

The sensitivity of the choice of chemical mechanism for Direct Numerical Simulation based analysis of NH₃/H₂ premixed turbulent flames

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The necessity of reducing greenhouse gas emissions has increased the importance of power generation using carbon-free fuels. Although H₂ is often identified as the fuel for the future, its wide flammability range, high ignitability and storage pose practical problems. In this respect, NH₃ has a better potential as an alternative fuel because of its higher volumetric energy density and the relative ease of its storage in comparison to H₂ [1]. Moreover, there is a well-established existing infrastructure for producing, storing, and transporting NH₃ due to its application in agriculture as a fertiliser. However, NH₃-air mixtures are significantly less reactive than H₂-air mixtures, exhibiting narrower flammability limits and lower laminar burning velocities. As a result, NH₃-air premixed flames are more susceptible to blowout and are more difficult to stabilize in practical combustion systems. To address these issues, NH₃ is often partially cracked to produce NH₃/H₂/N₂ mixtures or blended with H₂ generated via electrolysis. The addition of H₂ enhances the mixture's burning velocity, helping to mitigate the challenges posed by the inherently low reactivity of NH₃. As the use of NH₃ for combustion applications is relatively new in comparison to H₂ and hydrocarbon fuels, it is necessary to assess the sensitivity of the choice of the chemical mechanism in high-fidelity simulations of premixed turbulent combustion of NH₃/H₂ fuel blends. In order to address this objective, Direct Numerical Simulations of statistically planar turbulent premixed flames of NH₃/H₂/N₂ fuel blend with mole fraction ratio 40:45:15 have been considered for equivalence ratios 0.8 and 1.2 for two different chemical mechanisms [2,3]. One of these mechanisms was proposed by Stagni et al. [2] and consists of 31 species and 203 chemical reactions, whereas the other chemical mechanism, developed by Greenblatt et al. [3], includes 22 species and 104 chemical reactions. The DNS data has been analysed to assess the sensitivity of choice of the chemical mechanism on flame surface area, turbulent burning velocity, mode of combustion, heat release rate contribution by different species and production of NO_x and N₂O. Based on this exercise, it will be assessed whether the increased accuracy achieved from transporting additional species and utilising a more detailed model of chemical processes inherent to the larger mechanism outweighs the substantial computational efficiency and the significant saving in compute time when using the smaller mechanism.

References

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