Development and validation of a generic reduced chemical kinetic mechanism for CFD spray combustion modelling of biodiesel fuels

In this reported work, a generic reduced biodiesel chemical kinetic mechanism, with components of methyl decanoate (C_{11}H_{22}O_{2}, MD), methyl-9-decenoate (C_{11}H_{20}O_{2}, MD9D) and n-heptane (C_{7}H_{16}) was built to represent the methyl esters of coconut, palm, rapeseed and soybean. The reduced biodiesel mechanism with 92 species and 360 elementary reactions was developed using reduction techniques of directed relation graph (DRG), isomer lumping and temperature sensitivity analysis. The reduced biodiesel mechanism was then validated under various shock tube conditions against experimental measurements and detailed mechanism predictions, for each zero-dimensional (0D) auto-ignition and extinction process using CHEMKIN-PRO. Maximum percentage errors of less than 40.0% were recorded when the predicted ignition delay (ID) periods for coconut, palm, rapeseed and soybean methyl esters were compared to those of the respective detailed mechanisms. Predicted key species profiles in extinction process for each biodiesel fuel such as hydroxyl (OH), hydroperoxyl (HO_2), carbon dioxide (CO_2), ethylene (C_2H_4) were also found to be in reasonable agreement to those produced from the respective detailed mechanism, with a maximum deviation of 1 order in the mole fraction values. Meanwhile, satisfactory agreement was achieved when the predictions of reduced mechanism were compared against the measured ID periods of MD auto-ignition event in shock tube conditions and key species profiles of RME oxidation in jet stirred reactor (JSR). In the next stage of extended validation, the reduced biodiesel mechanism was implemented for two-dimensional (2D) computational fluid dynamics (CFD) spray combustion modelling, with initial temperatures of 900K and 1000 K at an ambient density of 22.8kgm^{-3}. Based on the simulation results, liquid penetration for soybean biodiesel was accurately predicted by the reduced mechanism as compared to the experimental data. Good agreements in the ID and lift-off length predictions were also achieved, where the ID was only advanced by 2.8% while the lift-off length was over-predicted by 17.3% from the experimental measurements when the initial temperature was 900K. Meanwhile, the predicted ID and lift-off length at the initial temperature of 1000K were both over-estimated by 29.8% and 43.4%, respectively. Thus, the reduced biodiesel mechanism formulated here is essentially accurate in predicting the in-cylinder ignition, combustion and extinction phenomena.

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