Development of comprehensive chemical kinetic mechanism for ammonia/methanol mixture

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Abstract

A thorough understanding of ignition delay time (IDT) is essential for engine design and validation of chemical kinetic mechanisms for alternative fuels such as ammonia (NH_3). The low reactivity of NH_3 restricts its application in the transport sector, whereas adding methanol (CH_3OH) as a combustion promoter enhances the reactivity. The fundamental chemistry in the combustion of newly proposed fuels can be studied using the detailed chemical kinetic mechanism. In this work, a kinetic model for auto-ignition of the NH_3/CH_3OH fuel blend was automatically generated by RMG, which contains four new reactions. Two of these estimated reactions by RMG are the H atom abstraction of CH_3OH by NH_2 radical, where the calculation of the reaction rates was repeated by ab-initio calculation. The ab-initio calculations showed more reliability than RMG results compared to the reaction rates of the same class of reactions in literature. Then an in-house algorithm was developed to reduce the size of the mechanism to 460 reactions.

The mechanism was validated using the experimental results for the IDT of NH_3/CH_3OH from the literature at high pressures and intermediate to high temperatures for fuel mixtures containing 1-20% CH_3OH. Also, numerical simulations of LBV of NH_3/CH_3OH mixtures containing 20-80% of CH_3OH at atmospheric pressure were compared to experimental data to help in the further validation of the generated mechanism. The model provided the analysis of reaction rates and sensitivity analyses. Further investigation with the kinetic model showed that the reactions involving C- and N-containing species are significant for the autoignition of different NH_3/CH_3OH mixtures.