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INSIGHT INTO NH₃ FORMATION CHARACTERISTICS AT RICH CONDITIONS IN 70/30 VOL% NH₃/H₂ FLAMES

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Abstract

Recent studies have highlighted that in fuel blends with a 70/30 vol% ratio of ammonia/hydrogen, the ratio of final to initial mole fractions of NH₃ is notably high. This finding underscores the importance of comprehensive understanding of the product gases, especially the residual NH₃, in NH₃/H₂ laminar flames. Such understanding is critical for designing NH₃-fueled combustors to comply with the stringent emission regulations. Understanding of the underlying chemistry in the oxidation of NH₃/H₂ mixtures is a pivotal factor for the flexible utilization of these mixtures in various applications, including propulsion systems and power generation. In this context, the current work investigates 70 kinetic reaction mechanisms from the literature in atmospheric conditions. This study aims to evaluate the effectiveness of these mechanisms in predicting the mole fraction of unburned NH₃ in a volumetric fuel mixture of 70% NH₃ and 30% H₂. The findings revealed that the Lamoureux kinetic model yielded reliable estimations of the unburned NH₃ within the equivalence ratio (ϕ) range of 1-1.2. However, its accuracy decreased around 1.4 of ϕ . Notable variations were observed in the reaction steps and rate parameters among these tested mechanisms. Predominantly, NH₃ was converted to NH₂ radicals through reactions with OH across all temperatures, with a secondary role played by O radicals at low to intermediate temperatures. At higher temperatures, NH₃ dehydrogenation also occurred via H radicals, as evidenced in the NH₃+H \rightleftharpoons NH₂+H₂ reaction. Additionally, at the combustion exit, NH₃ regeneration was primarily driven by the NH₃ \rightleftharpoons NH₂+H reaction at a temperature of 504 K.