Summary of New Species and Reactions for Isoprene and Monoterpene Oxidation

Table 1 – Species added or revised in GEOS-Chem

Species	FullName	Adv.?	Formula	MW_g	F0	H*_DD	H*_W	CR_W
ISOPRENE CHEMISTRY								
ACTA	acetic acid	**Yes**	$C_2H_4O_2$	60	1.0	4.1E3	4.1E3	6.3E3
HPALD	hydroperoxyaldehydes	Yes	$C_5H_8O_3$	116	0.0	4.0E4	NA	NA
HPC52O2	See MCM v3.3.1 for full structure	No	$C_5H_9O_6$	165	NA	NA	NA	NA
HC187	epoxide oxidation product m/z 187-189	No	NA	187	Scaled relative to HNO_3[2]		NA	NA
DHDN	c5 dihydroxydinitrate	Yes	$C_5H_{10}O_8N_2$	226	Scaled relative to ISOPN[3]		2E6	9.2E3
DHDC	di-hydroperoxide dicarbonyl	No	$C_5H_8O_6$	164	NA	NA	NA	NA
DHPCARP	dihydroxy α-formyl peroxy radical	No	$C_5H_9O_7$	181	NA	NA	NA	NA
ETHLN	ethanol nitrate	Yes	$C_2H_3O_3N$	105	Scaled relative to ISOPN[3]		2E6	9.2E3
GLYX	glyoxal	Yes	$C_2H_2O_2$	58	1.0	3.6E5	3.6E5	7.2E3
HCOOH	formic acid	Yes	CH_2O_2	46	1.0	8.9E3	8.9E3	6.1E3
H2O2	hydrogen peroxide	Yes	H_2O_2	34	1.0	5.0E7	5.0E7	7.4E3
IEPOXA	*trans*-β isoprene epoxydiol	Yes	$C_5H_{10}O_3$	118	1.0	8.0E7[8]	8.0E7	0d0
IEPOXB	*cis*-β isoprene epoxydiol	Yes	$C_5H_{10}O_3$	118	1.0	8.0E7[8]	8.0E7	0d0
IEPOXD	δ isoprene epoxydiol	Yes	$C_5H_{10}O_3$	118	1.0	8.0E7[8]	8.0E7	0d0
ISN1	nighttime isoprene nitrate	Yes	$C5H_8NO_4$	146	Scaled relative to ISOPN[3]		2.0E6	9.2E3
RIPA	1,2-ISOPOOH	Yes	$C_5H_{10}O_3$	118	1.0	1.7E6	1.7E6	0.0
RIPB	4,3-ISOPOOH	Yes	$C_5H_{10}O_3$	118	1.0	1.7E6	1.7E6	0.0
RIPD	δ(1,4 and 4,1)-ISOPOOH	Yes	$C_5H_{10}O_3$	118	1.0	1.7E6	1.7E6	0.0
SOAIE[6]	aerosol-phase IEPOX	Yes	$C_5H_{10}O_3$	118	0.0	NA	NA	NA
IMAE	C4 epoxide from oxidation of MPAN (PMN)	Yes	$C_4H_6O_3$	102	1.0	1.2E5	1.2E5	7.2E3
SOAME	aerosol-phase IMAE	Yes	$C_4H_6O_3$	102	0.0	NA	NA	NA
SOAGX	aerosol-phase glyoxal	Yes	$C_2H_2O_2$	58	0.0	NA	NA	NA
SOAMG	aerosol-phase methylglyoxal	Yes	$C_3H_4O_2$	72	0.0	NA	NA	NA
LVOC	gas-phase low-volatility non-IEPOX product of ISOPOOH (RIP) oxidation	Yes	$C_5H_{14}O_5$[7]	154	1.0	1E8	1E8	7.2E3
LVOCOA	aerosol-phase LVOC	Yes	$C_5H_{14}O_5$	154	0.0	NA	NA	NA
MGLY	methylglyoxal	Yes	$C_3H_4O_2$	72	1.0	3.7E3	3.7E3	7.5E3
ISN1OG	gas-phase second generation hydroxynitrates formed from ISOP+NO_3 reaction pathway	Yes	$C_5H_{10}O_8N_2$	226	1.0	2.3E4	2.3E4	9.2E3
ISN1OA	aerosol-phase ISN1OG	Yes	$C_5H_{10}O_8N_2$	226	0.0	NA	NA	NA

PMN	peroxymethacryloyl nitrate (MPAN)	Yes	$C_4H_5O_5N$	147	Scaled relative to PAN[4]		NA	NA
PPN	peroxypropionylnitrate	Yes	$C_3H_5O_5N$	135	Scaled relative to PAN[4]		NA	NA
MONOTERPENE CHEMISTRY								
API	alpha-pinene and other cyclic terpenes with one double bond	Yes	*Lumped APIN+BPIN +SABI+CA RE	136	0	0.049	0.049	0
APIO2	RO_2 from API	No	NA		NA	NA	NA	NA
LIM	limonene and other cyclic terpenes with two double bonds	Yes	*Lumped LIMO+MY RC+OCIM	136	0	0.07	0.07	0
LIMO2	RO_2 from LIM	No	NA		NA		NA	NA
PIP	peroxides from API & LIM	No	NA		NA		NA	NA
OLND	monoterpene-derived NO_3-alkene adduct that primarily decomposes	No	NA		NA		NA	NA
OLNN	monoterpene-derived NO_3 adduct that primarily retains NO_3	No	NA		NA		NA	NA
MONITS	saturated first generation monoterpene organic nitrate	Yes	NA	215	Scaled to ISOPN[3]		1.7E4	9200[5]
MONITU	Unsaturated first generation monoterpene organic nitrate	Yes	NA	215	Scaled to ISOPN[3]		1.7E4	9200[5]
HONIT	Second generation monoterpene organic nitrate	Yes	NA	215	Scaled to ISOPN[3]		2.69E13	5487[5]
ONITAam	Aerosol-phase organic nitrate formed from isoprene precursors[1]	Yes	NA					
ONITApm	Aerosol-phase organic nitrate formed from monoterpene precursors[1]	Yes	NA					

[1]Jenny Fisher: These names should be changed (they were originally daytime/nighttime species, but changed to isop/monot). I left them as is here because they'll need to change below as well and I didn't want to mess things. Scavenging efficiency = 0.8.

[2] DVZ = DVZ *sqrt(XMW(HNO3)/sqrt(XMW(N)) – based on Nguyen et al, 2015

[3] DVZ = DVZ *sqrt(XMW(ISOPN)/sqrt(XMW(N)) – based on Nguyen et al, 2015

[4] DVZ = DVZ *sqrt(XMW(PAN)/sqrt(XMW(N)) – based on Nguyen et al, 2015

[5]Browne et al, 2014

[6]The same gas-phase and aerosol-phase molecular weights areused for SOAIE because the organic and inorganic aerosol components are treated separately (externally mixed) in GC. The aerosol uptake mechanism takes into account aerosol-phase processing of IEPOX to form polyols, organosulfates, organonitrates. See Marais et al. (2016) for more details.

[7]The chemical formula is to represent the average molecular weight of a range of LVOC compounds identified by Krechmer et al. (2015).

[8]Uptake to aerosols is treated differently. H* for IEPOX uptake to aerosols is 3.3E7. From Eloise: odd though that it's lower than the dry dep value. I use 2.7E6 for IEPOX dry dep in my code. (Higher value comes from Nguyen et al, 2014). Possibly should reconsider H* for aerosol uptake.

Table 2- Updated Isoprene-Related Reactions to be added to GEOS-Chem

Old Reaction	Old Rate Constant	Reference	New Reaction	New Rate Constant	Reference
Reactions with OH					
-	-	-	HC187 + OH = 0.5MCO3+ 0.5MGLY + $0.5HO_2$ + 0.5CO + CH_2O	1.4E-11	*Reaction and Rate:* Bates et al. (2014)
-	-	-	HPALD + OH = 0.365HPC52O2 + 0.085GLYX + $0.085MCO_3$ + 0.55MGLY + 0.55 CO + $0.55CH_2O$ + $0.635OH + 0.085CO_2$[(n)]	5.1E-11	*Reaction:* Peeters and Müller, 2010 *Rate:* Wolfe et al., 2012
RIP + OH = $0.387RIO_2$ + 0.613OH + 0.613HC5	4.75E-12exp(200/T)	*Reaction and Rate:* Paulot et al. (2009b)	RIPA + OH = $0.750RIO_2$ + 0.250HC5 + $0.125(OH + H_2O)$	6.13E-12exp(200/T)	*Reaction*: St. Clair et al., 2016 *Rate:* St. Clair et al., 2016; Paulot et al., 2009b
-	-	-	RIPB + OH = $0.480RIO_2$ + 0.520HC5 + $0.26(OH + H_2O)$	4.14E-12exp(200/T)	*Reaction*: St. Clair et al., 2016 *Rate:* St. Clair et al., 2016; Paulot et al., 2009b
-	-	-	RIPD + OH = $0.250RIO_2$ + 0.750HC5 + $0.375 (OH + H_2O)$	5.11E-12exp(200/T)	*Reaction*: St. Clair et al., 2016 *Rate:* St. Clair et al., 2016; Paulot et al., 2009b
RIP + OH = OH + IEPOX	1.9E-11exp(390/T)	*Reaction and Rate:* Paulot et al. (2009b)	RIPA + OH = 0.850OH + 0.578IEPOXA + 0.272IEPOXB + 0.150HC5OO[(j)]	1.70E-11exp(390/T)	*Reaction*: St. Clair et al., 2016 *Rate:* St. Clair et al., 2016; Paulot et al., 2009b
-	-	-	RIPB + OH = 1.000OH + 0.680IEPOXA + 0.320IEPOXB	2.97E-11exp(390/T)	*Reaction*: St. Clair et al., 2016 *Rate:* St. Clair et al., 2016; Paulot et al., 2009b
-	-	-	RIPD + OH = 0.500OH + 0.500IEPOXD + 0.500HC5OO	2.92E-11exp(390/T)	*Reaction*: St. Clair et al., 2016 *Rate:* St. Clair et al., 2016; Paulot et al., 2009b
IEPOX + OH = IEPOXOO	5.78e-11exp(-400/T)	*Reaction and Rate:* Paulot et al. (2009b)	IEPOXA + OH = IEPOXOO	3.73E-11exp(-400/T)[(i)]	*Reaction*: Bates et al., 2014 *Rate:* Bates et al., 2014; Paulot et al., 2009b
-	-	-	IEPOXB + OH = IEPOXOO	5.79E-11exp(-400/T)	*Reaction*: Bates et al., 2014 *Rate:* Bates et al., 2014;

					Paulot et al., 2009b
-	-	-	IEPOXD + OH = IEPOXOO	3.20E-11exp(-400/T)	*Reaction*: Bates et al., 2014 *Rate:* Bates et al., 2014; Paulot et al., 2009b
ISOPND + OH =$ISOPNDO_2$	2.64E-11exp(380/T)	*Reaction and Rate:* Paulot et al. (2009a)	ISOPND + OH = 0.1IEPOX + 0.9$ISOPNDO_2$ + 0.1NO_2	1.2E-11exp(652/T)	*Reaction:* Jacobs et al., 2014 *Rate:* Lee et al., 2014
ISOPNB + OH =$ISOPNBO_2$	3.61E-12exp(380/T)	*Reaction and Rate:* Paulot et al. (2009a)	ISOPNB + OH = 0.1IEPOX +$ISOPNBO_2$+ 0.1NO_2	2.4E-12exp(745/T)	*Reaction:* Jacobs et al., 2014 *Rate:* Lee et al., 2014
PROPNN + OH = NO_2 + MGLY	8.0E-13	*Reaction and Rate:* Paulot et al. (2009a)	PROPNN + OH = NO_2 + MGLY	6.7E-13	*Reaction:* Same *Rate:* MCMv3.3
RO_2 + NO Reactions					
-	-	-	DHPCARP + NO = GLYX + MGLY + NO_2 + OH	2.7E-12exp(360/T)	*Reaction and Rate:* Jenkin et al., 2003, 2015
-	-	-	HPC52O2 + NO = GLYX + MGLY + NO_2 + OH	2.7E-12exp(360/T)	*Reaction and Rate:* Jenkin et al., 2003, 2015
RIO_2 + NO = 0.883NO_2 + 0.783HO_2 + 0.660CH_2O + 0.400MVK + 0.260MACR + 0.070ISOPND + 0.047ISOPNB + 0.123HC5 + 0.1DIBOO	2.7E-12 exp(350/T)	*Reaction and Rate:* Paulot et al. (2009a)	RIO_2 + NO = 0.91NO_2 + 0.82HO_2 + 0.82CH_2O + 0.476MVK + 0.344MACR + 0.058HC_5 + 0.03DIBOO + 0.009ISOPND + 0.081ISOPNB	2.7E-12 exp(350/T)	*Reaction:* Liu et al., 2013; Fisher et al., 2016 *Rate:* Paulot 2009a
IEPOXOO + NO = 0.725HAC+0.275GLYC+0.275GLYX +0.275MGLY +0.125OH+0.825HO_2+0.200CO_2+0.375CH_2O+0.074HCOOH +0.251CO +NO_2	2.7E-12exp(350/T)	*Reaction and Rate:* Paulot et al., 2009b	IEPOXOO + NO = 0.117HAC +0.088GLYC+0.088GLYX +0.088MGLY+ 0.125OH+ 0.825HO_2+0.8CO_2+0.375CH_2O +0.142HCOOH+0.678CO+NO_2+0.473HC187+0.058CO_2[(a)]	2.7E-12exp(350/T)	*Reaction:* Bates et al., 2014 *Rate:* Paulot et al., 2009b
$ISOPNDO_2$ + NO = 0.070MACRN + 0.310HCOOH + 0.440HAC + 0.130ETHLN + 0.650CH_2O + 1.340NO_2 + 0.150GLYC + 0.310NO_3 + 0.150PROPNN + 0.340MEK + 0.350HO_2	K* (1-YN) where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E	*Reaction and Rate:* Paulot et al. (2009a)	$ISOPNDO_2$ + NO = 0.019MACRN + 0.057HCOOH +0.27HAC + 0.210ETHLN + 0.15CH_2O + 0.790NO_2 + 0.3GLYC + 0.3PROPNN + 0.61HO_2 + 0.27DHDN + 0.075MVKN + 0.057$ISOPNDO_2$ [(b)]	2.4E-12exp(360/T)	*Reaction and Rate:* Lee et al., 2014

	00)				
$ISOPNBO_2$ + NO = 0.6GLYC + 0.6HAC + $0.4CH_2O$ + $1.6NO_2$ + 0.26MACRN + $0.4HO_2$ + 0.14MVKN	K* (1-YN) where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E 00)	*Reaction and Rate:* Paulot et al. (2009a)	$ISOPNBO_2$ + NO = 0.09GLYC + 0.09HAC + $0.70CH_2O^{(m)}$ + $0.88NO_2$ + 0.44MACRN + $0.69HO_2$ + 0.26MVKN + 0.21DHDN	2.4E-12exp(360/T)	*Reaction and Rate:* Lee et al., 2014
RO_2 + HO_2 Reactions					
-	-	-	DHPCARP + HO_2 = RCOOH	2.05E-13exp(1300/T)	*Reaction and Rate:* Jenkin et al., 2003, 2015
-	-	-	HPC52O2 +HO_2 = $RCOOH^{(o)}$	2.05E-13exp(1300/T)	*Reaction and Rate:* Jenkin et al., 2003, 2015
RIO_2 + HO_2= 0.88RIP + 0.12OH + 0.047MACR + 0.073MVK + $0.12HO_2$ + $0.12CH_2O$	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=5	*Reaction:* Paulot, et al. (2009b) *Rate:* Saunders et al. (2003)	RIO_2 + HO_2= 0.628RIPA + 0.272RIPB + 0.037RIPD + 0.063 (OH + CH_2O + HO_2) + 0.038MVK + 0.025MACR	2.06E-13*exp(1300/T)	*Reaction:* St. Clair et al., 2015; Liu et al., 2013 *Rate:* Saunders et al. (2003)
IEPOXOO + HO_2 = 0.725HAC + 0.275GLYC + 0.275GLYX + 0.275MGLY + 1.125OH + $0.825HO_2$ + $0.200CO_2$ + $0.375CH_2O$ + 0.074HCOOH + 0.251CO	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=5	*Reaction:* Paulot, et al. (2009b) *Rate:* Saunders et al. (2003)	IEPOXOO + HO_2 = 0.085HAC +0.025GLYC + 0.085GLYX+ 0.085MGLY + 1.125OH+ $0.825HO_2$+ $1.1CO_2$+$0.375CH_2O$ + 0.278HCOOH + 0.6CO + 0.44HC187+$0.072CO_2^{(a)}$	2.06E-13*exp(1300/T)	*Reaction:* Bates et al., 2014 *Rate:* Saunders et al. (2003)
$ISOPNDO_2$ + HO_2 = 0.035MACRN + 0.155HCOOH + 0.22HAC + 0.065ETHLN + $0.325CH_2O$ + $0.170NO_2$ + 0.075GLYC + $0.155NO_3$ + 0.075PROPNN + 0.170MEK + $0.175HO_2$ + 0.5OH + 0.5ISNP	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=5	*Reaction:* Paulot, et al. (2009b) *Rate:* Saunders et al. (2003)	$ISOPNDO_2$ + HO_2 = 0.01MACRN + 0.2HAC + 0.2ETHLN + $0.07CH_2O$ + 0.23GLYC + 0.23PROPNN + $0.5HO_2$ + 0.5OH + 0.06MVKN + $0.5ISNP^{(c)}$	8.7E-14*exp(1650/T)	*Reaction and Rate:* Lee et al., 2014
$ISOPNBO_2$ + HO_2 = 0.3GLYC + 0.3HAC + $0.2CH_2O$ + 0.13MACRN + 0.07MVKN + $0.3NO_2$ + $0.2HO_2$ + 0.5OH + 0.5ISNP	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=5	*Reaction:* Paulot, et al. (2009b) *Rate:* Saunders et al. (2003)	$ISOPNBO_2$ + HO_2 = 0.06GLYC + 0.06HAC + $0.44CH_2O$ + 0.28MACRN + 0.16MVKN + $0.06NO_2$ + $0.44HO_2$ + 0.5OH + $0.5ISNP^{(c)}$	8.7E-14*exp(1650/T)	*Reaction and Rate:* Lee et al., 2014

RO_2 + MO_2/RO_2 Reactions					
RIO_2 + RIO_2 = 1.28HO_2 + 0.92CH_2O + 0.56MVK + 0.36MACR + 0.48ROH + 0.5HC5	1.54E-13	No reference cited on wiki page?	RIO_2 + RIO_2 = 0.91HO_2 + 0.75CH_2O + 0.45MVK + 0.29MACR + 0.09DIBOO + 1.11HC5+ 0.29CO	2.3E-12	*Reaction and Rate:* Xie et al., 2013
Reactions with O_3					
ISOPNB + O_3 = 0.610MVKN + 0.390MACRN + 0.27OH + CH_2O	1.06E-16	*Reaction and Rate:* Lockwood et al., 2010	ISOPNB + O_3 = 0.05HO_2 + 0.11MVKN + 0.32MACRN + 0.16HCOOH + 0.0.05OH + 0.62CH_2O + 0.36CO_2 + 0.21CO + 0.06PROPNN + 0.36PROPNN[(d)] + 0.1MVKN + 0.41HNO_3 [(e)]	3.7E-19	*Reaction and Rate:* Lee et al., 2014
ISOPND + O_3 = 0.5PROPNN + 0.5ETHLN + 0.27OH + 0.5GLYC + 0.5HAC	5.3E-17	*Reaction and Rate:* Lockwood et al., 2010	ISOPND + O_3 = 0.06NO_2 +0.24PROPNN + 0.26ETHLN + 0.37OH + 0.24GLYC + 0.26HAC + 0.63CO_2 + 0.24MOH + 0.09EOH + 0.2CH_2O + 0.1MCO_3 + 0.06GLYX + 0.16HAC + 0.14PROPNN + 0.3HNO_3[(e)]	2.9E-17	*Reaction and Rate:* Lee et al., 2014
ISN1 + O_3 = 0.3R4N_2 + 0.7GLYX + 0.7NO_2 + 0.25CH_2O + 0.25MOH + 0.5HO_2 + 0.5CH_2O	4.15E-15*exp(-1520/T)	**No reference cited on wiki page?**	ISN1 + O_3 = 0.3PROPNN + 0.7GLYX + 0.7NO2 + 0.25CH2O + 0.25MOH + 0.5HO2 + 0.5CH2O	4.15E-15*exp(-1520/T)	*Reaction:* Change R4N2 to PROPNN as we now track the specific species formed[(g)]
Reactions with NO_3 leading to ISN1OG aerosol precursor					
ISNOHOO + NO → 0.934R4N2 + 0.934HO_2 + 0.919GLYX	2.6E-12*exp(380/T)	*Reaction and Rate:* Xie et al., 2012	ISNOHOO + NO → 0.894PROPNN + 0.934HO_2 + 0.919GLYX + 0.04ISN1OG	No change	*Reaction:* Redistribute carbons to form 4% low-volatility 2nd generation hydroxynitrate aerosol precursor (Yield measured by Rollins et al. 2009).
ISNOHOO + HO_2 → INPN	2.06E-13*exp(1300/T)	*Reaction and Rate:* Xie et al., 2012	ISNOHOO + HO_2 → 0.96INPN + 0.04ISN1OG	No change	*Reaction:* Same as above
ISNOHOO + MO_2 → 0.7R4N2 + 0.7GLYX + 1.2HO_2 + 0.75CH_2O	2E-13	*Reaction and Rate:* Xie et al., 2012	ISNOHOO + MO_2 → 0.660PROPNN + 0.7GLYX + 1.2HO_2 + 0.75CH_2O + 0.04ISN1OG	No change	*Reaction:* Same as above.
ISNOOA + NO_3 → NO_2 +	4E-12	*Reaction and*	ISNOOA + NO_3 → NO_2 +	No change	*Reaction:* Same as above.

R4N2 + CO + HO_2		*Rate:* Xie et al., 2012	0.96PROPNN + CO + HO_2 + 0.04ISN1OG		
ISNOOA + NO → NO_2 + R4N2 + CO + HO_2	6.7E-12*exp(340/T)	*Reaction and Rate:* Xie et al., 2012	ISNOOA + NO → NO_2 + 0.96PROPNN + CO + HO_2 + 0.04ISN1OG	No change	*Reaction:* Same as above.
ISNOOA + HO_2 → 0.75RP + 0.25RCOOH + 0.25O_3	5.2E-13*exp(980/T)	*Reaction and Rate:* Xie et al., 2012	ISNOOA + HO_2 → 0.75RP + 0.25RCOOH + 0.25O_3 + 0.96NO_2 + 0.04ISN1OG	No change	*Reaction:* Same as above. Also included NO_2 as product. N not balanced in original reaction.
ISNOOB + NO_3 → R4N2 + GLYX + 2NO_2	2.3E-12	*Reaction and Rate:* Xie et al., 2012	ISNOOB + NO_3 → 0.94PROPNN + GLYX + 2NO_2 + 0.04ISN1OG	No change	*Reaction:* Same as above.
ISNOOB + NO → 0.94R4N2 + 0.94GLYX + 1.88NO_2	2.6E-12*exp(380/T)	*Reaction and Rate:* Xie et al., 2012	ISNOOB + NO → 0.9PROPNN + 0.94GLYX + 1.88NO_2 + 0.04ISN1OG	No change	*Reaction:* Same as above.
ISNOOB + HO_2 → INPN	2.06E-13*exp(1300/T)	*Reaction and Rate:* Xie et al., 2012	ISNOOB + HO_2 → 0.96INPN + 0.04ISN1OG	No change	*Reaction:* Same as above.
ISNOOB + MO_2 → 0.7R4N2 + 0.7GLYX + 0.7NO_2 + 0.75CH_2O + 0.25MOH + 0.5HO_2	2E-13	*Reaction and Rate:* Xie et al., 2012	ISNOOB + MO_2 → 0.66PROPNN + 0.7GLYX + 0.7NO_2 + 0.75CH_2O + 0.25MOH + 0.5HO_2+ 0.04ISN1OG	No change	*Reaction:* Same as above.
Isomerization Reactions					
-	-	-	DHPCARP = RCOOH + CO + OH	2.9E7*exp(-5300/T)	*Reaction and Rate:* Crounse et al., 2012
-	-	-	DHPCARP = DHDC	1.28E7*exp(-5300/T)	*Reaction and Rate:* Crounse et al., 2012, 2013
RIO_2 = 2HO_2 + CH_2O + 0.5MGLY + 0.5GLYC + 0.5GLYX +0.5HAC + OH	4.07E+08 exp(-7694/T)	*Reaction:* Stavrakou et al. (2010). *Rate:* Crounse et al. (2011)	RIO_2 = 0.5HPALD + 0.5DHPCARP	4.07E8*exp(-7694/T)[k]	*Reaction:* Peeters et al. (2014) *Rate:* Crounse et al. (2011)
Photolysis Reactions					
-	-	-	DHDC = MGLY + GLYX + 2OH[f]	J_{HPALD}	*Reaction and Rate:* Crounse et al., 2012
HPALD = OH + HO_2 + 0.5GLYC + 0.25GLYX +	Rate is equivalent to	*Reaction:* Stavrakou et	HPALD = 0.5MGLY + 0.39HAC + 0.11GLYC + 0.11MCO_3 + 1.89CO +	Rate is equivalent to MACR photolysis	*Reaction:* Peeters et al., 2014 *Rate:* Peeters and Müller,

0.25MGLY + CH_2O + 0.5HAC	MACR photolysis	al., 2010 *Rate:* Peeters and Müller, 2010	0.89HO_2 + 2OH		2010
-	-	-	ISN1 = NO_2 + HO_2 + 0.5GLYC + 0.25GLYX + 0.25MGLY + CH_2O + 0.5HAC	Rate is equivalent to MACR photolysis	*Reaction:* Products based on HPALD (Muller et al., 2014, Stavrakou et al., 2010) but with NO_2 instead of HO_2 *Rate*: Same as HPALD (Chris Chan Miller suggestion)
Hydrolysis Reactions					
-	-	-	ONITAam = INDIOL + HNO_3	2.78e-04 s^{-1}	*Reaction:* *Rate:* imposed lifetime = 1 hour (Fisher et al, 2016)
-	-	-	ONITApm = INDIOL + HNO_3	2.78e-04 s^{-1}	*Reaction:* *Rate:* imposed lifetime = 1 hour (Fisher et al, 2016)

[a]*IEPOXOO + NO2*: Other organic products were identified by Bates et al. (2014). These structural isomers are replaced with CO for the epoxide product, peroxyacetyl nitrate. The product "0.058CO_2" is a placeholder to balance carbon. *IEPOXOO + HO2:* The product "0.072CO_2" is a placeholder to balance carbon.

[b]The yields are not identical to the Lee et al. (2014) values, and there is artificial recycling of $ISOPNDO_2$ to account for non-unity reactants (i.e. in Lee et al. (2014), one $ISOPNDO_2$ reacts with 1.06$ISOPNDO_2$).

[c]In Lee et al. (2014), a C5 hydroperoxide is formed (ROOH). In order to close the nitrogen budget, this would have to be ISNP.

[d]Replace C4NACID in Lee et al. (2014) with PROPNN.

[e]HNO_3 added to this reaction to close the nitrogen budget, as we replace ethyl nitrate with its oxidation product, peroxyacetyl nitrate.

[f]Reaction is assumed to proceed through the same mechanism as HPALD.

[g]Jenny Fisher: We updated this in SEAC4RS to reflect that PROPNN is formed from this nighttime pathway (not generic species R4N2) – same for subsequent reactions. I can't remember the reference, I think it may have been in conversation with the Wennberg group.

[i]Eloise Marais: In my mechanism I used the Jacobs et al., 2013 A-value of 1.37E-10. If the mechanism is used as presented here, I might need to calculate a new Henry's Law constant for IEPOX uptake.

[j] In my mechanism I form 0.005LVOC from RIP oxidation, where LVOC is the aerosol precursor. Your reactions could be rewritten to form 0.005LVOC (some 5-carbon low volatility aerosol precursor) from RIPA, RIPB, and RIPD by taking 0.005IEPOX away from the products. Something like this: RIPA + OH 0.850OH + 0.576IEPOXA + 0.269IEPOXB + 0.150HC5OO + 0.005LVOC. This would have little impact on gas-phase IEPOX concentrations. Jason St. Clair/Kelvin Bates may be able to provide you with a more rigorous suggestion.

[k]For this reaction, we might also consider a different rate constant from Peeters et al. (2014) that is 1.8 times faster than Crounse et al. (2011).

[0.62*(9.5E7*exp(-7009/T) + 1.79E-7*exp(3722.5/T)*ktr)] + [0.31*(3.80E13*exp(-10745/T) + 5.82E-2*exp(476.3/T)*ktr)]; ktr = 0.01 for low NOx; ktr = 0.1 for high NOx

[m] This CO_2 is to balance carbon. The reason for the carbon balance issue is that the coproduce of GLYX is the MCMv3.3.1 species HYPERACET (CH3CHOCH2OOH). Perhaps hydroxyacetone (HAC) is a better proxy for this product. (From Chris Miller). Its not that hard to include HYPERACET in the simulation if you want to be really pedantic. The main two pathways look like reaction with OH and photolysis, using the MEK photolysis rate http://mcm.leeds.ac.uk/MCM/browse.htt?species=HYPERACET. (KRT, future work can address this, or we can use future Caltech recommendations).
[o] Carbon is not balanced. This is just a placeholder reaction (It forms a >C2 organic acid). The real structure is much more complicated, but not really worth including in a reduced mechanism.

Table 3- Updated Monoterpene-related Reactions to be added to GEOS-Chem

Old Reaction	**Old Rate Constant**	**Reference**	**New Reaction**	**New Rate Constant**	**Reference**
API/APIO2 Reactions					
$APIO_2 + HO_2$	1.50E-11	*Reaction and Rate:* Roberts and Bertman (1992)	No Change	No Change	No Change
$APIO_2$+NO = 0.82HO_2 + 0.82NO_2 + 0.23HCHO+ 0.43 RCHO + 0.11 ACET + 0.44MEK + 0.07 HCOOH + 0.18ONIT	4.0E-12	*Reaction:* Atkinson and Avery (2003) *Rate:* Roberts and Bertman (1992)	$APIO_2$+NO = 0.82HO_2 + 0.82NO_2 + 0.23HCHO+ 0.43 RCHO + 0.11 ACET + 0.44MEK + 0.07 HCOOH + 0.12MONITS + 0.06MONITU	No Change	*Reaction:* Browne et al. (2014) *Rate:* Roberts and Bertman (1992)
$APIO_2 + MO_2 = HO_2$ + 0.75HCHO + 0.25 MOH + 0.25 ROH	3.56E-14exp(708/T)	*Reaction:*Browne et al. (2012)? *Rate:* Roberts and Bertman (1992)	$APIO_2 + MO_2 = HO_2$ + 0.75HCHO + 0.25 MOH + 0.25 ROH + 0.75RCHO + 0.75MEK	No Change	*Reaction and Rate:* Roberts and Bertman (1992)
$APIO_2 + MCO_3 = 0.5HO_2$ + 0.5MO_2 + RCHO + MEK + RCOOH	7.40E-13exp(765/T)	*Reaction and Rate:* Roberts and Bertman (1992)	No Change	No Change	No Change
$APIO_2 + NO_3 = HO_2 + NO_2$ + RCHO + MEK	1.20E-12	*Reaction and Rate:* Roberts and Bertman (1992)	No Change	No Change	No Change
API + OH = $APIO_2$	1.21E-11exp(440/T)	*Reaction and Rate:* IUPAC	No Change	No Change	No Change

		Web version Jan 2010			
API + O_3 = 0.85OH + 0.1HO_2 + 0.62KO_2 + 0.14CO + 0.02H_2O_2 + 0.65RCHO + 0.53MEK	5.3E-16*exp(-530/T)	*Reaction:* Goliff et al. (2013) *Rate:* Atkinson et al. (2003) *?*	No Change	5.0E-16*exp(-530/T)	*Reaction and Rate:* Atkinson and Arey (2003)
API + NO_3 = 0.1OLNN + 0.9OLND	1.19E-12exp(490/T)	*Reaction and Rate:* Atkinson and Arey (2003)	No Change	8.33E-13exp(490/T)	*Reaction:* Atkinson and Arey (2003) *Rate*: Average of α- and β-pinene values in MCMv3.3; See Fisher et al. (2016)
LIM/LIMO2/PIP Reactions					
LIM + OH = $LIMO_2$	4.02E-11*exp(-401/T)	*Reaction and Rate:* Gill and Hites (2002)	No Change	4.20E-11exp(401/T)	Same reference as the old rate; believed to be a typo in the old rate
LIM + O3 = 0.85OH + 0.1HO_2 + 0.62KO_2 + 0.02H_2O_2 + 0.14CO + 0.46PRPE + 0.04HCHO + 0.79MACR + 0.01HCOOH + 0.07RCOOH	2.95E-15exp(-783/T)	*Reaction and Rate:* Atkinson and Arey (2003)	LIM + O_3 = 0.85OH + 0.1HO_2 + 0.16ETO_2 + 0.42KO_2 + 0.02H_2O_2 + 0.14CO + 0.46PRPE + 0.04HCHO + 0.79MACR + 0.01HCOOH + 0.07RCOOH	No Change	Same reference; believe to be a typo in the old reaction product yield
LIM + NO_3 = 0.71OLNN + 0.29OLND	1.22E-11	*Reaction:* Spittler et al. (2006) *Rate*: Atkinson and Arey (2003)	LIM + NO_3 = 0.5OLNN + 0.5OLND	No Change	*Reaction:* Fry et al. (2014) *Rate:* Atkinson and Arey (2003)
$LIMO_2$ + NO = HO_2 + 0.65NO_2 + 0.35ONIT + 0.05PRPE + 0.43HCHO + 0.68RCHO + 0.07HCOOH	4.0E-12	*Reaction:* Ito et al. (2007) ONIT yield; Atkinson and Arey (2003) *Rate:* Roberts and Bertman (1992)	$LIMO_2$ + NO = 0.686HO_2 + 0.78NO_2 + 0.22MONITU + 0.289PRPE + 0.231HCHO + 0.491RCHO + 0.058HAC + 0.289MEK	No Change	*Reaction:* Browne et al. (2014) *Rate:* Roberts and Bertman (1992)

$LIMO_2 + HO_2 = PIP$	1.5E-11	*Reaction and Rate:* Roberts and Bertman (1992)	No Change	No Change	No Change
$LIMO_2 + MO_2 = HO_2 + 0.192PRPE + 1.04HCHO + 0.308MACR + 0.25MOH + 0.25ROH$	3.56E-14exp(708/T)	*Reaction and Rate:* Roberts and Bertman (1992)	No Change	No Change	No Change
$LIMO_2 + MCO_3 = 0.5HO_2 + 0.5MO_2 + 0.192PRPE + 0.385HCHO + 0.308MACR + 0.5RCOOH$	7.40E-13*exp(765/T)	*Reaction and Rate:* Roberts and Bertman (1992)	No Change	No Change	No Change
$LIMO_2 + NO_3 = HO_2 + NO_2 + RCHO + MEK$	1.20E-12	*Reaction and Rate:* Roberts and Bertman (1992) ?	$LIMO_2 + NO_3 = HO_2 + NO_2 + 0.385PRPE + 0.385HCHO + 0.615MACR$	No Change	Same reference, but replaced RCHO and MEK with PRPE, HCHO, and MACR.
$PIP + OH = 0.5APIO_2 + HO_2 + 0.5RCHO + 0.5MEK$	3.8E-12exp(200/T)	*Reaction and Rate:* Ito et al. (2007)	$PIP + OH = 0.49OH + 0.44R_4O_2 + 0.08RCHO + 0.41MEK$	3.4E-12exp(190/T)	*Reaction and Rate:* Goliff et al. (2013)
OLNN/OLND Reactions					
$OLNN + NO = HO_2 + NO_2 +$ ONIT	4.0E-12	*Reaction and Rate:* Goliff et al. (2013)	$OLNN + NO = HO_2 + NO_2 +$ MONITS	No Change	*Reaction*: Browne et al. (2014) *Rate:* Goliff et al. (2013)
$OLND + NO = 2.0NO_2 + 0.287HCHO + 1.24RCHO + 0.464MEK$	4.0E-12	*Reaction and Rate:* Goliff et al. (2013)	No Change	No Change	No Change
$OLNN + HO_2 =$ ONIT	1.66E-13exp(1300/T)	*Reaction and Rate:* Roberts and Bertman (1992)	$OLNN + HO_2 = 0.7$MONITS + 0.3MONITU	No Change	*Reaction:* Browne et al. (2014) *Rate:* Roberts and Bertman (1992)
$OLND + HO_2=$ ONIT	1.66E-13exp(1300/T)	*Reaction and Rate:* Roberts and Bertman (1992)	$OLND + HO_2 = 0.7$MONITS + 0.3MONITU	No Change	*Reaction:* Browne et al. (2014) *Rate:* Roberts and Bertman (1992)
$OLNN + MO_2 = 2.0HO_2 +$ HCHO + ONIT	1.60E-13exp(708/T)	*Reaction and Rate:* Roberts and Bertman	$OLNN + MO_2 = 2.0HO_2 +$ HCHO + 0.7MONITS + 0.3MONITU	No Change	*Reaction:* Browne et al. (2014) *Rate:* Roberts and Bertman

		(1992)			(1992)
OLND + MO_2 = 0.5HO_2 + 0.5NO_2 + 0.965HCHO + 0.93RCHO + 0.348MEK + 0.25MOH + 0.25ROH + 0.5ONIT	9.68E-14exp(708/T)	*Reaction and Rate:* Roberts and Bertman (1992)	OLND + MO_2 = 0.5HO_2 + 0.5NO_2 + 0.965HCHO + 0.93RCHO + 0.348MEK + 0.25MOH + 0.25ROH + 0.35MONITS + 0.15MONITU	No Change	*Reaction:* Browne et al. (2014) *Rate:* Roberts and Bertman (1992)
OLNN + MCO_3 = HO_2+ MO_2 + ONIT	8.85E-13exp(765/T)	*Reaction and Rate:* Roberts and Bertman (1992)	OLNN + MCO_3 = HO_2 + MO_2 + 0.7MONITS + 0.3MONITU	No Change	*Reaction:* Browne et al. (2014) *Rate:* Roberts and Bertman (1992)
OLND + MCO_3 = 0.5MO_2 + NO_2 + 0.287HCHO + 1.24RCHO + 0.464MEK + 0.5RCOOH	5.37E-13exp(765/T)	*Reaction and Rate:* Roberts and Bertman (1992)	No Change	No Change	No Change
OLNN + NO_3 = HO_2 + NO_2 + ONIT	1.20E-12	*Reaction and Rate:* Roberts and Bertman (1992)	OLNN + NO_3 = HO_2 + NO_2 + 0.7MONITS + 0.3MONITU	No Change	*Reaction:* Browne et al. (2014) *Rate:* Roberts and Bertman (1992)
OLND + NO3 = 2.0NO_2 + 0.287HCHO + 1.24RCHO + 0.464MEK	1.20E-12	*Reaction and Rate:* Roberts and Bertman (1992)	No Change	No Change	No Change
OLNN + OLNN = HO_2 + 2.0ONIT	7.0E-14exp(1000/T)	*Reaction and Rate:* Roberts and Bertman (1992)	OLNN + OLNN = HO_2 + 1.4MONITS + 0.6MONITU	No Change	*Reaction:* Browne et al. (2014) *Rate:* Roberts and Bertman (1992)
OLNN + OLND = 0.5HO_2 + 0.5NO_2 + 0.202HCHO + 0.64RCHO + 0.149MEK + 1.5ONIT	4.25E-14exp(1000/T)	*Reaction and Rate:* Roberts and Bertman (1992)	OLNN + OLND = 0.5HO_2 + 0.5NO_2 + 0.202HCHO + 0.64RCHO + 0.149MEK + 1.05MONITS + 0.45MONITU	No Change	*Reaction:* Browne et al. (2014) *Rate:* Roberts and Bertman (1992)
OLND + OLND = NO_2 + 0.504HCHO + 1.21RCHO + 0.285MEK	2.96E-14exp(1000/T)	*Reaction and Rate:* Roberts and Bertman (1992)	OLND + OLND = NO_2 + 0.504HCHO + 1.21RCHO + 0.285MEK + 0.7MONITS + 0.3MONITU	No Change	*Reaction:* Browne et al. (2014) *Rate:* Roberts and Bertman (1992)
MONITS/MONITU/HONIT Reactions					
-	-	-	MONITS + OH = HONIT	4.80E-12	*Reaction and Rate:* Browne et al. (2014)

-	-	-	MONITU + OH = HONIT	7.29E-11	*Reaction and Rate:* Browne et al. (2014)
-	-	-	MONITU + O_3 = HONIT	1.67E-16	*Reaction and Rate:* Browne et al. (2014)
-	-	-	MONITU + NO_3 = HONIT	3.15E-13exp(-448/T)	*Reaction and Rate:* Fisher et al. (2016); This is the same rate constant as used for nighttime isoprene nitrates
-	-	-	MONITS + NO_3 = HONIT	3.15E-13exp(-448/T)	*Reaction and Rate:* Fisher et al. (2016); This is the same rate constant as used for nighttime isoprene nitrates
-	-	-	HONIT + OH = NO_3 + HKET	Same as HNO_3 + OH	*Reaction and Rate:* Browne et al. (2014)
Photolysis Reactions					
PIP = OH + HO_2 + RCHO	J(H_2O_2)	*Reaction and Rate:* Goliff et al. (2013)	No Change	No Change	No Change
-	-	-	MONITS = MEK + NO_2	J(ONIT1)[(a)]	*Reaction and Rate:* Browne et al. (2014)
-	-	-	MONITU = RCHO + NO_2	J(ONIT1)[(a)]	*Reaction and Rate:* Browne et al. (2014)
-	-	-	HONIT = HKET + NO_2	J(ONIT1)[(a)]	*Reaction and Rate:* Browne et al. (2014)

[(a)]MCM tert-butyl nitrate photolysis cross-section, divided by 3 due to the hydroxyl group (Roberts and Fajer, 1989).
Note: Roberts and Bertman (1992), Atkinson and Arey (2003), IUPAC Web Jan. (2010), Gill and Hites (2002), Spittler et al. (2006), and Ito et al. (2007) were incorporated into Goliff et al. (2013).

Aerosol Uptake

Species	Gamma	Aerosol Type	Reference
IEPOX → SOAIE	EPOXUPTK[b]	inorganic[a]	Gaston et al, 2014
IMAE → SOAME	EPOXUPTK[c]	inorganic[a]	Lin et al., 2013; Pye et al., 2013; Marais et al., 2016
GLYX → SOAGX	2.9E-3[(h)]	inorganic[a]	Marais et al, 2016
MGLY → SOAMG	2.9E-5	inorganic[a]	Marais et al, 2016
LVOC → LVOCOA[d]	1.0	inorganic[a]	Krechmer et al., 2015; Marais et al., 2016
ISN1OG → ISN1OA[e]	1.0	inorganic[a]	Ng et al., 2008; Rollins et al., 2009; Marais et al., 2016

ISOPNB = ONITAam[f]	5E-3		
ISOPND = ONITAam[f]	5E-3		
MACRN = ONITAam	5E-3		
MVKN = ONITAam	5E-3		
R4N2 = ONITAam	5E-3		
ISN1 = ONITAam	5E-3[(g)]		
DHDN = ONITAam[f]	5E-3		
MONITS = ONITApm	1E-2		
MONITU = ONITApm	1E-2		
HONIT = ONITApm	1E-2		

[(a)]Only for relative humidity greater than 35%.

[(b)]First-order particle phase reaction rate. K_HPLUS = 3.6E-2, K_NUC = 2.0E-4, K_HSO4 = 7.3E-4, HSTAR = 3.3E7.

[(c)]MEPOX in Marais et al. (2016). At pH < 4 MEPOX uptake is calculated as 30 times slower than that of IEPOX. At pH > 4 MEPOX and IEPOX uptake are assumed equal (but they are then both very low). IMAE is a minor isoprene SOA component (<0.1% mass yield), so the gas-phase chemistry for IMAE formation is not included in the standard mechanism.

[(d)]Low volatility non-IEPOX oxidation product of ISOPOOH (C_5-LVOC in Marais et al., 2016).

[(e)]Low volatility second-generation hydroxynitrate formed from the ISOP+NO_3 reaction pathway (NT-ISOPN in Marais et al., 2016).

[(f)]Alternate representation of ISOPNB, ISOPND, and DHDN aerosol uptake is by reactive uptake using Henry's Law constant of 3.3E5 M/atm for all 3 compounds and aqueous-phase hydrolysis rate of 1.6E-5 s^{-1} for ISOPNB and 6.8E-3 s^{-1} for ISOPND and DHDN (Hu et al., 2011; Jacobs et al., 2014). Resultant mass yields are <0.01% for ISOPNs and 0.05% for DHDN in the Southeast US in summer 2013 (Marais et al., 2016).

[(g)] *Jenny Fisher*: This is what I used, but is this double counting the ISN1OG → ISN1OA above? Or maybe not as ISN1 is 1st generation product of ISOP + NO3 while ISN1OG is second(?)?

Eloise Marais: ISN1OG is second generation. My impression from Rollins (2009) and maybe also Ng et al. (2008) is that most ISOP+NO3 aerosol is from second-generation products.

Jenny Fisher: I don't see why this would apply only for ISOPN(B/D) + DHDN – wouldn't something similar apply for other organic nitrates species (MACRN, MVKN, R4N2, MONITS, MONITU)? Eloise might be able to advise on appropriate parameters here.

Eloise Marais: I parameterized MACRN, MVKN, and other organonitrates following the same approach, but don't include them here. When I developed the mechanism, I could not find hydrolysis reaction rate constants to parameterize all organonitrates. You constrained their uptake with measurements, so my approach may under/overestimate these. For ISN1OG uptake I set gamma to 1 (i.e., assume aerosol precursors are non-volatile and so all partition to the aerosol phase).

[(h)] This is the daytime value. Nighttime value is 5E-6.

References

Atkinson, R. and Arey, J.: Gas-phase tropospheric chemistry of biogenic volatile organic compounds: a review, Atmos. Environ., 37 Supplement No. 2, S197 – S219, doi:10.1016/S1352-2310(03)00391-1, 2003.

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and Subcommittee, 20 I.: Evaluated kinetic and photochemical data for atmospheric chemistry: Volume II -gas phase reactions of organic species, Atmos. Chem. Phys., 6, 3625–4055, 2006.

Bates, K. H., Crounse, J. D., St Clair, J. M., Bennett, N. B., Nguyen, T. B., Seinfeld, J. H., Stoltz, B. M., and Wennberg, P. O.: Gas Phase Production and Loss of Isoprene Epoxydiols, Journal of Physical Chemistry A, 118, 1237-1246, 2014.

Browne, E. C., Wooldridge, P. J., Min, K.-E., and Cohen, R. C.: On the role of monoterpene chemistry in the remote continental boundary layer, Atmos. Chem. Phys., 14, 1225–1238, doi:10.5194/acp-14-1225-2014, 2014.

Crounse, J. D., Paulot, F., Kjaergaard, H. G., and Wennberg, P. O.: Peroxy radical isomerization in the oxidation of isoprene, Phys. Chem. Chem. Phys., 13, 13 607–13 613, 2011.

Crounse, J. D., Knap, H. C., Ørnsø, K. B., Jørgensen, S., Paulot, F., Kjaergaard, H. G., and Wennberg, P. O.: Atmospheric Fate of Methacrolein. 1. Peroxy Radical Isomerization Following Addition of OH and O2, The Journal of Physical Chemistry A, 116, 5756–5762, 2012.

Crounse, J. D., Nielsen, L. B., Jørgensen, S., Kjaergaard, H. G., and Wennberg, P. O.: Autoxidation of Organic Compounds in the Atmosphere, The Journal of Physical Chemistry Letters, 4, 3513–3520, 2013.

Fisher, J. A., Jacob, D. D., Travis, K. R., Kim, P. S., Marais, E., Miller, C. C., Yu, K., Zhu, L., Yantosca, R. M., Sulprizio, M. P., Mao, J., Wennberg, P. O., Crounse, J. D., Teng, A. P., Nguyen, T. B., St Clair, J. M., Romer, P., Nault, B. A., Wooldridge, P. J., Jimenez, J. L., Campuzano-Jost, P., Day, D. A., Shepson, P. B., Xiong, F., Blake, D. R., Goldstein, A. H., Misztal, P. K., Hanisco, T. F., Wolfe, G. M., Ryerson, T. B., Wisthaler, A., and Mikoviny, T.: Organic nitrate chemistry and its implications for nitrogen budgets in an isoprene- and monoterpene-rich atmosphere: constrains from aircraft (SEAC^{4}RS) and ground-based (SOAS) observations in the Southeast US, Atmos. Chem. Phys., 16, 5969–5991, 2016.

Fry, J. L., Draper, D. C., Barsanti, K. C., Smith, J. N., Ortega, J., Winkler, P. M., Lawler, M. J., Brown, S. S., Edwards, P. M., Cohen, R. C., and Lee, L.: Secondary Organic Aerosol Formation and Organic Nitrate Yield from NO3 Oxidation of Biogenic Hydrocarbons, Environ. Sci. Technol., 48, 11944–11953, doi:10.1021/es502204x, 2014.

Gaston, C. J., Riedel, T. P., Zhang, Z., Gold, A., Surratt, J. D., and Thornton, J. A.: Reactive uptake of an isoprene-derived epoxydiol to submicron aerosol particles, Environ. Sci. Technol., 48, 11178–11186, 2014.

Gill, K.J., and Hites, R.A.: Rate Constants for the Gas-Phase Reactions of the Hydroxyl Radical with Isoprene, α- and β-Pinene, and Limonene as a Function of Temperature, Journal of Physical Chemistry A, 106, 2538 – 2544, doi:10.1021/jp013532q, 2002.

Goliff, W. S., Stockwell, W. R., and Lawson, C. V.: The regional atmospheric chemistry mechanism, version 2, Atmos. Environ., 68, 174–185, doi:10.1016/j.atmosenv.2012.11.038, 2013.

Hu, K. S., Darer, A. I., and Elrod, M. J.: Thermodynamics and kinetics of the hydrolysis of atmospherically relevant organonitrates and organosulfates, Atmos. Chem. Phys., 11, 8307–8320, 2011.

Ito, A., Sillman, S., and Penner, J. E.: Effects of additional nonmethane volatile organic compounds, organic nitrates, and direct emissions of oxygenated organic species on global tropospheric chemistry, J. Geophys. Res., 112, D06309, doi:10.1029/2005jd006556, 2007.

Jacobs, M. I., Burke, W. J., and Elrod, M. J.: Kinetics of the reactions of isoprene-derived hydroxynitrates: gas phase epoxide formation and solution phase hydrolysis, Atmos. Chem. Phys., 14,8933-8946, 2014.

Jenkin, M. E., Saunders, S. M., Wagner, V., and Pilling, M. J.: Protocol for the development of the Master Chemical Mechanism, MCM v3 (Part B): tropospheric degradation of aromatic volatile organic compounds, Atmos. Chem. Phys., 3, 181–193, 2003.

Jenkin, M. E., Young, J. C., and Rickard, A. R.: The MCM v3.3.1 degradation scheme for isoprene, Atmospheric Chemistry and Physics, 15, 11,433–11,459, 2015.

Krechmer, J. E., Coggon, M. M., Massoli, P., Nguyen, T. B., Crounse, J. D., Hu, W., Day, D. A., Tyndall, G. S., Henze, D. K., Rivera-Rios, J. C., Nowak, J. B., Kimmel, J. R., Mauldin, III, R. L., Stark, H., Jayne, J. T., Sipilä, M., Junninen, H., St. Clair, J. M., Zhang, X., Feiner, P. A., Zhang, L., Miller, D. O., Brune, W. H., Keutsch, F. N., Wennberg, P. O., Seinfeld, J. H., Worsnop, D. R., Jimenez, J. L., and Canagaratna, M. R.: Formation of low volatility organic compounds and secondary organic aerosol from isoprene hydroxyhydroperoxide low-NO oxidation, Environ. Sci. Technol., 49, 10330–10339, 2015.

Lee, L., Teng, A. P., Wennberg, P. O., Crounse, J. D., and Cohen, R. C.: On Rates and Mechanisms of OH and O_3 Reactions with Isoprene-Derived Hydroxy Nitrates, The Journal of Physical Chemistry. A, 118, 1622-1637, 10.1021/jp4107603, 2014.

Lin, Y.-H., Zhang, H., Pye, H. O. T., Zhang, Z. F., Marth, W. J., Park, S., Arashiro, M., Cui, T., Budisulistiorini, S. H., Sexton, K. G., Vizuete, W., Xie, Y., Luecken, D. J., Piletic, I. R., Edney, E. O., Bartolotti, L. J., Gold, A., and Surratt, J. D.: Epoxide as a precursor to secondary organic aerosol formation from isoprene photooxidation in the presence of nitrogen oxides, P. Natl. Acad. Sci. USA, 110, 6718–6723, 2013.

Liu, Y. J., Herdlinger-Blatt, I., McKinney, K. A., and Martin, S. T.: Production of methyl vinyl ketone andmethacrolein via the hydroperoxyl pathway of isoprene oxidation, Atmos. Chem. Phys., 13, 5715-5730, 2013.

Lockwood, A. L., Shepson, P. B., Fiddler, M. N., and Alaghmand, M.: Isoprene nitrates: preparation, separation, identification, yields, and atmospheric chemistry, Atmospheric Chemistry and Physics, 10, 6169-6178, 2010.

Marais, E A, D. J. Jacob, J. L. Jimenez, P. Campuzano-Jost, D. A. Day, W. Hu, J. Krechmer, L. Zhu, P. S. Kim, C. C. Miller, J. A. Fisher, K. Travis, K. Yu, T. F. Hanisco, G. M. Wolfe, H. L. Arkinson, H. O. T. Pye, K. D. Froyd, J. Liao, and V. F. McNeill, Aqueous-phase mechanism for secondary organic aerosol formation from isoprene: application to the southeast United States and co-benefit of SO_2 emission controls. Atmos. Chem. Phys., 16, 1603-1618, 2016.

Miller, C., C., D. J. Jacob, E. A. Marais, K. Yu, K. R. Travis, P. S. Kim, J. A. Fisher, L. Zhu, G. M. Wolfe, F. N. Keutsch, J. Kaiser, K.-E. Min, S. S. Brown, R. A. Washenfelder, G. Gonzalez Abad, and K. Chance, Glyoxal yield from isoprene oxidation and relation to formaldehyde: chemical mechanism, constraints from SENEX aircraft observations, and interpretation of OMI satellite data, Atmos. Chem. Phys. Discuss., 2016.

Müller, J.-F., Peeters, J., and Stavrakou, T.: Fast photolysis of carbonyl nitrates from isoprene, Atmos. Chem. Phys., 14, 2497–2508, 2014.

Ng, N. L., Kwan, A. J., Surratt, J. D., Chan, A. W. H., Chhabra, P. S., Sorooshian, A., Pye, H. O. T., Crounse, J. D., Wennberg, P. O., Flagan, R. C., and Seinfeld, J. H.: Secondary organic aerosol (SOA) formation from reaction of isoprene with nitrate radicals (NO_3), Atmos. Chem. Phys., 8, 4117–4140, 2008.

Nguyen, T. B., Crounse, J. D., Teng, A. P., St Clair, J. M., Paulot, F., Wolfe, G. M., and Wennberg, P. O.: Rapid deposition of oxidized biogenic compounds to a temperate forest, P. Natl. Acad. Sci USA, 112, E392-401, doi:10.1073/pnas.1418702112, 2015.

Paulot, F., Crounse, J. D., Kjaergaard, H. G., Kroll, J. H., Seinfeld, J. H., and Wennberg, P. O.: Isoprene photooxidation: new insights into the production of acids and organic nitrates, Atmospheric Chemistry and Physics, 9, 1479-1501, 2009a.

Paulot, F., Crounse, J. D., Kjaergaard, H. G., Kurten, A., St Clair, J. M., Seinfeld, J. H., and Wennberg, P. O.: Unexpected Epoxide Formation in the Gas-Phase Photooxidation of Isoprene, Science, 325, 730-733, 2009b.

Peeters, J., Nguyen, T. L., and Vereecken, L.: HOx radical regeneration in the oxidation of isoprene, Physical Chemistry Chemical Physics: PCCP, 11, 5935-5939, 2009.

Peeters, J., and Muller, J. F.: HO(x) radical regeneration in isoprene oxidation via peroxy radical isomerisations. II: experimental evidence and global impact, Physical Chemistry Chemical Physics: PCCP, 12, 14227-14235, 2010.

Pye, H. O. T., Pinder, R. W., Piletic, I. R., Xie, Y., Capps, S. L., Lin, Y.-H., Surratt, J. D., Zhang, Z., Gold, A., Luecken, D. J., Hutzell, W. T., Jaoui, M., Offenberg, J. H., Kleindienst, T. E., Lewandowski, M., and Edney, E. O.: Epoxide pathways improve model predictions of isoprene markers and reveal key role of acidity in aerosol formation, Environ. Sci. Technol., 47, 11056– 11064, 2013.

Roberts, J.M., Bertman, S.B., 1992. The thermal decomposition of peroxyacetic nitric anhydride (PAN) and peroxymethacrylic nitric anhydride (MPAN). International Journal of Chemical Kinetics 24, 297– 307.

Rollins, A. W., Kiendler-Scharr, A., Fry, J. L., Brauers, T., Brown, S. S., Dorn, H.-P., Dubé, W. P., Fuchs, H., Mensah, A., Mentel, T. F., Rohrer, F., Tillmann, R., Wegener, R., Wooldridge, P. J., and Cohen, R. C.: Isoprene oxidation by nitrate radical: alkyl nitrate and secondary organic aerosol yields, Atmos. Chem. Phys., 9, 6685–6703, 2009.

Saunders, S. M., Jenkin, M. E., Derwent, R. G., and Pilling, M. J.: Protocol for the development of the Master Chemical Mechanism, MCM v3 (Part A): tropospheric degradation of non-aromatic volatile organic compounds, Atmos. Chem. Phys., 3, 161-180, 2003.

Spittler, M., Barnes, I., Bejan, I., Brockmann, K.J., Benter, T., and Wirtz, K.: Reactions of NO_3 radicals with limonene and α-pinene: Product and SOA formation, Atmos. Environ., 40, S116 – S127, :10.1016/j.atmosenv.2005.09.093, 2006.

St. Clair, J. M., Rivera-Rios, J.C., Crounse, J.D., Knap, H.C., Bates, K.H., Teng, A.P., Jorgensen, S., Kjaergaard, H.G., Keutsch, F.N., and Wennberg, P.O.: Kinetics and Products of the Reaction of the First-Generation Isoprene Hydroxy Hydroperoxide (ISOPOOH) with OH: J. Phys. Chem. A, 120, 1441 – 1451, 2016.

Stavrakou, T., Peeters, J., and Muller, J. F.: Improved global modelling of HOx recycling in isoprene oxidation: evaluation against the GABRIEL and INTEX-A aircraft campaign measurements, Atmos. Chem. Phys.,10, 9863-9878, 2010.

Travis, K. R., Jacob, D. J., Fisher, J. A., Kim, P. S., Marais, E. A., Zhu, L., Yu, K., Miller, C. C., Yantosca, R. M., Sulprizio, M.P., Thompson, A. M., Wennberg, P. O., Crounse, J. D., St. Clair, J. M., Cohen, R. C., Laugher, J. L., Dibb, J. E., Hall, S. R., Ullmann, K., Wolfe, G. M., Pollack, I. B., Peischl, J., Neuman, J. A., and Zhou, X.: Why do models overestimate surface ozone in the Southeast United States? Atmos. Chem. Phys.,16, 2016.

Wolfe, G. M., Crounse, J. D., Parrish, J. D., St Clair, J. M., Beaver, M. R., Paulot, F., Yoon, T. P., Wennberg, P. O., and Keutsch, F. N.: Photolysis, OH reactivity and ozone reactivity of a proxy for isoprene-derived hydroperoxyenals (HPALDs), Physical Chemistry Chemical Physics: PCCP, 14, 7276-7286, 2012.

Xie, Y., Paulot, F., Carter, W. P. L., Nolte, C. G., Luecken, D. J., Hutzell, W. T., Wennberg, P. O., Cohen, R. C., and Pinder, R.W.: Understanding the impact of recent advances in isoprene photooxidation on simulations of regional air quality, Atmos. Chem. Phys., 13, 8439-8455, 2013.