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Can chemiluminescence be used as preferential diffusion indicator in partially cracked ammonia flames on a Bunsen burner?

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Ammonia as a fuel has become a topic of wide interest in recent years, aligning with initiatives on mitigating carbon-based emissions. Despite its potential as a fuel for spark-ignition engines due to certain beneficial properties, the laminar flame speeds of ammonia-air mixtures are notably low. It is often combined with hydrogen to overcome some unwanted properties of both fuels when employed independently. Since every mole of ammonia contains 3 moles of H atom, it is often considered as hydrogen carrier. Researchers have come up with a solution to use the best of both fuels by partially cracking ammonia to have mixtures of ammonia/hydrogen/nitrogen. As the cracking percentage changes, the blended fuel properties differ. There are multiple methods to crack ammonia, including thermal, thermo-chemical, and catalytic cracking, all of which can yield hydrogen. There is a wealth of literature available on measuring various parameters such as flame speed, flame stretch, NO_x emissions, and chemiluminescence for ammonia/hydrogen flames. The presence of hydrogen in the initial mixture significantly modifies the diffusive transfers. Coulon et al. (1) show the preferential diffusion of H₂ and H especially in highly curved flames via DNS. Another DNS study (2) highlighted the effect of the preferential diffusion of H atoms on NO production.

The main objective is to identify markers that would indicate the presence of preferential diffusion. Additional goals encompass the qualitative use of chemiluminescence to assess NO_x levels and to investigate the chemistry of NO_x formation as the radical pool alters when the composition of the fresh gas mixture changes. Spectroscopic measurements are recorded to compare NO* quantities and to establish correlations with other excited species and NO_x (from simulations) NH₂* has been identified as an indicator of preferential diffusion for pure ammonia-air flames. It has been noted that ammonia decomposes into hydrogen which diffuses faster than the fresh gas mixture leading to a local enhanced reactivity. It was also found that for those flames whose $Le > 1$, negative curvature tends to promote hydrogen production leading to increased local reactivity and vice versa. For cracked premixed ammonia-air flames, both NH₂* and OH* have been selected as potential tracers. Zhu et al.(3) suggest OH* as a substitute for NO in very lean to stoichiometric ammonia-hydrogen-air flames. The experiments were performed at $\phi = 1.1$ for a cracking percentage of 0-40% leading to χ_{H_2} in fuel (ammonia + hydrogen) of 0-0.5 on a Bun-

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sen burner at atmospheric conditions. The mixtures were diluted with an excess of nitrogen to stabilize these flames once it was established that the addition of nitrogen didn't affect the point of preferential diffusion. Upon diluting the mixtures, the intensity and thickness of the excited species changed as the flame temperature decreased. Identical patterns were observed in both NH_2^* and OH^* inverse Abel-transformed 2D images. A shift in the local intensity along the flame contour was observed at the same point for both species, with this transition point being dependent on the fresh gas mixture. Finally, a 1D profile of both species was extracted for the different cases and compared with a 1D simulation using Ansys Chemkin. Both the simulation and experimental profiles of the species showed an increase in intensity and narrower profiles (low FWHM) when the fresh gas had a higher hydrogen content. The intensity of both NH_2^* and OH^* decreased with an increase in thickness as the content of H_2 dropped. As the flame temperature rises (with higher hydrogen content in fresh gases), the probability of collisions also increases, leading to an increase in the quantities of both species. Simulations also revealed that the non-excited state of both species increases with the rise in hydrogen content. This high concentration also explains the trend observed in the case of the excited species. Emission spectroscopy was also performed for the UV-VIS range and it was observed that the emission spectra of NO^* increased as the emission of both OH^* and NH_2^* increased. On probing into NO , N_2O , and NO_2 concentrations as provided by the simulations, it was seen that as the mole fraction of H_2 increases, the concentration of these species also increases.

In summary, as the hydrogen content in the fresh gas increased, the excited species (NH_2^* and OH^* , NO^*), non-excited species (NH_2 , OH , NO , N_2O , and NO_2) all increased, as observed in both the experiment and simulation.

References:

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