Supplementary Material: Understanding the oxidation behavior of automotive LPG fuels: Experimental and kinetic analysis

A.K. Ramalingam[1*], M. Krieck[2,3], S. Pischinger[2], K.A. Heufer[1]

[1] Physico-Chemical Fundamentals of Combustion, RWTH Aachen University, Germany

[2] Institute for Combustion Engines (VKA), RWTH Aachen University, Germany

[3] FEV Europe GmbH, Germany

List of Species in different mechanisms

Mechanism	AM 2.0	AM 1.3	USC II	San Diego	Creck	GRI	Seidel	Konnov
Ethane	C2H6	C2H6	C2H6	C2H6	C2H6	C2H6	C2H6	C2H6
Propane	C3H8	C3H8	C3H8	C3H8	C3H8	C3H8	C3H8	C3H8
Propene	C3H6	C3H6	C3H6	C3H6	C3H6	-	C3H6	C3H6
Isobutane	IC4H10	IC4H10	iC4H10	-	IC4H10	-	I-C4H10	-
n-Butane	C4H10	C4H10	C4H10	C4H10	NC4H10	-	C4H10	-
trans-2-Butene	C4H8-2	C4H8-2	C4H82	-	-	-	2-C4H8	T2C4H8
1-Butene	C4H8-1	C4H8-1	C4H81	C4H8	NC4H8	-	1-C4H8	C4H8
Isobutene	IC4H8	IC4H8	iC4H8	-	IC4H8	-	I-C4H8	
cis-2-Butene	-	-	-	-	-	-	C-2-C4H8	C2C4H8
1,3-Butadiene	C4H6	C4H6	C4H6	C4H6	C4H6	-	C4H6	C4H6

Table S1: List of species available in the different mechanism that were considered in this study

Production	LPG 1	HO2	OH
others		0.4596	0.5223
C3H8	48.439	0.3655	0.0378
C3H6	50.0045	0.1194	0.3221
IC4H10			
C4H10			
2-C4H8			
1-C4H8			

OH Radical Pool		800
H2O2 (+M) <=> 2 OH (+M)		0.3658
CH3 + HO2 <=> CH3O + OH		0.0215
CH3O2H <=> CH3O + OH		0.0736
CH2CHO + O2 => CH2O + CO + OH		0.0354
HO2CH2CO => CH2O + CO + OH		0.026
C3H6OOH1-2 <=> C3H6O1-2 + OH		0.1272
C3H6OOH1-3O2 <=> C3KET13 + OH		0.0187
C3KET13 => CH2CHO + CH2O + OH		0.0191
C3H6 + HO2 <=> C3H6O1-2 + OH		0.0401
C3H5-A + HO2 <=> C3H5O + OH		0.0409
AC3H5OOH <=> C3H5O + OH		0.0721
C3H6OH1-2 + O2 <=> CH2O + CH3CHO + OH		0.0305
CH3COCH2 + HO2 <=> CH3COCH2O + OH		0.0113

HO2 radical Pool		800
H2O2 + OH <=> H2O + HO2		0.0114
H2O2 + OH <=> H2O + HO2		0.0109
H + O2 (+M) <=> HO2 (+M)		0.0799
CH3O2 + H2O2 <=> CH3O2H + HO2		0.0206
CH3O + O2 <=> CH2O + HO2		0.0568
HCO + O2 <=> CO + HO2		0.253
C2H5 + O2 <=> C2H4 + HO2		0.027
IC3H7 + O2 <=> C3H6 + HO2		0.1346
NC3H7O2 <=> C3H6 + HO2		0.0766
IC3H7O2 <=> C3H6 + HO2		0.1543
C3H6OH1-2 + O2 <=> C2H5CHO + HO2		0.0285
C3H6OH2-1 + O2 <=> HO2 + IC3H5OH		0.0909

Production	LPG 2	HO2	OH
others		0.373	0.4989
C3H8	66.1776	0.3794	0.1411
C3H6		0.02	0.0808
IC4H10	10.7234	0.061	
C4H10	22.2613	0.0994	0.0644
2-C4H8			
1-C4H8			

OH Radical Pool		800
H2O2 (+M) <=> 2 OH (+M)		0.3195
CH3 + HO2 <=> CH3O + OH		0.0108
CH3O2H <=> CH3O + OH		0.0851
CH2CHO + O2 => CH2O + CO + OH		0.0402
HO2CH2CO => CH2O + CO + OH		0.0433
C3H6OOH1-2 <=> C3H6O1-2 + OH		0.036
C3H6OOH1-3O2 <=> C3KET13 + OH		0.0554
C3KET13 => CH2CHO + CH2O + OH		0.0563
NC3H7O2H <=> NC3H7O + OH		0.0181
IC3H7O + OH <=> IC3H7O2H		0.0113
C3H5-A + HO2 <=> C3H5O + OH		0.011
AC3H5OOH <=> C3H5O + OH		0.0338
C4H8OOH1-3 <=> C4H8O1-3 + OH		0.0197
C4H8OOH1-3O2 <=> NC4KET13 + OH		0.0166
NC4KET13 => CH2CHO + CH3CHO + OH		0.0166
C4H8OOH2-3 <=> C4H8O2-3 + OH		0.0115

HO2 radical Pool		800
H2O2 + OH <=> H2O + HO2		0.0138
H2O2 + OH <=> H2O + HO2		0.0108
H + O2 (+M) <=> HO2 (+M)		0.0597
CH3O2 + H2O2 <=> CH3O2H + HO2		0.0288
CH3O + O2 <=> CH2O + HO2		0.0543
HCO + O2 <=> CO + HO2		0.1753
C2H5 + O2 <=> C2H4 + HO2		0.0303
IC3H7 + O2 <=> C3H6 + HO2		0.1063
NC3H7O2 <=> C3H6 + HO2		0.1003
IC3H7O2 <=> C3H6 + HO2		0.1728
C3H6OH2-1 + O2 <=> HO2 + IC3H5OH		0.02
PC4H9O2 <=> C4H8-1 + HO2		0.0109
SC4H9O2 <=> C4H8-1 + HO2		0.0495
IC4H9O2 <=> HO2 + IC4H8		0.012
HO2 + IC4H8 <=> TC4H9O2		0.03
HO2 + IC4H8 <=> IC4H8O2H-T	0.00597	0.019
SC4H9O2 <=> C4H8-2 + HO2	0.0076	0.0242
SC4H9O2 <=> C4H8-2 + HO2	0.00465	0.0148

Production	LPG 3	HO2	OH
others		0.4003	0.5064
C3H8	81.118	0.4818	0.1728
C3H6		-0.0136	0.1056
IC4H10			
C4H10			
2-C4H8	5.0300		
1-C4H8	8.4456		0.0124

OH Radical Pool		800
H2O2 (+M) <=> 2 OH (+M)		0.3189
CH3 + HO2 <=> CH3O + OH		0.0132
CH3O2H <=> CH3O + OH		0.0905
CH2CHO + O2 => CH2O + CO + OH		0.0415
HO2CH2CO => CH2O + CO + OH		0.0423
NC3H7O2 <=> C3H6O1-2 + OH		0.0119
C3H6OOH1-2 <=> C3H6O1-2 + OH		0.0455
C3H6OOH1-3O2 <=> C3KET13 + OH		0.0629
C3KET13 => CH2CHO + CH2O + OH		0.064
NC3H7O2H <=> NC3H7O + OH		0.0211
IC3H7O + OH <=> IC3H7O2H		0.0129
C3H6 + HO2 <=> C3H6O1-2 + OH		0.0112
C3H5-A + HO2 <=> C3H5O + OH		0.012
AC3H5OOH <=> C3H5O + OH		0.0369
C4H72-1OOH => C3H5-S + CH2O + OH		0.0124

HO2 radical Pool		800
H2O2 + OH <=> H2O + HO2		0.0125
H2O2 + OH <=> H2O + HO2		0.01
H + O2 (+M) <=> HO2 (+M)		0.064
CH3O2 + H2O2 <=> CH3O2H + HO2		0.0285
CH3O + O2 <=> CH2O + HO2		0.0583
HCO + O2 <=> CO + HO2		0.1967
C2H5 + O2 <=> C2H4 + HO2		0.0303
NC3H7 + O2 <=> C3H6 + HO2		0.01
IC3H7 + O2 <=> C3H6 + HO2		0.133
NC3H7O2 <=> C3H6 + HO2		0.1231
IC3H7O2 <=> C3H6 + HO2		0.2056
C3H6OOH1-3O2 <=> AC3H5OOH + HO2		0.0101
C3H5-A + HO2 <=> AC3H5OOH		-0.0366
C3H6OH2-1 + O2 <=> HO2 + IC3H5OH		0.023

Production	LPG 4	HO2	OH
others		0.3929	0.3798
C3H8	15.3121	0.1136	0.0324
C3H6	7.5745	0.0212	0.0839
IC4H10	24.8286	0.1483	0.0478
C4H10	51.7654	0.24	0.2305
2-C4H8			
1-C4H8			0.0106

OH Radical Pool		800
H2O2 (+M) <=> 2 OH (+M)		0.1991
CH3 + HO2 <=> CH3O + OH		0.0108
CH3O2H <=> CH3O + OH		0.0986
CH2CHO + O2 => CH2O + CO + OH		0.0328
HO2CH2CO => CH2O + CO + OH		0.0385
C3H6OOH1-2 <=> C3H6O1-2 + OH		0.0234
C3H6OOH1-3O2 <=> C3KET13 + OH		0.0161
C3KET13 => CH2CHO + CH2O + OH		0.0163
C3H5-A + HO2 <=> C3H5O + OH		0.0125
AC3H5OOH <=> C3H5O + OH		0.0305
CH3COCH2 + HO2 <=> CH3COCH2O + OH		0.0175
OH + SC4H9O <=> SC4H9O2H		0.0164
C4H8OOH1-3 <=> C4H8O1-3 + OH		0.0443
C4H8OOH1-4 <=> C4H8O1-4 + OH		0.0103
C4H8OOH2-4 <=> C4H8O1-3 + OH		0.012
C4H8OOH1-3O2 <=> NC4KET13 + OH		0.0437
C4H8OOH2-4O2 <=> NC4KET24 + OH		0.017
C4H72-1OOH => C3H5-S + CH2O + OH		0.0106
NC4KET13 => CH2CHO + CH3CHO + OH		0.0438
NC4KET24 => CH2O + CH3COCH2 + OH		0.017
IC4H8O2H-T <=> IC4H8O + OH		0.0149
IC4H8OOH-IO2 <=> IC4KETII + OH		0.0113
IC4KETII => C2H5CO + CH2O + OH		0.0113
TC4H8O2H-I <=> IC4H8O + OH		0.0103
C4H8OOH2-3 <=> C4H8O2-3 + OH		0.026

HO2 radical Pool		800
H2O2 + OH <=> H2O + HO2		0.0115
H + O2 (+M) <=> HO2 (+M)		0.0689
CH3O2 + H2O2 <=> CH3O2H + HO2		0.0294
CH3O + O2 <=> CH2O + HO2		0.0712
HCO + O2 <=> CO + HO2		0.1679
C2H5 + O2 <=> C2H4 + HO2		0.0328
C2H5O2 <=> C2H4 + HO2		0.0112
IC3H7 + O2 <=> C3H6 + HO2		0.0318
NC3H7O2 <=> C3H6 + HO2		0.0261
IC3H7O2 <=> C3H6 + HO2		0.0557
C3H6OH2-1 + O2 <=> HO2 + IC3H5OH		0.0212
PC4H9O2 <=> C4H8-1 + HO2		0.0258
SC4H9O2 <=> C4H8-1 + HO2		0.1196
IC4H9O2 <=> HO2 + IC4H8		0.029
HO2 + IC4H8 <=> TC4H9O2		0.071
HO2 + IC4H8 <=> IC4H8O2H-T		0.0483
SC4H9O2 <=> C4H8-2 + HO2		0.0588
SC4H9O2 <=> C4H8-2 + HO2		0.0358

Table S 2. Radical pool flux analysis at 800K, 20 bar stoichiometric conditions with regard to production of OH and HO2 radicals and individual components in the different LPG mixtures.

Consumption	LPG 1	HO2	OH	LPG 2	HO2	OH	LPG 3	HO2	OH	LPG 4	HO2	OH
Others		-0.3352	-0.1254		-0.4729	-0.105		-0.4395	-0.1105		-0.4139	-0.0928
C3H8	48.439	-0.199	-0.3732	66.1776	-0.1077	-0.487	81.118	-0.1249	-0.611	15.3121	-0.0149	-0.114
C3H6	50.0045	-0.3853	-0.4266		-0.163	-0.0595		-0.1318	-0.0718	7.5745	-0.2	-0.0571
IC4H10				10.7234	-0.0193	-0.0756				24.8286	-0.0518	-0.1784
C4H10				22.2613	-0.0499	-0.1732			-0.0121	51.7654	-0.1159	-0.4132
2-C4H8							5.03	-0.0367	-0.0149			
1-C4H8							8.4456	-0.0844	-0.0533			
IC4H8											-0.015	-0.0174
	OH Radical Pool		800	OH Radical Pool		800	OH Radical Pool		800	OH Radical Pool		800
	H2O2 + OH <=> H2O + HO2		-0.0122	H2O2 + OH <=> H2O + HO2		-0.0157	H2O2 + OH <=> H2O + HO2		-0.0146	H2O2 + OH <=> H2O + HO2		-0.0122
	H2O2 + OH <=> H2O + HO2		-0.0116	H2O2 + OH <=> H2O + HO2		-0.0122	H2O2 + OH <=> H2O + HO2		-0.0117	CH2O + OH <=> H2O + HCO		-0.0692
	CH2O + OH <=> H2O + HCO		-0.1016	CH2O + OH <=> H2O + HCO		-0.0771	CH2O + OH <=> H2O + HCO		-0.0842	CH3CHO + OH <=> CH3CO + H2O		-0.0114
	C3H8 + OH <=> H2O + NC3H7		-0.1826	C3H8 + OH <=> H2O + NC3H7		-0.2314	C3H8 + OH <=> H2O + NC3H7		-0.2915	C3H8 + OH <=> H2O + NC3H7		-0.0538
	C3H8 + OH <=> H2O + IC3H7		-0.1906	C3H8 + OH <=> H2O + IC3H7		-0.2556	C3H8 + OH <=> H2O + IC3H7		-0.3195	C3H8 + OH <=> H2O + IC3H7		-0.0602
	C3H6O1-2 + OH => C2H3 + CH2O + H2O		-0.032	C3H6 + OH <=> C3H5-A + H2O		-0.0312	C3H6 + OH <=> C3H5-A + H2O		-0.0382	C3H6 + OH <=> C3H5-A + H2O		-0.0293
	C3H6 + OH <=> C3H5-A + H2O		-0.1763	C3H6 + OH <=> C3H6OH1-2		-0.014	C3H6 + OH <=> C3H6OH1-2		-0.0169	C3H6 + OH <=> C3H6OH1-2		-0.0133
	C3H6 + OH <=> C3H5-T + H2O		-0.0197	C3H6 + OH <=> C3H6OH1-2		-0.0143	C3H6 + OH <=> C3H6OH1-2		-0.0167	C3H6 + OH <=> C3H6OH1-2		-0.0145
	C3H6 + OH <=> C3H5-S + H2O		-0.0251	C4H10 + OH <=> H2O + PC4H9		-0.0636	C4H10 + OH <=> H2O + SC4H9		-0.0121	C4H10 + OH <=> H2O + PC4H9		-0.1514
	C3H6 + OH <=> C3H6OH1-2		-0.0715	C4H10 + OH <=> H2O + SC4H9		-0.1096	C4H8-1 + OH <=> C4H71-3 + H2O		-0.0236	C4H10 + OH <=> H2O + SC4H9		-0.2618
	C3H6 + OH <=> C3H6OH1-2		-0.056	IC4H10 + OH <=> H2O + IC4H9		-0.0532	C4H8-1 + OH <=> C4H71-4 + H2O		-0.0142	IC4H10 + OH <=> H2O + IC4H9		-0.1251
	C3H6 + OH <=> C3H6OH2-1		-0.0202	IC4H10 + OH <=> H2O + TC4H9		-0.0224	C4H8-1 + OH <=> PC4H8OH-2		-0.0155	IC4H10 + OH <=> H2O + TC4H9		-0.0533
	C3H6 + OH <=> C3H6OH2-1		-0.0258				C4H8-2 + OH <=> C4H71-3 + H2O		-0.0149	IC4H8 + OH <=> H2O + IC4H7		-0.0174
	HO2 radical Pool		800	HO2 radical Pool		800	HO2 radical Pool		800	HO2 radical Pool		800
	2 HO2 <=> H2O2 + O2		-0.0586	2 HO2 <=> H2O2 + O2		-0.0782	2 HO2 <=> H2O2 + O2		-0.0716	2 HO2 <=> H2O2 + O2		-0.0624
	2 HO2 <=> H2O2 + O2		-0.1048	2 HO2 <=> H2O2 + O2		-0.2021	2 HO2 <=> H2O2 + O2		-0.1753	2 HO2 <=> H2O2 + O2		-0.1745
	CH3 + HO2 <=> CH3O + OH		-0.0301	CH3 + HO2 <=> CH3O + OH		-0.0176	CH3 + HO2 <=> CH3O + OH		-0.0198	CH3 + HO2 <=> CH3O + OH		-0.0175
	CH3O2 + HO2 <=> CH3O2H + O2		-0.038	CH3O2 + HO2 <=> CH3O2H + O2		-0.0589	CH3O2 + HO2 <=> CH3O2H + O2		-0.0572	CH3O2 + HO2 <=> CH3O2H + O2		-0.073
	CH2O + HO2 <=> H2O2 + HCO		-0.1037	CH2O + HO2 <=> H2O2 + HCO		-0.1161	CH2O + HO2 <=> H2O2 + HCO		-0.1156	CH2O + HO2 <=> H2O2 + HCO		-0.0865
	CH3CHO + HO2 <=> CH3CO + H2O2		-0.0233	CH3CHO + HO2 <=> CH3CO + H2O2		-0.0289	CH3CHO + HO2 <=> CH3CO + H2O2		-0.0295	CH3CHO + HO2 <=> CH3CO + H2O2		-0.0392
	C3H8 + HO2 <=> H2O2 + NC3H7		-0.0184	C3H8 + HO2 <=> H2O2 + NC3H7		-0.0299	C3H8 + HO2 <=> H2O2 + NC3H7		-0.0351	C3H8 + HO2 <=> H2O2 + IC3H7		-0.0149
	C3H8 + HO2 <=> H2O2 + IC3H7		-0.0428	C3H8 + HO2 <=> H2O2 + IC3H7		-0.0778	C3H8 + HO2 <=> H2O2 + IC3H7		-0.0898	C3H6OOH1-2 <=> C3H6 + HO2		-0.0333
	C3H6OOH1-2 <=> C3H6 + HO2		-0.1377	C3H6OOH1-2 <=> C3H6 + HO2		-0.0356	C3H6OOH1-2 <=> C3H6 + HO2		-0.0369	C3H6 + O2 <=> C3H5-A + HO2		-0.0102
	C3H6O1-2 + HO2 => C2H3 + CH2O + H2O2		-0.0486	C3H6 + HO2 <=> C3H6O1-2 + OH		-0.0151	C3H6O1-2 + HO2 => C2H3 + CH2O + H2O2		-0.0111	C3H6 + HO2 <=> C3H6O1-2 + OH		-0.0118
	C3H6 + O2 <=> C3H5-A + HO2		-0.0285	C3H5-A + HO2 <=> C3H5O + OH		-0.0181	C3H6 + HO2 <=> C3H6O1-2 + OH		-0.0168	C3H5-A + HO2 <=> C3H5O + OH		-0.0201
	C3H6 + HO2 <=> C3H5-A + H2O2		-0.0289	C3H5-A + HO2 <=> AC3H5OOH		-0.038	C3H5-A + HO2 <=> C3H5O + OH		-0.018	C3H5-A + HO2 <=> AC3H5OOH		-0.0445
	C3H6 + HO2 <=> C3H6O1-2 + OH		-0.0563	CH3COCH2 + HO2 <=> CH3COCH2O + OH		-0.0139	C2H3CHO + HO2 <=> C2H3CO + H2O2		-0.0195	CH3COCH2 + HO2 <=> CH3COCH2O + OH		-0.0283
	C3H5-A + HO2 <=> C3H5O + OH		-0.0574	C2H3CHO + HO2 <=> C2H3CO + H2O2		-0.0134	C4H8-1 + HO2 <=> C4H71-3 + H2O2		-0.02	C2H3CHO + HO2 <=> C2H3CO + H2O2		-0.0126
	C3H5-A + HO2 <=> AC3H5OOH		-0.0943	C4H10 + HO2 <=> H2O2 + SC4H9		-0.0499	C4H71-3 + HO2 <=> C4H72-1OOH		-0.0207	C4H10 + HO2 <=> H2O2 + PC4H9		-0.0185
	CH3COCH2 + HO2 <=> CH3COCH2O + OH		-0.0158	HO2 + IC4H10 <=> H2O2 + TC4H9		-0.0193	C4H71-3 + HO2 <=> C4H7O2-1 + OH		-0.0114	C4H10 + HO2 <=> H2O2 + SC4H9		-0.0974
	C2H3CHO + HO2 <=> C2H3CO + H2O2		-0.0322				C4H71-3 + HO2 <=> C4H71-3OOH		-0.0198	HO2 + IC4H10 <=> H2O2 + IC4H9		-0.0138
							C4H71-3 + HO2 <=> C4H71-O + OH		-0.0125	HO2 + IC4H10 <=> H2O2 + TC4H9		-0.038
							C4H8-2 + HO2 <=> C4H71-3 + H2O2		-0.0105	HO2 + IC4H7 <=> IC4H7OOH		-0.015
							C4H8-2 + HO2 <=> C4H8O2-3 + OH		-0.0131			
							C4H64,2-1OH + HO2 <=> C4H6OHOOH1-4-3		-0.0131			

Table S 3. Radical pool flux analysis at 800K, 20 bar stoichiometric conditions with regard to consumption of OH and HO2 radicals and individual components in the different LPG mixtures.