Manifold modeling of tangential diffusion effects in lean ammonia/hydrogen/nitrogen-air premixed flames

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Partially cracked ammonia is a promising hydrogen-carrying fuel with logistical advantages compared to pure hydrogen. Ammonia/hydrogen/nitrogen-air premixed flames can be thermodiffusively unstable under fuel lean conditions. These instabilities affect the flame propagation speeds as well as the local formation of nitrogen oxides and nitrous oxide. To assess the viability of partially cracked ammonia as a zero-carbon fuel, understanding and modeling these pollutants in thermodiffusively unstable flames is critical. In previous work [1], detailed two-dimensional simulations of laminar premixed flames were conducted to understand the development of thermodiffusive instabilities in flames of ammonia/hydrogen/nitrogen mixtures and air. The degree of ammonia cracking was varied to understand the influence of fuel composition on the instability behavior and subsequent formation of nitrogen oxides and nitrous oxide. The databases from these detailed simulations were used to evaluate a premixed manifold model in progress variable that includes differential diffusion and flame curvature effects [2]. Manifold models significantly decrease computational cost by mapping the high-dimensional thermochemical state to a lower-dimensional manifold. With the existing formulation, the premixed manifold model cannot accurately predict these pollutants in these flames. Strong differential diffusion effects leading to significant diffusive transport in the direction orthogonal to the progress variable gradient, so-called tangential diffusion, are responsible for this model failure. Analysis of the diffusive fluxes showed that direct tangential diffusion effects are strongest for highly cracked fuel mixtures, and both the radical pool and pollutant species are impacted. Even in the less cracked mixtures, there is a non-negligible direct effect of tangential diffusion on important radicals, which indirectly effects the pollutant species, and explains the model failure at both high and low cracking ratios.

In this work, these detailed simulations are used to extract the tangential diffusion terms and quantify how they depend on progress variable and its dissipation rate and curvature. Based on these results, a general, explicit model is developed for tangential diffusion effects. This model is implemented in a premixed manifold solver and evaluated against the detailed simulation databases. With this explicit model for tangential diffusion, both direct and indirect effects of tangential diffusion are captured by the manifold model, without having to resort to a mixture fraction variable to account for indirect tangential diffusion effects, leaving such a variable available for modeling other phenomena.

References

[1] S. L. Rzepka, K. VanderKam, M. E. Mueller, Tangential diffusion effects in thermodiffusively unstable ammonia/hydrogen/nitrogen-air laminar premixed flames (2025) submitted.
[2] M. E. Mueller, Physically-derived reduced-order manifold-based modeling for multi-modal turbulent combustion, Combust. Flame 214 (2020) 287-305.