A DNS STUDY OF TURBULENT PREMIXED AMMONIA-AIR FLAMES

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Abstract

In the current energy transition process, *ammonia* (NH_3) is gaining momentum as a fuel for carbon-free combustion, owing to properties such as high bulk energy density, relatively simple storage if compared with pure hydrogen (H_2), and a global developed economy. Still, given its toxic and corrosive nature, and its unfavorable combustion properties, research is needed to make it a feasible solution [1]. As part of the PRIN PNRR 2022 *"Reactant"* Project, the present work proposes a numerical study to characterize the combustion properties of perfectly premixed NH_3 (pure or doped with H_2) flames when submitted to Homogeneous Isotropic Turbulence (HIT). First, few recent detailed reaction mechanisms [2-3] are compared with an experimental dataset to select the most suitable scheme to predict NH_3/air laminar combustion properties, i.e., laminar flame speed (Fig. 1) and adiabatic flame temperature. Then, an Analytically Reduced Chemistry (ARC) version of the selected mechanism is used in the high-fidelity CFD code AVBP (https://www.cerfacs.fr/avbp7x/) to perform Direct Numerical Simulations (DNS) of a turbulent 3D stochiometric flat ammonia flame, a canonical configuration commonly adopted in the literature [4]. Preliminary results (Fig. 1) show hydrogen preferential diffusion on positively wrinkled regions, impacting local equivalence ratio, Heat Release Rate (HRR) and NO_x concentration. Multiple turbulence levels ranging from low to high Karlovitz numbers will be investigated in the future.

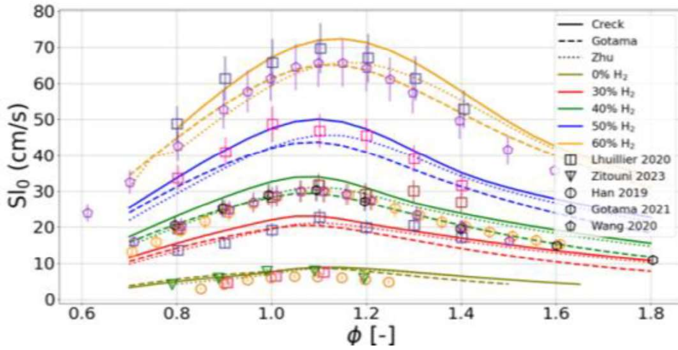

Figure 1. Flame speed for different schemes and comparison with experiments.

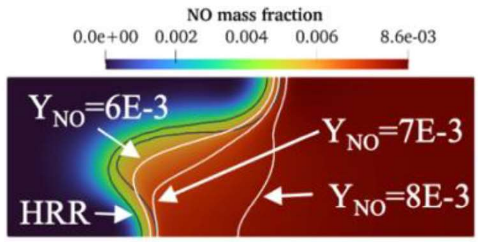

Figure 2. NO mass fraction for ($70\%NH_3+30\%H_2$)/air flame at $\phi = 1$ (HRR = 1.9 GW/m^3).

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