

Supplementary Material:

A first evaluation of butanoic acid oxidation kinetics

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1. Additional comparisons of model simulation and measurements of minor species.

Butanoic Acid

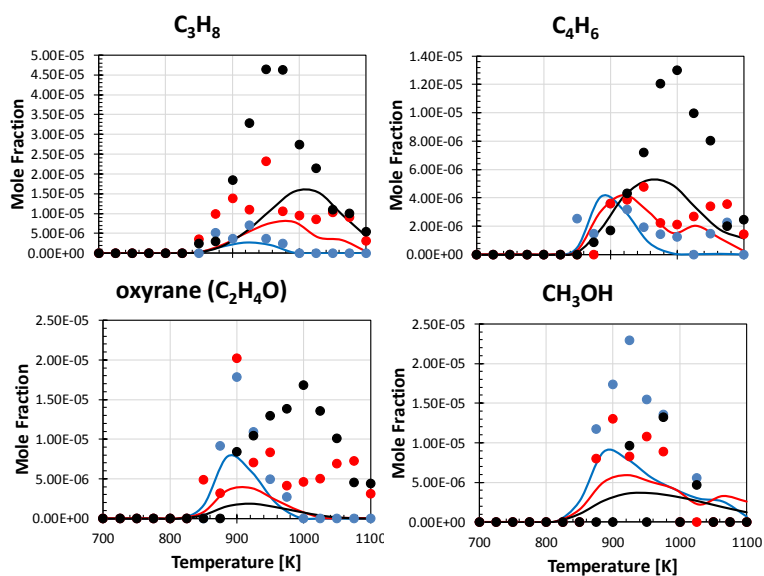


Figure S1: Additional comparison of measured species and model results in butanoic acid oxidation in JSR. Blue: $\phi=0.5$, red: $\phi=1$ and black: $\phi=2$.

Pentanoic Acid

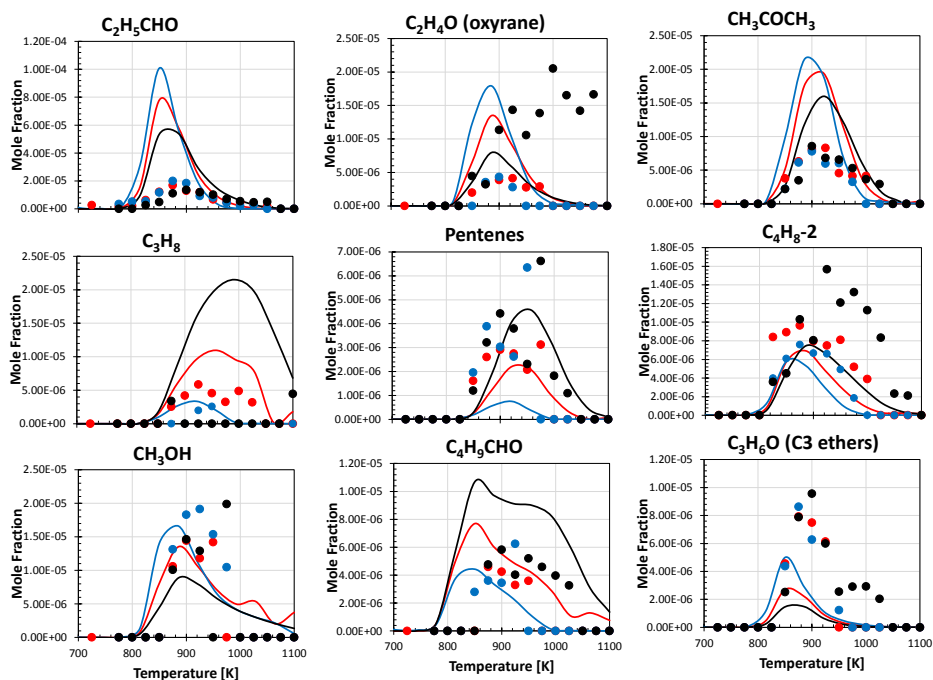


Figure S2: Additional comparison of measured species and model results in pentanoic acid oxidation in JSR. Blue: $\phi=0.5$, red: $\phi=1$ and black: $\phi=2$.

2. Main Species nomenclature

Table s1: Nomenclature of main species added to the CRECK model to describe butanoic and pentanoic acids oxidation.

	Name in mechanism	Brute Formula	Structure
Butanoic Acid and Radicals			
	C3H7COOH	C4H8O2	CH3-CH2-CH2-(C=O)OH
	RBUTANOICA	C4H7O2	CH3-CH2-*CH-(C=O)OH
	RBUTANOICB	C4H7O2	CH3-*CH-CH2-(C=O)OH
	RBUTANOICC	C4H7O2	*CH2-CH2-CH2-(C=O)OH
	C2H5CHCO (Ethylketene)	C4H6O	CH3-CH2-CH=C=O
	C3H5COOH-1 (Butenoic Acid isomers)	C4H6O2	CH2=CH-CH2-(C=O)OH CH3-CH=CH-(C=O)OH
	RO2BUTANOIC	C4H7O4	RO2 _{lumped} in Figure S3
	QBUTANOIC	C4H7O4	QOOH _{lumped} Figure S3

	ZBUTANOIC	C ₄ H ₇ O ₆	OOQOOH _{lumped} in Figure S3
	KBUTANOIC	C ₄ H ₆ O ₅	KHP _{lumped} in Figure S3
Pentanoic Acid and Radicals			
	C₄H₉COOH	C ₅ H ₁₀ O ₂	CH ₃ -CH ₂ -CH ₂ -CH ₂ - (C=O)OH
	RPENTANOICA	C ₅ H ₉ O ₂	CH ₃ -CH ₂ -CH ₂ -*CH- (C=O)OH
	RPENTANOICB	C ₅ H ₉ O ₂	CH ₃ -CH ₂ -*CH-CH ₂ - (C=O)OH
	RPENTANOICC	C ₅ H ₉ O ₂	CH ₃ -*CH-CH ₂ -CH ₂ - (C=O)OH
	RPENTANOICD	C ₅ H ₉ O ₂	*CH ₂ -CH ₂ -CH ₂ -CH ₂ - (C=O)OH
	C ₃ H ₇ CHCO (Propylketene)	C ₅ H ₈ O	CH ₃ -CH ₂ -CH ₂ -CH=C=O
	C ₄ H ₇ COOH-1 (Pentenoic Acid Isomers)	C ₅ H ₈ O ₂	CH ₃ -CH ₂ -CH=CH-(C=O)OH CH ₃ -CH=CH-CH ₂ -(C=O)OH CH ₂ =CH-CH ₂ -CH ₂ - (C=O)OH
	RO ₂ PENTANOIC	C ₅ H ₉ O ₄	RO ₂ _{lumped} in Figure S3
	QPENTANOIC	C ₅ H ₉ O ₄	QOOH _{lumped} Figure S2
	ZPENTANOIC	C ₅ H ₉ O ₆	OOQOOH _{lumped} in Figure S2
	KPENTANOIC	C ₅ H ₈ O ₅	KHP _{lumped} in Figure S2
	C ₂ H ₃ COOH (propenoic acid)	C ₃ H ₄ O ₂	CH ₂ =CH-(C=O)OH
	CH ₂ COOH (acetic acid primary radical)	C ₂ H ₃ O ₂	*CH ₂ -(C=O)OH
	CH ₂ CH ₂ COOH (propanoic acid primary radical)	C ₃ H ₅ O ₂	*CH ₂ -CH ₂ -(C=O)OH

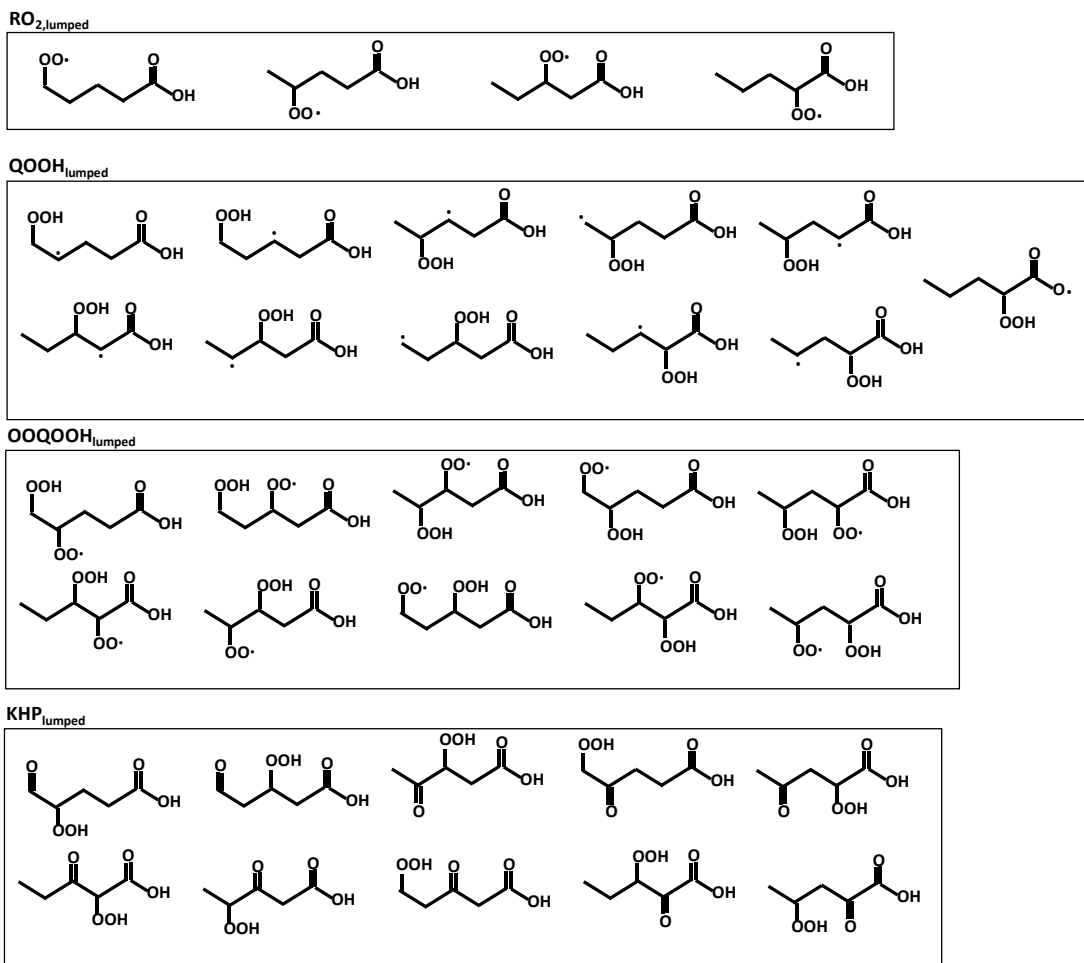


Figure S3: Lumped species in the low temperature oxidation of pentanoic acid.

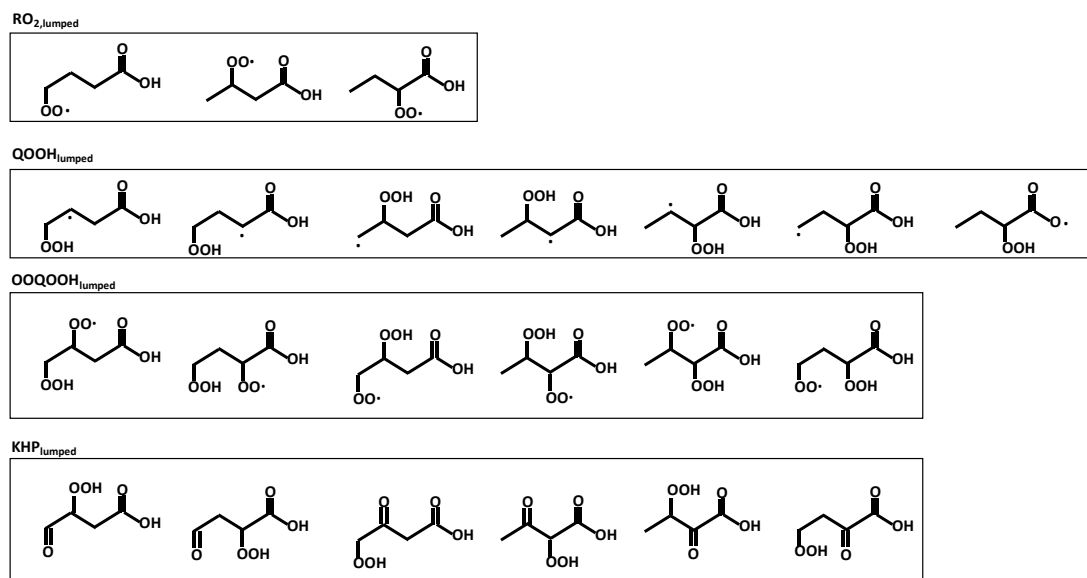


Figure S4: Lumped species in the low temperature oxidation of butanoic acid.

3. Effect of the residence time on the simulations

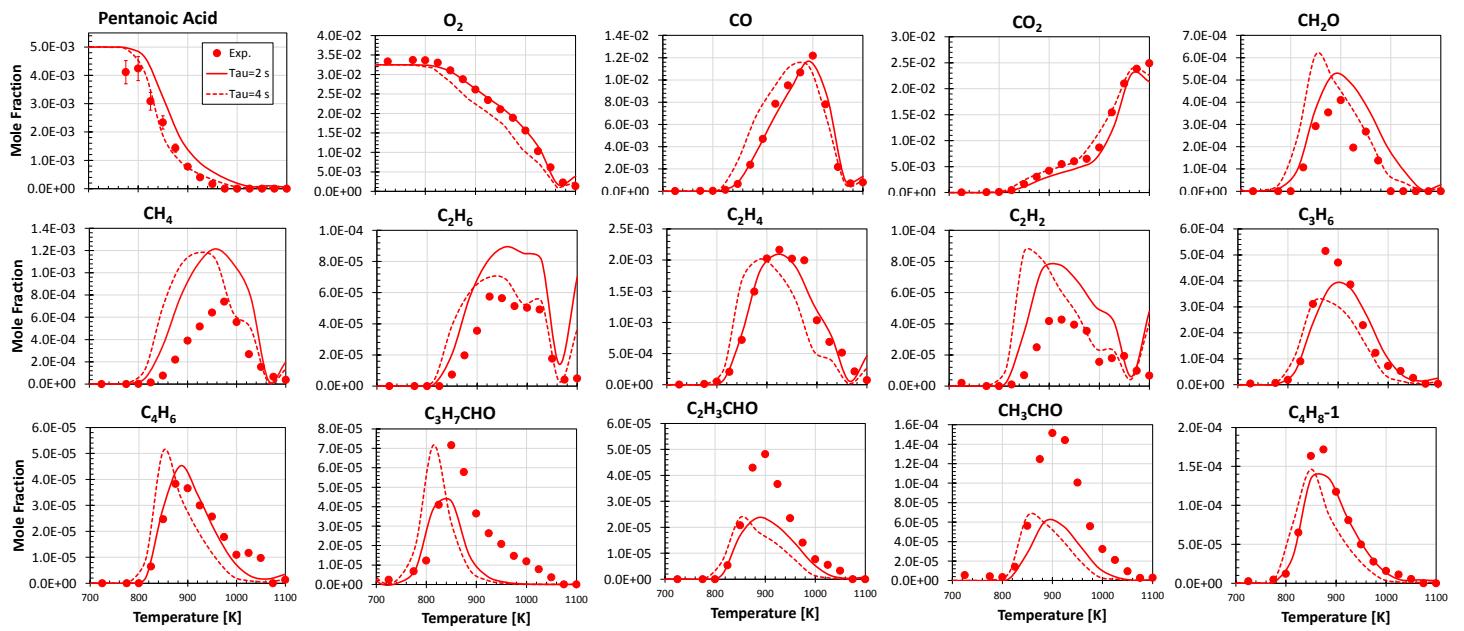


Figure S5: Effect of the residence time on the simulations for pentanoic acid at $\phi=1$ and $\tau=2$ and 4 s.