

Experimental and modeling oxidation study of alkyl-aromatics in a jet-stirred reactor at pressures up to 10 bar

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Supplementary Material

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Scheme of the new jet-stirred reactor

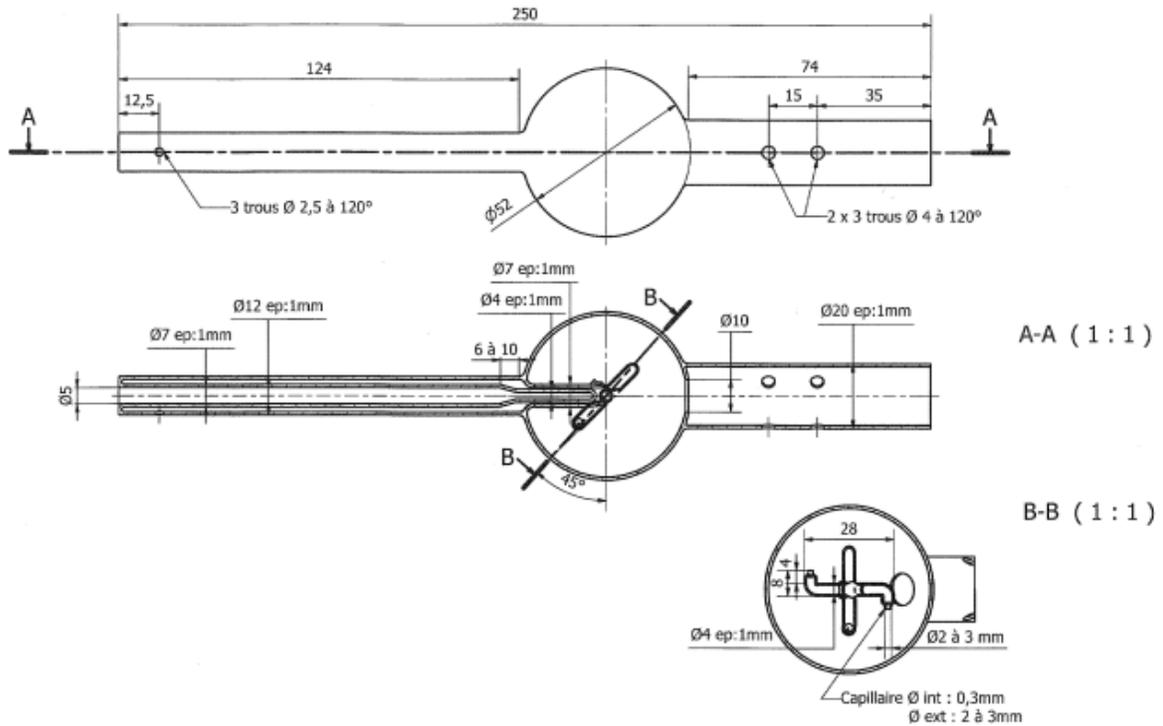


Figure S1: Scheme of the new jet-stirred reactor developed for experiments up to 10 bar.

Potential problems detected when using a sonic probe for sampling

The use of a capillary tube instead of a sonic probe was preferred during this work as the first tentative with a sonic probe led to the observation of strange phenomena. The first was the observation of the formation of many reaction products at the lowest pressure (2 bars) whereas no conversion was observed for *n*-heptane and oxygen (the calibration of the gas chromatograph was checked and could not be responsible). The second phenomenon was the occurrence of an unexpected break between 5 and 6 bars in the profiles of mole fractions of species. These two phenomena were not observed with the use of the capillary tube. Especially, the conversion of *n*-heptane was consistent with the formation of reaction products à 2 bars as illustrated in Figure S2. Further reactions in the probe due to an ineffective cooling cannot explain the inconsistency observed for the conversion of *n*-heptane (mass balance non-closure).

Sonic probes are made by hand by a glass blower and it is impossible to control their final geometry. Each piece is different. The advantage of a capillary tube is that the geometry is better defined as it is machine made. It is relatively easy to have a nice cut, which can be controlled using a magnifying glass.

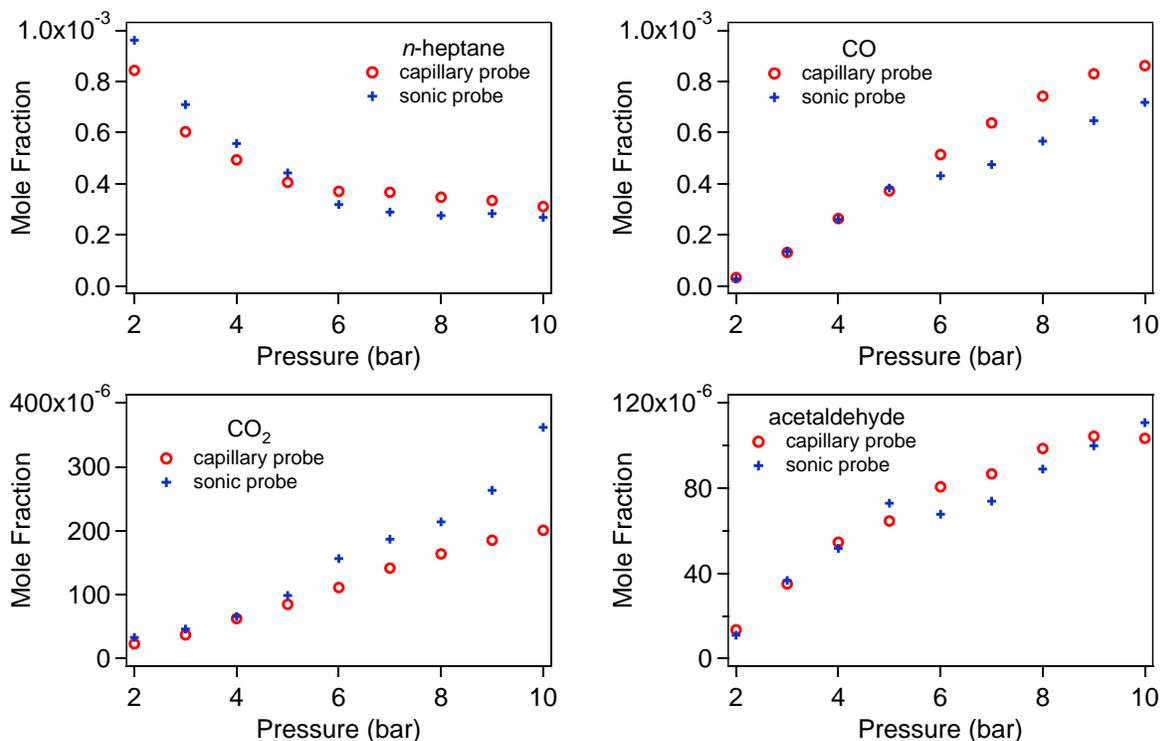


Figure S2: Comparison of data obtained with two different sampling methods during the oxidation of *n*-heptane in a jet-stirred reactor.

Data comparison between data obtained at 1 bar with the atmospheric pressure JSR and the 10 bar JSR devices

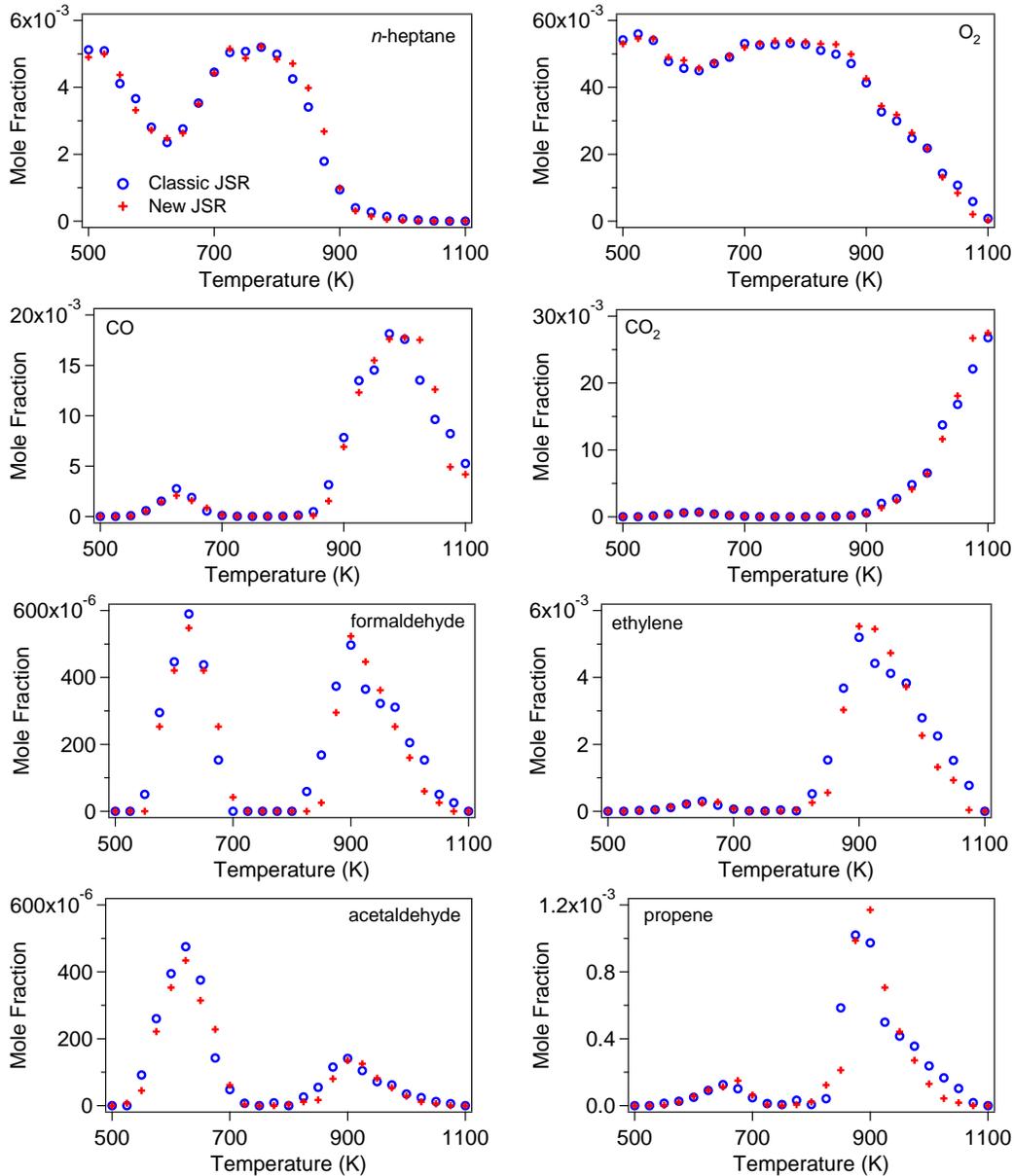


Figure S3: Comparison of data obtained with the classic JSR for studies at pressure close to the atmosphere and the new JSR for studies up to 10 bar ($P = 1.09$ bar, $\tau = 2.0$ s, $\varphi = 1$ and $x_{fuel}^{inlet} = 0.005$).

Reactions considered in the model of Zhang et al. [1]

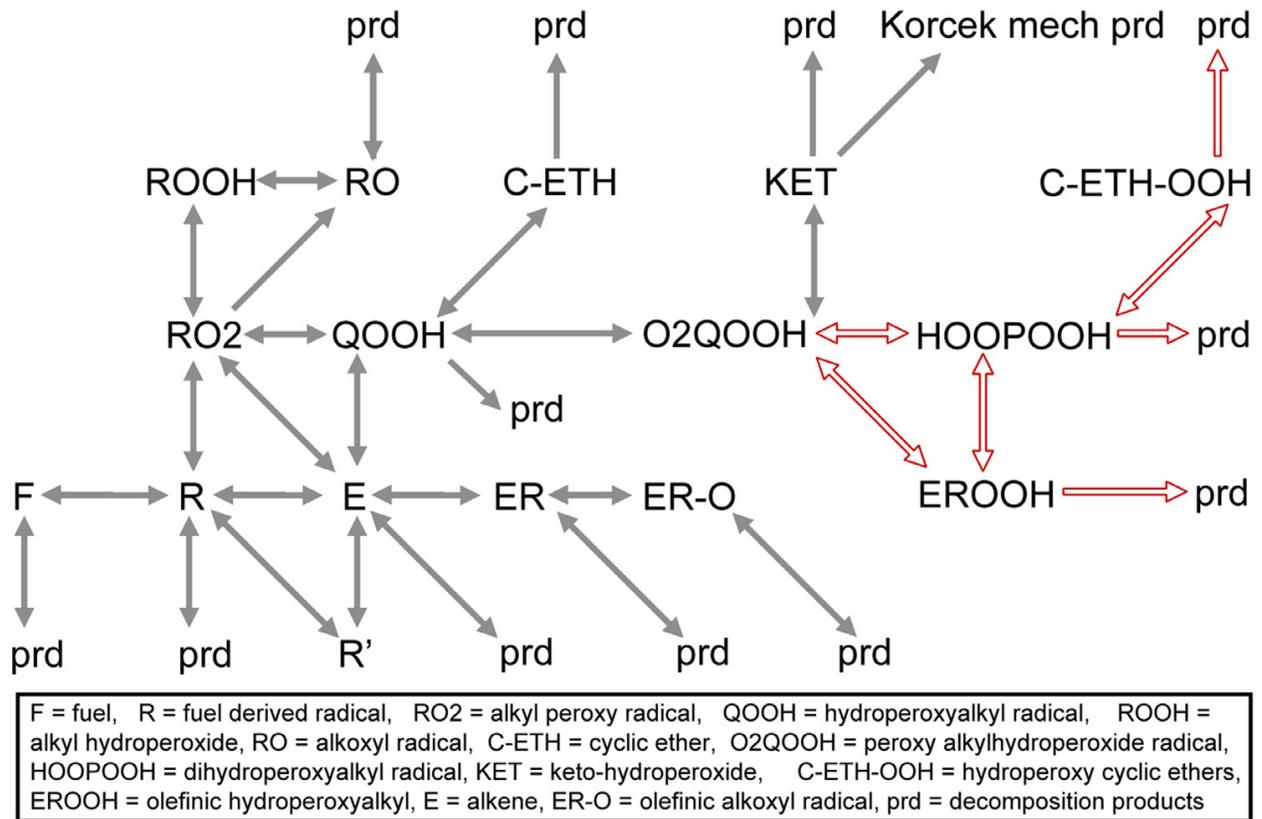


Figure S4: Reaction pathways considered in the development of this model as reproduced from [1].

References

- [1] K. Zhang, C. Banyon, J. Bugler, H.J. Curran, A. Rodriguez, O. Herbinet, F. Battin-Leclerc, C. B'Chir, K.A. Heufer, An updated experimental and kinetic modeling study of *n*-heptane oxidation, *Combust. Flame*. 172 (2016) 116–135.