Supplementary material for "Global Mechanistic Model of SOA Formation: Effects of Different Chemical Mechanisms"

Guangxing Lin[1], Joyce E. Penner[1], Sanford Sillman[1], Domenico Taraborrelli[2], and Jos Lelieveld[2,3]

[1]Department of Atmospheric, Oceanic, and Space Sciences, University of Michigan, Ann Arbor, Michigan, USA.

[2]Department of Atmospheric Chemistry, Max Planck Institute for Chemistry, Mainz, Germany.

[3]The Cyprus Institute, Nicosia, Cyprus.

Correspondence to: Guangxing Lin (gxlin@umich.edu)

This supplementary material includes four tables. Table S1 lists oxidation products that partition to aerosol phase through gas-particle partitioning, parent VOCs, partitioning coefficients (K), production rates and relative contributions (annual mean) to ne_oSOA in three different simulations. The other three tables describe the chemical species (Table S2) and reactions (Table S3 and S4) used in the HO_x recycling mechanism in Simulation B and C.

Table S1. Oxidation products that partition to aerosol phase through gas-particle partitioning, parent VOCs, partitioning coefficients (K), production rates and relative contributions (annual mean) to ne_oSOA in three different simulations.

Short name	Chemical formula	Parent VOC	K ($m^3/\mu g$)	Production (Tg/year)			% contribution to ne_oSOA		
				Simulation A	Simulation B	Simulation C	Simulation A	Simulation B	Simulation C
A-DI	C6H5OH(OH)CHO	aromatics	1.47E-03	8.11E-02	5.12E-02	6.32E-02	3.31E-01	3.39E-01	2.38E-01
AD2P	C6H4(CH3)OH(OH)OOH	aromatics	1.01E-1	1.59E+00	1.47E+00	1.53E+00	6.47E+00	9.71E+00	5.74E+00
AP	C6H5OH(OH)C(O)OOH	aromatics	8.34E-1	1.35E+00	1.26E+00	1.30E+00	5.52E+00	8.35E+00	4.87E+00
APAN	C6H5OH(OH)CO3NO2	aromatics	1.76E-1	6.85E-01	6.43E-01	6.74E-01	2.80E+00	4.26E+00	2.53E+00
DPAN	CHOCH=CHCO3NO2	aromatics	4.34E-07	3.79E-05	3.43E-05	3.83E-05	1.55E-04	2.27E-04	1.44E-04
GPAN	HOCH2C(O)OONO2	isoprene	6.33E-07	1.72E-03	1.05E-08	1.32E-08	7.04E-03	6.96E-08	4.94E-08
NITP	C6H5ONO2	aromatics	3.24E-07	7.76E-05	3.66E-05	5.05E-05	3.17E-04	2.42E-04	1.90E-04
XAP	CH3COCH=CHC(O)OOH	aromatics	1.12E-05	1.21E-04	7.09E-05	8.89E-05	4.93E-04	4.69E-04	3.34E-04
XPAN	CH3COCH=CHCO3NO2	aromatics	1.81E-06	4.56E-05	3.64E-05	4.20E-05	1.86E-04	2.41E-04	1.58E-04
YAP	CHOCH=C(CH3)C(O)OOH	aromatics	7.24E-06	8.54E-05	4.78E-05	6.10E-05	3.49E-04	3.16E-04	2.29E-04
YPAN	CHOCH=C(CH3)CO3NO2	aromatics	1.33E-06	3.43E-05	2.66E-05	3.10E-05	1.40E-04	1.76E-04	1.17E-04
ZAP	CHOC(CH3)=CHC(O)OOH	aromatics	7.54E-06	8.90E-05	4.97E-05	6.36E-05	3.63E-04	3.29E-04	2.39E-04
ZPAN	CHOC(CH3)=CHCO3NO2	aromatics	1.38E-06	3.56E-05	2.76E-05	3.22E-05	1.45E-04	1.83E-04	1.21E-04
IAP	HOCH2C(CH3)(OOH)CH(OH)CHO	isoprene	7.77E-02	4.58E+00	8.71E-01	2.12E+00	1.87E+01	5.76E+00	7.97E+00
INPN	O2NOCH2C(OOH)(CH3)CH=CH2	Isoprene	1.83E-05	3.91E-03	2.77E-03	3.43E-03	1.60E-02	1.83E-02	1.29E-02
ISNP	HOCH2C(OOH)(CH3)CH(ONO2)CH2OH	Isoprene	3.39E+00	1.06E+00	4.51E-01	6.79E-01	4.32E+00	2.98E+00	2.55E+00
LIP	HOC10H16OOH	Limonene	2.54E-02	8.10E-01	1.07E+00	1.07E+00	3.30E+00	7.09E+00	4.01E+00
MRP	HOCH2C(OOH)(CH3)CHO	from MACR, isoprene, limonene, alpha pinene	6.15E-05	9.94E-03	2.00E-03	3.39E-03	4.06E-02	1.33E-02	1.27E-02
PINT	ONO2C10H16OOH	alpha pinene and limonene	1.55E-02	2.05E-01	1.11E-01	1.57E-01	8.37E-01	7.37E-01	5.92E-01
PIP	HOC10H16OOH	alpha pinene	7.58E-03	7.87E-01	8.02E-01	8.63E-01	3.21E+00	5.31E+00	3.24E+00
VRP	HOCH2CH(OOH)C(O)CH3	Isoprene	9.90E-05	2.01E-02	4.25E-03	7.75E-03	8.21E-02	2.81E-02	2.91E-02
DB1OOH	HOCH=C(CH3)CH(OOH)CH2OH + HOCH2C(CH3)(OOH)CH=CHOH	Isoprene	6.40E-03	-	5.22E-01	1.41E+00	-	3.45E+00	5.30E+00
DB2OOH	CHOC(CH3)(OOH)CHOHCH2OH + HOCH2C(CH3)(OH)CH(OOH)CH2OH	Isoprene	1.10E-01	-	2.47E+00	6.34E+00	-	1.63E+01	2.38E+01
TRIOL	HOCH=C(CH3)CH(OH)CH2OH + HOCH2C(CH3)(OH)CH=CHOH	isoprene	4.78E-06	-	1.67E-06	5.16E-06	-	1.10E-05	1.94E-05
PRN2	C4H7O6N	Isoprene	4.42E-02	1.34E+01	8.07E+00	1.04E+01	5.45E+01	5.34E+01	3.91E+01
RIP	HOCH2C(OOH)(CH3)CH=CH2	isoprene	1.77E-05	7.04E-03	1.09E-03	3.28E-03	2.87E-02	7.21E-03	1.23E-02
Total anthropogenic sources			-	3.7	3.4	3.6	15.1	19.1	13.5
Total biogenic sources			-	20.8	14.4	23.0	84.9	80.9	86.5

Table S2. Additional species used in the HO_x recycling mechanism

Symbol	Formula	Description
RIPEEO2	Z-HOCH2C(CH3)=CHCH2O2 + Z-CH2O2C(CH3)=CHCH2OH	Z isomers of the internally double bonded isoprene peroxy radicals
RIPEEOOH	Z-HOCH2C(CH3)=CHCH2OOH + Z-CH2OOHC(CH3)=CHCH2OH	Hydroperoxide from RIPEEO2
DB1O2	HOCH=C(CH3)CH(O2)CH2OH + HOCH2C(CH3)(O2)CH=CHOH	first-generation RO2 from Dibble mechanism (Paulot et al., 2009a)
DB2O2	CHOC(CH3)(O2)CHOHCH2OH + HOCH2C(CH3)(OH)CH(O2)CH2OH	second-generation RO2 from Dibble mechanism (Paulot et al., 2009a)
DB1OOH	HOCH=C(CH3)CH(OOH)CH2OH + HOCH2C(CH3)(OOH)CH=CHOH	Hydroperoxide from DB1O2
DB2OOH	CHOC(CH3)(OOH)CHOHCH2OH + HOCH2C(CH3)(OH)CH(OOH)CH2OH	Hydroperoxide from DB2O2
TRIOL	HOCH=C(CH3)CH(OH)CH2OH + HOCH2C(CH3)(OH)CH=CHOH	Triol from the molecular channel of DB1O2 permutation reaction
ZCO3HC23DBCOD	HOCH=C(CH3)CH(OH)CH2OH + HOCH2C(CH3)(OH)CH=CHOH	Acylhydroperoxyaldehydes (PACALD) predicted by Peeters et al., (2009)
ZCODC23DBCOOH	CHOC(CH3)=CHCH2OOH + HOOCH2C(CH3)CHCHO	Hydroperoxyaldehydes (HPALD) predicted by Peeters et al., (2009)

Table S3. Additional reactions for HO_x recycling mechanism

Reaction	Rate constant	References	Notes
RIPEEO2 => ZCODC23DBCOOH + HO2	9.82E8 * EXP(-6303/T)	Peeters et al. (2009)	1,6-H-shift
RIO2 => 0.864 HO2 + 0.690 HCHO + 0.402 MVK + 0.288 MACR + 0.136 RIO1 + 0.127 IALD	6.08E10 * EXP(-8893/T)	Peeters et al. (2009)	1,5-H-shift for MVK and MACR precursors; Although the parent RO2 of IALD do not undergo 1,5-H-shift, for simplicity the products of RIO2 + NO are taken except NO2
RIPEEO2 + HO2 => RIPEEOOH	2.91E-13 * EXP(1300./T) * 0.706		MCM rate constant
RIPEEO2 + MO2 => IAP + HO2 + HCHO + HO2	K same as for IAO2 + MO2		
RIPEEO2 + NO => IAP + HO2 + NO2	2.54E-12 * EXP(360./T)		Rate constant as for the others first-generation RO2 from isoprene
RIPEEOOH + hv => OH + IAP + HO2	J(CH3OOH)		
RIPEEOOH + OH => 0.5 IEPOX + 0.25MGLY + 0.25GLYX + 0.25HOOCH2CHO + 0.25CH3COCH2OOH	k= same as for RIP + OH		approximation: a carbonyl function should have been an -OH functional group
ZCODC23DBCOOH + OH => 0.5MGLY + 0.5 HOOCH2CHO + 0.5CH3COCH2OOH + 0.5GLYX	4.50E-11	SAR (Taraborrelli et al., in prep.)	rate constant calculated by SAR by and similar to the estimate of Peeter and Mueller, PCCP 2010
ZCODC23DBCOOH + hv => OH + IAO2	J(CH3OOH)+J(MACR)/0.004		J value for MACR photolysis assuming IMPACT has a quantum yield of 0.004 (as recommended by IUPAC). IAO2 should represent LHC4ACCO3 of MIM2
CH3COCH2OOH + OH => ATO2	1.90E-12 * EXP(190/T)	IUPAC	H-abstraction channel from the –OOH group
CH3COCH2OOH + OH => MGLY + OH	8.39E-12	SAR (Taraborrelli et al., in prep.)	H-abstraction from the –CH2OOH group with following prompt OH-elimination
CH3COCH2OOH + hv => MCO3 + HCHO + OH	J(MEK) + J(CH3OOH)		Structural analogy to methyl ethyl ketone and methyl hydroperoxide
IAO2 => ZCO3HC23DBCOD +	7.32E8 * EXP(-	Peeters et al. (2009)	1, 6-H-shift

HO2	5556./T)		
ZCO3HC23DBCOD + hv => MCO3 + 2CO2 + 2OH + HO2 + CO	J(CH3OOH)+J(MACR)/0.004	Peeters et al. (2009)	enhanced photolysis
VRO2 => 0.7MGLY + 0.7HCHO + 0.3HOOCH2CHO + 0.3MCO3 + OH	5.1E10 * EXP(-8893/T)	Peeters et al. (2009)	1,5-H-shift
MRO2 => 0.830 HCHO + 0.830 MGLY1 + 0.170 + HAC + 0.170 CO + .17 HO2 + OH	4.5E10*EXP(-8893/T)	Peeters et al. (2009)	1,5-H-shift
HOOCH2CHO + OH => OH + 0.44HCHO + 0.44CO + 0.56GLYX	2.081E-11		0.29 HCOCH2O2 neglected and the other two yields re-scaled with a factor of 1/(1-.29)
HOOCH2CHO + hv => OH + HCHO + CO + HO2	J(CH3OOH)+J(GLYC)		Structural analogy to glycolaldehyde and methyl hydroperoxide
DB1O2 + MO2 => 0.8 DB2O2 + 0.2 TRIOL + HCHO + HO2	2.9E-12		MCM rata constant for a secondary RO2
DB1O2 + HO2 => DB1OOH	0.706 * 2.91E-13 * EXP(1300./T)		MCM rate constant
DB1O2 + NO => DB2O2 + NO2	2.54E-12 * EXP(360./T)		Rate constant as for the others first-generation RO2 from isoprene
DB2O2 + MO2 => 0.5 HAC + 0.5 GLYC + 0.5 MGLY + 0.5 GLYX + HO2 + HCHO + HO2	2.9E-12		MCM rata constant for a secondary RO2
DB2O2 + HO2 => DB2OOH	0.706 * 2.91E-13 * EXP(1300./T)		MCM Rate constants
DB2O2 + NO => 0.5 HAC + 0.5 GLYC + 0.5 MGLY + 0.5 GLYX + HO2 + NO2	2.54E-12 * EXP(360./T)		Rate constant as for the others first-generation RO2 from isoprene
DB1OOH + OH = >DB1O2	0.4*k_CH3OOH_OH		
DB1OOH + hv => DB2O2 + OH	J(CH3OOH)		Structural analogy to methyl hydroperoxide
DB2OOH + OH => DB2O2	0.4*k_CH3OOH_OH		
DB2OOH + hv => 0.5 HAC + 0.5 GLYC + 0.5 MGLY + 0.5 GLYX + HO2 + OH	J(CH3OOH)		Structural analogy to methyl hydroperoxide
TRIOL + OH => IAO2	1E-11	SAR (Taraborrelli et al., in prep.)	Triol from permutations reactions of DB1O2

Table S4. Modified reactions in HOx recycling mechanism

Modified reactions	Original reactions	References	Notes
MAO3 + HO2 => 0.44 OH + 0.44 HO2 + 1.76HCHO + 0.350 MAOP + 0.150 RCOH	MAO3 + HO2 => 0.7MAOP + 0.30 RCOH + 0.3O3		Structural analogy to MCO3
MCO3 + HO2 => 0.44 OH + 0.44 MO2 + 0.35 MAP + .15 ACTA + .15 O3	MCO3 + HO2 => O3 + ACTA MCO3 + HO2 => MAP	IUPAC, 2009	
RIO2 + NO => NO2 + 0.864 HO2 + 0.690 HCHO + 0.402 MVK + 0.288 MACR + 0.09 DB1O2 + 0.046 RIO1 + 0.127 IALD	RIO2 + NO => NO2 + 0.864 HO2 + 0.690 HCHO + 0.402 MVK + 0.288 MACR + 0.136 RIO1 + 0.127 IALD	Paulot et al., (2009a)	
MO2 + RIO2 => 1.864 HO2 + 1.690 HCHO + 0.402 MVK + 0.288 MACR + 0.09 DB1O2 + 0.046 RIO1 + 0.127 IALD	MO2 + RIO2 => 0.25MOH + 0.92HO2 + HCHO +0.2MVK + 0.14MACR +0.07RIO1 + 0.06IALD +0.25MEK +0.25ROH	This work	Consistent with Paulot et al., (2009a)
MCO3 + RIO2 => MO2 + 0.864 HO2 + 0.690 HCHO + 0.402 MVK + 0.288 MACR + 0.09 DB1O2 + 0.046 RIO1 + 0.127 IALD	MCO3 + RIO2 => MO2 + 0.864HO2 + 0.690HCHO + 0.402MVK + 0.288MACR + 0.136RIO1 + 0.127IALD	This work	Consistent with Paulot et al., (2009a)
RIO2 + RIO2 => 1.728 HO2 + 1.38 HCHO + 0.804 MVK + 0.576 MACR + 0.18 DB1O2 + 0.092 RIO1 + 0.254 IALD	RIO2 + RIO2 => 0.680MVK + 0.390MACR + 0.930IPRD +0.40HCHO + 1.380HO2	This work	Consistent with Paulot et al., (2009a)
RIO2 + HO2 => RIP	RIO2 + HO2 => 0.88RIP + 0.12OH + 0.047MACR + 0.073MVK + 0.120HCHO + 0.120HO2		the 12% yield of OH was used in Paulot et al., (2009b) in order to account for the initial NOx present in the "low-NOx" experiments
RIO1 + HO2 => RIP	RIO1 + HO2 => 0.88RIP + 0.12OH + 0.047MACR + 0.073MVK + 0.120HCHO + 0.120HO2		The same above
GLYX + OH => 1.8 CO + 0.8 HO2 + 0.2 OH	GLYX + OH => HO2 +2CO	This work	Combination of results from Orlando and Tyndall, (2001), Feierabend et al., (2008)
GLYC + OH => 0.75 HO2 + 0.25 OH + 0.13 GLYX + 0.52 CO + 0.16 HCOOH + 0.71 HCHO	GLYC + OH => 0.80GCO3 + 0.20 GLYX + 0.20HO2	Butkovskaya et al., (2006a)	
HAC + OH => 0.75 MGLY + 0.825 HO2 + 0.125	HAC + OH => MGLY + HO2	Butkovskaya et al., (2006b)	

HCOOH + 0.1 OH +0.125 MO2 + 0.05 CO + 0.125 ACTA			
RIP + OH => 0.5 IAO2 + 0.50MGLY + 0.50GLYX + 0.50CH3COCH2OOH + 0.50HOOCH2CHO	RIP + OH => 0.50IAO2 + 0.4RIO2 + 0.2RIO1	This work	Approximation regarding the degradation products

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