Effect of reaction scheme on the structure of ammonia turbulent flame

Tomohiro Tsubota[1], Naoya Matsuda[1], & Yukihiko Okumura[1]
Kagawa University Faculty of Engineering and Design, Takamatsu, Kagawa 761-0396, Japan[1]
s20g516@stu.kagawa-u.ac.jp

Ⅰ. Abstract

In recent years, global environmental problems, particularly global warming due to carbon dioxide (CO_2), have become substantially evident. It is therefore necessary to investigate novel and efficient energy utilization methods, to significantly suppress CO_2 emission, and thus preserve the environment. Ammonia (NH_3) is a fuel that does not emit greenhouse gases. However, the burning velocity of NH_3 is below 0.06 m/s, which is much lower than that of conventional hydrocarbon fuels (oil-based fuels), making it difficult to achieve stable combustion of NH_3. If NH_3 is forcibly combusted, a large amount of NO_X (toxic substance) will be generated. In this study, the calculations were performed using three chemical kinetic mechanisms (GRI Mech 3.0, Okafor Mech, Creck Mech), and the best mechanism was selected by comparing the experimental and calculation results. The GRI Mech 3.0 (Smith, et al) has a common reaction that has been used for the combustion calculation of many hydrocarbon fuels. The Okafor Mech (Okafor, et al, 2018) was improved NH_3 reactivity based on GRI Mech 3.0 and Tian Mech. The Creck Mech (Stagni, et al, 2020) was a newly created mechanism and the mechanism for promoting the NH_3/H_2 reactions was added to the conventional scheme. By comparing the experimental and numerical data (i.e., flame structure and laminar burning velocity), it is found that that the Creck Mech was judged to be the most suitable chemical kinetic mechanism for ammonia burner with hydrogen flame stabilizer.

Ⅱ. Results & Discussion

The analysis object of ammonia burner is shown in Figure 1. A stable flame was obtained by separately supplying ammonia, hydrogen, and air in central, duplex, and triple tubes, respectively (Figure 1). The burner developed in this study can supply a high-velocity airflow (8m/s). Figure 2 shows the comparison of flame structure between experimental and numerical result. In particular, NH_3 consumption height from burner rim well agreed, and the distributions of temperature and chemical species by Creck Mech well agreed with experimental result. Figure 3 (a), (b) shows laminar burning velocities S_h of NH_3-H_2 (50-50:vol%) /Air flame, and stoichiometric NH_3-H_2/Air flame, respectively. X_{H_2} represents the ratio of H_2 in NH_3-H_2 mixture fuel. From Figure 3 (a), (b), the Creck Mech can takes account of the improvement of burning velocity and reactivity when H_2 is added to NH_3.

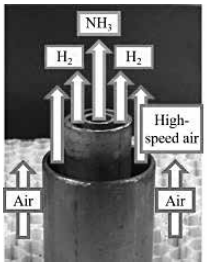

Figure 1. Ammonia burner

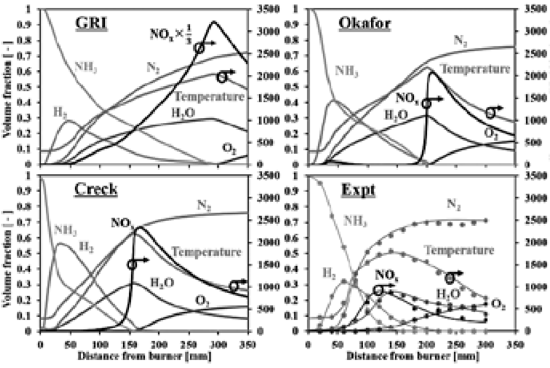

Figure 2. Flame structure at central axes of flame

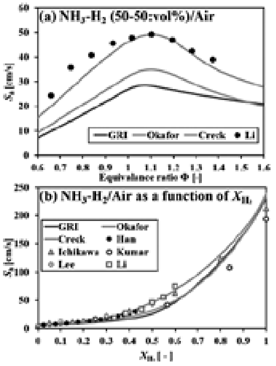

Figure 3. Laminar burning velocity S_h

Ⅲ. Conclusion

(1) From a point of view with the flame structure and laminar burning velocity, the calculation results obtained using the Creck Mech well agreed with the experimental results.

(2) In GRI Mech 3.0 and Okafor Mech, the flame length became longer because the burning velocity (NH_3/H_2) due to the addition of H_2 was not taken into consideration. Then, the GRI Mech 3.0 and Okafor Mech are underestimate reactivity when H_2 are added to NH_3.

Ⅳ. References

Smith, GP., Golden, DM., Frenklach, M., Moriarty, NW., Eiteneer, B., ... & Goldenberg, M., URL:http://www.me.berkeley.edu/gri_mech/.

Okafor, E. C., Naito, Y., Colson, S., Ichikawa, A., Kudo, T., Hayakawa, A., & Kobayashi, H. (2018). Experimental and numerical study of the laminar burning velocity of CH_4–NH_3–air premixed flames. *Combustion and flame, 187,* 185-198.

Stagni, A., Cavallotti, C., Arunthanayothin, S., Song, Y., Herbinet, O., Battin-Leclerc, F., & Faravelli, T. (2020). An experimental, theoretical and kinetic-modeling study of the gas-phase oxidation of ammonia. Reaction Chemistry & Engineering, 5(4), 696-711.