INSIGHT INTO NH_3 FORMATION CHARACTERISTICS AT RICH CONDITIONS IN 70/30 VOL% NH_3/H_2 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 NH_3 is notably high. This finding underscores the importance of comprehensive understanding of the product gases, especially the residual NH_3, in NH_3/H_2 laminar flames. Such understanding is critical for designing NH_3-fueled combustors to comply with the stringent emission regulations. Understanding of the underlying chemistry in the oxidation of NH_3/H_2 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 NH_3 in a volumetric fuel mixture of 70% NH_3 and 30% H_2. The findings revealed that the Lamoureux kinetic model yielded reliable estimations of the unburned NH_3 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, NH_3 was converted to NH_2 radicals through reactions with OH across all temperatures, with a secondary role played by O radicals at low to intermediate temperatures. At higher temperatures, NH_3 dehydrogenation also occurred via H radicals, as evidenced in the $NH_3+H \rightleftharpoons NH_2+H_2$ reaction. Additionally, at the combustion exit, NH_3 regeneration was primarily driven by the $NH_3 \rightleftharpoons NH_2+H$ reaction at a temperature of 504 K.