

Supplemental Material

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New insights in the oxidation of *n*-butane in a jet stirred reactor using cw-CRDS measurements

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I/ Evolution with temperature of concentration of minor compounds of the oxidation of *n*-butane measured by gas chromatography

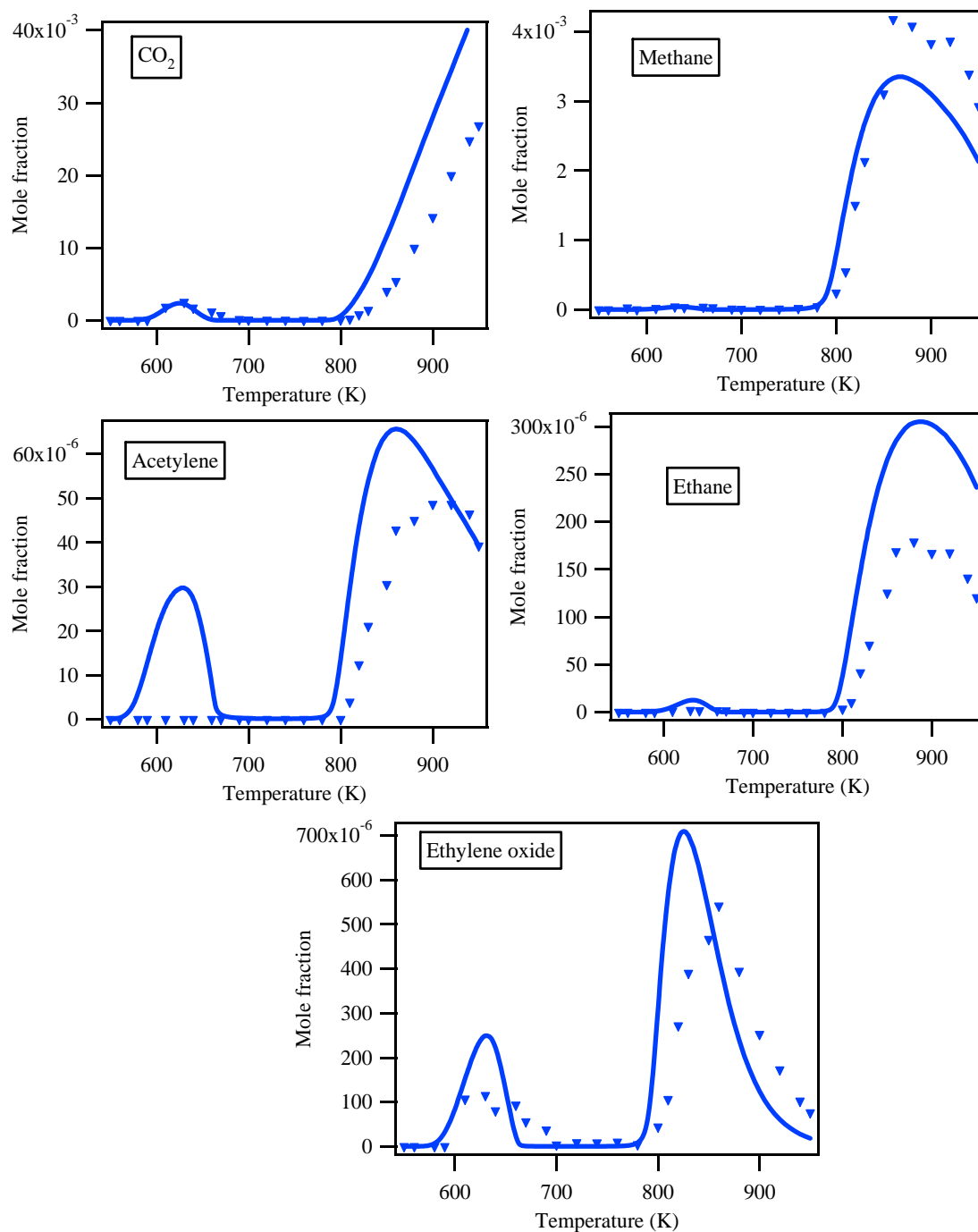


Figure S1: Evolution with temperature of the experimental (blues triangles) and simulated (full line) mole fractions of carbon dioxide, methane, acetylene and ethane.

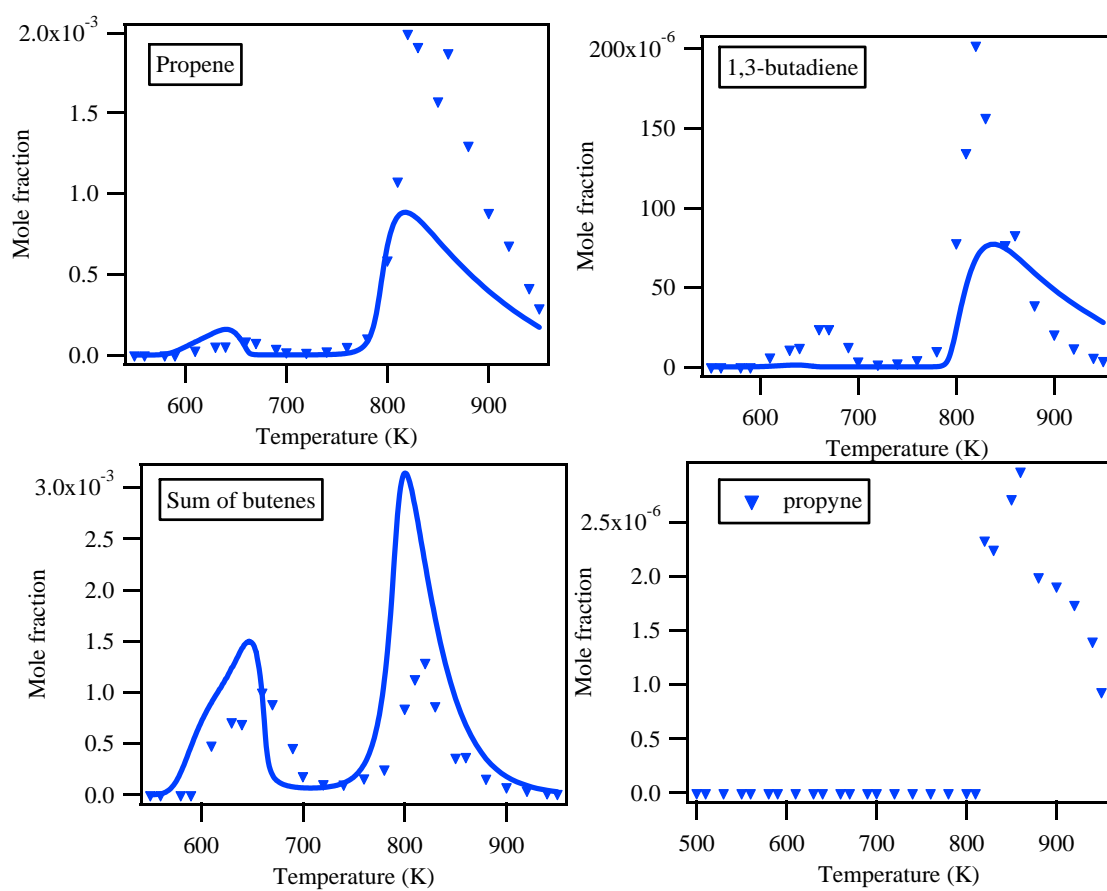


Figure S2: Evolution with temperature of the experimental (blues triangles) and simulated (full line) mole fractions of C₃-C₄ hydrocarbons. Propyne is not included in the used model.

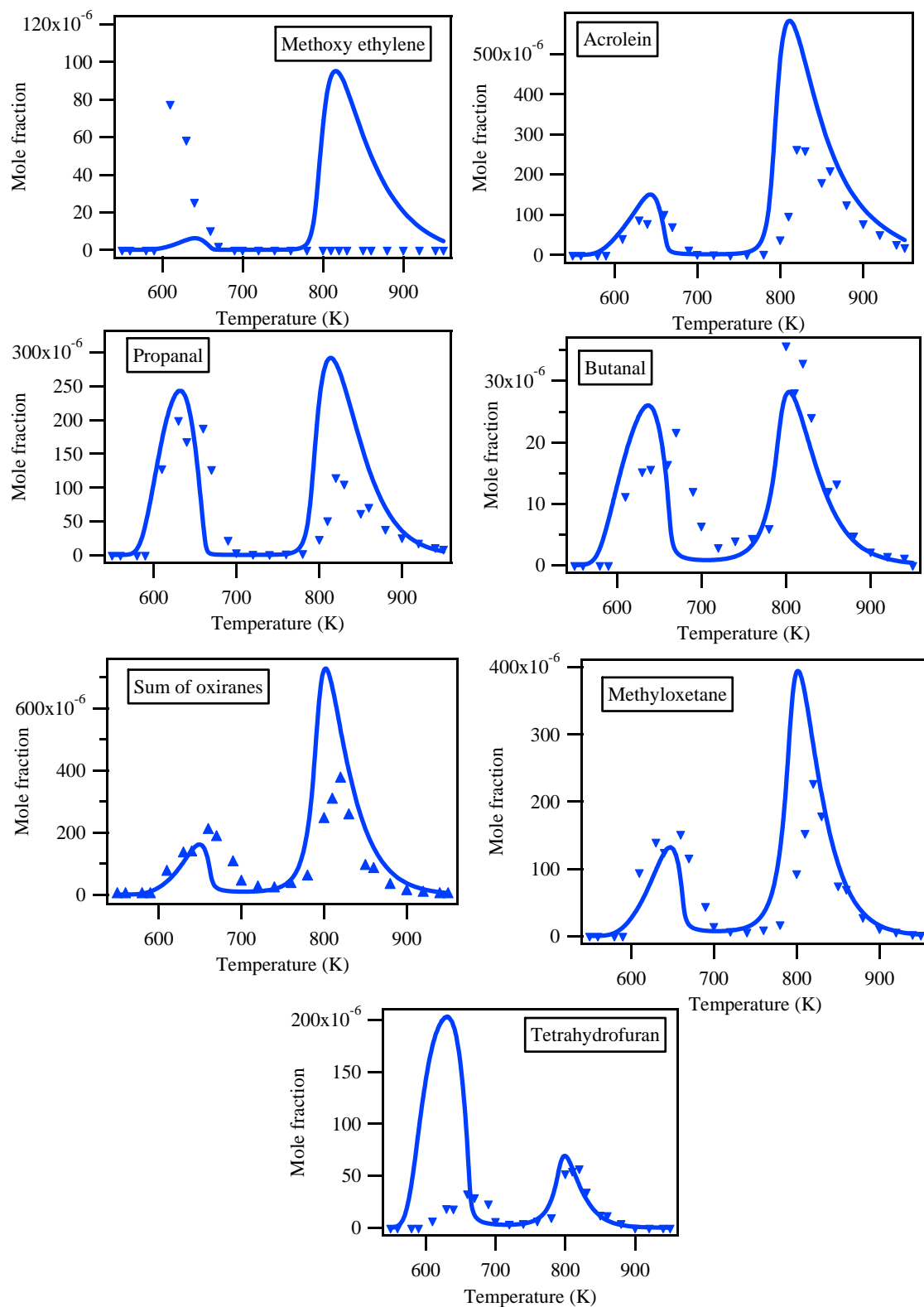
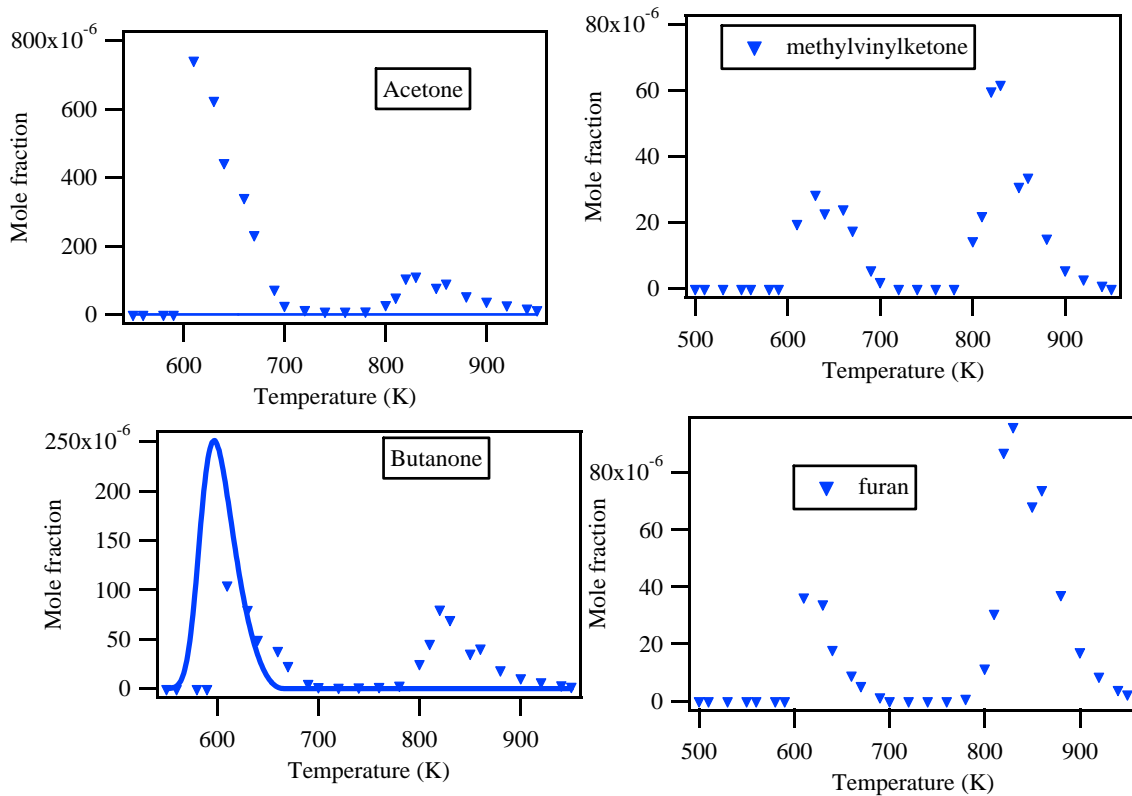


Figure S3: Evolution with temperature of the experimental (blues triangles) and simulated (full line) mole fractions of minor oxygenated species – part 1.

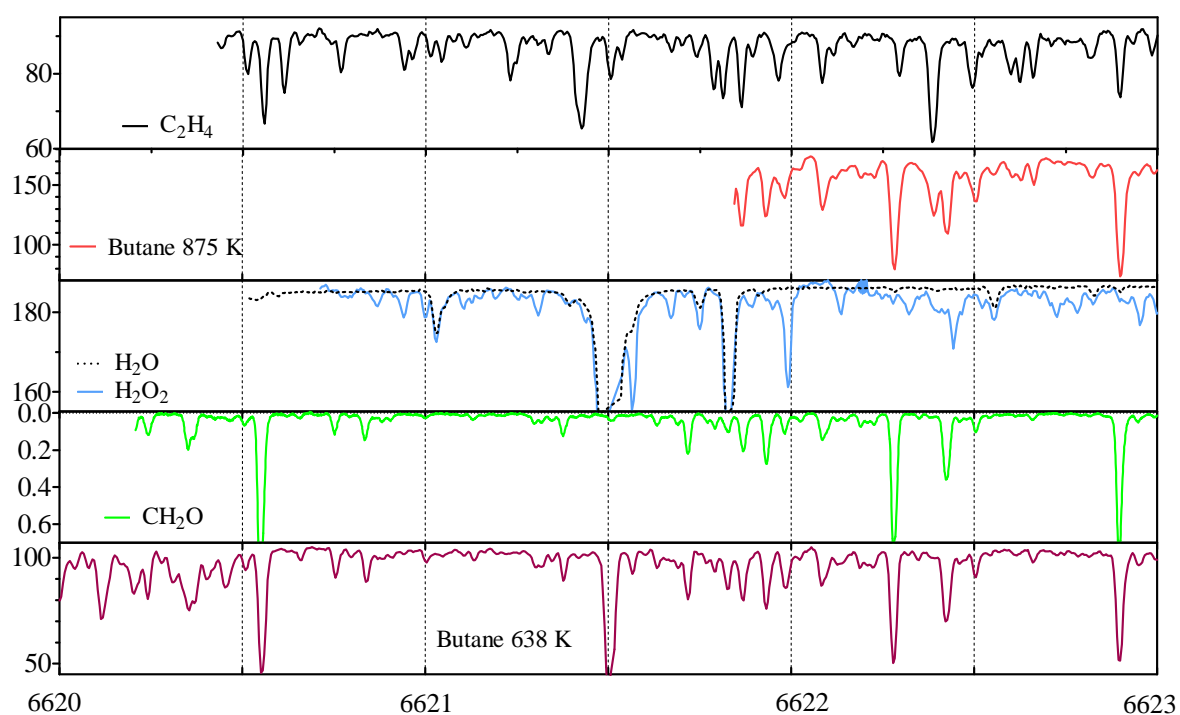


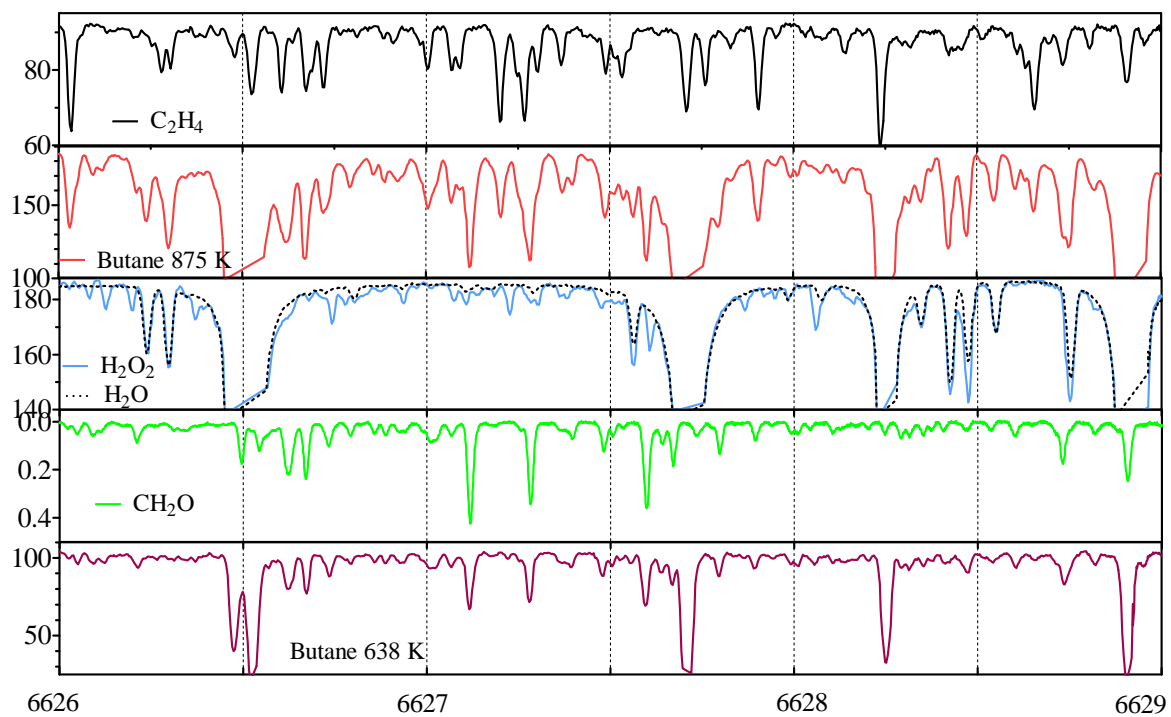
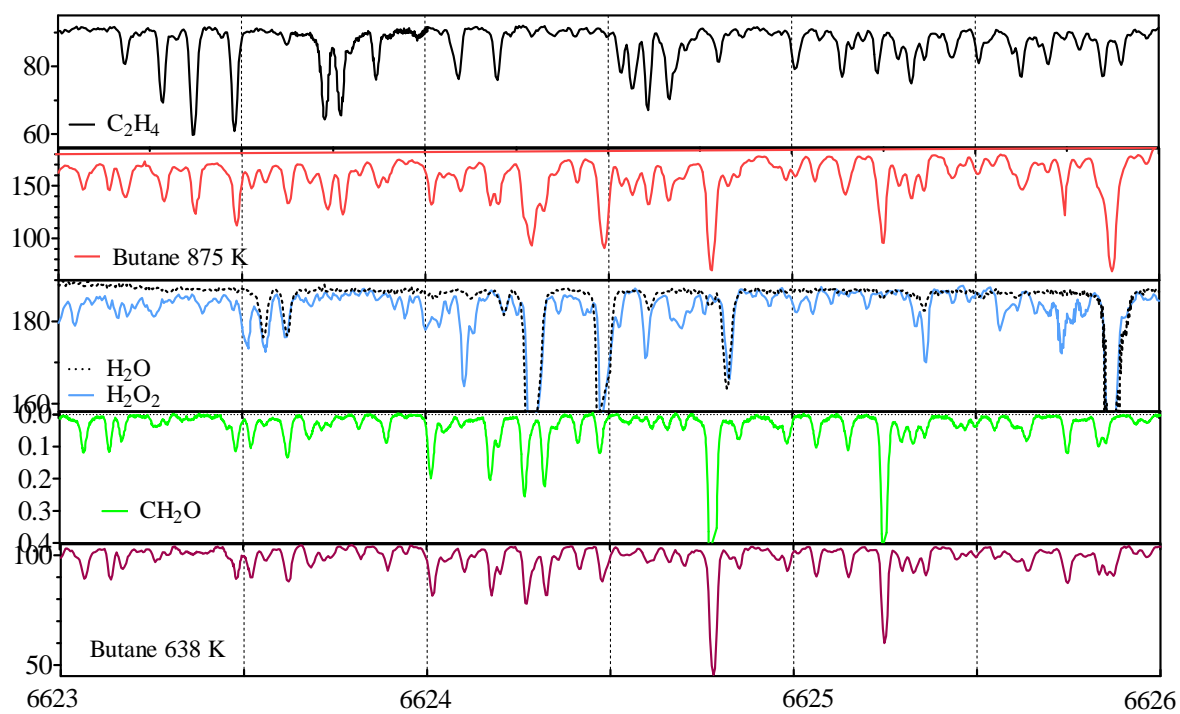
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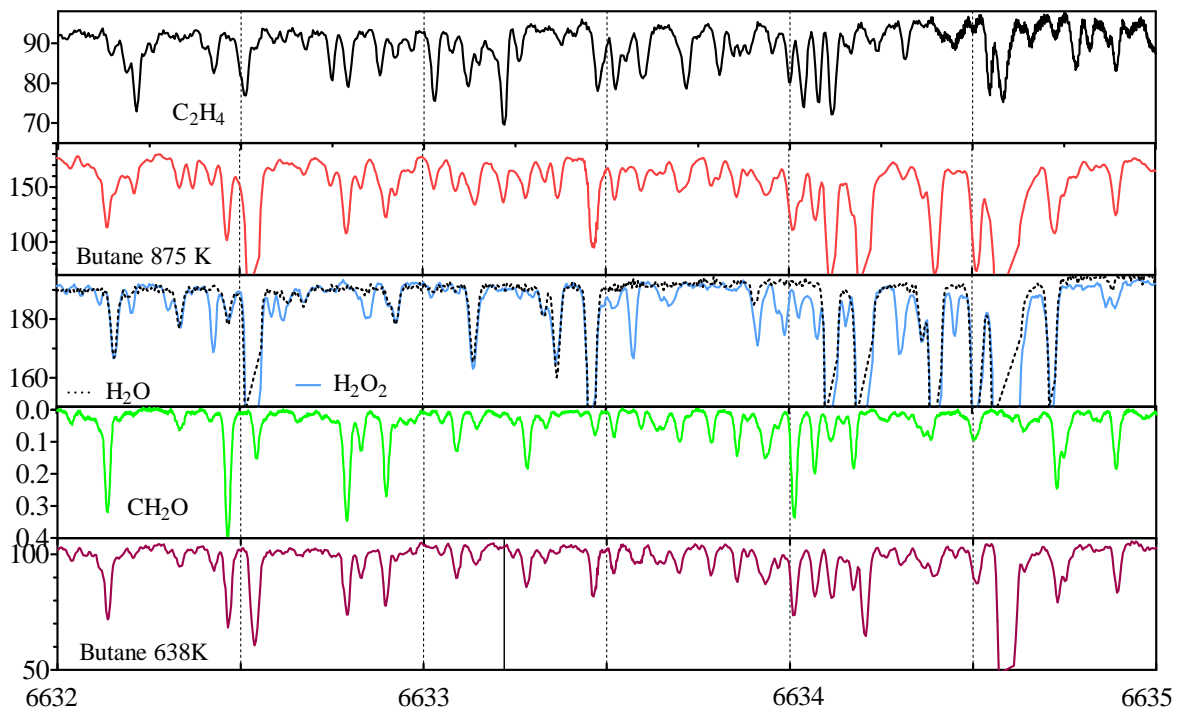
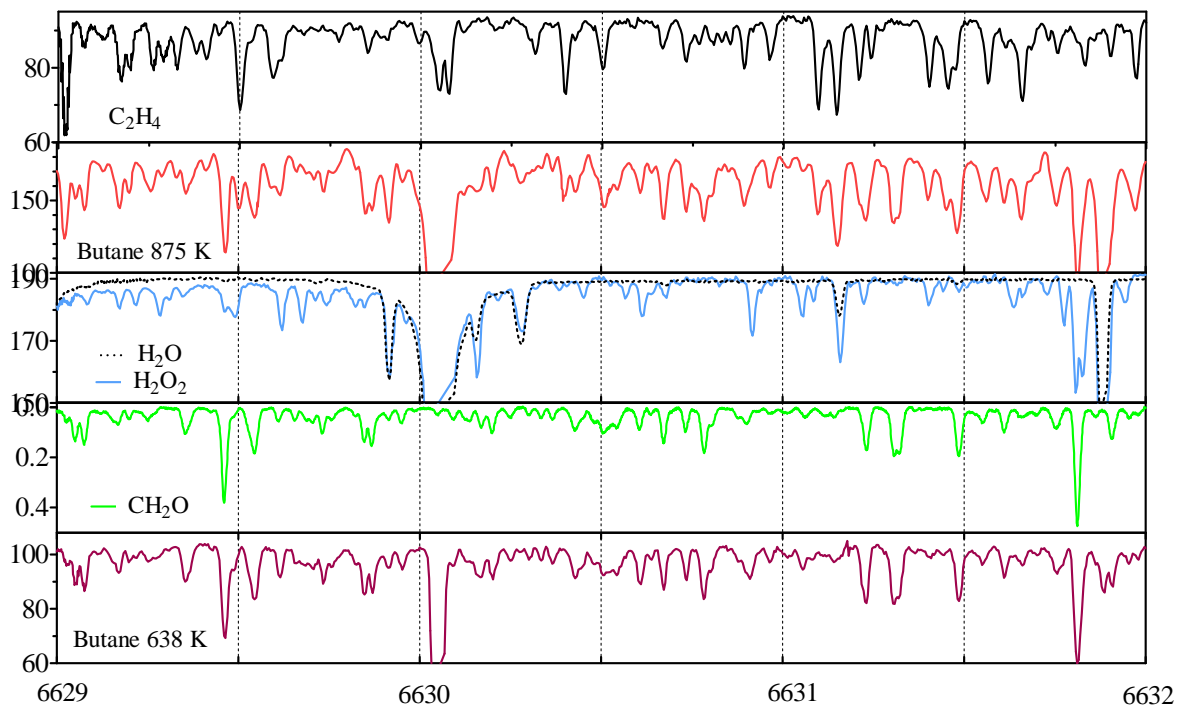
figure S4: Evolution with temperature of the experimental (blues triangles) and simulated (full line) mole fractions of minor oxygenated species – part 2. Acetone, methylvinylketone and furan are not included in the used model.

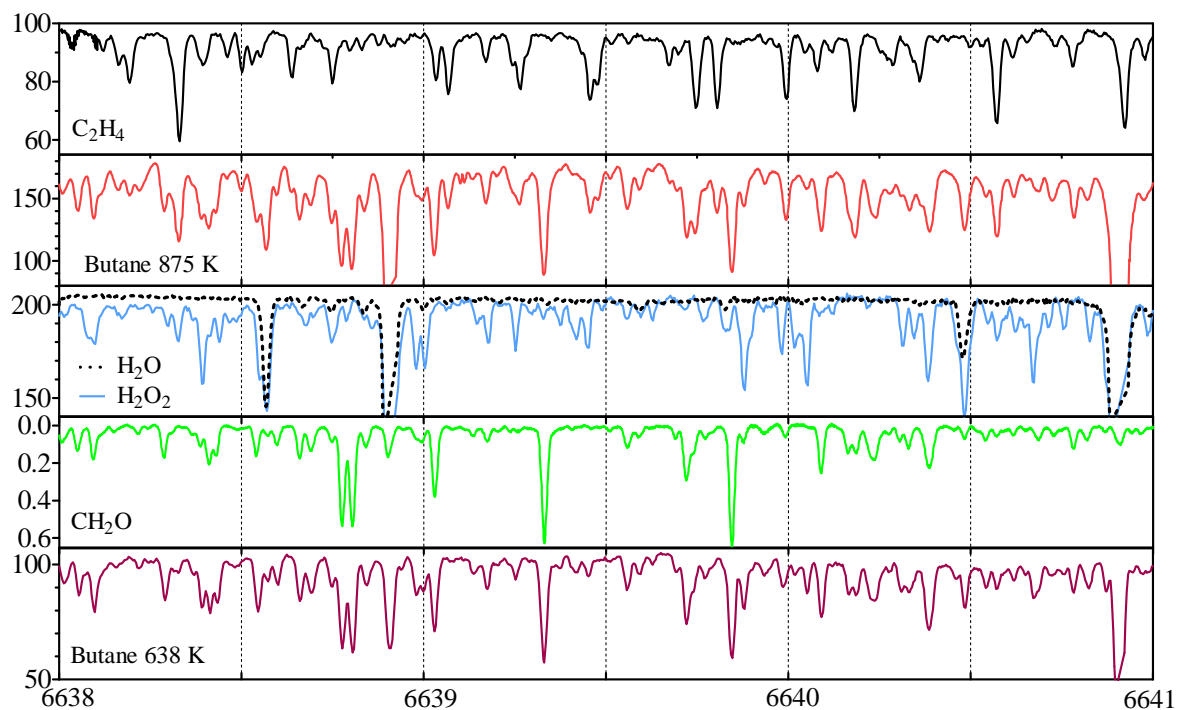
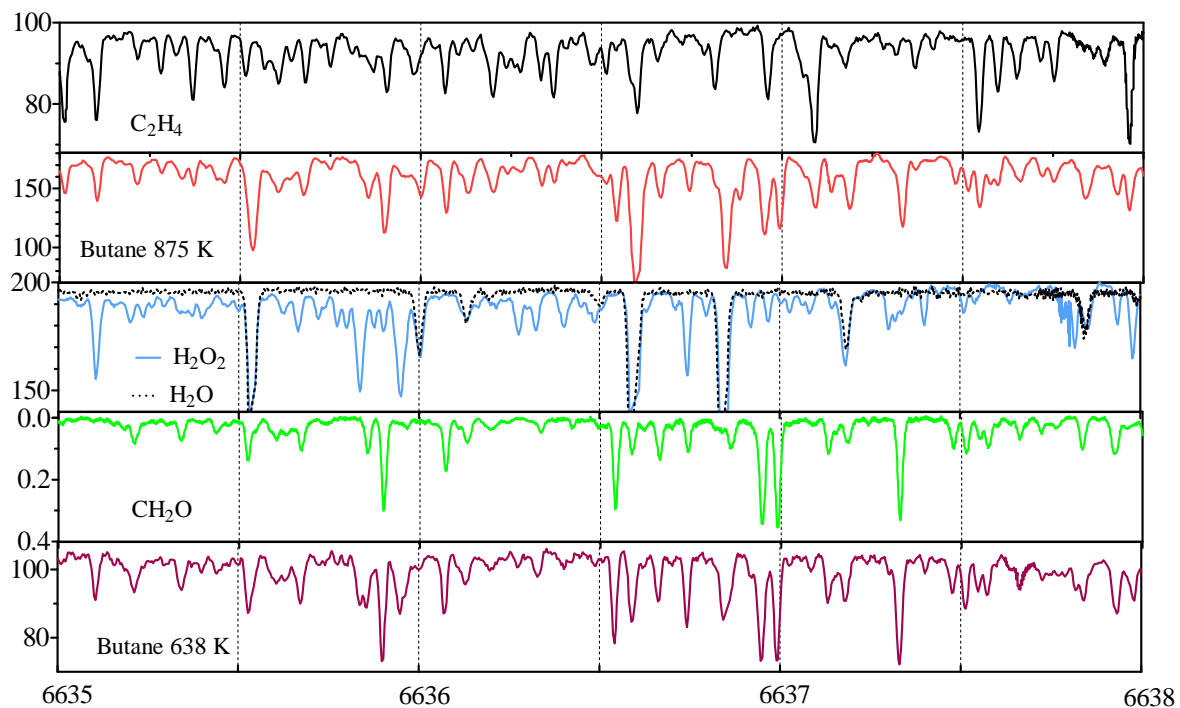
II/ Full absorption spectra

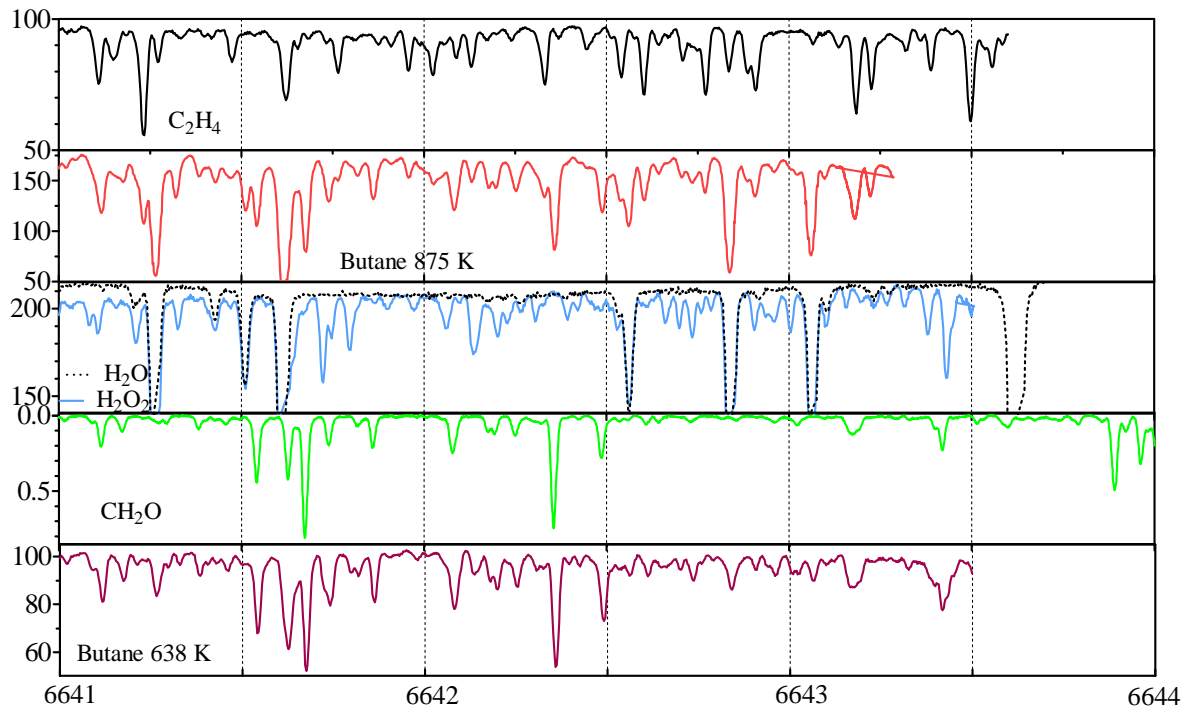
Figure S5 Absorption spectrum in the range 6620 - 6644 cm^{-1} for the major absorbing reaction products: units are ring down time τ as a function of wavenumber for H_2O_2 , H_2O and C_2H_4 , as well as the spectrum such as observed from the oxidation of n-butane at 638 K and 875 K, absorption cross sections σ in 10^{-21} cm^2 taken from Staak *et al*¹ for CH_2O











III/ Comparison between simulations using different mechanisms of the literature

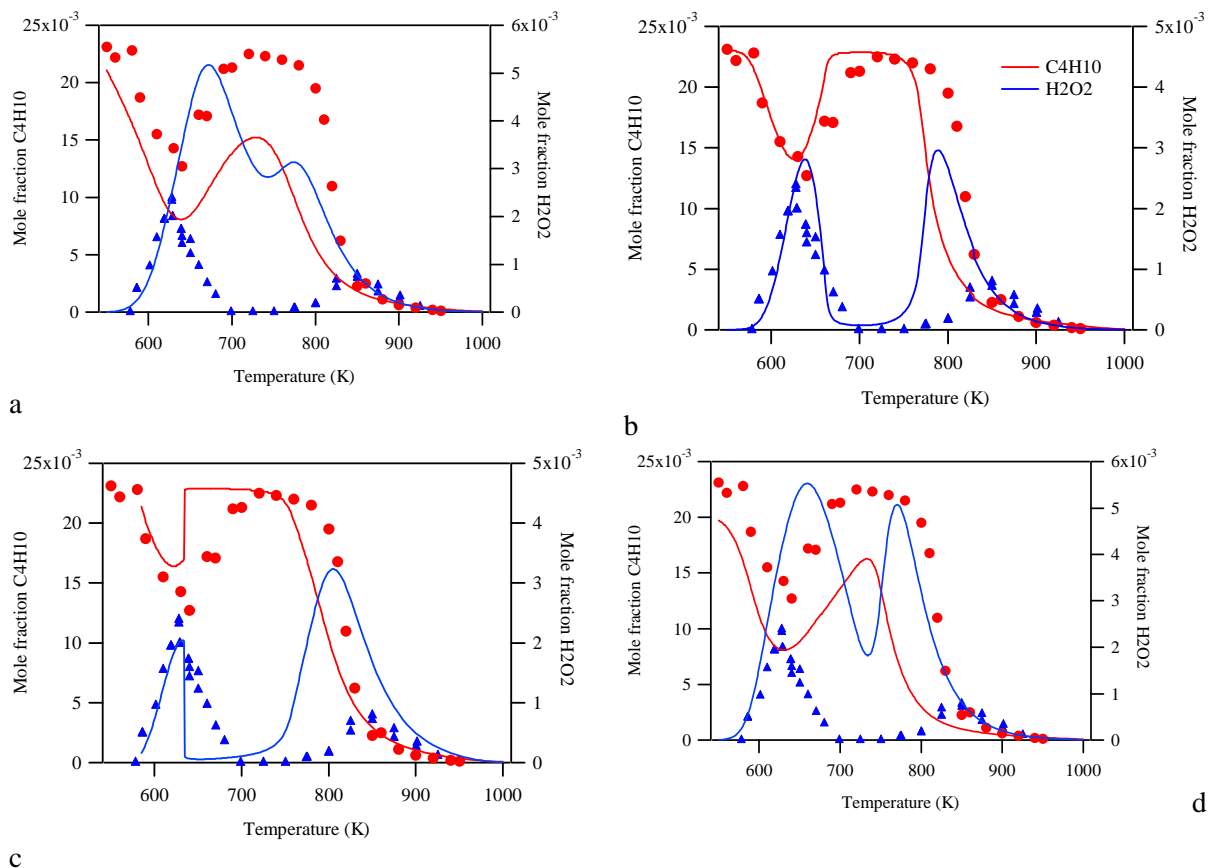


Figure S6: Comparisons between the experimental results (symbols) presented in this paper for the consumption of *n*-butane and the formation of H₂O₂ with simulations (lines) performed using different mechanisms of the literature: (a) a model automatically generated by software EXGAS as described by Buda et al.² and by Biet et al.³, (b) the mechanism of Battin-Leclerc et al.⁴, (c) the mechanism of Cord et al.⁵, and (d) the mechanism of Healy et al.⁶

IV/ Inert coating of the wall of the reactor



Figure S7. Photography of the treated reactor.

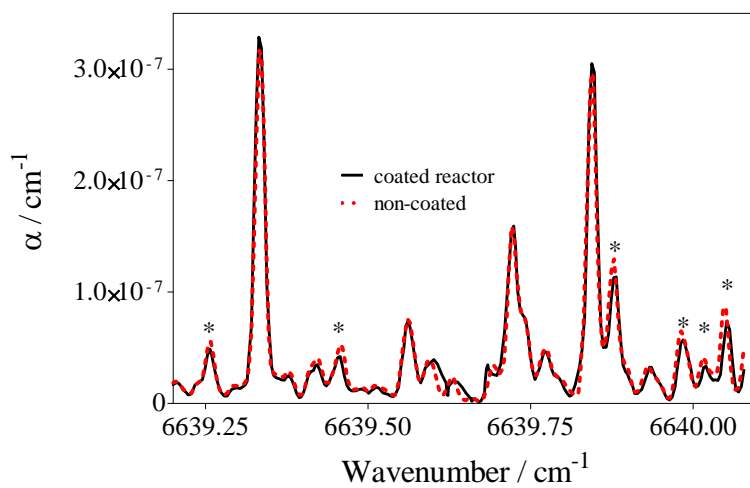


Figure S8. CRDS spectra obtained with reactor walls fully covered by the SilcoNert™ 2000 surface treatment and with reactor walls without any special treatment.

V/ Effect of wall reactions at different residence times and fuel initial mole fractions

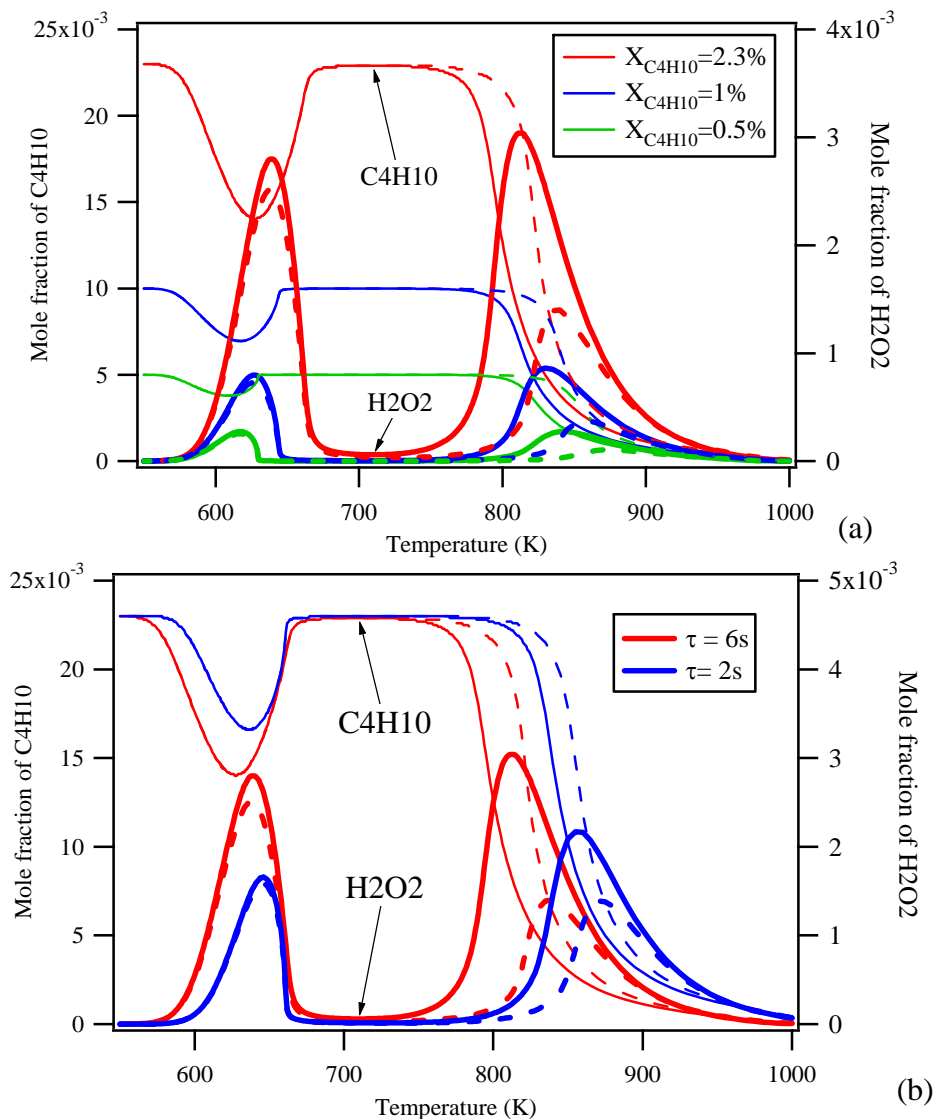


Figure S9: Influence of the wall reactions for the simulated consumption of *n*-butane (thin lines) and the formation of H_2O_2 (thick lines) for (a) different fuel initial mole fractions for a residence time of 6s and (b) different residence times (τ) for an initial fuel mole fraction of 2.3%. Full lines are simulation with the initial gas-phase mechanism dotted lines are simulations considering wall reactions.

VI/ Supplementary references

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