Multi-Fidelity Numerical Simulations of a Swirled Turbulent Spray Flame: Impact of Chemical Reaction Modelling

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Abstract
Aviation, before COVID-19, was responsible for 2.5 - 4% of the total CO_2 emissions and recent projections report that the demand for air transport is expected to double by 2040 [1]. In this scenario, Sustainable Aviation Fuels (SAFs) represent the solution in the near-term, since their adoption does not require any modification of existing propulsive systems. Therefore, numerous experimental campaigns based on the SAF surrogates defined by the National Jet Fuels Combustion Program (NJFCP) have been conducted, offering a basis for evaluating the physical and chemical properties of SAFs [2]. Experimental investigations carried out with laboratory-scale burners with jet-engine combustors-like conditions and spray injectors are essential to understanding the flame dynamics and the interaction between the liquid droplets, the turbulent flow field, and combustion phenomena. Aiming at the same purpose, Computational Fluid Dynamics (CFD) can be employed to analyze the wide range of alternative fuels, exploiting the reduced time requirements and versatility with respect to experimental testing. The authors present a comprehensive analysis of the effects of the chemical reaction modelling on the n-heptane spray flame of the Cambridge burner [3]. Firstly, adopting an Eulerian-Lagrangian numerical framework, both the URANS and LES model are compared to the experimental data. Thus, the efficacy of the well-established Flamelet-Generated Manifold (FGM) model is examined. To take into account the droplet evaporation phenomenon and its coupling with the gaseous phase, non-adiabatic flamelets are employed in the tabulation process. Results revealed an optimal alignment with experimental data regarding flame topology for both the URANS and LES models. Finally, a finite-rate chemistry approach is investigated. The computational expense associated with using the same chemical mechanism used for flamelet tabulation would be excessive. Hence, a mechanism reduction driven by Computational Singular Perturbation (CSP) is proposed. This reduction specifically focuses on the Low-Temperature Chemistry (LTC) pathway, which is indicative of the spray-flame interaction, as well as multi-regime combustion in the lab-scale burner under consideration. Research on numerical simulations with finite-rate chemistry is currently underway.

[1] IATA, “Global outlook for air transport: highly resilient, less robust”, 2024
[2] Edwards, J., “Reference jet fuels for combustion testing”, AIAA, 2017.
[3] Yuan R., Kariuki J., Mastorakos E. , “Measurements in swirling spray flames at blow-off”, Int. J. of Spray and Comb. Dyn. 10.3, 2018.