

# Experimental and modeling investigation of the low-temperature oxidation of 1-hexene

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Olefins are an important class of molecules which can be found in fuels and which are also intermediates observed in oxidation reactions. Double bonds are also present in esters present in biodiesel fuels. The number and position of double bonds in molecules strongly affect the reactivity of the species as well as the nature of reaction products (1). It is then of importance to better understand the specific oxidation chemistry of molecules having double bonds. In the present work, a new set of experiments was carried out using a jet-stirred reactor with a particular care taken to the detection of branching agents (species with hydroperoxide groups) formed in the oxidation of 1-hexene. Hydrogen peroxide was quantified using cw-cavity ring-down spectroscopy. Other hydroperoxides were quantified using time-of-flight mass spectrometry combined with laser photoionization (10.6 eV). These species were methyl-hydroperoxide ( $\text{CH}_3\text{OOH}$ ), ethyl-hydroperoxide ( $\text{C}_2\text{H}_5\text{OOH}$ ), propyl-hydroperoxide isomers ( $\text{C}_3\text{H}_7\text{OOH}$ ), allyl-hydroperoxide ( $\text{C}_3\text{H}_5\text{OOH}$ ), hexenyl-hydroperoxide isomers ( $\text{C}_6\text{H}_{11}\text{OOH}$ ) and possibly  $\text{C}_6\text{H}_{10}\text{O}_3$  keto- / aldo-hydroperoxide isomers. This method enabled the detection of both propene and ketene which have close atomic mass.

A new detailed kinetic model, based on a previous work (2), was developed. Kinetic parameters of sensitive reactions were updated from recent literature theoretical calculations. These sensitive reactions are mainly those concerning the system composed of the fuel and OH radicals. The new set of kinetic parameters enabled a better prediction of the reactivity, especially at low temperature. The keto- and aldo-hydroperoxides, which were initially lumped into one virtual species, were considered individually. This led to a better prediction of aldehydes.

## References

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- (2) Bounaceur, R.; Warth, V.; Sirjean, B.; Glaude, P. A.; Fournet, R.; Battin-Leclerc, F. *Proceedings of the Combustion Institute* **2009**, 32 (1), 387–394.