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Numerical Simulation of Combustion Dynamics and NOx Emissions in NH_3/CH_4/Air Flames Using Integrated Detailed Chemistry and Flamelet-Generated Manifold

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ABSTRACT

Ammonia/methane (NH_3/CH_4) flames have emerged as a promising pathway toward achieving a sustainable, carbon-free energy economy. This study presents a detailed numerical investigation into the combustion and emissions characteristics of ammonia-methane blends in a swirl burner, focusing on understanding the effects of varying ammonia doping ratios (%NH_3) on flame dynamics and pollutant formation. The chemistry of the combustion process is comprehensively addressed utilizing a detailed mechanism, featuring 957 reaction steps and 128 species, integrated within the flamelet generated manifold (FGM) model framework. The analysis evaluates ammonia doping ratios (%NH_3) ranging from 20% to 50% at equivalence ratios (φ) of 1.0 and 1.2. The results indicate that ammonia doping has a negligible effect on the overall flow field, including velocity distributions and recirculation zones. However, it profoundly influences combustion and emissions characteristics. As the ammonia fraction increases, the peak flame temperature decreases due to ammonia's lower heat release rates and reduced flame speed. For instance, a 20% ammonia blend at an equivalence ratio of 1.0 achieves a peak flame temperature of 2207 K, which drops to 2167 K when the ammonia content is increased to 50%. This flame temperature reduction significantly impacts the flame's thermal structure and downstream pollutant formation. Carbon-based emissions, such as carbon monoxide (CO) and carbon dioxide (CO_2), show a substantial decline as ammonia content increases. For example, a 40% ammonia blend reduces the peak CO mass fraction by 32.25% compared to a 20% blend at an equivalence ratio of 1.0. This reduction is attributed to the lower carbon availability in the fuel blend, which inherently limits the formation of carbon-based pollutants. Nitrogen oxides (NOx), including NO, N_2O, and NO_2, exhibit a more complex behavior with increasing ammonia content. At an equivalence ratio of 1.0, NOx emissions increase by 9.46% when the ammonia fraction rises from 20% to 30%, driven by enhanced thermal and prompt NO formation mechanisms. However, as the ammonia content is further increased to 40%, NOx emissions decrease by 3.72%, attributed to lower flame temperatures and shifts in chemical pathways that suppress NO formation. Among all tested cases, the highest NOx emissions are consistently observed at a 30% ammonia blend with an equivalence ratio of 1.0. These findings underscore the significant challenge posed by NOx emissions in achieving environmentally sustainable ammonia combustion. To address this issue, advanced combustion strategies, such as rich-lean two-stage combustion and extended residence times, are proposed.