Detailed Kinetic Model for *Iso*-Butanol Pyrolysis and Combustion

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Despite the extensive use of ethanol as a renewable transportation fuel, it is believed that it is not the ideal alternative to gasoline (1, 2). Higher chain alcohols (C3-C5) are considered best options because they have higher energy densities, lower vapor pressures and lower hygroscopicity, with several practical positive effects on combustion engines (2-4). *Iso*-butanol not only presents all the aforementioned advantages when compared to ethanol, but its "production process has already reached near-industrial level" (4).

In the current investigation we present a comprehensive kinetic mechanism for iso-butanol combustion. The kinetic mechanism is generated using the open source software package Reaction Mechanism Generator (RMG) and includes pressure-dependent kinetics. The mechanism is tested against a large number of new and recently published data including – pyrolysis product profiles in plug flow reactor and shock tube, jet-stirred reactor mole fraction profiles, opposed flow diffusion flame mole fraction profiles, laminar flame speeds at different pressures and autoignition delays in rapid-compression machine and high-pressure shock tubes. The isobutanol model predicts with great fidelity on all the above mentioned datasets – ignition delays and major product species are predicted within a factor of two in most cases, for low pressure flame the major radicals are within a factor of three of experimental measurements. A flux and sensitivity analysis is performed for the different datasets to reveal important pathways; of note is the pathway for keto-enol tautomerization in low pressure flames. It is seen in order to reasonably predict the keto- enol product distribution in low pressure flames it is essential to include accurate pressure dependent kinetics for direct and assisted tautomerization for various isomers in the model. To the author's knowledge this is one of the first mechanisms to accurately predict iso-butanol combustion over a wide range of conditions.

References

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