

An Experimental Ignition Delay Time and Chemical Kinetic Modelling Study of 1-hexene

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Many liquid transportation fuels (e.g. gasoline) quickly decompose to the intermediate 1-hexene during oxidation, which subsequently limits the reaction progress of the charge towards ignition. The development of a chemical kinetic mechanism for the oxidation of 1-hexene at engine relevant conditions is therefore essential in order to accurately simulate the ignition chemistry for larger fuels; the aim of *this study* is to do so. To facilitate this study an experimental campaign was conducted where chemically isolated ignition delay times were measured for 1-hexane mixtures at $\phi = 1, 0.5$ and 2.0 , $p = 15$ and 30 bar, $T = 600 - 1300$ K in a shock tube and rapid compression machine. A chemical kinetic mechanism for the oxidation of 1-hexene, which has previously been validated against low-pressure laminar flame experiments, has been updated to account for the ignition chemistry of 1-hexene at the thermodynamic states of the newly reported experiments. In particular, reactions were added to the mechanism that consider the addition of molecular oxygen to fuel radicals, along with the subsequent isomerization and decomposition reactions toward stable products, in order to match simulation results with the ignition delay time measurements within the negative temperature coefficient regime. An overall good agreement is observed between simulations with the newly developed kinetic mechanism and the newly reported ignition delay time experiments.