Carrier-phase direct numerical simulation of a laboratory-scale liquid ammonia jet flame

Zhenhua An[1]*, Jiangkuan Xing[1], Meng Zhang[2], Abhishek Lakshman Pillai[1], Ryoichi Kurose[1]

[1]*Department of Mechanical Engineering and Science, Kyoto University, Kyoto, daigaku-Katsura, Nishikyo-ku, Kyoto 615–8540, Japan*
[2]*State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, Xi'an 710049, China*

Abstract: A laboratory-scale liquid ammonia jet flame is investigated using Carrier-Phase Direct Numerical Simulation (CP-DNS) with a detailed reaction mechanism (Combust. Flame 204(2019)162175), which includes 42 chemical species and 130 reactions. The validity of the CP-DNS is evaluated by comparing the simulation results with the experimental data. Subsequently, flame structure and combustion characteristics are explored in detail. The results show that strong heat loss caused by the flash boiling significantly reduces the local heat release. From upstream to downstream, the combustion reactions are affected by different degrees of phase change. Notably, NO formation is much more significant in the downstream due to the higher ammonia concentration and local temperature. (108 words)

Keywords: Liquid ammonia jet flame, CP-DNS, Detailed chemistry, Heat loss, Combustion modes

1. Introduction

Ammonia has broad prospects in the long-term goal of reducing carbon emissions. Remarkable progress has been made in recent decades. Much basic and applied research has been carried out on ammonia combustion. For example, the fundamental combustion characteristics of ammonia [1], ammonia/methane [2], and ammonia/hydrogen [3] flames, such as flame speed and emission, have been advanced on various fronts. Ammonia is usually stored in the liquid phase, then direct combustion of liquid ammonia can reduce the cost and complexity of fuel supply systems for engineering devices, which reduces about 7-9 % of the consumption of generated power for the vaporization process and the start-up time in gas turbines [4].

However, relatively little effort has been devoted to the study of liquid ammonia combustion because it is a relatively new topic. There are some differences between gaseous and liquid phase ammonia combustion in terms of droplets-flame interaction, heat loss from the phase change process, and non-uniform mixing during evaporation [5]. It is essential to analyze the combustion characteristics of liquid ammonia flames. As a novel liquid fuel, the turbulent combustion dynamics of liquid ammonia jet flames, which involve the interplay of flash boiling, heat loss, mass transfer, reaction thermal chemistry, and flame surfaces, have not been fully understand and explored. Therefore, the aim of the present study is to conduct a Direct Numerical Simulation (DNS) of a laboratory-scale ammonia flash spray flame to investigate the combustion characteristics.

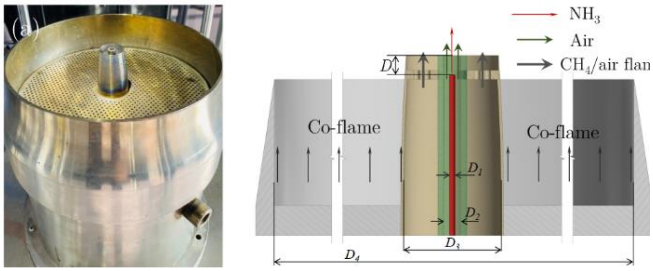
2. Numerical methods

For the gas phase, the conservation equations of mass, momentum, enthalpy, and species are directly calculated in an Euler manner without any averaging and filtering. For the dispersed phase, the Lagrangian method is used to capture the dynamics of droplets. The two-way coupling approach is used to consider the interaction between the gas and dispersed phases as our previous studies [6-8]. The Zuo boiling model combined with the non-equilibrium Langmuir–Knudsen evaporation model is used in this study, which has been validated under flash boiling conditions in our previous study [6], by comparing with the experimental data. Those governing equations are not detailed here for brevity, and the interested readers can refer to our previous studies [6,9].

3. Computational details

3.1. Experiment and simulation set up

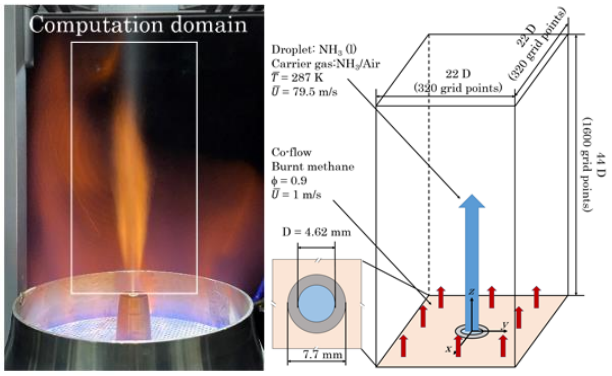
The experiment was conducted based on a laboratory-scale liquid ammonia jet flame burner [10], as shown in Fig. 1. This burner can realize a stable liquid ammonia jet spray and spray flame. Liquid ammonia is injected through the center tube, shown by red color, which is installed in a coaxial air tube. The horizontal position of the liquid ammonia injector is adjustable for controlling the degree of the mixing between fuel and air. Annual pilot co-flow is used to ignite the liquid ammonia/air mixture. The co-flow provides the hot atmosphere using the burnt gas of methane/air.



(a) (b)

Figure 1 (a) The photograph of burner, (b) the schematic and dimensions of burner [10].

The target flame and computational domain are shown in Fig. 2. The computational domain is located in the white box with size of 102×102×204 mm^3 in the digital photo in Fig. 2 (a). In the present study, the mesh is 320×320×1600, as shown in Fig. 2 (b). A detailed mechanism (59 species and 356 reactions) [2] is used for the combustion chemistry. The mean jet velocity is 79.5 m/s, and the corresponding Reynold number is 20000. The computational grid at the center is refined and stretched in the radical and axial direction, and the grid size is comparable to the Kolmogorov scale and could have about ten points across the flame thickness. A fully turbulent pipe flow carrying ammonia droplets is injected into the domain through the center nozzle.



(a) (b)

Figure 2 (a) digital photo of liquid ammonia jet spray flames captured in the experiment [10], (b) Schematic diagram of the DNS configuration and burner details. The gray circle represents a wall between the center jet and pilot co-flow.

3.2. Simulation parameters

The data processing of droplet diameter and number is shown in Fig. 3. The position with the strongest gradient change in the image is usually the object on the focal plane. Using image gradient information for image binarization and extracting the boundaries of droplets.

(a) (b) (c)

Figure 3 (a) Original image. (b) Binary images drawn through gradient information. (c) Droplet image.

The percentage of non-evaporation droplets mass, $m_{NH3(l)}$, which represents the percentage of liquid ammonia without pre-evaporation in the inlet tube, is obtained from Fig. 3, and the droplet sizes are descried with a Rosin-Rammler (R-R) distribution whose parameters have been fitted from the experimental identified data.

4. Results and discussion

Figure 4 shows the comparison of instantaneous droplet distribution between the experiment employing Mie scattering and the present DNS. These results show the same trend that the intensity decreases from upstream to downstream, which means the droplet continue to evaporate. However, there are some differences on the width. More validation will be carried out in future study.

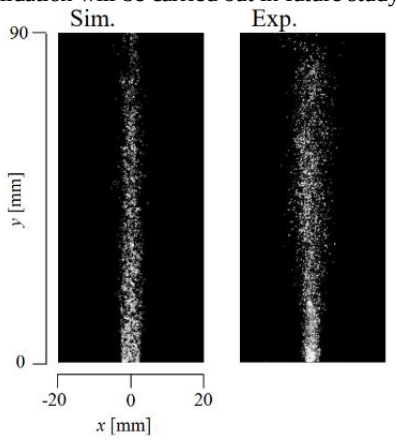


Figure 4 The comparison of droplet distribution represented by Mei scattering (left) measured from experiment and Lagrangian fields (right) calculated from DNS.

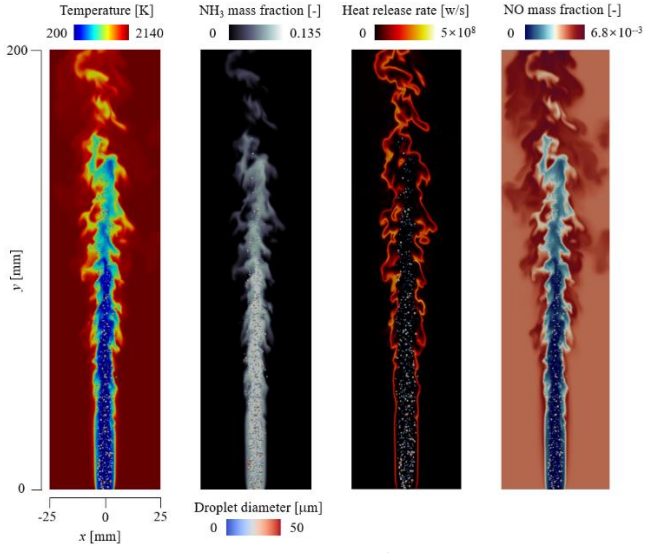


Figure 5 Instantaneous distributions of (a) gas temperature, and (b) NH_3 mass fraction, (c) heat release rate, and (d) NO mass fraction. The liquid ammonia droplets are shown by relatively size.

Figure 5 shows the instantaneous fields of liquid ammonia jet flame. It can be found that the temperature of co-flow is always larger than the central jet, as shown in Fig. 5 (a). Figure 5 (b) shows the distribution of NH_3 mass fraction. Figure 5 (c) shows the HRR, the maximum value of HRR is 5 $\times 10^8$ W/m^3, which is limited by large heat loss from flash boiling of liquid ammonia. The HRR will be higher downstream because liquid ammonia evaporates rapidly upstream and the heat loss downstream is relatively small, resulting in a relatively high HRR. This also leads to NO aggregation downstream, as shown in Fig. 5 (d).

5. Conclusions

A laboratory-scale liquid ammonia jet flame was investigated using DNS method coupled with detail chemistry. The parameters used in simulation were all measured from experiment. The results showed that rapid heat loss from flash boiling considerably reduced the local heat release. From upstream to downstream, combustion reactions experience varying extents of phase change. Importantly, NO production is more pronounced downstream because of elevated ammonia concentrations and local temperatures.

Acknowledgement

This work was partially supported by MEXT as “Program for Promoting Researches on the Supercomputer Fugaku” (Development of the Smart design system on the supercomputer “Fugaku” in the era of Society 5.0) (JPMXP1020210316). This research used the computational resources of supercomputer Fugaku provided by the RIKEN Center for Computational Science (Project ID: hp220180, hp230193).

Reference

[1] Hayakawa, A., Goto, T., Mimoto, R., et al., ***Fuel*** 2015; 159: 98-106.

[2] Okafor, E.C., Naito, Y., Colson, S., et al., ***Combustion and Flame*** 2018; 187: 185-98

[3] Honzawa, T., Kai, R., Okada, O., et al., ***Energy*** 2019; 186: 115771.

[4] Okafor, E.C., Yamashita, H., Hayakawa, A., et al., ***Fuel*** 2021; 287: 119433.

[5] Ozel, E.G., Hasslberger, J., Klein, M., et al., ***Combustion Science and Technology*** 2019; 191: 833-67.

[6] An, Z.H., Xing, J.K., Kurose, R., ***Fuel*** 2023; 345: 128229.

[7] Xing, J.K., Luo, K., Kurose, R., Fan, J., ***Proceedings of the Combustion Institute***, 2023, 39(3): 3227-3237.

[8] Hu, Y., Kurose, R., ***Combustion and Flame***, 2018, 188: 227-242.

[9] An, Z.H., Xing. J.K., Pillai, A., Kurose, R., Fuel, 2023, 357: 129660.

[10] Zhang, M., Wang, R., An, Z.H., et al., ***Fuel*** under review, 2023.