SUPPLEMENTARY MATERIAL:

An experimental and kinetic modelling study of *n*-C_4-C_6 aldehydes oxidation in a jet-stirred reactor.

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1. Results

This Section presents additional comparisons of experimental measurements carried out in this study with model results.

1.1 *n*-butanal

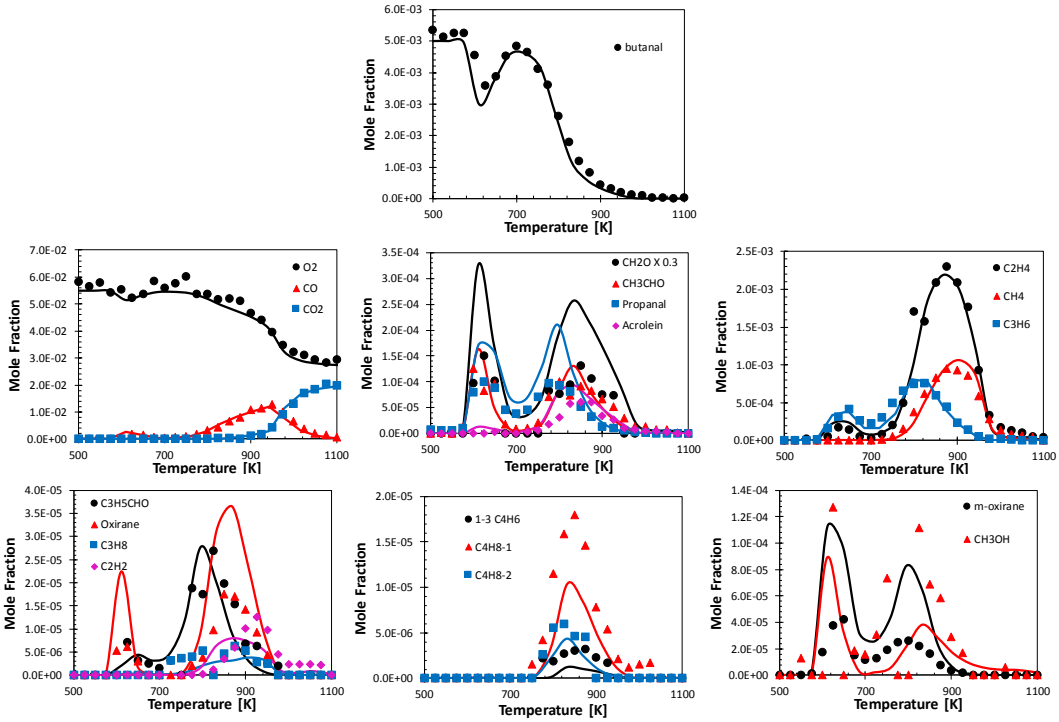

Figure S 1: n-butanal/O_2/He oxidation in a JSR at 1 atm, τ = 2.0 s, and φ = 0.5. The initial fuel (C_3H_7CHO) mole fraction is 0.5%. Symbols: experimental data from this study, lines: model results.

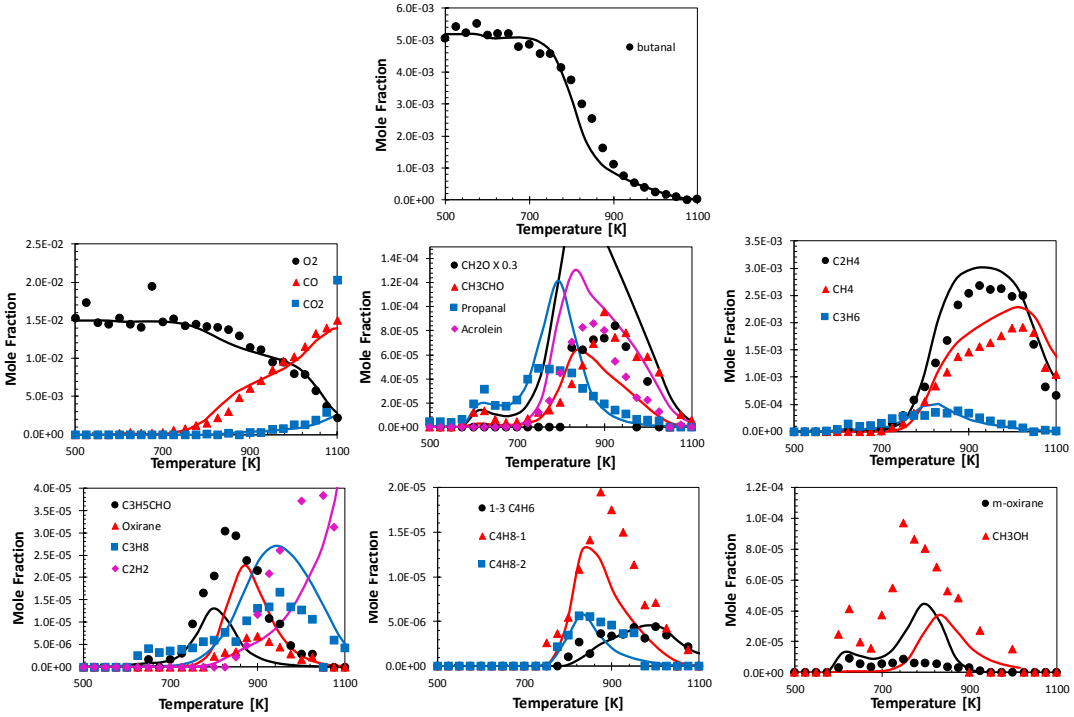

Figure S 2: n-butanal/O_2/He oxidation in a JSR at 1 atm, τ = 2.0 s, and φ = 2.0. The initial fuel (C3H7CHO) mole fraction is 0.5%. Symbols: experimental data from this study, lines: model results.

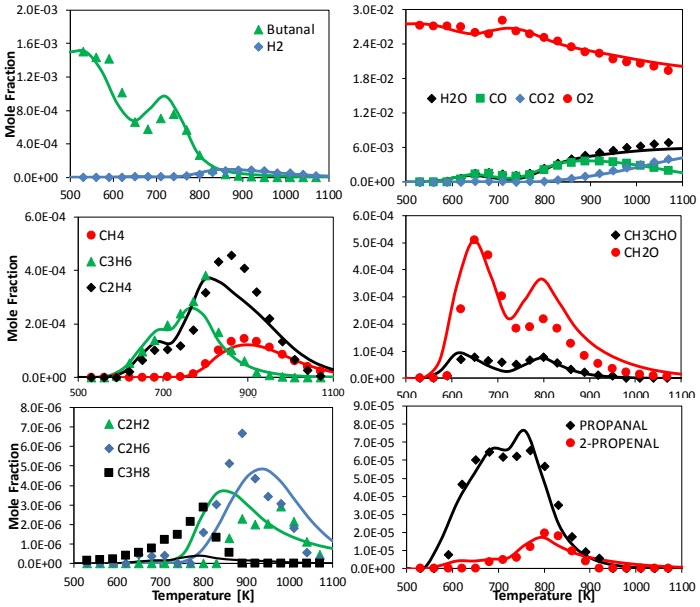

Figure S 3: n-butanal/O_2/N_2 oxidation in a JSR at 10 atm, τ = 0.7 s, and φ = 0.3. The initial fuel (C_3H_7CHO) mole fraction is 0.15%. Symbols: experimental data from Veloo et al., lines: model results.

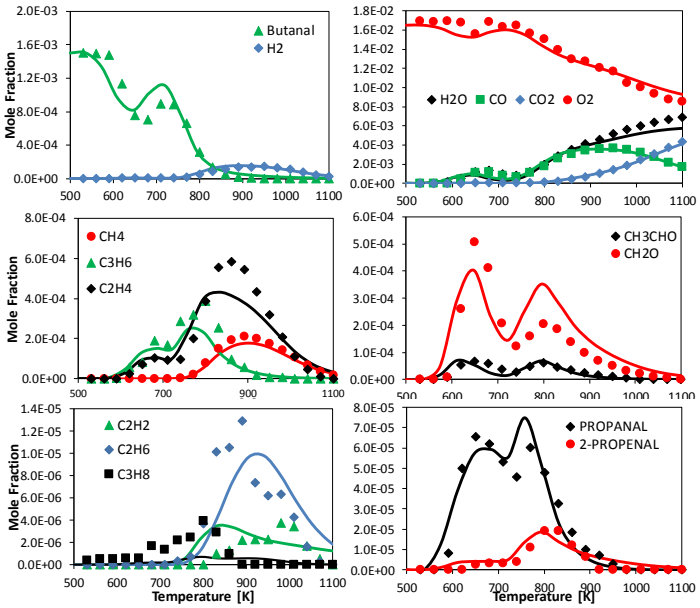

Figure S 4: n-butanal/O_2/N_2 oxidation in a JSR at 10 atm, τ = 0.7 s, and φ = 0.5. The initial fuel (C_3H_7CHO) mole fraction is 0.15%. Symbols: experimental data from Veloo et al., lines: model results.

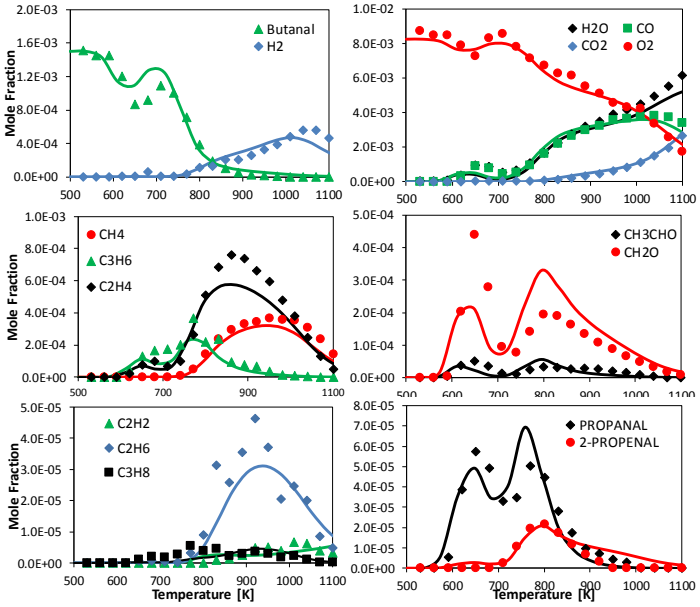

Figure S 5: n-butanal/O_2/N_2 oxidation in a JSR at 10 atm, τ = 0.7 s, and φ = 1.0. The initial fuel (C_3H_7CHO) mole fraction is 0.15%. Symbols: experimental data from Veloo et al., lines: model results.

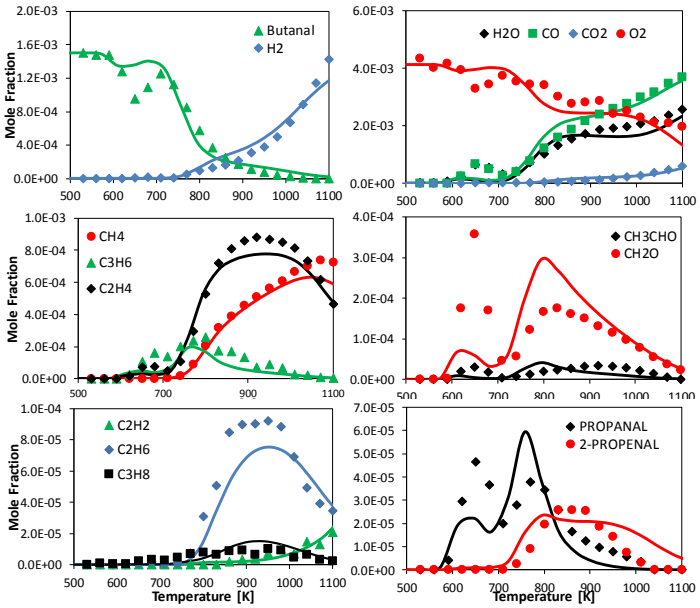

Figure S 6: n-butanal/O_2/N_2 oxidation in a JSR at 10 atm, τ = 0.7 s, and φ = 2.0. The initial fuel (C_3H_7CHO) mole fraction is 0.15%. Symbols: experimental data from Veloo et al., lines: model results.

1.2 *n*-pentanal

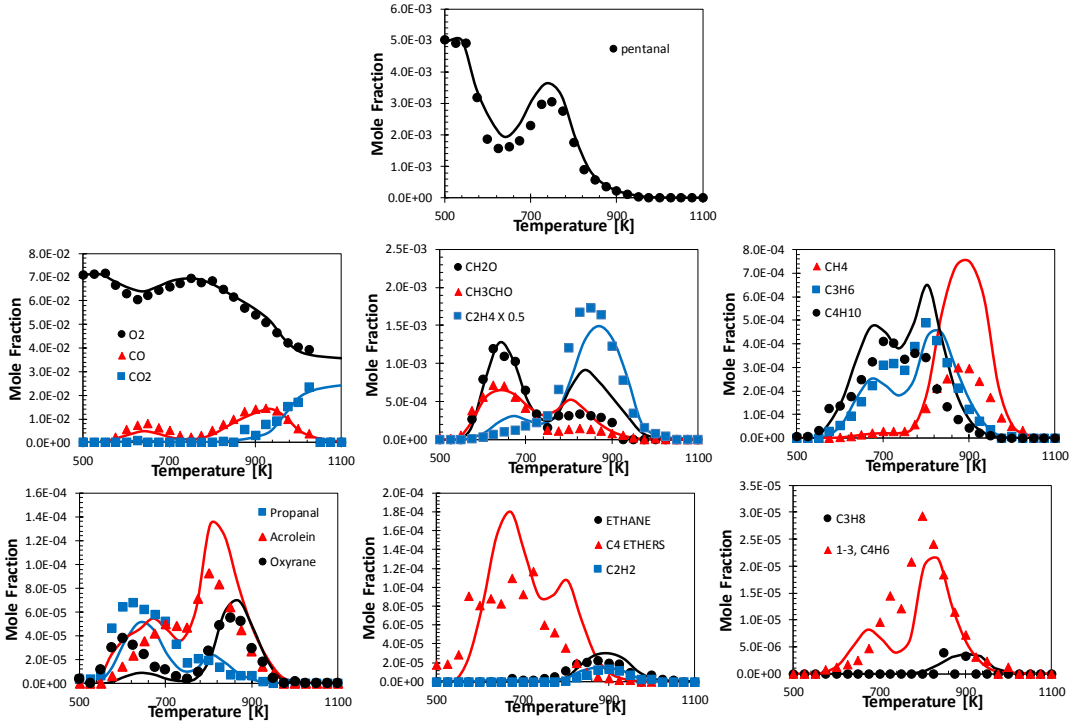

Figure S 7: n-pentanal/O_2/He oxidation in a JSR at 1 atm, τ = 2.0 s, and φ = 0.5. The initial fuel (C_4H_9CHO) mole fraction is 0.5%. Symbols: experimental data from this study, lines: model results.

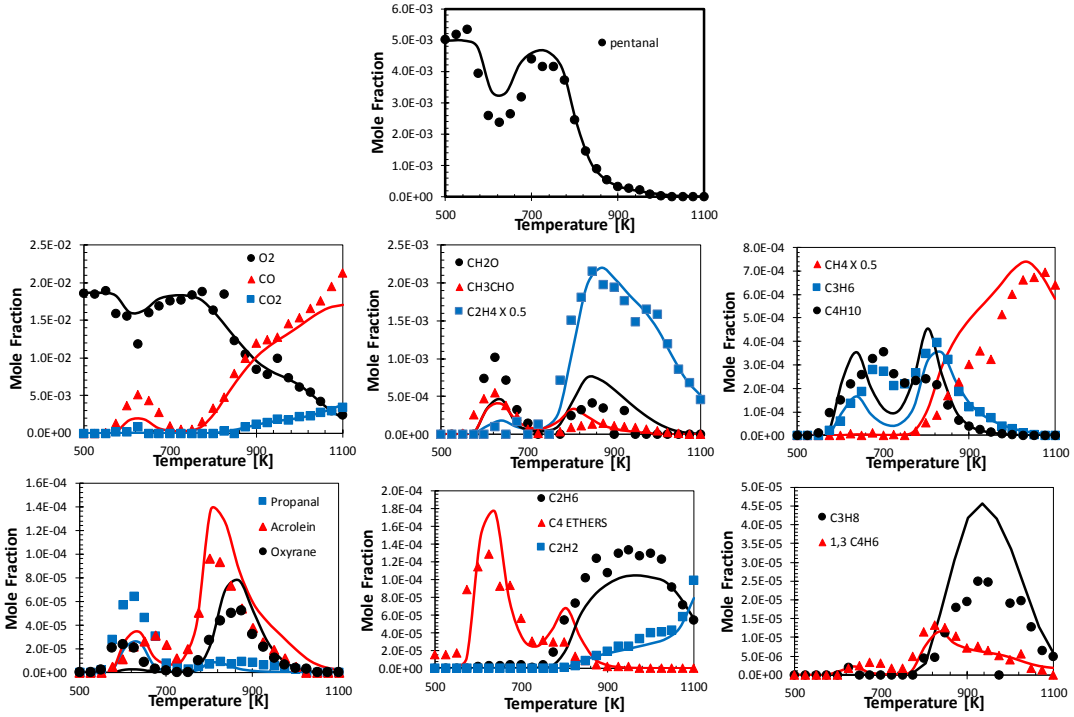

Figure S 8: n-pentanal/O_2/He oxidation in a JSR at 1 atm, τ = 2.0 s, and φ = 2.0. The initial fuel (C_4H_9CHO) mole fraction is 0.5%. Symbols: experimental data from this study, lines: model results.

1.3 *n-hexanal*

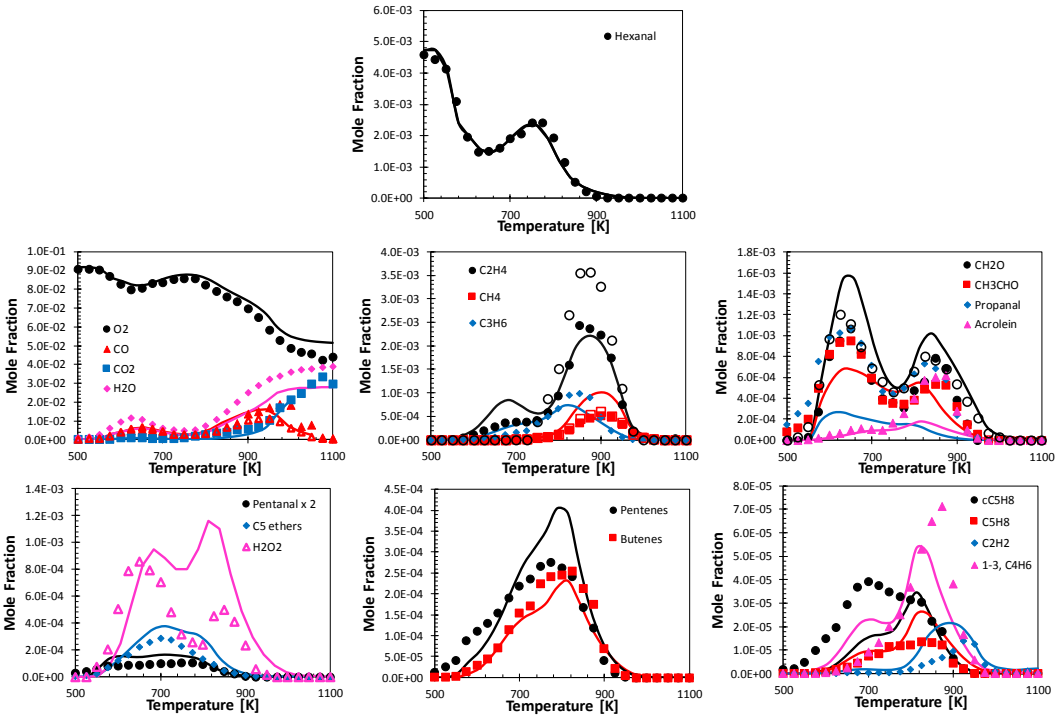

Figure S 9: n-hexanal/O_2/He oxidation in a JSR at 1 atm, τ = 2.0 s, and φ = 0.5. The initial fuel (ALDC6) mole fraction is 0.5%. Symbols: experimental data from this study, lines: model results.

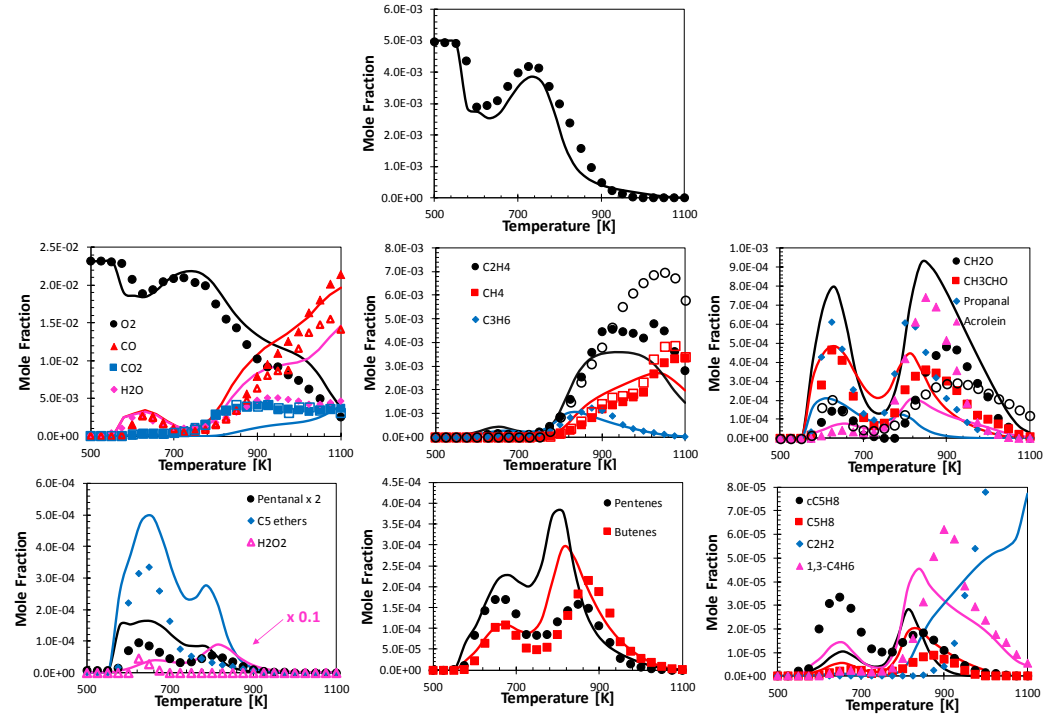

Figure S 10: n-hexanal/O_2/He oxidation in a JSR at 1 atm, τ = 2.0 s, and φ = 2.0. The initial fuel (ALDC6) mole fraction is 0.5%. Symbols: experimental data from this study, lines: model results.

Additional comparisons

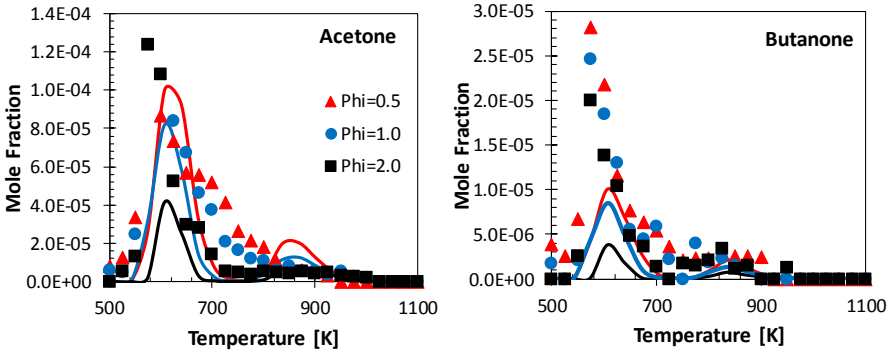

Figure S 11: Acetone and butanone formation in n-pentanal oxidation. Symbols: experimental data from this study, lines: model predictions.

The decomposition of butane ketohydroperoxides through the Korcek mechanism (*Combust. Flame*, 162 (2015) 1679-1691) explains the low temperature formation of acetone in n-pentanal oxidation. However, formic acid that should be formed together with acetone was not detected.

Butanone formation is explained on the basis of recombination/disproportionation reactions of peroxy radicals butyl radicals, as discussed in Ranzi et al. (*Combust. Flame*, 162 (2015) 1679-1691).

2. Lumped Low Temperature Mechanism and Species Nomenclature

Table S1: Kinetic parameters of the lumped low temperature reactions of n-butanal and n-hexanal.

	n-butanal		n-hexanal	
Lumped Reactions	**A**	**Ea (cal/mol)**	**A**	**Ea (cal/mol)**
OH+ALD = H_2O + CO + $R_{Cn-1,\ alkyl}$	2.00E+13	630	2.00E+13	630
OH+ALD = H_2O + RALD	2.00E+13	1700	3.40E+13	1700
O2+RALD => RALDOO	4.00E+12	0	4.00E+12	0
RALDOO => O2+RALD	1.00E+13	31500	1.00E+13	31500
RALDOO => QALDX	1.50E+12	25000	3.00E+12	24000
QALDX => RALDOO	3.00E+10	15000	3.00E+10	15000
RALDOO => OH + CO+ $C_{n-1,aldehyde}$	6.00E+11	23500	6.00E+11	23500
RALDOO => CO + $C_{nalkane}$ QOOH	3.00E+10	19000	3.00E+10	19000
QALDX =>OH + C_nLactone	1.00E+12	18000	1.00E+12	17000
QALDX =>HO2 + C_n Unsat. Ald.	4.00E+13	23500	4.00E+13	23500
QALDX => OH + $C_{l\ Dione}$ + $C_{m\ olefin}$	2.40E+13	23000	2.40E+13	23000

QALDX => OH + $C_{l\ Sat.\ Aldehyde}$ + $C_{m\ Unsat.\ Aldehyde}$	2.40E+13	23000	2.40E+13	23000
O2 + QALDX => QALDX	4.00E+12	0	4.00E+12	0
ZALDX => O2 + QALDX	1.00E+13	31500	1.00E+13	31500
ZALDX => OH + KEALD	1.00E+11	18000	1.00E+11	18000
ZALDX => OH + CO+$C_{n-1,alkane}$ KHYP	1.00E+11	18000	1.00E+11	18000
KEALD => OH + Products	3.80E+15	41000	3.80E+15	41000

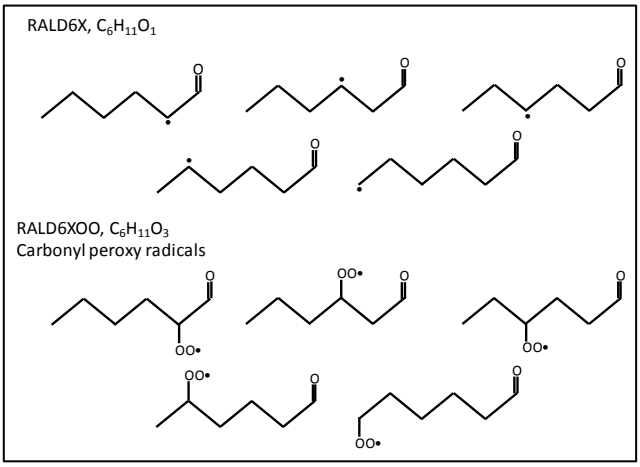

Figure S 12: alkyl radicals (RALD6X) and peroxy carbony radicals (RALD6XOO) from n-hexanal (ALDC6) LT oxidation.

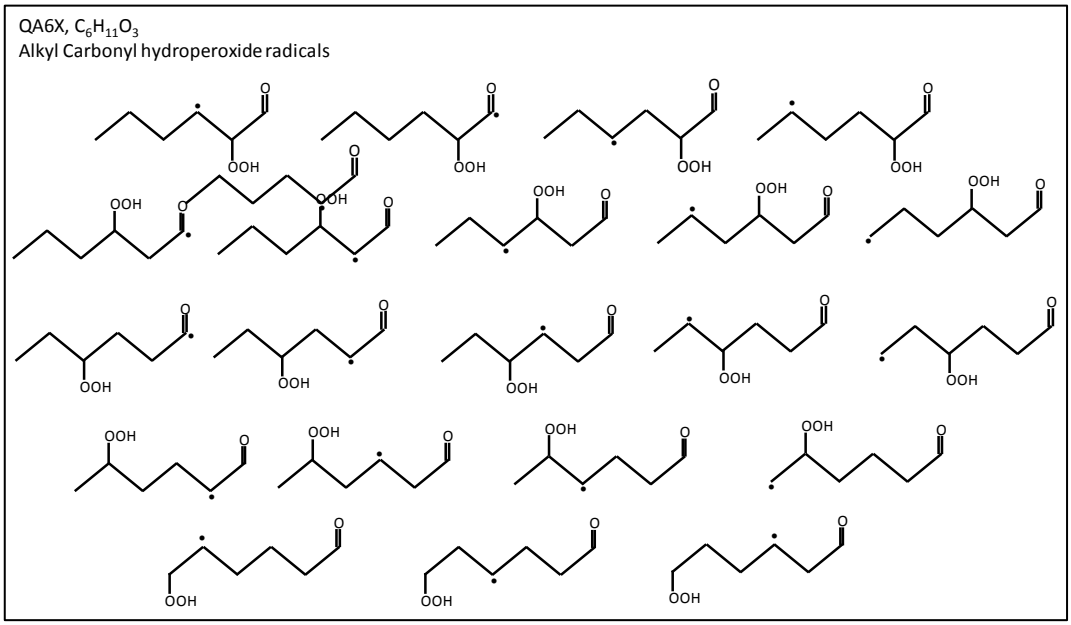

Figure S 13: alkyl carbony hydroperoxide radicals (QA6X) from n-hexanal LT oxidation.

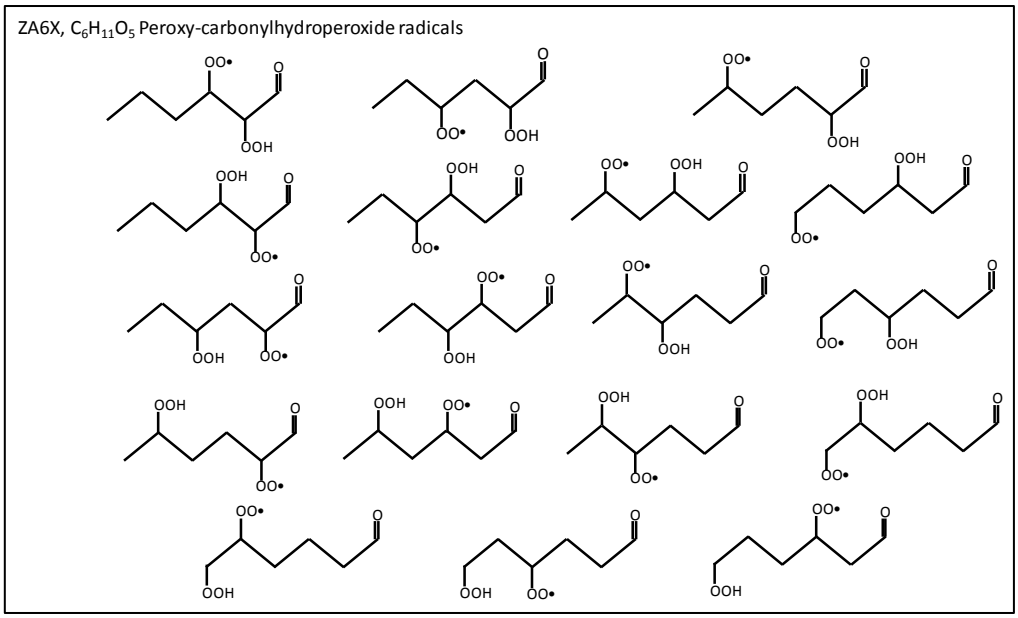

Figure S 14: Figure S 15: Peroxy carbony hydroperoxide radicals (ZA6X) from n-hexanal LT oxidation.

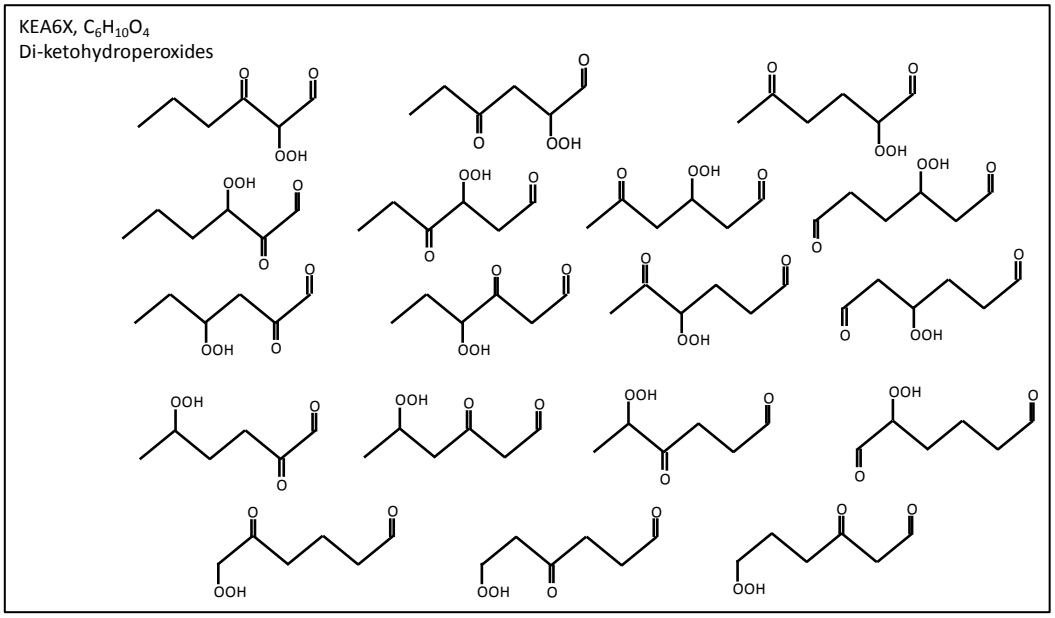

Figure S 16: Di-ketohydroperoxides (KEA6X) from n-hexanal LT oxidation.

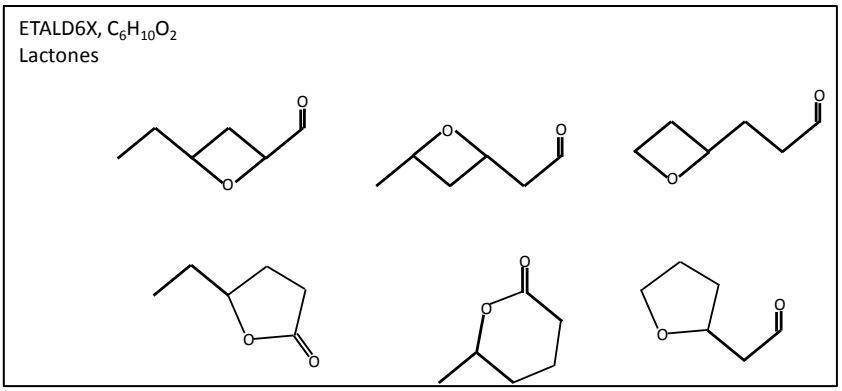

Figure S 17: Lactones (ETALD6X) from n-hexanal LT oxidation.

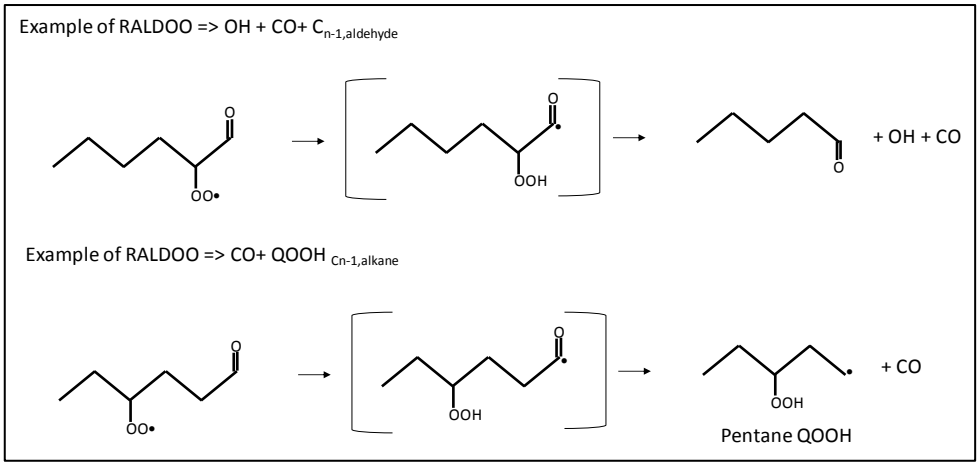

Figure S 18: Example of decomposition reactions of RALD6OOX radical.

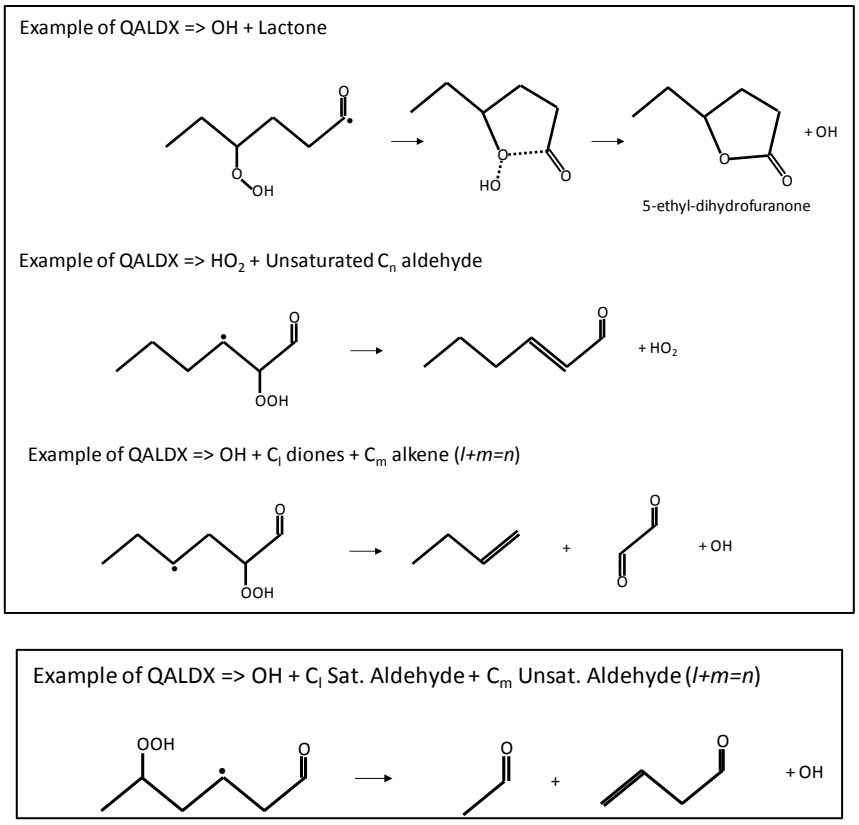

Figure S 19: Example of decomposition reactions of QA6X radical.

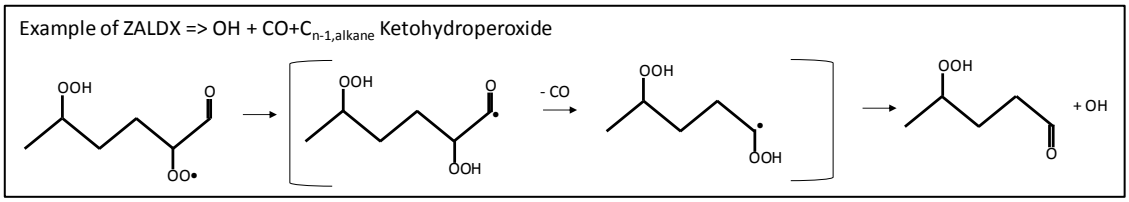

Figure S 20: Example of decomposition reactions of ZA6X radical.

Table S2: nomenclature of other relevant species.

Formula	Name	Nomenclature
n-butanal (C3H7CHO)		
C4H8O3	Carbonyl peroxy radical	RALD4OOX
C4H8O3	Alkyl Carbonyl hydroperoxide radicals	QA4X
C4H8O5	Peroxy-carbonylhydroperoxide radicals	ZA4X
C4H6O4	Di-ketohydroperoxides	KEA4X
C4H6O2	Butyrolactones	ETALD4X
n-pentanal (C4H9CHO)		
C5H11O2	Pentyl peroxy radical	NC5H11-OO
C5H11O2	Pentyl hydroperoxide radical	NC5-QOOH
C5H11O4	Peroxy pentyl hydroperoxide radical	NC5-OOQOOH
C5H10O1	C5 cyclic ethers	NC5H10-O
C5H10O3	Pentane ketohydroperoxide	NC5-OQOOH
Other species relevant to the LT combustion of n-aldehydes		
C4H6O2	Butanedione	C4H6O2
C3H4O2	Propanedial	CHOCH2CHO
C2H2O2	Glyoxal	CHOCHO
C4H6O1	Butenal isomers	C3H5CHO
C3H4O1	Acrolein (propenal)	C2H3CHO
C6H10O1	Hexenal isomers	C5H9CHO

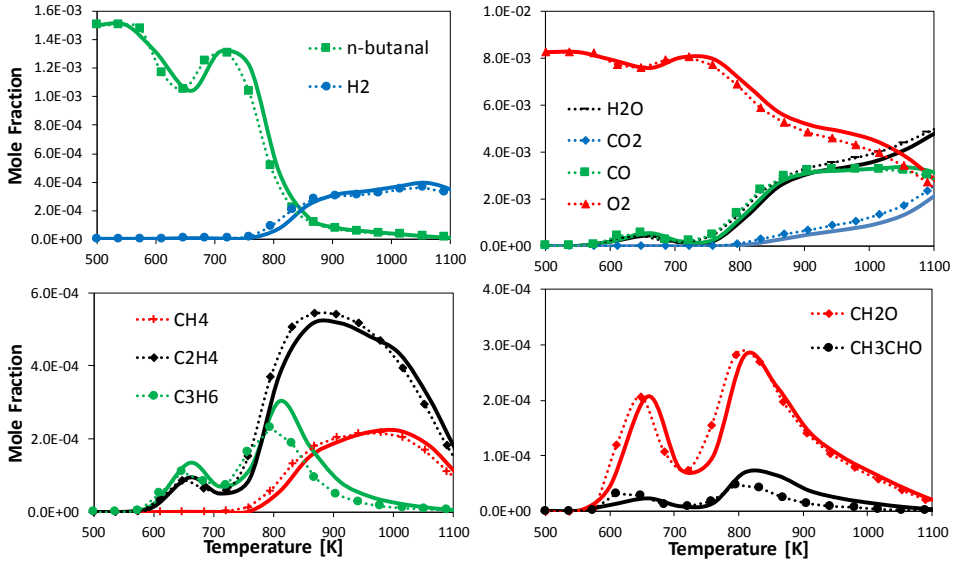

Figure S 22: Comparison between detailed n-butanal model (solid lines) (Pelucchi et al. Proceedings of the Combustion Institute 36.1 (2017): 393-401) and its lumped version (dashed lines with symbols). Conditions as in Figure S5.