Nitrogen Oxides Chemical Pathway Identification in a Partially Premixed NH_3-H_2 Swirled Flame

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Abstract

The mechanisms of NO_x formation in a partially premixed ammonia-hydrogen swirled flame with differentiated fuel injection are investigated using Large Eddy Simulations (LES). Ammonia is first injected perfectly premixed with air, and hydrogen injected 4 cm upstream of the burner lips, resulting in a flame with heterogeneous fuel composition. Four operating points corresponding to distinct equivalence ratios were examined maintaining a fixed global fuel composition of 70/30 (vol.) NH_3/H_2 blend at 288 K and atmospheric pressure. The swirled flames were studied experimentally obtaining NO Planar Laser Induced Fluorescence (PLIF) measurements and OH* chemiluminescence imaging. The study employed the multi-fuel thickened flame (MF-TFLES) turbulent combustion model along with the NH3H2N2_15_211_5_HV reduced mechanism for ammonia-hydrogen flames. The effect of the equivalence ratio on NO_x formation was thoroughly analyzed and the contribution of distinct nitrogen oxide formation path in each case was quantified.

Introduction

The ubiquitous need to decarbonize the current energy mix and mitigate carbon dioxide emissions in transport applications underscores ammonia as a viable alternative to fossil fuels, particularly in sectors such as power generation through gas turbines. Employing ammonia-hydrogen blends combines the advantages of ammonia's efficient transport and storage with the high reactivity of hydrogen. However, the combustion of these blends can result in the formation of nitrogen oxides (NO_x), including NO and NO_2, both toxic to human health, but also N_2O, a highly potent greenhouse gas (GHG) with a global warming potential (GWP) that is 273 times greater than that of CO_2. Thus, managing nitrogen oxides emissions is critical to mitigate their adverse effects on climate and public health. The Cardiff burner with differentiated fuel injection [1] is used to investigate the effect of the equivalence ratio on the NO_x formation chemical pathways in an ammonia-hydrogen swirling flame. The study investigated, experimentally and numerically, four different operating conditions while keeping all parameters constant but setting the equivalence ratio to 0.65 (TP01), 0.8 (TP03), 1.0 (TP05), and 1.2 (TP07).

Experimental and Numerical Setup

The flames' topology is first experimentally studied by collecting OH* chemiluminescence signals and NO PLIF images. More information on the experimental setup can be found in previous studies on the Cardiff burner [1]. The compressible solver AVBP (www.cerfacs.fr/avbp7x/) was used to perform 4 reactive Large Eddy Simulations (LES) corresponding to the previously mentioned operating points. The modeling strategy presented in our previous work [2], consisting of the MF-TFLES turbulent combustion model and the NH3H2N2_15_211_5_HV chemical kinetics model, was employed in all simulations. Indeed, this approach is particularly well-suited for flames with differentiated fuel injection due to its ability to accurately capture local variations in equivalence ratio and fuel composition that are critical for the correct parameterization of the turbulent combustion model. The significance of heat losses was accounted for through the implementation of a Heat Resistivity Tuning (HRT) approach [3] with reference temperature profiles retrieved during the experimental campaign.

Reactive LES Validation

The validation of numerical predictions against experimental measurements is presented in Fig. 1, comparing the heat release rate (HRR*$\mathcal{F}$) with OH* chemiluminescence signals. The normalization by $\mathcal{F}$ ensures proper comparison of heat release rate distributions across all operating conditions. Both HRR* $\mathcal{F}$ and OH* fields are self-normalized to enable qualitative comparison of flame structure.

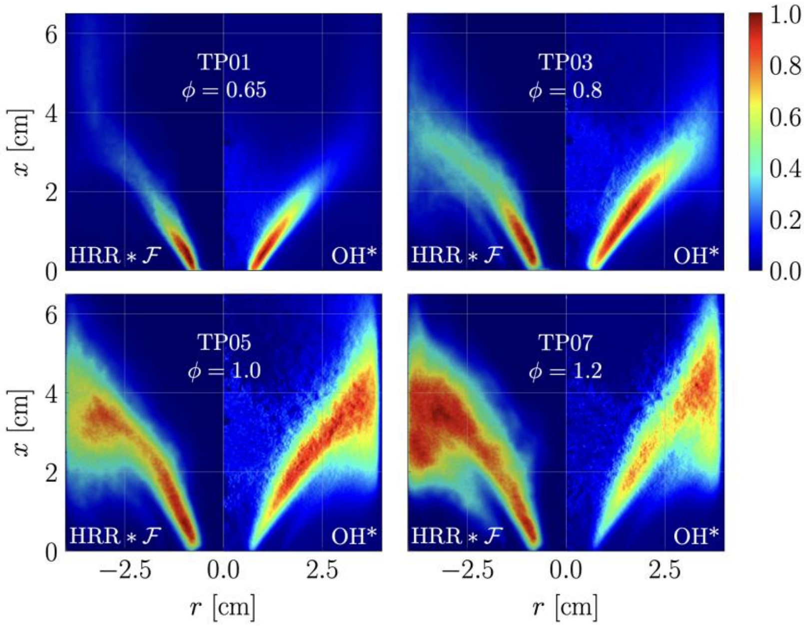

Figure 1. Comparison between numerical heat release rate (left half) and experimental OH* chemiluminescence (right half).

NO_x Production Pathway Analysis

The relative importance of various NO production pathways is illustrated in Fig. 2, showing the NO formation rates for major submechanisms across the four test points.

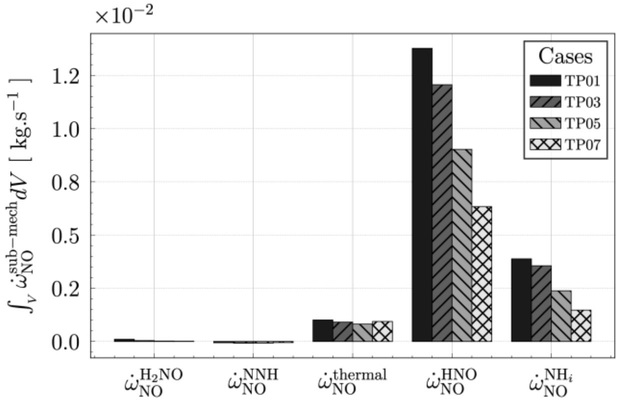

Figure 2. Contribution of the major NO production submechanisms.

Conclusion

A joint experimental and numerical study was conducted on NH_3/H_2 swirling flames, including a parametric study of four operating points with varying equivalence ratios. The Cardiff burner with differentiated fuel injection was employed for the study. Flame topology was successfully validated by comparing predicted fields to OH* chemiluminescence data. Once validated, the modeling approach allowed retrieval of the contributions from different NO production chemical submechanisms for each operating point studied. The most active submechanisms were the two fuel-NO pathways: the HNO and NH_i routes. While thermal NO was present, it contributed only a small percentage to overall NO production.

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