Experimental and numerical study of the structure of $NH_3/H_2/O_2/Ar$ flames at elevated pressures

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Transition to the carbon-free fuels is one of the most important problems for modern energetics. Despite hydrogen use can mitigate the zero-carbon target its direct application in transportation systems is associated with problems of fire and explosion safety. Hydrogen carriers, for example, ammonia are considered as a prospective solution. Unlike hydrogen the infrastructure of ammonia storage, transportation and distribution is well established and has many years of experience. Nevertheless, pure ammonia has poor combustion properties, which can be improved by hydrogen addition. Moreover, hydrogen can be produced via ammonia cracking.

The scope of the present work was to obtain new experimental data on the structure of $NH_3/H_2/O_2/Ar$ flames (φ=0.8, 1.0 and 1.2) at 4 and 6 atm and to compare them with numerical results obtained using four published mechanisms (Models).

For flame structure measurement molecular beam mass-spectrometric setup with soft electron impact ionization was used. Flames were stabilized on the flat burner (T_0=368K). For high-pressure measurements, the burner was placed at the chamber pressurized with N_2. Temperature profiles were measured using thin S-type thermocouples with a diameter of 0.03 mm. PREMIX code from CHEMKIN package was used for numerical modeling. The comparison with experimental data revealed that recently developed Model 4 [1] has the best predictive capability.

Ammonia molecule has fuel-bonded nitrogen, which inevitably enhances NO_x formation. Both experimental and numerical data showed that NO is mainly present in the post-flame zone while concentration of N_2O and NO_2 is negligible. Moreover, the transition to rich blends reduces NO concentration in the post-flame zone as well as peak-concentration of NO, N_2O and NO_2. The pressure increase has the same effect on NO_x concentration. Model 4 showed good agreement for NO mole fraction profile, however, for N_2O and NO_2 larger discrepancies are observed. Numerical analysis indicated that N_2O and NO_2 mainly form from NO. Thus, the NO- submechanism needs to be refined.

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