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Modeling local extinction and differential diffusion in turbulent ammonia-hydrogen jet flames using principal component transport

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Partial cracking of ammonia (NH_3) into hydrogen (H_2) and nitrogen (N_2) improves flame stability in carbon-neutral combustion systems by mitigating NH_3's inherently low reactivity. However, modeling turbulent NH_3/H_2/N_2-air jet flames at high Reynolds numbers remains challenging due to complex extinction dynamics and the insufficiently understood role of differential diffusion. Recent joint experimental–numerical investigations of the KAUST piloted flames [1], presented at the TNF workshop, revealed persistent discrepancies, including over-predicted flame height, inaccurate radial decay of the mixture fraction, and under-prediction of local extinction.

To address these challenges, we propose a reduced-order large eddy simulation (LES) framework that integrates principal component (PC) transport with deep neural networks (PC-DNN). Thermochemical states and source terms are projected onto a reduced PC basis and regressed using DNNs, which are trained on counterflow diffusion flame data. Retaining only the first two PCs captures over 99% of the total variance, significantly reducing computational cost while preserving predictive fidelity.

Differential diffusion is explicitly modeled using a VARIMAX-rotated PC basis, derived from mixture-averaged transport counterflow simulations. This rotation yields a diagonally dominant diffusion matrix, enabling accurate species-specific transport modeling. In addition, the combustion subgrid-scale closure is incorporated through a presumed β-PDF under the assumption of statistical independence of the PCs. Through *a priori* analysis of direct numerical simulation (DNS) data from a temporally evolving NH_3/H_2/N_2-air jet flame with detailed chemistry and transport, we demonstrate that the assumption of PCs independence is appropriate, as the PCs—being inherently uncorrelated by definition—exhibit significantly weaker statistical dependence in the combustion zone compared to traditional flamelet-based approaches using mixture fraction and progress variable pairs.

Validation against high-resolution experimental data from Tang et al. [1], including Raman/Rayleigh scattering and NH_2/OH-LIF diagnostics, confirms that the PC-DNN model with VARIMAX-enhanced diffusion treatment satisfactorily captures key flame features, including temperature, species concentrations, and extinction/reignition behavior. Compared to unity-Lewis-number models, this framework significantly improves local extinction predictions, provides new insight into differential diffusion effects, and advances reduced-order modeling of ammonia-based turbulent combustion.

References

[1] Tang, H., Barlow, R., and Magnotti, G., Local extinction in piloted turbulent partially premixed ammonia/hydrogen/nitrogen-air jet flames. *Proc. Combust. Inst.*, 40 (2024) 105472.