Spray Combustion and Emission Characteristics of Ammonia–Hydrocarbon Blends under Engine-Equivalent Conditions: A CFD Study with Detailed Chemistry

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Ammonia is gaining attention as a zero-carbon fuel, and in particular, the spray combustion of liquid ammonia could serve as an attractive alternative to conventional high-output diesel engines. However, ammonia's low reactivity and high latent heat of vaporization pose challenges for its application in high-output diesel engines. Directly mixing hydrocarbons such as propane, which exhibits similar liquefaction properties to ammonia, or liquid fuels like methanol with ammonia is a promising approach to improve ammonia liquid spray combustion. In this study, we analyzed the spray combustion behavior of mixed fuels containing ammonia and either methanol or propane under engine-equivalent conditions involving compression and expansion using three-dimensional RANS CFD.

The analysis employed a Euler–Lagrange approach-based spray model and a combustion model incorporating a detailed chemical reaction mechanism (112 species and 597 reactions)[1][2]. The target fuels were pure ammonia (A100), ammonia–methanol (M30A70), and ammonia–propane (P30A70). The calculations were performed under two conditions: with constant input heat and with constant injection parameters, allowing for a comprehensive comparison of the effects of mixed fuel composition on combustion behavior and exhaust emissions.

The simulation results accurately reproduced the heat release rate history obtained from a rapid compression expansion machine (RCEM)[3], demonstrating the validity of our CFD. Furthermore, the calculations enabled quantitative and detailed capture of changes in flame structure, transition of flame liftoff length, mixture formation, and formation behavior of emissions such as NO_x (NO and NO_2) and N_2O. In particular, with propane-blended fuels, the formation of a high equivalence ratio region around the spray axis caused fuel to remain unburned, resulting in significant afterburning. Furthermore, hydrocarbon blending altered the spatial distribution of nitrogen-based emissions, leading to an increase in NO_x (NO and NO_2) formation while promoting the oxidation of N_2O and thereby reducing N_2O emissions.

In this presentation, we report the results of a systematic analysis of the spray combustion behavior and emission characteristics of ammonia–hydrocarbon mixed fuels under engine-equivalent conditions, based on two comparative designs (input heat and injection conditions).

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References
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