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High-fidelity numerical simulations of diesel-ammonia dual-fuel ignition in internal combustion engines

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Decarbonizing heavy-duty transportation, which is challenging to electrify, often involves retaining internal combustion engines (ICE) while replacing hydrocarbon fuels with carbon-free alternatives. Among the carbon-free fuels, ammonia emerges as a promising candidate for long-range transportation applications due to its higher energy density compared to hydrogen and its ease of storage. However, ammonia's inherently low reactivity and its nitrogen content pose challenges associated with combustion efficiency and fuel-bound NO_x emissions. In particular, there are concerns that nitrous oxide (N_2O) emissions from ammonia combustion could offset its climate benefits considering N_2O has approximately 300 times higher global warming potential (GWP) over CO_2. This study investigates the feasibility of partially replacing diesel with ammonia in ICEs, focusing on thermal performance, emissions characteristics, and the impact of ammonia substitution on overall greenhouse gas emissions.

To explore this, downsized and gas-phase direct numerical simulations (DNS) of turbulent reactive flows under engine-relevant conditions were performed using an open-source CFD solver PeleLMeX [1]. Specifically, simulations replicate the ECN Spray H condition with a light-diesel fuel modeled as n-heptane, and combustion chamber set to approximately 40 atm and 1000 K. In the dual-fuel approach, ignition of the ammonia main charge is achieved by first injecting a diesel pilot charge to initiate a robust pilot flame. Ammonia is then injected immediately after the end of the diesel injection to leverage the pilot flame as an ignition source. The results of the dual-fuel ignition were compared against a baseline light-diesel flame for the same amount of energy injected.

Results indicate that 70% of diesel energy content can be replaced with ammonia. However, a significant amount of unburned ammonia is found to remain in the combustion chamber. Although late oxidation of the residual ammonia can (in principle) contribute to increased combustion efficiency, it also leads to increased emissions, particularly of N_2O. Interestingly, it is observed that NO_x emissions are higher in the case of the diesel-only flame. This is primarily due to 1) the stronger thermal NO_x due to high temperature present in the diesel-only flame and 2) the NO-to-N_2O conversion process taking place in the dual-fuel flame. This ultimately results in significant N_2O emissions for the latter case. While the overall GWP was found higher for the dual-fuel configuration, the potential for significant N_2O emissions from dual-fuel configurations suggest the need for careful assessment and optimization of ammonia-fired engines.

References

[1] Esclapez L. et al., PeleLMeX: an AMR Low Mach Number Reactive Flow Simulation Code without level sub-cycling. *The Journal of Open Source Software*. 2023;8:5450.