Development of multi-component diesel surrogate fuel models – Part II: Validation of the integrated mechanisms in 0-D kinetic and 2-D CFD spray combustion simulations

The aim of this study is to develop compact yet comprehensive multi-component diesel surrogate fuel models for computational fluid dynamics (CFD) spray combustion modelling studies. The fuel constituent reduced mechanisms including n-hexadecane (HXN), 2,2,4,4,6,8,8-heptamethylnonane (HMN), cyclohexane (CHX) and toluene developed in Part I are applied in this work. They are combined to produce two different versions of multi-component diesel surrogate models in the form of MCDS1 (HXN + HMN) and MCDS2 (HXN + HMN + toluene + CHX). The integrated mechanisms are then comprehensively validated in zero-dimensional chemical kinetic simulations under a wide range of shock tube and jet stirred reactor conditions. Subsequently, the fidelity of the surrogate models is further evaluated in two-dimensional CFD spray combustion simulations. Simulation results show that ignition delay (ID) prediction corresponds well to the change of fuel constituent mass fraction which is calculated to match the cetane number (CN). In addition, comparisons of the simulation results to the experimental data of #2 diesel fuel (D2) in a constant volume combustion chamber show that IDs and lift-off lengths are reasonably well replicated by the models. The MCDS2 model is also found to perform better in the soot formation prediction in D2 fuel combustion as the model contains aromatic and cyclo-alkane components which provide an additional pathway to the formation of rich species such as C2H2 and C6H6. Implementation of MCDS2 predicts an increase of maximum local soot volume fraction by a factor of 2.1 when the ambient temperature increases from 900 K to 1000 K, while the prediction by MCDS1 is lower at 1.6. This trend qualitatively agrees with the experimental observation. This work demonstrates that MCDS1 serves as a potential surrogate fuel model for diesel fuels with CN values ranging from 15 to 100. It also shows that MCDS2 is a more appropriate surrogate model for fuels with aromatics and cyclo-paraffinic contents, particularly when soot calculation is of main interest.

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