

## **A comparative study of direct moment closure and flamelet-based models for piloted turbulent partially cracked ammonia flames**

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Ammonia ( $\text{NH}_3$ ) is considered a promising hydrogen carrier and carbon-free fuel. Large eddy simulation (LES) is an important tool for studying turbulent ammonia combustion. To accurately simulate turbulent ammonia combustion, high-fidelity turbulent combustion models are required to account for the complex turbulence-chemistry interactions. In our previous studies, we proposed a direct moment closure (DMC) model [1, 2] for modeling turbulence-chemistry interactions with direct closure of the chemical source term. In addition, as well-known tabulation methods, flamelet/progress variable (FPV) [3] and flamelet-generated manifold (FGM) [4] models are efficient methods to be used with LES considering detailed reaction mechanisms. The objective of this work is to compare the performance of these three models in predicting turbulent ammonia combustion. To this end, LESs of the KAUST piloted turbulent partially cracked ammonia flames D and F are performed using these three models, and the simulation results are compared with experimental data.

The results show that all the three models perform well in predicting temperature and major species, and their results are highly consistent. This suggests that for partially premixed flames, the prediction results may be insensitive to the development basis (premixed or non-premixed modes) of combustion models. However, the DMC model is significantly better than the FPV and FGM models in predicting minor species like OH. This suggests that finite-rate chemistry models have an advantage over flamelet-based models in predicting minor species. In addition, it is observed that LES-FGM predicts stronger turbulent fluctuations near the pilot flame compared to LES-DMC and LES-FPV, even with the same turbulent inlet settings. This further leads to faster auto-ignition of the main jet fuel in the LES-FGM simulation. As a result, LES-FGM's prediction performs excellently in the upstream region of the flame but slightly overestimates in the downstream region. On the other hand, all the three models underestimate the local extinction extent in flame F with a high Reynolds number. This leads to deviations in the regions with significant extinction phenomena. It emphasizes that accurately capturing local extinction in high Reynolds number turbulent flames remains a challenge in turbulent combustion modeling. Improving modeling to enhance the predictive capability for unsteady phenomena is a focus for future study.

### **References**

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