Development of multi-component diesel surrogate fuel models – Part I: Validation of reduced mechanisms of diesel fuel constituents in 0-D kinetic simulations

In the present work, development and validation of reduced chemical kinetic mechanisms for several different hydrocarbons are performed. These hydrocarbons are potential representative for practical diesel fuel constituents. n-Hexadecane (HXN), 2,2,4,4,6,8,8-heptamethylnonane (HMN), cyclohexane (CHX) and toluene are selected to represent straight-alkane, branched-alkane, cyclo-alkane and aromatic compounds in the diesel fuel. A five-stage chemical kinetic mechanism reduction scheme formulated in the previous work is applied to develop the reduced HMN and CHX models based on their respective detailed mechanisms. Alongside with the development of the reduced CHX model, a skeletal toluene sub-mechanism is constructed since the elementary reactions for toluene are subset of the detailed CHX mechanism. The final reduced HMN mechanism comprises 89 species with 319 elementary reactions, while the final reduced CHX mechanism which includes the toluene sub-mechanism consists of 80 species with 287 elementary reactions. Both reduced models are approximately 92% smaller than their respective detailed models in terms of total number of species and elementary reactions. Following that, both the newly developed fuel constituent reduced mechanisms, together with the formerly derived reduced HXN mechanism are comprehensively validated in zero-dimensional chemical kinetic simulations under a wide range of shock tube and jet-stirred reactor (JSR) conditions. Well agreement between the reduced and detailed mechanisms is achieved for ignition delay (ID) and species concentration predictions under both auto-ignition and JSR conditions, with a maximum relative error of 40%. In addition, the reduced models are further validated against the JSR experimental results for each diesel fuel constituents. The surrogate models are able to reasonably reproduce the experimental species concentration profiles in view of their simplified fuel chemistries. Deviations within one order of magnitude in the absolute values are recorded between the computations and measurements. Validation of these reduced models for each diesel fuel constituents in this work serves as a prerequisite for constructing a multicomponent diesel surrogate fuel model. The compact yet accurate chemical models proposed here aid to reduce the chemistry size of the final multi-component diesel surrogate model such that it remains computationally efficient when it is incorporated with multi-dimensional CFD simulations. The reduced mechanism of each fuel constituent can also be used individually for other CFD applications.
Mechanism reduction, Diesel fuel, Branched-alkanes, Cyclo-alkanes, Aromatics

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