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Direct Numerical Simulation of a Multicomponent Alcohol-to-Jet Fuel Droplet Cloud Autoignition

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Spray combustion plays a key role in various industrial and transportation systems, including diesel engines and aircraft combustors. In light of increasingly strict regulations on greenhouse gas (GHG) emissions, sustainable aviation fuels (SAFs) have emerged as the most practical short-term pathway for decarbonizing aviation. These bio- and e-fuels exhibit distinct physicochemical properties compared to conventional kerosene-based jet fuels, making it crucial to investigate their combustion behavior, particularly in view of increasing the blending ratio beyond the current 50% limit. A widely used test case to study the interplay between droplet evaporation and autoignition in practical systems is the combustion of a droplet cloud in a hot environment [1]. In this work, a numerical experiment of this nature is adopted to assess how the preferential evaporation characteristics of the alcohol-to-jet (ATJ) C1 POSF-11498 influence the combustion mode of the droplet cloud. To this end, a Direct Numerical Simulation (DNS) of a droplet cloud in a quiescent, atmospheric-pressure environment has been carried out using a two-component C1-surrogate composed of two highly-branched C_{12} and C_{16} iso-paraffins [2]. The numerical framework accounts for differential diffusion and evaporation effects, and employs Adaptive Mesh Refinement (AMR) to resolve the flame structure while ensuring that the Δ/d_p ratio remains above the dilute regime threshold, where Δ is the grid size and d_p the droplet diameter. The results reveal the development of a distinct combustion mode, deviating from the single- and two-stage ignition modes found in literature for single-component fuels. As the more volatile C_{12} component begins to evaporate, a flame front forms at the outer edge of the droplet cloud and propagates inward. Owing to the bimodal distillation curve of C1, the residual droplets, depleted of C_{12}, continue to evaporate in the surrounding hot environment, releasing the heavier C_{16} iso-paraffin. The low cetane number of C1 inhibits the formation of a cool flame typically associated with two-stage ignition. Instead, localized flame fronts are observed around droplets actively evaporating C_{16}, indicating a heterogeneous combustion mode. When compared to the autoignition of n-heptane clouds under the same initial conditions, C1 exhibits significantly longer ignition delay times τ_{ign}, which could compromise the reliability of aeronautical engines by increasing the risk of local extinctions or blow-off events during operation.

References

[1] *Zhou, H. & Liu, Y. External group combustion of droplet clouds under two-stage autoignition conditions.* Combustion And Flame. ***234*** *pp. 111689 (2021)*

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