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Development of Simplified Reaction Models for Natural Gas Combustion Using Combined Global Optimization Methods

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Detailed chemical kinetic mechanisms are wildly used to simulate the combustion of hydrocarbons. However, the simulation tasks can become expensive or even unfeasible as the complexity, i.e. the number of carbon atoms in the fuel increases. It can be particularly problematic in large-scale CFD simulations. Thus, several methods were introduced to create simpler models and decrease the computational demand, such as developing skeletal mechanisms, optimization, lumping or tabulation approaches. In our previous works [1,2] Genetic Algorithm (GA) and Simplified Reaction Pathway (SRP) methods were used successfully to generate simplified reaction models for methane, natural gas and ammonia.

This method involves setting up a simplified reaction scheme for the hydrocarbon oxidation consisting of virtual species and reactions, and the detailed chemistry of H_2/CO/O_2 system. A simplified 14-species model was created for natural gas oxidation with the following virtual reaction scheme: FUEL→R→IO→CO, where FUEL, R, and IO are virtual species for the fuel, fuel radical, and aldehyde, respectively. CH_4 was used as FUEL in the mechanism, and an ideal surrogate mixture of $CH_4/C_2H_6/C_3H_8/n\text{-}C_4H_{10}/i\text{-}C_4H_{10}$ = 96.91/2.33/0.54/0.10/0.12 was assumed for the thermodynamic and transport properties which were taken from AramcoMech 3.0 [3] mechanism. For R and IO, the properties of CH_3, and CH_2O were used, respectively. GA was used to determine the rate parameters of 30 virtual reactions by minimizing an error function characteristic for the difference between the simulation results of the detailed and the simplified mechanisms. This method could feasibly provide a model of which performance well approached the performance of the detailed model on simulating ignition delay times and laminar burning velocities. Though, this method can provide feasible parameter set, it can be time consuming to find the best set with the lowest objective function value.

Thus, after finding an appropriate parameter set for the virtual reactions, the FOCTOPUS [4] global optimization method developed by Turányi and coworkers [5] were used to find the best parameter set more efficiently. This method was developed for the optimization of detailed models with systematic search of Arrhenius parameters of the most influential reactions within their uncertainty domain. It was now successfully applied for the optimization of a simplified reaction model. The model, generated with GA-SRP and optimized with FOCTOPUS, could well reproduce the simulation results of the detailed mechanism for speciation data in perfectly stirred reactors for major species, e.g. CO and CO_2, in addition to ignition delay times and laminar burning velocities which were used in the objective function value in GA.

References

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