

**TNF target flame:** Turbulent piloted jet flames of partially cracked ammonia

## Authors

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## Introduction

Partially cracking technology is considered a promising strategy to enhance ammonia (NH<sub>3</sub>) combustion. The KAUST piloted turbulent flames of partially cracked ammonia are investigated using Direct Numerical Simulations (DNS) coupled with detailed chemistry. Two cases are considered: flames D and F with Reynolds numbers of 24000 and 36000, respectively. The predicted mean and root mean square profiles of temperature and major/minor species are compared with the experimental data in the physical and mixture fraction spaces. Good agreement for flame D could be achieved. While the local extinctions in the midstream regions have not been sufficiently reproduced for flame F. The statistics and analyses on combustion modes and their heat release contributions demonstrate that premixed and diffusion modes appear in the inner and outer layers, respectively, and the heat release contribution from each mode is comparable.

## DNS configuration and methods

The governing equations of mass, momentum, species, and energy are solved for the turbulent reacting flows without introducing any filtering and averaging. A detailed chemical reaction mechanism developed by Shrestha et al. [1] is used to describe the combustion kinetics, including 33 species and 253 reactions (with carbon-related species and reactions removed). The mixture-averaged method is used to account for the species diffusivity [2]. The Soret effect is not considered. The radiation effect is considered with the P1 model [3].

The DNS calculations are performed with an in-house solver developed based on OpenFOAM-8 [4]. The spatial integration terms are discretized using the cubic scheme, as suggested by Zirwes et al. [5]. and the time integration terms are handled with a Crank-Nicolson scheme. To ensure numerical stability during the calculations, the Courant number is maintained to be less than 0.5, and the corresponding time step is less than 0.1 micro-seconds. The first 10 flow periods are used to develop the flames. Another 8 flow periods are used to get the mean and *rms* statistics.

## Operation conditions

The flames D and F of the KAUST piloted turbulent jet flames of partially cracked ammonia are investigated as shown in Figure 1. The burner has three streams: the central fuel stream, the annular pilot stream, and the surrounding co-flow stream. The central fuel stream is composed of a premixed mixture of partially cracked ammonia and air. The cracking ratio is 43%, the equivalence ratio is 3.0, and the mixture temperature is 293.5 K. The pilot stream features a burnt mixture of 43% partially cracked

ammonia and air at an equivalence ratio of 0.9, and the velocity is 6.55 m/s which is determined by mass conservation considering the density difference between the fresh and equilibrium gases. The temperature and compositions of the mixture are obtained by equilibrium calculations. The co-flow stream is cold air with a velocity of 0.8 m/s and a temperature of 296.6 K. The configurations of flames D and F are identical with different central jet velocities (62.2 m/s and 93.3 m/s). Fully developed turbulent pipe flows, which are obtained by performing cold flow DNS calculations for the corresponding jet velocities, are sampled and used as the inflow velocity profiles.

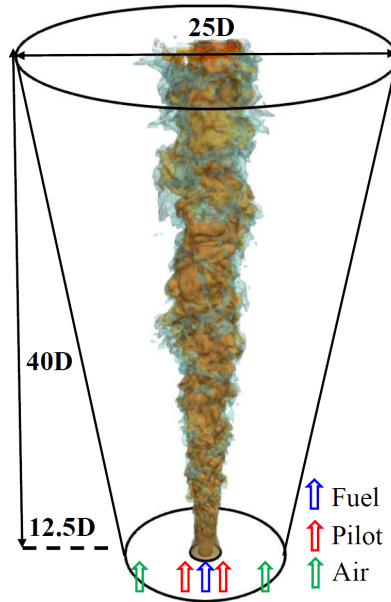


Figure 1. Computational schematic of turbulent piloted jet flames.

The computational domain is a cylinder with a length of  $40 D$ , and its diameter gradually varies from  $15 D$  to  $25 D$ , as shown in Figure 1. For the flame D, in the core flame region, the computational grids are uniform in the central jet region ( $r/D < 1$ ) with a resolution of  $20 \mu\text{m}$  and radially stretched from  $20 \mu\text{m}$  to  $80 \mu\text{m}$  in the region of  $1 < r/D < 2$ . As for the Flame F, the computational grids are uniform in the central jet region ( $r/D < 1$ ) with a resolution of  $15 \mu\text{m}$  and radially stretch from  $15 \mu\text{m}$  to  $60 \mu\text{m}$  in the region of  $1 < r/D < 2$ . The computational grids are also stretched in the streamwise direction with a resolution from  $20 \mu\text{m}$  near the jet nozzle to  $200 \mu\text{m}$  at  $z/D = 40$ . The total grid numbers are 0.112 billion and 0.265 billion for the flames D and F, respectively, providing 8 to 22 grid points across the thinnest flame thickness and well resolve the Kolmogorov scale in the core flame region.

### Exemplary results

Figure 2 shows the flame structure represented by distributions of gas temperature,  $Y_{\text{H}_2}$ ,  $Y_{\text{H}_2\text{O}}$ , and  $Y_{\text{NH}_2}$ .

Figure 3 demonstrates the distribution of combustion mode represented by Takeno's flame index [6] as well as quantitative statistics on their proportions/heat release contribution.

### How to get access to the data

Upon request.

Contact Ryoichi Kurose ([kurose.ryoichi.6x@kyoto-u.ac.jp](mailto:kurose.ryoichi.6x@kyoto-u.ac.jp)) or Jiangkuan Xing ([zjuxjk@zju.edu.cn](mailto:zjuxjk@zju.edu.cn))

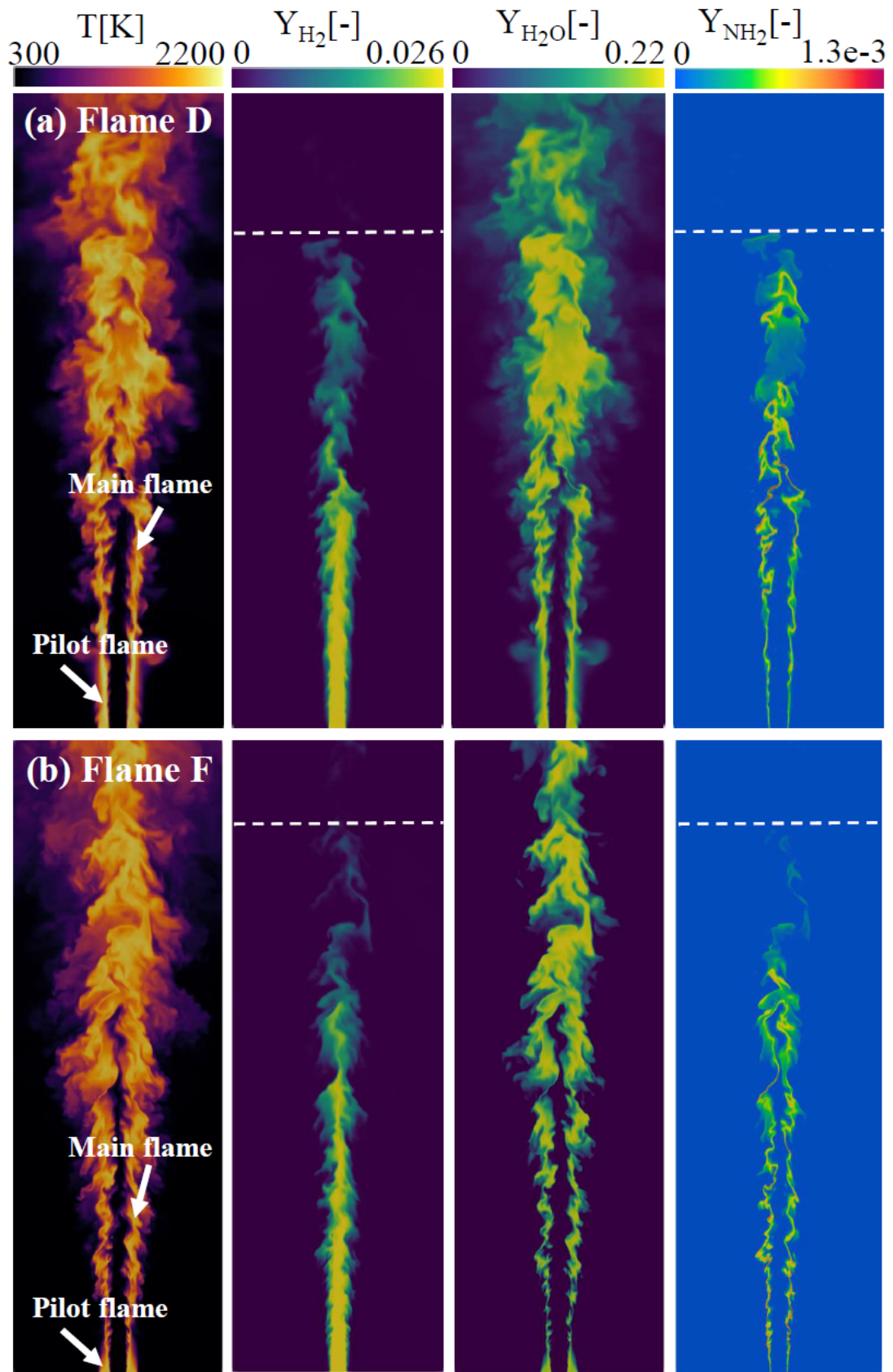


Figure 2. Flame structures of (a) flame D and (b) flame F. Note that only gas temperature,  $Y_{H_2}$ ,  $Y_{H_2O}$ , and  $Y_{NH_2}$  are shown here for brevity, and the computational domain is cut into a square shape for a better presentation ( $r/D \in [0, 12.5]$  and  $z/D \in [0, 40]$ ). The white dashed lines represent the position where fuels are fully consumed.

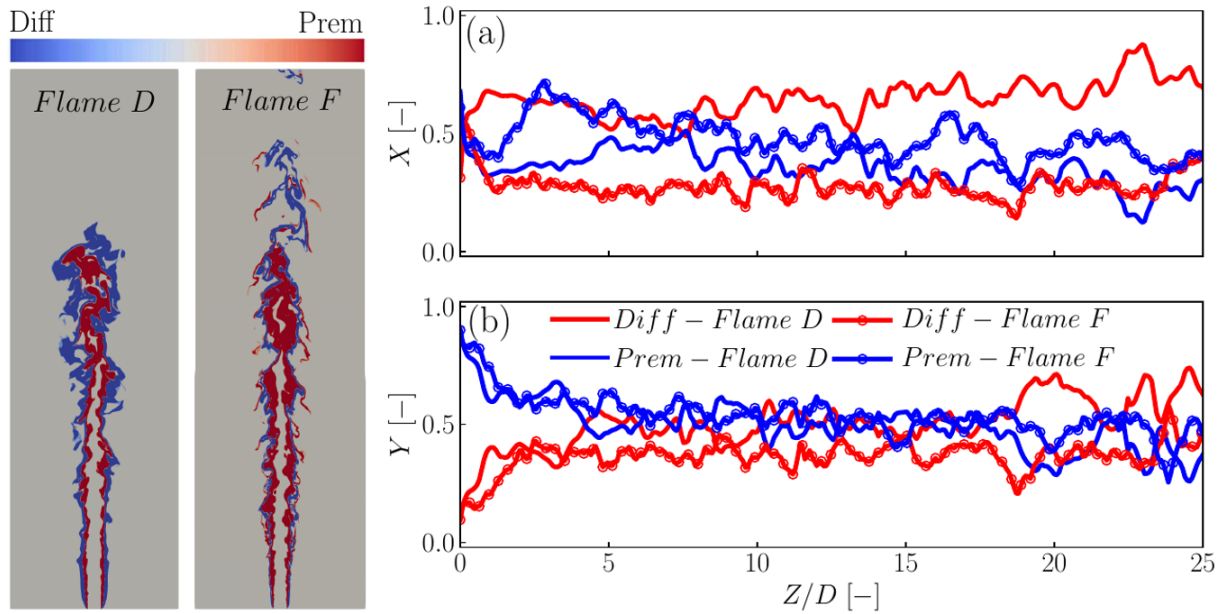


Figure 3. Left: combustion mode indicated by flame index in flames D and F. Right: statistics of the stream-wise mean proportions of (a) combustion mode and (b) heat release contribution of each combustion mode.

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