Experimental and simulated OH and NO mole fraction profiles in low-pressure ammonia flames

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Motivations and Objectives

- ❑ As NH_3 is a carbon-free fuel, it is envisaged as combustible, mostly for marine engines since they can operate in a wide range of fuel composition from heavy-petrol to ammonia
- ❑ NH_3 is a poor fuel (low LBV, high ignition *T*) and requires to be blended with conventional hydrocarbons, or hydrogen to maintain the advantage of carbon-free blends
- ❑ NO_x are expected to be emitted at high levels compared to hydrocarbons
- ❑ But detailed kinetic models have been mostly validated against Laminar Burning Velocities (LBV), Ignition Delay Times (IDT), while only few experimental species data are reported in literature
  - Flame structures in Ar diluted mixtures were performed by MBMS at low-pressure (Duynslaegher et al. ProCI32(2009), CF159(2012)), at atmospheric pressure (Osipova et al. IJHE46(2021))
  - Recent works reported in JSR apparatus in temperature range (700-1300K), (Zhang et al. CF234(2021), Tang et al. CF240(2022), Osipova et al. Fuel310(2022), Manna et al. CF(2022) in press)
  - The synergic effects between NH_3 and H_2 still require to be examined

• NO and OH profiles have been measured in low-pressure flames using in situ Laser Induced Fluorescence (LIF) and Absorption techniques

• Effect of H_2 addition on NO formation

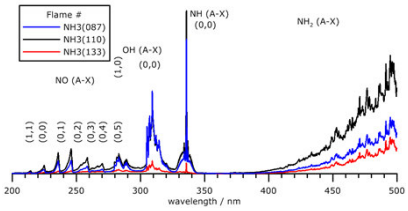
Experimental approaches

Low-Pressure McKenna Burner

- Laminar premixed flames $NH_3/O_2/N_2$ (Φ = 0.87, 1.10, 1.33), dilution 24% with N_2, and $NH_3/H_2/O_2/N_2$ (10%H_2, Φ = 0.87, 40%N_2)
- Stainless-steel burner vertically mobile
- Low-pressure chamber at p = 10 kPa

Flame #	NH_3	H_2	O_2	N_2
NH3(087)	1.07		0.92	0.64
NH3(110)	1.23		0.84	0.64
NH3(133)	1.29		0.73	0.64
NH3-10H2(087)	1.16	0.13	1.07	1.58

Emission spectra @ 9 mm



Laser Diagnostics

frequency-doubled seeded Nd:YAG laser pumping a tunable dye laser

- at around 615 nm providing after doubling wavelengths around 307.5 nm,
- At around 572 nm providing 225 nm wavelength after doubling and mixing with the residual IR of the Nd:YAG,

T and OH quantification using Single-pass absorption

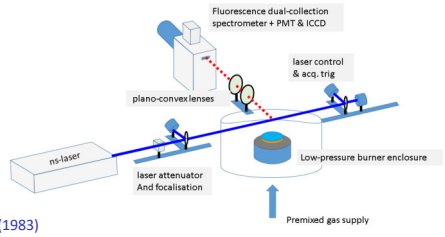
- OH absorption (single-pass) along the line $R_2(7)$ at 307.01 nm
- Integrated spectral absorption to determine the absolute density of OH
- Scan of absorption spectra to determine the absolute temperature from Boltzmann plot

A-X(0,0) OH LIF

- LIF excitation of OH along the line $R_{21}(7)$ at 306.53 nm,
- Fluorescence detection at 309 nm (BP 3 nm) of the Q-branch of the (0-0) vibrational band of OH, to prevent the collection of the excited wavelength

NO LIF

- LIF excitation of NO along the line A-X(0,0) $Q_2(26.5)$ at 225.58 nm,
- Fluorescence detection at 245 nm (BP 9 nm) of the A-X(0,2) band
- WIP; calibration from previous measurements performed in a CH_4 flame at p=10.6 kPa using NO addition method (Lamoureux et al., EF35(2021))

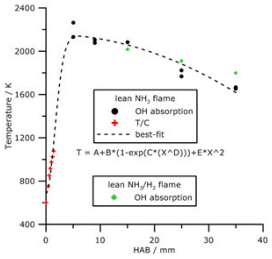


- Strong absorption in the UV due to NH_3 as mentioned by Chou et al. in JCP 78, 5962 (1983)

Results

Temperature determination

- The temperature in the burnt gases area is determined from the OH absorption spectra with respect to the Boltzmann plot
- The onset of the temperature increase close to the burner surface is measured using type-K thermocouple
- Performed in the lean NH_3 flame only (WIP)

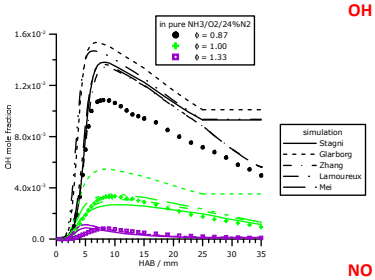


OH and NO profiles using LIF

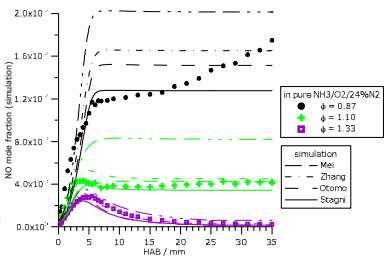
- The maximum mole fraction of both NO and OH decreases with the increase of the equivalence ratio
- The shape of the OH mole fraction profiles is similar in all studied flames
- With the H_2 addition, a slight increase of OH and NO is observed
- In the lean NH_3 flames, the NO profiles increase in the burned gases up to 1.8% in mole fraction
- In the near stoichiometric NH_3 flame, the profile of NO remains flat in the burned gases
- In the rich NH_3 flame, the NO profile presents a peak value (0.3%) and decreases close to 0 in the burned gases

In $NH_3/O_2/N_2$ flames

OH profiles

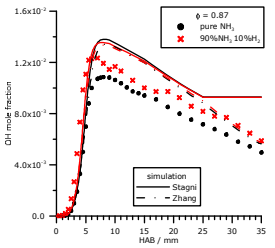


NO profiles

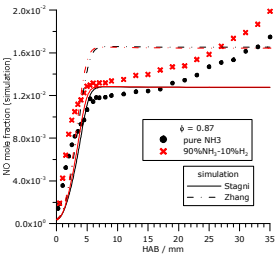


H_2 addition

OH profiles



NO profiles



Simulation of OH and NO profiles using different detailed kinetic models

- 5 kinetic models have been used with Chemkin-Pro software to simulate the 4 flames **but** considering the same temperature profile (measured in the lean NH_3 flame only)
- Calculations indicate a strong NH_3 consumption at the burner surface
- Globally, the OH experimental species profiles are well predicted by the 5 models
- The comparison between the predicted NO profiles and the experimental ones shows that :
  - In the lean NH_3 flames (with and w/o H_2) the predicted NO profiles remain flat in the burned gases contrary to the increase observed experimentally
  - In the near stoichiometric flame, 2 of the examined models predict well the small hump of the NO profile around 5 mm (Stagni, Zhang)

References

Lamoureux, CF163(2016)
Glarborg et al., PECS67(2018)
Meiet al., CF210(2019)
Stagniet al., React. Chem. Eng5(2020)
Zhang et al., CF234(2021)

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