

TESTING OF REACTION MECHANISMS FOR THE COMBUSTION OF NH₃/H₂ MIXTURES USING A LARGE AMOUNT OF EXPERIMENTAL DATA

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BACKGROUND-AIM

Due to the global climate change, it is extremely important to find alternative fuels to reduce the utilization of fossil fuels and the emission of air pollutants such as carbon dioxide (CO₂), hydrocarbon pollutants, and soot. Ammonia (NH₃) is a promising carbon free fuel candidate that can store and transport renewable hydrogen (H₂) energy.

Although ammonia has several advantages over hydrogen in practical applications, the combustion properties of NH₃ are different from traditional hydrocarbon fuels. A possible solution to improve the disadvantageous combustion properties of ammonia is to blend it with other fuels. For this purpose, one of the most usually used co-fuels is hydrogen.

METHODS

In this work, 19 detailed reaction mechanisms were investigated that had been published in the last 13 years. Their performance was quantitatively assessed based on how well they can reproduce the results of published experimental data. Almost 4000 experimental data points were utilized from the literature including ignition delay times measured in shock tubes, concentration measurements in jet stirred and flow reactors, and laminar burning velocity measurements. Local sensitivity analysis was carried out on the kinetic and thermodynamic parameters of the best performing mechanisms.

RESULTS

It can be concluded that there are significant differences between the performances of the different models, and the performance of a mechanism may also vary largely with the type of experiments. Even though the investigated mechanisms are different, sensitivity analysis identified almost the same set of important reactions and thermodynamic data in these mechanisms.

CONCLUSIONS

Results presented in this work can help in the selection of the best performing reaction mechanism and may serve as a good basis of combustion mechanism development for NH₃/H₂ fuel systems.