



Development and Validation of Combustion Kinetic Mechanisms for Ammonia-Diesel Dual-Fuel Engines

Dong Han, Zhiyu Shang, Yuxiao Qiu, Zhen Huang

*Dong Han, dong_han@sjtu.edu.cn

Key Laboratory for Power Machinery and Engineering, Ministry of Education, Shanghai Jiao Tong University, Shanghai 200240, China

The application of ammonia as a carbon-free fuel in internal combustion engine can effectively solve the carbon emissions problem in the transportation sector. To accurately predict the combustion process and emissions characteristics of ammonia/diesel dual fuel engines, an ammonia/n-heptane combustion mechanism consisting of 138 species and 963 reactions was constructed. The zero-dimensional homogeneous reactor from CHEMKIN with variable volume profile was used for ignition delay verification against experimental results of ammonia/diesel blends. By coupling the combustion mechanism with a three-dimensional numerical model, the engine combustion and emissions of diesel-ammonia fuels with different ammonia energy ratios (AERs) were compared. The results show that this mechanism has more satisfactory predictive effects than the literature existing mechanisms in the fuel ignition delay time (IDT) at engine operation conditions, especially at high pressure and high AERs conditions. Through a kinetic analysis, ammonia inhibits ignition by competing with n-heptane in low-temperature reactions for radicals such as OH and HO₂, leading to weakened combustion intensity. Furthermore, the numerical calculations for engine combustion were conducted with different AERs, in which gaseous ammonia was injected into the intake port and mixed with air, and then ignited by diesel direct injection. The simulated cylinder pressures and heat release rates were in well accordance with the experimental results, and the trend of nitrogen-based emissions was also generally consistent with the experimental phenomena. As the AER increases, the ignition time of pre-injection fuel is retarded, and the peak heat release rate of pre-injected fuel gradually decreases. It is indicated that the weakened combustion intensity increases unburned NH₃ by 62% and fuel-source NO_x by 37%.