

Experimental and modeling investigation of the effect of the unsaturation degree on the gas-phase oxidation of fatty acid methyl ester found in biodiesel fuels

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Supplemental Material

1) Lumped species introduced in the model for the Waddington mechanism	2
2) Stoichiometric oxidation of n-decane/Methyl-Oleate mixture [1].	3
3) Comparison of data computed using the model developed in this study and that of Westbrook et al. [2].	4
4) Comparison with experimental data of the oxidation of neat n-decane and n-decane/benzene mixtures in a JSR [3].	5
References.....	6

1) Lumped species introduced in the model for the Waddington mechanism

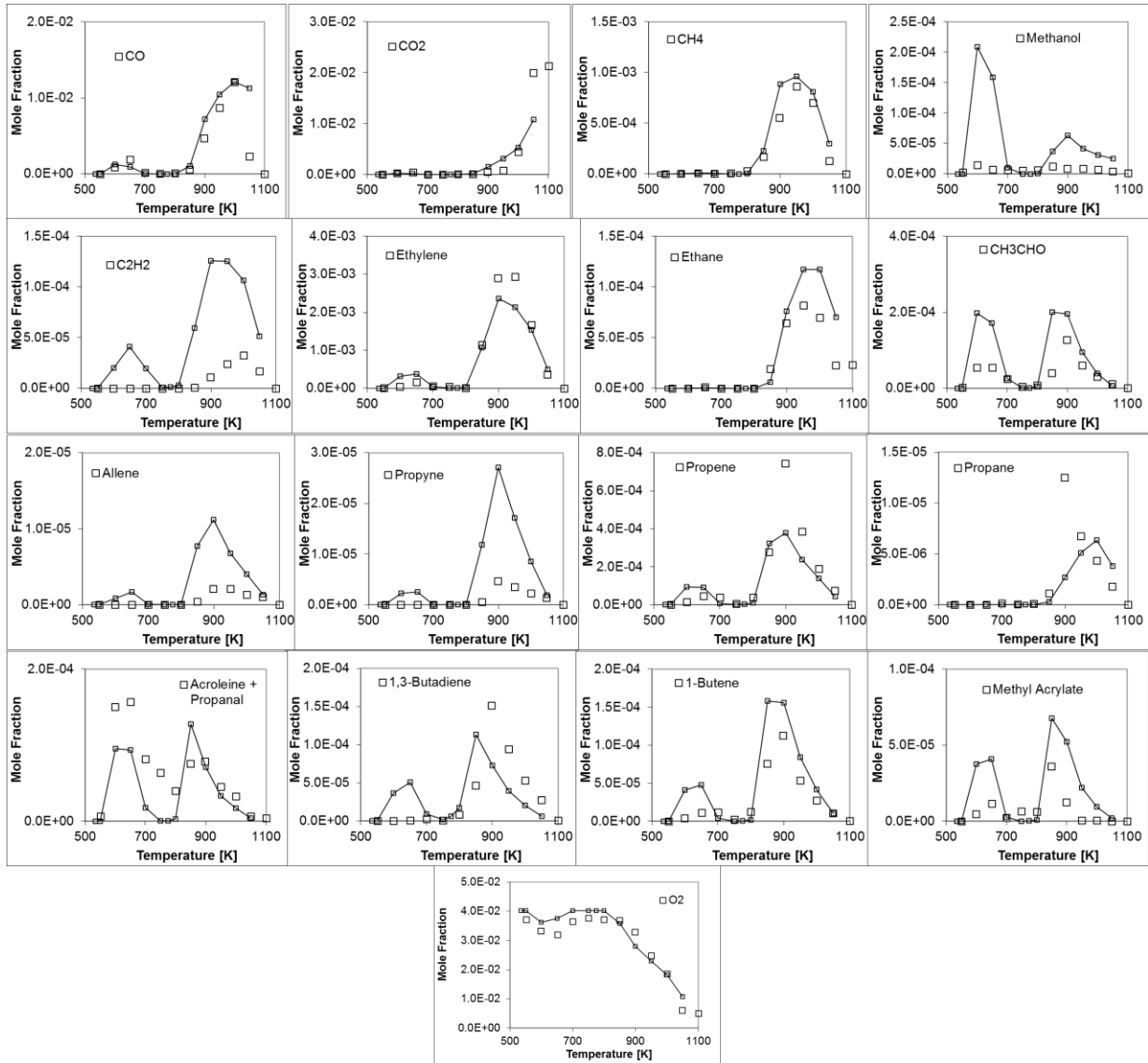
2

3 Table S1: Lumped species introduced in the model for the Waddington mechanism

Name in the model	Formula	Structure
RMEOLEOH	$C_{19}H_{37}O_3$	
RMEOLEOHO	$C_{19}H_{37}O_5$	
ALD9	$C_9H_{18}O$	
MEALD9	$C_{10}H_{18}O_3$	
RMLIN1OH	$C_{19}H_{33}O_3$	
RMLIN1OHO	$C_{19}H_{33}O_5$	
MEALDU12	$C_{13}H_{22}O_3$	
HEXENAL	$C_6H_{10}O$	

4 2) Stoichiometric oxidation of *n*-decane/Methyl-Oleate mixture [1].

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Figure S1: Mole fraction profiles of atmospheric and stoichiometric oxidation of methyl oleate /*n*-decane (26 mol%/74 mol%) mixtures at 1.5 s ($x_{fuel} = 0.002$). Comparisons of experimental (symbols) and predicted conversions (lines).

3) Comparison of data computed using the model developed in this study and that of Westbrook et al. [2].

a) JSR at 1 atm, 1.5 s, 0.2% fuel at $\phi = 1$, with He diluent.

b) Shock tube device, air/fuel mixtures in stoichiometric conditions, at 13.5 atm.

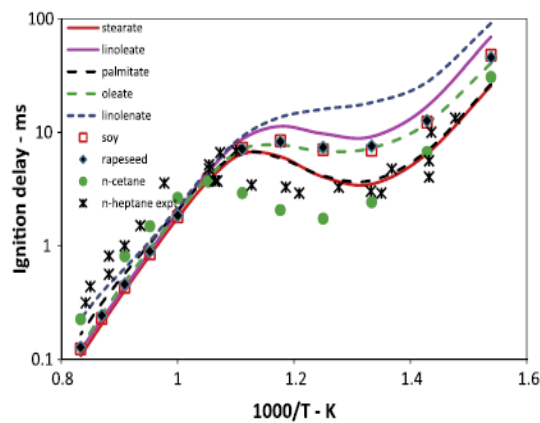
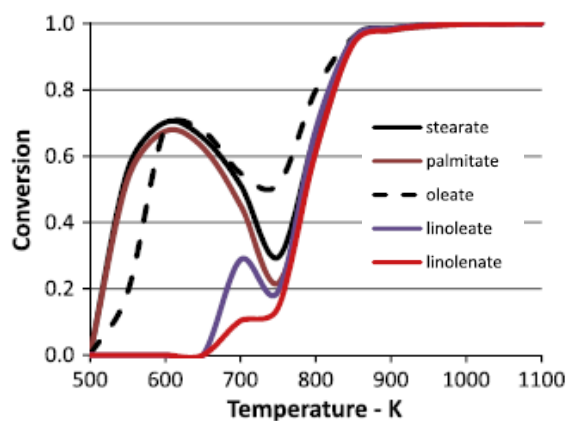
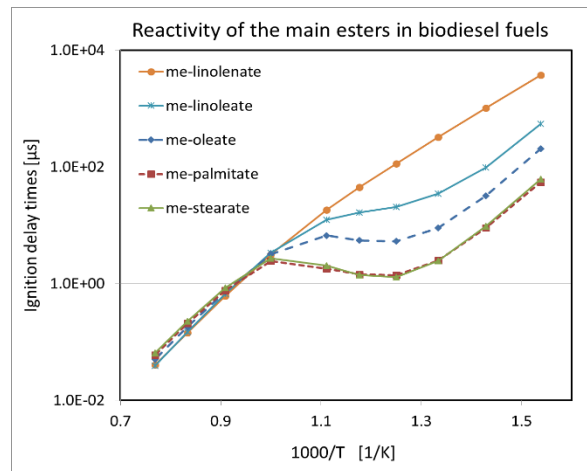
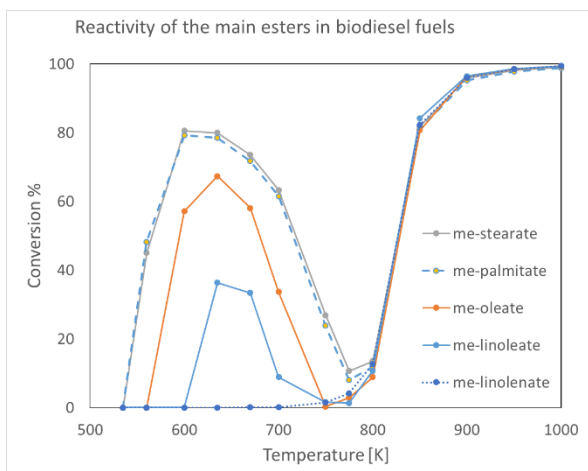


Figure S2: Comparison of data computed using the model developed in this study (upper panels) and that of Westbrook et al. [2] (lower panels). JSR conditions: $P = 1 \text{ bar}$, $\tau = 1.5 \text{ s}$, $x_{\text{ester}} = 2 \times 10^{-3}$, $\phi = 1$. Shock tube conditions: stoichiometric air/fuel mixtures at 13.5 bars.

4) Comparison with experimental data of the oxidation of neat n-decane and n-decane/benzene mixtures in a JSR [3].

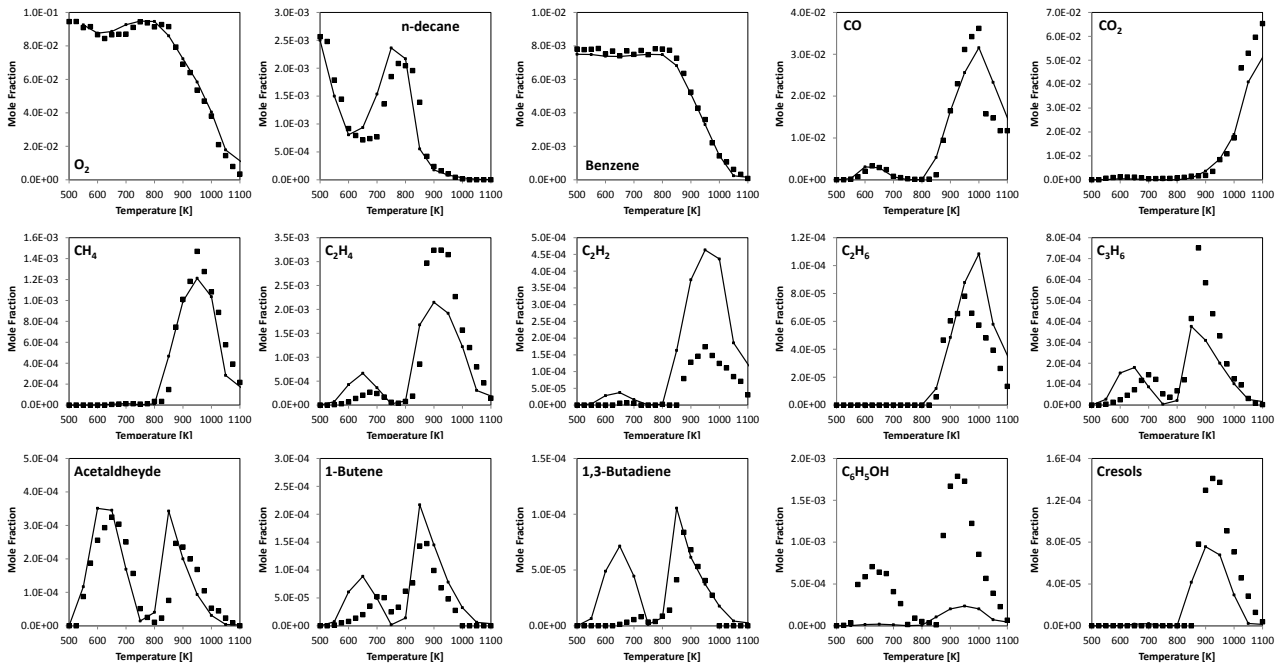


Figure S3: Mole fractions of relevant species in the oxidation of the benzene/*n*-decane mixture at 800 torr and a residence time of 2 s. Experimental (symbols) and model predictions (lines with small symbols)[3].

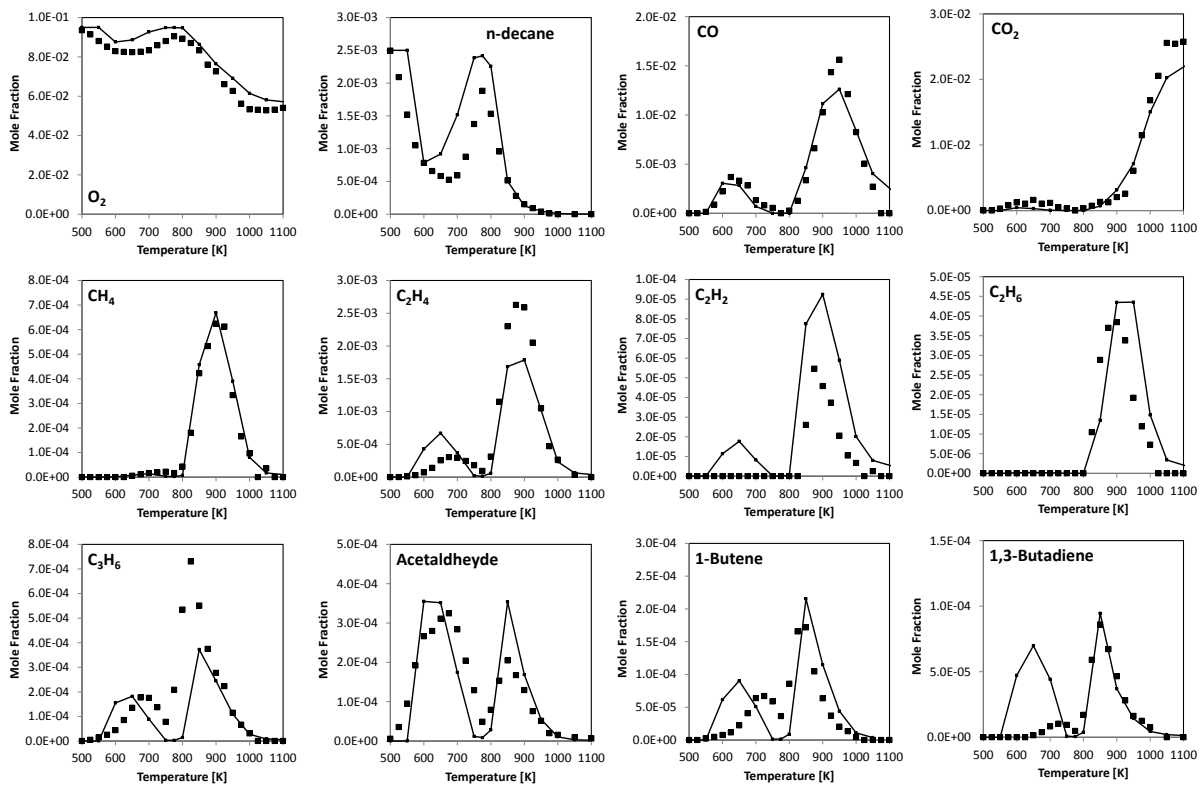


Figure S4: Mole fractions of relevant species in the oxidation of neat *n*-decane at 800 torr and a residence time of 2 s. Experimental (symbols) and model predictions (lines with small symbols)[3].

32 [References](#)

- 33 [1] S. Bax, M.H. Hakka, P.-A. Glaude, O. Herbinet, F. Battin-Leclerc, *Combust. Flame* 157 (2010) 1220.
34 [2] C.K. Westbrook, C.V. Naik, O. Herbinet, W. Pitz, M. Mehl, S.M. Sarathy, H.J. Curran, *Combust. Flame* 158 (2011)
35 742.
36 [3] O. Herbinet, B. Husson, M. Ferrari, P.A. Glaude, F. Battin-Leclerc *Proc. Combust. Inst.*, 34 (1) (2013), pp. 297–305]

37