Pareto-efficient combustion modeling for extinction prediction in LES of a piloted partially premixed NH3/H2/N2-air turbulent jet flame

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Ammonia is an appealing carbon free fuel alternative for energy production and industrial burners due to its mature production and storage capability, high hydrogen density, and ability to be cracked into hydrogen through in-situ pyrolysis or catalysis. However, NH3/H2 fuel blends have been observed to exhibit significantly different dynamics in turbulent environments due to localized diffusion and preferential consumption. Extinction events remain difficult to accurately predict. The fundamental behavior of turbulent ammonia flame extinction must be understood to enable analysis driven design of future ammonia combustors. Large-eddy simulation (LES) is used to simulate ammonia combustion. Using a flamelet-progress variable (FPV) model, the LES is shown to reasonably predict global flame behavior. However, there are large deviations in local temperature and ammonia slip in the extinction regions compared to experiments. To address this with a reasonable computational cost, the Pareto efficient combustion (PEC) framework is implemented, combining an FPV approach with local dynamic assignment of finite rate chemistry to study extinction behavior in highly turbulent and strained flames. LES-PEC is used to predict turbulent partially premixed 40:45:15 NH3/H2/N2 piloted jet flames at Reynolds numbers of 24,000 and 36,000, corresponding to 59% and 89% of the extinction Reynolds number, respectively.