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Effects of differential diffusion and reaction in premixed turbulent combustion of NH3/H2/N2 blends

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The concept of NH3 as a potential fuel source has been endorsed to facilitate fuel transition in the power generation and propulsion sectors in the framework of a net-zero economy and meet increasingly strict pollution control regulations [1]. However, the reactivity of NH3 is comparatively low, and thus pure NH3-air flames are prone to blow-off. Therefore, NH3 alone is often not directly suitable for reliable industrial operations. This aspect can be improved through the catalytic production of H2 via partial thermal decomposition from waste heat to form an NH3/H2/N2 mixture. The effects of the differences in reactivity and diffusion characteristics between NH_3 and H_2 in globally lean, premixed turbulent flames of NH_3/H_2 fuel blends have been analysed using a Direct Numerical Simulation (DNS) database from statistically planar turbulent flames [2]. Two fuel mixtures were analyzed—60% NH_3 / 25% H_2 / 15% N_2 and 40% NH_3/45% H_2/15% N_2—both with an equivalence ratio of 0.81, within the thin reaction zones regime. Variations in chemical reactivity and differential diffusion between NH_3 and H_2 result in local fluctuations in equivalence ratio throughout the flame, leading to significant deviations in species distribution compared to one-dimensional (1D) laminar premixed flames. The increased H_2 content in the 40% NH_3/ 45%H_2 blend intensifies differential diffusion effects, giving rise to locally stoichiometric or even fuel-rich zones despite the overall lean condition. This also promotes localized diffusion-mode combustion—primarily involving H_2 in the 60% NH_3/25% H_2 /15% N_2 blend and NH_3 in the 40% NH_3 / 45% $H_2$15% N_2 blend. The transition from lean premixed to non-premixed combustion at the trailing edge of the flame causes misalignment among the isosurface normals of NH_3, H_2, and temperature, thereby affecting the reaction–diffusion balance. The displacement speed of the H_2 isosurface surpasses that of NH_3, leading to differing effective normal strain rates, which along with equivalence ratio variation influences the behaviour of the scalar gradient magnitude. These results underscore the importance of accounting for variable equivalence ratios and non-premixed combustion modes in numerical models of NH_3/H_2 premixed flames, even under globally lean conditions.

References

[1] H. Kobayashi, A. Hayakawa, K.D.K.A. Somarathne, E.C. Okafor, Science and technology of ammonia combustion, Proc, Combust. Inst., 37, 109-133, 2019.
[2] R. Khamedov, M. R. Malik, F.E. Hernandez-Perez, H.G. Im, Propagation characteristics of lean turbulent premixed ammonia–hydrogen flames, Proc. Combust. Inst. 40, 105736, 2024.