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Reduced chemistry development for numerical combustion and topological analysis of hydrogen-blended ammonia flame

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Growing interest in reducing carbon emissions from hard-to-decarbonize sectors has increasingly turned scientific community interest toward zero-carbon fuels like ammonia (NH_3) and hydrogen (H_2). Hydrogen blended with ammonia improves the fuel's flammability but significantly influences nitrogen oxide (NO_x) emissions. The combustion behavior of ammonia—especially in mixtures with hydrogen—is notably complex due to the broad range of time scales involved. Oxidation reactions occur in about 0.1 milliseconds, whereas DeNOx processes can take several seconds in large-scale furnaces. This complexity presents major difficulties in creating kinetic models for computational fluid dynamics (CFD) that can reliably represent all relevant reaction pathways with a limited amount of species and reactions.

In this study, two simplified chemical mechanisms (RmAH-1 and RmAH-2) were developed from a detailed kinetic model (C3MECHV3.3[1] from NUI Galway) through ORCh [2] and implemented in direct numerical simulations (DNS) of reactive mixing layer. These mechanisms were generated using the Directed Relation Graph with Error Propagation (DRGEP) method and a Genetic Algorithm (GA) to refine reaction rate parameters and improve predictions. The models share 19 chemical species and 75 reactions, though they differ in the specific rate constants used.

This work highlights how a methodical optimization strategy—applied across a series of 0D and 1D benchmark scenarios, potentially involving turbulent mixing—can lead to the creation of reliable and efficient reduced kinetic models. The study is furtherly validated with 2D high-fidelity simulations of turbulent NH_3/H_2-air mixing layers, providing useful information on accuracy and computational stiffness. These simulations highlight the critical role of hydrogen as a flame enhancer, with ignition dynamics largely governed by its rapid diffusion toward the air stream. This fast diffusion significantly influences both flame initiation and stabilization. Detailed analyses of differential diffusion effects and flame anchoring were also performed, revealing the formation of unique and complex structures in the stabilization region. These findings underscore the strong coupling between fuel composition, transport properties, and combustion dynamics in ammonia-hydrogen systems.

References

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