A Detailed Kinetics Model for the Combustion of Diisopropyl Ketone

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Recently, several classes of endophytic fungi have been identified that convert cellulosic biomass to a variety of oxygenated molecules, including several ketones and cyclic ethers, which are potentially viable as biofuels [1,2]. To evaluate the viability of these candidate biofuels, their combustion chemistry must be understood. This understanding will allow for identification of the most promising candidates, which can then become the focus of efforts to biologically engineer the production of these species. A detailed kinetics model for the combustion of novel fuels is also important for use in the development of the next generation of engines, such as the homogenous charge compression ignition (HCCI) engine.

This work presents a new detailed kinetics model for the combustion of diisopropyl ketone (2,4-dimethylpentanone), generated automatically using the Reaction Mechanism Generator (RMG) software package. RMG estimates the thermodynamic and kinetic parameters needed for detailed kinetics models by querying a database of rules and heuristics for similar species and reactions. Several new and improved rate rules have been added to the RMG database in order to improve the performance of the diisopropyl ketone model. The model has been evaluated against experimental ignition delays from our team's rapid compression machine measurements, which show a significant region of negative temperature coefficient (NTC) behavior. Autoignition chemistry is of vital importance in modeling the NTC region, particularly R + O_2 peroxy chemistry and pressure dependent rate coefficients. The model has also been evaluated using Multiplexed Photoionization Mass Spectrometry (MPIMS) measurements by our team.

References

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