

## Large-eddy simulations of liquid ammonia direct injection: Hydrogen impact on ignition and emissions in hot ambient conditions

Waseeq Siddiqui<sup>1\*</sup>, Ville Vuorinen<sup>1</sup>
\*lead presenter: waseeq.siddiqui@aalto.fi
1 Aalto University, Finland

In recent years, liquid ammonia has attracted increasing interest as a potential alternative fuel due to its ability to combust without emitting carbon. Despite challenges with ignitability, ammonia holds promise when blended with other renewable or low-carbon fuels, paving the way for cleaner combustion technologies. This study investigates the potential of liquid ammonia in combustion engines using large-eddy simulations conducted with OpenFOAM. Both non-reacting and reacting scenarios are explored.

Initially, the study validates an inert benchmark case, focusing on the injection of liquid ammonia into a constant volume chamber. It then compares the ignition characteristics of pure ammonia with those of pure ammonia in a premixed H2/air mixture during combustion in engine-like environments. The numerical validation includes simulations for a single-hole nozzle based on the work of R. Payri et al. [1], inspired by Engine Combustion Network (ECN) conditions with hot ambient and vaporizing environments. The numerical setup considers factors such as mesh strategy, injection angle and breakup models.

The study investigates the combustion characteristics of liquid ammonia under conditions similar to ECN's Spray-D, both with and without hydrogen present in the ambient environment. The mechanism developed by Otomo et al. [2], consisting of 32 species, is utilized, with the in-house dynamic load balancing model DLBFOAM [3] employed to accelerate chemical reactions. Key aspects, including pollutant formation, ignition properties, and spray characteristics, are investigated.

## References

- [1] Payri, R., García-Oliver, J. M., Bracho, G., & Cao, J. (2024). Experimental characterization of direct injection liquid ammonia sprays under non-reacting diesel-like conditions. Fuel, 362, 130851.
- [2] Otomo, J., Koshi, M., Mitsumori, T., Iwasaki, H., & Yamada, K. (2018). Chemical kinetic modeling of ammonia oxidation with improved reaction mechanism for ammonia/air and ammonia/hydrogen/air combustion. International Journal of Hydrogen Energy, 43(5), 3004-3014.
- [3] Tekgül, B., Peltonen, P., Kahila, H., Kaario, O., & Vuorinen, V. (2021). DLBFoam: An open-source dynamic load balancing model for fast reacting flow simulations in OpenFOAM. Computer Physics Communications, 267, 108073.