Global Sensitivity Analysis of the Butanol Combustion Mechanism

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Butanol has become the focus of recent interest as a potential biofuel. As such, it is important to develop reliable butanol combustion models to aid in the optimization of the combustion conditions and the design of fuel blends. We have recently developed a new technique to systematically improve chemical kinetic models using first global sensitivity analysis to identify key reaction steps, followed by high level theoretical modeling to improve the rate coefficients for targeted reactions.(1,2) In the present work we apply this mechanism improvement scheme to the 1600 reversible-step butanol combustion model of Curran and coworkers (3). It is found that the HO_2+n-C_4H_9OH reaction is most crucial in setting the ignition delay time. However, other steps are identified as more important for the growth of measurable intermediate species in the pre-ignition phase of the kinetics. It is shown that model is improved by the theoretical update of the targeted reactions.

References

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