochemical state accounts for the liquid phase by simply reducing the fuel temperature, effectively ignoring relevant phase change physics and treating the liquid as an equivalent enthalpy gas [2].

In this work, a physically-derived approach to manifold-based spray modeling is developed. A set of boundary conditions for a spherically-symmetric vaporizing droplet is derived in manifold coordinates to exactly describe the gaseous composition at the droplet surface. An exact formulation for the mixture fraction dissipation rate profile is also derived to close the manifold equations. With two additional inputs—droplet radius and droplet surface temperature—the manifold model predicts a more physically accurate thermochemical profile compared to the traditional approach. Furthermore, the multi-phase combustion model provides as outputs the droplet vaporization and heating rates, which are quantities typically obtained from empirical expressions. The model is validated against Direct Numerical Simulation studies of spherically symmetric *n*-heptane droplets. Additionally, the approach is extended to capture multi-component droplet vaporization and combustion through the consideration of additional mixture fractions for each fuel component. Finally, differential diffusion effects, consideration of multi-modal combustion, and proposed implementation into Large Eddy Simulation are discussed.

References

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