Mass-Consistent Manifold Modeling for Large Eddy Simulation of Turbulent Sooting Flames

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Large Eddy Simulation (LES) combined with reduced-order, manifold-based combustion models represents a computationally efficient approach to turbulent reacting flows. Reduced order, manifold-based combustion models project the thermochemical state onto a low-dimension manifold, which can be solved independently from the flow solver. Manifold-based models have been extended to a variety of complex, multi-physics reacting flows including soot evolution in turbulent flames. In sooting flames, an additional consideration is the coupling of the soot with the gas phase. Previous manifold models for sooting flames, e.g. [1], have considered the consumption of Polycyclic Aromatic Hydrocarbons (PAH) since this consumption rate only depends on the gas phase and can be computed in the manifold model a priori without knowledge of soot, which is computed during the LES. However, these approaches have neglected the gas-phase source terms for species participating in soot surface chemistry, notably acetylene, since these rates depend on soot, which is not known when the manifold equations are solved. Neglecting to account for changes in the gas-phase concentration of these other species violates mass conservation and could lead to inaccurate soot volume fraction predictions (e.g., via overprediction of acetylene). This effect is expected to be more pronounced in conditions with higher soot loading, such as in aircraft combustors, where these gas-phase sources are expected to be larger.

In this work, a fully mass-consistent manifold model is developed for turbulent sooting flames. The approach relies on In-Situ Adaptive Manifolds (ISAM) [2], in which necessary manifold solutions are computed on-the-fly and stored with ISAT for reuse. ISAM allows for an increase in the dimensionality of the manifold model (i.e., more inputs) without excessive memory or precomputation requirements. For non-adiabatic, nonpremixed turbulent sooting flames, in addition to inputs to ISAM of the mixture fraction dissipation rate and a heat loss parameter, the soot surface area, evaluated locally from LES, is incorporated into the manifold solution to allow for the addition and removal of species from the gas phase due to soot surface reactions. Closure of these gas-phase source terms within the manifold model is consistent with the underlying presumed subfilter PDF for soot [3]. The Sandia ethylene-air turbulent nonpremixed piloted jet flame, as described in [4], is simulated with both the new fully mass-consistent manifold model and the traditional approach that considers only the removal of PAH from the gas phase in order to evaluate the impact of mass consistency.

References

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