The flame structure of ammonia/hydrogen/oxygen/argon blends at 4 and 6 atm

Ksenia Osipova [1,2], Artëm Dmitriev[1,2], Oleg Korobeinichev[1], Andrey Shmakov[1,2]

[1] Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, 3, Institutskaya str., Novosibirsk, Russia, 630090

[2] Novosibirsk State University, 2, Pirogova str., Novosibirsk, Russia, 630090

k.n.osipova23@gmail.com

One of the key problem of the modern energy systems is the transition to zero-carbon fuels. Hydrogen is the most perspective one. However, the application of pure hydrogen due to its specific properties inevitably encounters the problems of fire and explosion safety. The use of hydrogen carriers, in particular, ammonia, enables to solve these problems. Ammonia has well established infrastructure of its storage, transportation and distribution. Nevertheless, ammonia has high ignition energy and ammonia/air flames have very low burning velocity. The addition of hydrogen could improve ammonia combustion properties. Moreover, hydrogen can be produced via ammonia decomposition.

The aim of the present work is to obtain new experimental data on the flame structure of ammonia/hydrogen/oxygen/argon blends with different stoichiometry (φ=0.8, 1.0 and 1.2) at the pressure of 4 and 6 atm and to compare experimental results with numerical data obtained with four published chemical kinetic mechanisms (Models).

The experiments on the flame structure at elevated pressures were performed using molecular beam mass-spectrometric setup with soft electron impact ionization. Flames were stabilized on the flat burner. The burner temperature was 368K throughout the experiment. The burner was placed at high-pressure chamber. Nitrogen was used to maintain the pressure value. Temperature profiles were measured with thin S-type thermocouples made from the wire with a diameter of 0.03mm.

Numerical simulations were performed using PREMIX code from CHEMKIN package. The comparison of experimental and numerical data showed that the Model 4 recently developed in the work [1] showed the best predictive capability.

One of the key problems of the potential application of ammonia is fuel-nitrogen, which enhances NOx formation. The experimental data showed that the main nitrogen-containing species, which are present in the post-flame zone are N_2 and NO whereas concentration of N_2O and NO_2 is negligible. The analysis showed that the transition to rich fuel blends is more effective in terms of reduction of NO concentration in the post-flame zone as well as peak-concentration of NO, N_2O and NO_2. The pressure increase also results into the decrease of NO concentration in the post-flame zone as well as the decrease of NO, N_2O and NO_2 peak mole fractions.

The obtained data showed that mole fraction profile of NO is described well with the Model 4. However, there are larger discrepancies for N_2O and NO_2 peak mole fraction is significantly overpredicted. Numerical analysis revealed that N_2O and NO_2 form from ammonia molecule via NO. Thus, to improve the agreement of experimental and numerical data for N_2O and NO_2 it is necessary to refine rate constants of reactions involving NO.

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References

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