Numerical investigation of soot production in a two-phase gas turbine combustor model

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Spray combustion remains a major challenge in the development of cleaner and more efficient energy systems due to the complex interactions between spray dynamics, turbulence, combustion, and pollutant formation. This study focuses on n-heptane turbulent spray combustion and soot emissions in the atmospheric, non-swirled Coria Rouen Spray Burner (CRSB) [1], a configuration characterized by a dual reaction zone structure: an outer laminar diffusion flame and an inner wrinkled, partially premixed flame that is susceptible to local extinction. Extending previous work [2], which showed that large-eddy simulations (LES) with tabulated chemistry can capture unsteady extinction events, this study incorporates a more detailed chemical mechanism including polycyclic aromatic hydrocarbons (PAHs) to enable soot predictions via a sectional method.

The numerical results show good agreement with experimental data for both gas- and liquid-phase statistics, including mean and root-mean-square quantities. The predicted flame lift-off length is also consistent with measurements. Soot formation is found to be dominated by surface growth reactions, with peak source terms exceeding PAH condensation rates by at least two orders of magnitude. The current results indicate that the predicted soot volume fraction field extends over a wider region than observed experimentally, with the peak located further upstream. This study also evaluates the impact of solving a dedicated transport equation for pyrene, the PAH species used for nucleation and condensation in this work, as a means to capture its slower evolution compared to major species [3].

References

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