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Chemical Flame Structure Analysis of Laminar Premixed Ammonia and Ammonia/Hydrogen Flames

Analyse de la Structure Chimique des Flammes d'Ammoniac et d'Ammoniac/Hydrogène Prémélangés Laminaires

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Abstract

With the continuous rise in the global carbon emissions and the ongoing global warming, several regulations such as the Paris Agreement have been adopted worldwide to achieve carbon neutrality by 2030/2050. To meet these goals, significant reductions in greenhouse gas (GHG) emissions are required across all sectors, including transportation, energy production, and industry. Among these sectors, maritime transport is recognized as a major contributor to global CO_2 emissions, accounting for nearly 3% of the total anthropogenic output. In response, the International Maritime Organization (IMO) has implemented a series of regulations to reduce the carbon intensity of international shipping. Achieving these targets requires adopting alternative low/zero-carbon fuels capable of replacing conventional fossil-based marine fuels.

One promising emerging candidate is ammonia (NH_3) due to its carbon-free composition, high hydrogen content, and relatively mature production and storage technologies. While ammonia combustion does not produce CO_2, it presents other challenges, notably the formation of nitrogen oxides (NO_x), which are potent air pollutants contributing to acid rain and ozone depletion. To minimize NO_x emissions, a thorough understanding of ammonia's combustion chemistry is essential. This can be achieved through chemical kinetic models validated against a wide range of experimental data, including both global combustion parameters such as laminar burning velocity and ignition delay time, and speciation measurements obtained in well-characterized reactors like jet-stirred reactors, flow reactors, and burner-stabilized flames (BSF).

While extensive datasets exist for many of these configurations, there remains a significant lack of BSF data for NH_3 and NH_3/H_2 mixtures in the literature. Such data are crucial, as BSFs provide valuable insights into the chemical flame structures under a variety of conditions. To address this gap, the present thesis work focuses on providing a new reliable dataset of speciation measurements in laminar premixed $NH_3/O_2/N_2$ and $NH_3/H_2/O_2/N_2$ flat flames at low pressure (10 kPa). In the context of this study, temperature and species profiles (NO, OH, NH, and H_2O) were measured using in-situ (calibrated Laser-Induced Fluorescence) and ex-situ (using Fourier Transform Infrared Spectroscopy) laser diagnostic techniques. Five different flames were investigated, covering a range of equivalence ratios (0.87, 1.1, 1.3) and ammonia/hydrogen blends (0-10%) to explore their effect on NH_3 oxidation and NO_x formation.

The obtained experimental species profiles were then compared to simulations of different detailed kinetic models available in the literature. A satisfactory agreement between the experimental and simulated profiles was observed. Using the best performing model (Mei_2021), a detailed pathway analysis was conducted to elucidate the main reactions controlling ammonia oxidation, NO formation, in addition to the effect of hydrogen addition. The results presented in this study provide a dataset that can be used to validate and refine the literature chemical kinetic mechanisms of ammonia oxidation. Such validated models are indispensable for the design and optimization of next-generation ammonia combustion systems, enabling the safe and efficient utilization of ammonia as a marine fuel an-d supporting the transition towards carbon-neutral maritime transport. This work is a contribution to the ANR-SIAC (ANR-22-CE50–0022) project, and is funded by the LabEx CaPPA (ANR-11-LABX-0005–01) and ADEME (Agence de la transition écologique).

Keywords: Ammonia, combustion, laminar premixed flames, laser diagnostics, laser-induced fluorescence, NOx emissions, kinetic modeling