

## Kinetic Modelling of the Oxidation of Large Aliphatic Hydrocarbons Using an Automatic Mechanism Generation

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A mechanism generator code to automatically generate mechanisms for the oxidation of large hydrocarbons has been successfully modified and considerably expanded in this work. The modification was through (1) improvement of the existing rules such as cyclic-ether reactions and aldehyde reactions, (2) inclusion of some additional rules to the code, such as ketone reactions, hydroperoxy cyclic-ether formations and additional reactions of alkenes, (3) inclusion of small oxygenates, produced by the code but not included in the handwritten C<sub>1</sub>–C<sub>4</sub> sub-mechanism yet, to the handwritten C<sub>1</sub>–C<sub>4</sub> sub-mechanism. In order to evaluate mechanisms generated by the code, simulations of observed results in different experimental environments have been carried out. Experimentally derived and numerically predicted ignition delays of *n*-heptane–air and *n*-decane–air mixtures in high-pressure shock tubes in a wide range of temperatures, pressures and equivalence ratios agree very well. Concentration profiles of the main products and intermediates of *n*-heptane and *n*-decane oxidation in jet-stirred reactors at a wide range of temperatures and equivalence ratios are generally well reproduced. In addition, the ignition delay times of different normal alkanes was numerically studied.