A Chemical Kinetic Modeling Study for Enhancing the Combustion Properties of Ammonia: A Zero-Carbon Fuel

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Ammonia has been considered an encouraging substitute for fossil fuels in hopes of decreasing greenhouse gas emissions. Although ammonia is promising, it still has the issue of low reactivity, which can be addressed by introducing additives. Ignition delay times (IDTs) of neat ammonia and various blends (ammonia/methane [NH3/CH4], ammonia/hydrogen [NH3/H2], and ammonia/dimethyl ether [NH3/DME]) were calculated using the reaction mechanism of Issayev et al., with the use of the software Chemkin Pro. The simulations were performed at 20 and 40 bar, with equivalence ratios of 0.5 and 1. The temperatures ranged from 909 - 1500 K. The simulations were then validated in the lab against pure ammonia data acquired from a high-pressure shock tube in a temperature range of 1100 – 1600 K, pressures of 20 and 40 bar, and equivalence ratios of 0.5 and 1.0. The simulations resulted in a conclusion that additives are needed for the use of NH3 as a fuel due to its low reactivity and high IDTs. The NH3/H2 fuel blend was found to be the most optimal in high-temperature internal combustion engines, and NH3/DME blends were determined to be the most viable for low-temperature internal combustion engines due to their high reactivity. Shock tube experimental results will be compared with the kinetic modeling results to gauge the reliability of the predictions. In addition, the influence of diethyl ether addition to the combustion behavior of ammonia will be compared with other blends, and discussed accordingly.

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