Large Eddy Simulations for Ammonia/Hydrogen/n-Dodecane Combustion

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To investigate the behavior of ammonia (NH_3) in dual-fuel and tri-fuel combustion systems, this study offers Large Eddy Simulation (LES) findings of spray combustion under engine-relevant conditions. Using the ECN Spray A configuration [1] as a validated reference case, the simulations performed in OpenFOAM with the updated Aalto75 skeletal mechanism which is specifically designed for n-dodecane/ammonia blends [2]. The study investigates the effects of adding ammonia into the ambient environment to simulate advanced dual-fuel and tri-fuel techniques after a successful validation of spray penetration and ignition delay in both non-reactive and reactive situations. A test matrix of LES is built in order to observe the influence of different ambient equivalence ratios (φ=0.5,0.7,1.0) and temperatures (900-950K) on ignition behavior, reaction front development, and emissions. To help overcome ammonia's slow flame speed, hydrogen was also added to the mixture to observe the reactivity boost and support more stable combustion. The results show that higher levels of ammonia in the ambient environment tend to slow down ignition and change the balance between NO and N_2O emissions, whereas adding hydrogen helps speed up ignition and makes the combustion process more stable. These findings serve increase our understanding of how ammonia can be used more effectively in cleaner engine technologies aimed at reducing carbon emissions.

References

[1] Pickett LM et al. "Comparison of Diesel Spray Combustion in Different High-Temperature, High-Pressure Facilities". SAE International Journal of Engines 2010.
[2] Kurumus AT et al. "A skeletal mechanism for n-dodecane/ammonia combustion and an open-source reaction scheme optimization tool". Fuel 2024;373, p. 132168.