

# Direct kinetic measurements of 1-butyl + O<sub>2</sub> reaction: capturing pressure and temperature dependencies

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Reactions of propyl and larger saturated free radicals R with O<sub>2</sub> are important reactions under low-temperature combustion conditions ( $T \approx 500 - 900$  K) due to their propensity to lead ketohydroperoxide formation.<sup>[1]</sup> Thermal decomposition of ketohydroperoxide leads to chain-branching that, in competition with chain termination and chain propagation reactions, initiates autoignition of hydrocarbon(fuel) – air mixture.<sup>[2]</sup>

In order to simulate a complex oxidation chemistry leading to ketohydroperoxide formation and subsequent autoignition, kinetics of R + O<sub>2</sub> reaction is required. However, very little is still known experimentally on kinetics of R + O<sub>2</sub> reactions for propyl and larger radicals based on direct measurements performed as a function of temperature and pressure.

In the current work we have measured kinetics of 1-butyl + O<sub>2</sub> reaction over a wide temperature and pressure range by employing excimer laser photolysis at 193 nm for the radical production and photoionization mass-spectrometer for following radical decays as a function of [O<sub>2</sub>] under pseudo-first-order conditions. Experiments were performed at low-pressures (~ 0.5 – 15 Torr) and temperature range extended well below room temperature. Master-equation calculations for the system will also be performed.

## References

- [1] a) S. S. Merchant, C. F. Goldsmith, A. G. Vandeputte, M. P. Burke, S. J. Klippenstein, W. H. Green, *Combust. Flame* **2015**, 162, 3658-3673; b) A. J. Eskola, O. Welz, J. Zador, I. O. Antonov, L. Sheps, J. D. Savee, D. L. Osborn, C. A. Taatjes, *Proceedings of the Combustion Institute* **2015**, 35, 291-298.
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