International Conference on Numerical Combustion
Rome, Italy, October 14-17, 2025
www.icnc2025.com

Comprehensive numerical investigation of detailed NH_3 and NH_3/H_2 combustion kinetic mechanisms: testing and development

Szanthoffer AG[1,2,*] , Papp M[1], Nagy T[3], Turányi T[1]
* andras.gyorgy.szanthoffer@ttk.elte.hu
1 Institute of Chemistry, ELTE Eötvös Loránd University, Hungary
2 Hevesy György PhD School of Chemistry, ELTE Eötvös Loránd University, Hungary
3 Institute of Materials and Environmental Chemistry, HUN-REN RCNS, Hungary

Ammonia (NH_3) is a promising carbon-free fuel candidate, gaining increasing interest in the combustion community. The combustion properties of NH_3 are less favorable than those of traditional hydrocarbon fuels; therefore, NH_3 is usually mixed with other fuels (e.g. H_2) in practical applications. To facilitate the development of new ammonia-based reciprocating engines and gas turbines, accurate chemical kinetic models are needed that can quantitatively predict the combustion characteristics of NH_3 and its fuel mixtures. In recent years, many new NH_3 combustion mechanisms have been published, but the performance of these models has not been tested against experimental data covering wide ranges of experimental conditions.

In this work, the performance of 36 recent, detailed combustion mechanisms was systematically evaluated against a large collection of experimental data on NH_3 and NH_3/H_2 combustion. The experimental data collection includes shock tube ignition delay times (IDT), laminar burning velocities (LBV), and concentrations measured in flow reactors, jet stirred reactors, and shock tubes. With 17,242 data points in 1,327 data series (collected from 110 publications), this is the largest data collection ever used for NH_3/H_2 mechanism testing. A novel approach was proposed to propagate the uncertainty of temperature to the measured concentrations, which resulted in more realistic errors for the concentration data than in previous studies. These uncertainties were considered in assessing the performance of the mechanisms. The results showed that there is no existing mechanism that can reproduce the experimental data well under all available experimental conditions. The overall best-performing mechanism is NUIG-2024 [1], which has the best performance for IDT (Fig. 1) and concentration measurements and has medium performance for LBV data.

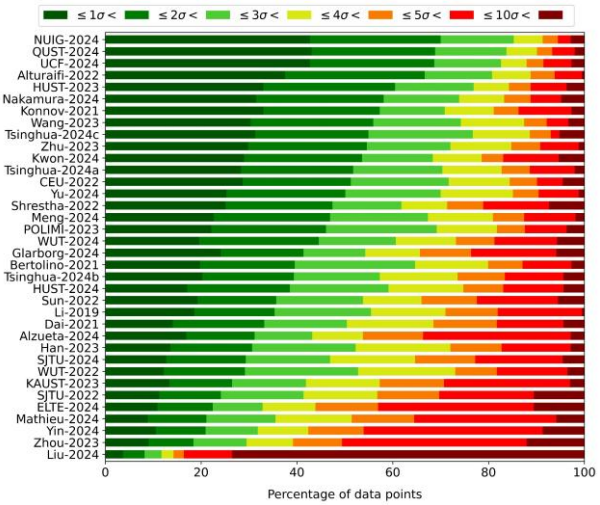

Fig. 1. Performance of the mechanisms for IDT data based on the percentage of the experimental data that they reproduced within given multiples of the standard deviation (σ) of the experimental data.

The NUIG-2024 mechanism was selected for further mechanism development. Reaction rate coefficients whose values influenced the performance of the mechanism the most were identified, and they were optimized within their physically allowed uncertainty range to match the experimental data better than the original model. The optimized model can be considered the most accurate NH_3 combustion mechanism in wide ranges of experimental conditions.

References

[1] Zhu Y et al. The combustion chemistry of ammonia and ammonia/hydrogen mixtures: A comprehensive chemical kinetic modeling study. Combust. Flame. 2024;260:113239.