

A flow reactor study of NH₃/DEE oxidation

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Introduction

Ammonia (NH₃) is a **carbon-free fuel** with strong potential for clean energy systems, though its **low reactivity limits** practical use.



Ammonia (NH₃) is a carbon-free fuel with strong potential for **low-emission** energy systems. However, its combustion is hindered by **poor thermochemical properties**, such as high ignition temperature, low flame speed, and narrow flammability limits, as well as the formation of significant NO_x emissions.

Blending with diethyl ether (DEE), a highly reactive oxygenated fuel, enhances ignition. This fuel mixture offers a promising enhances in key parameters such as ignition delay time (IDT) and laminar burning velocity (LBV).

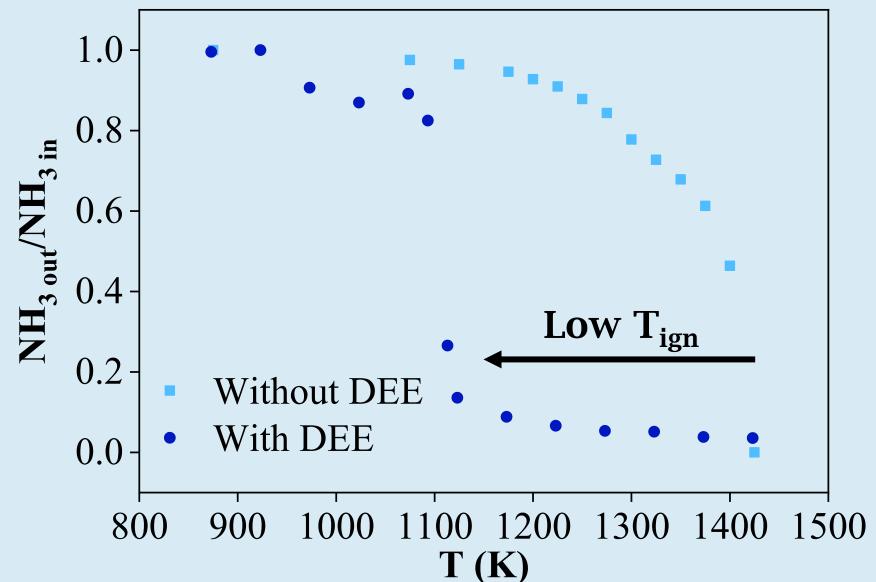
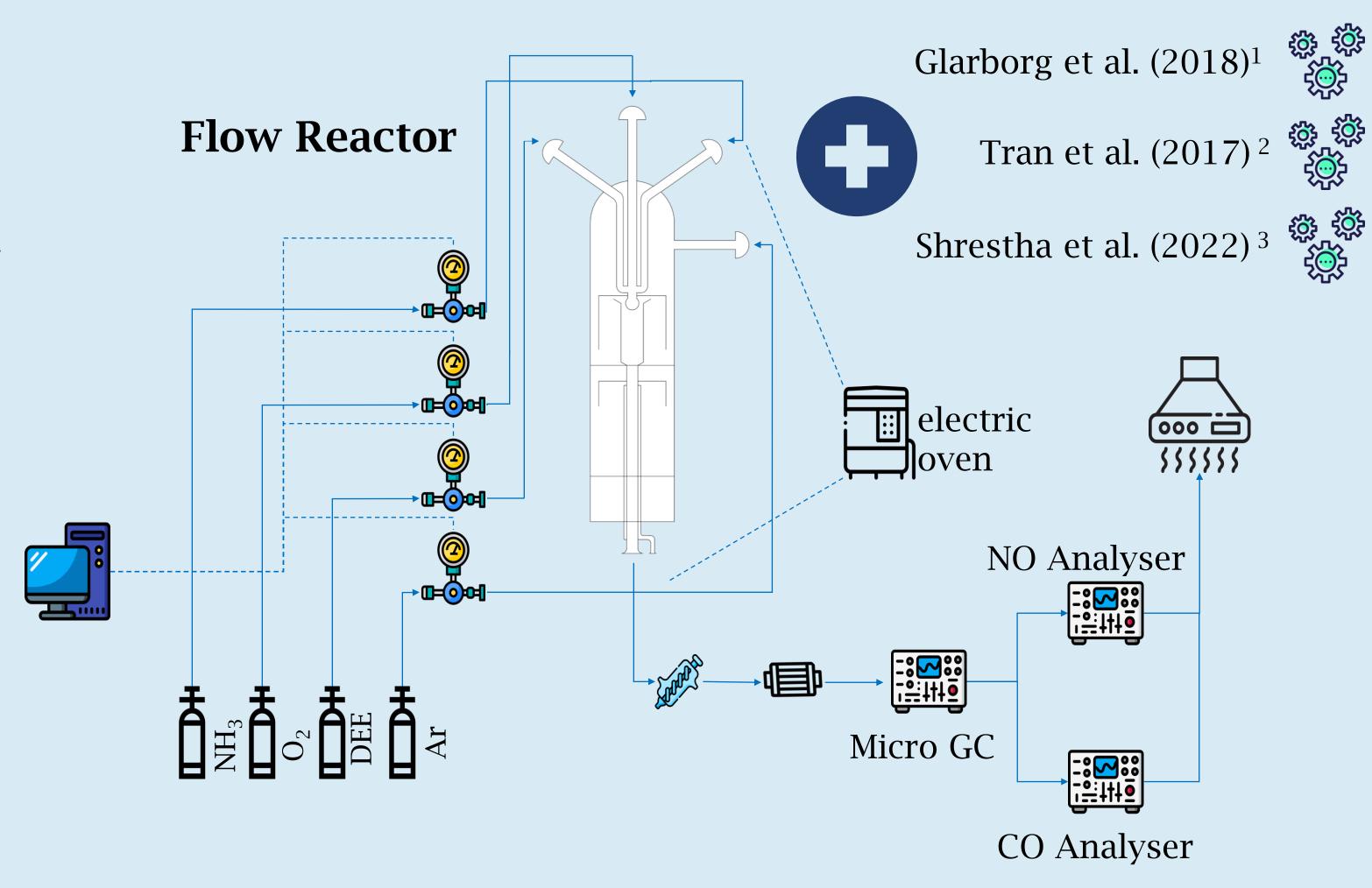


Figure 1. NH₃ profiles.

Methodology

Detailed kinetic mechanism



Results

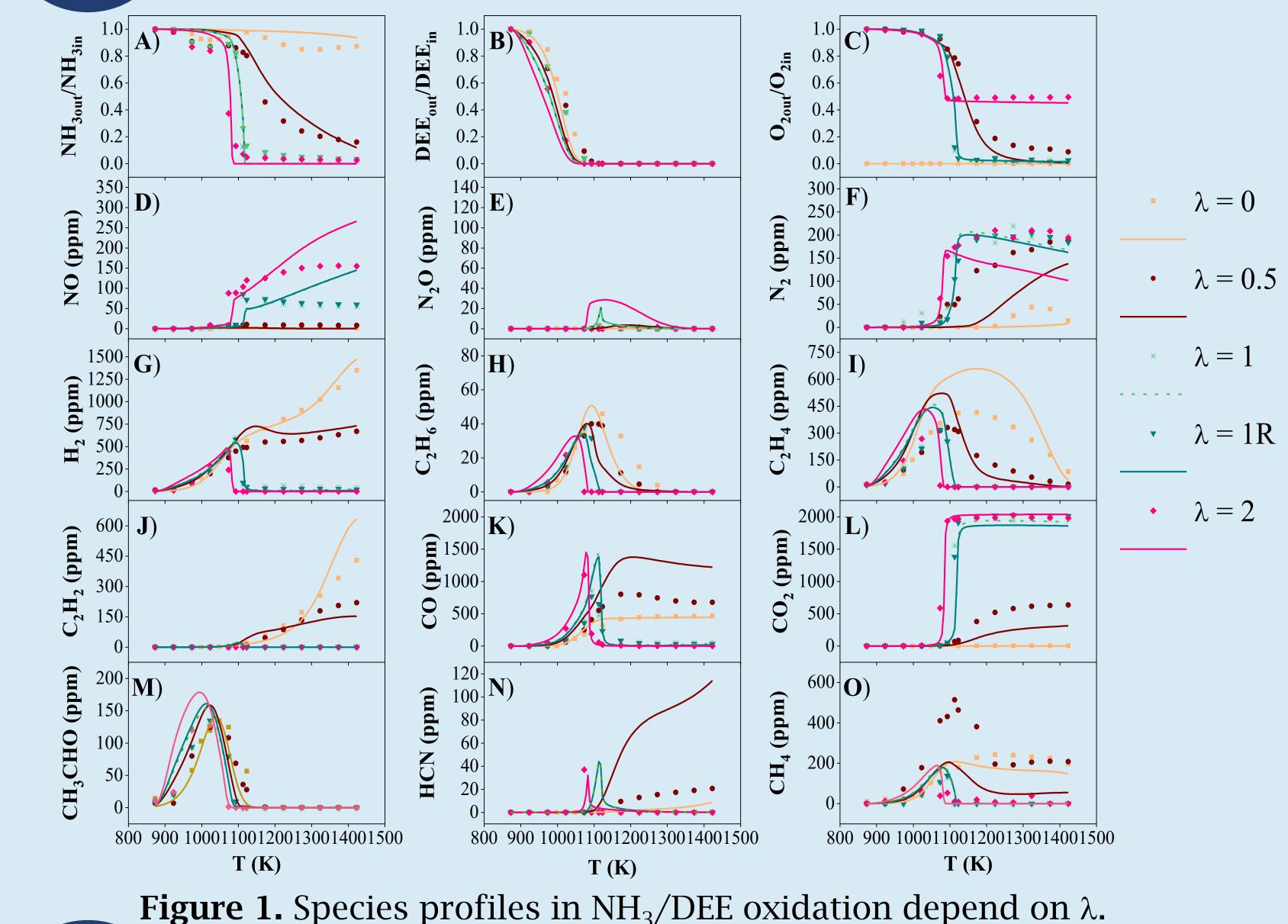


Figure 2. Reaction Pathway of A) DEE and B) NH₃

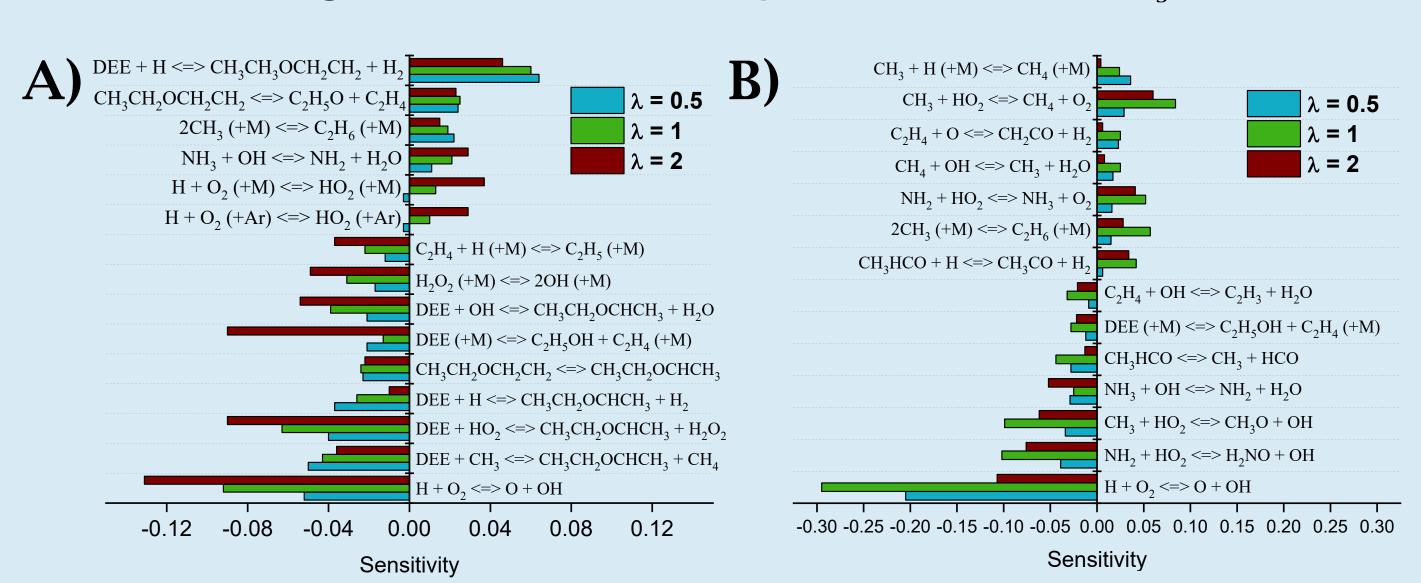


Figure 3. Sensitivity analysis of A) DEE and B) NH₃.

Conclusion

- The oxidation of both fuels shifts to lower temperatures as the equivalence ratio (λ) increases. This effect is especially pronounced at higher λ values, with a notable temperature drop observed for NH₃ when λ is below 1.
- Radical pool dynamics plays a key role in NH₃ oxidation, with OH and O radicals being the primary contributors. Additionally, interactions with DEE-derived species have been observed to enhance the oxidation process.
- Variations in the equivalence ratio (λ) influence the prominence of specific reaction pathways, a trend observed in both fuels.
- \triangle A kinetic model has been developed, offering reasonably accurate predictions across a wide range of conditions.

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