New isoprene scheme

From Geos-chem

This page is for documentation of the isoprene chemistry mechanism (cf. Fabien Paulot) included in GEOS-Chem v9-02. This update was tested in the 1-month benchmark simulation v9-02g and approved on 24 Mar 2013.

Previous page of description can be found here New isoprene scheme prelim.

— Bob Yantosca, 28 May 2014

Contents

Implementation of the Paulot isoprene scheme

This chemistry is largely base on Paulot et al.(2009a, ACP) for high-NOx regime and Paulot et al.(2009b, Science) for low-NOx regime. Other additions include:

1. Isomerization of RIO2 base on Peeters et al. (2009, 2010) an Crounse et al. (2011).
2. Isomerization of MRO2 base on Crounse et al. (2012).
3. Nighttime isoprene oxidation based on Rollins et al. (2009) and Xie et al. (2012).
4. Updates to the reactions of isoprene nitrates + O3 base on Lockwood et al. (2010).

Evaluation of this chemical mechanism is described here (http://dx.doi.org/10.1002/jgrd.50817). If you have any questions, please let us know (Fabien Paulot (mailto:paulot@seas.harvard.edu), Jingqiu Mao (mailto:jmao@seas.harvard.edu)).

--Bob Y. 13:47, 12 May 2014 (EDT)

Species information

The following tables list the species that comprise the Paulot isoprene chemistry mechanism:

Species

Species	Formula	Note
A3O2	CH3CH2CH2OO	primary RO2 from C3H8
ACET	CH3C(O)CH3	acetone

ACTA	CH3C(O)OH	acetic acid
ALD2	CH3CHO	acetaldehyde
ALK4	RH	≥C4 alkanes
ATO2	CH3C(O)CH2O2	RO2 from acetone
ATOOH	CH3C(O)CH2OOH	ATO2 peroxide
B3O2	CH3CH(OO)CH3	secondary RO2 from C3H8
C2H6	C2H6	ethane
C3H8	C3H8	propane
CH2O	CH2O	formaldehyde
CH4	CH4	methane
CO	CO	carbon monoxide
CO2	CO2	carbon dioxide
DHMOB	HOCH2C(CH3)(OH)C(=O)CHO	See Paulot et al., ACP (2009)
DIBOO		Dibble peroxy radical
EOH	C2H5OH	ethanol
ETHLN	CHOCH2ONO2	Ethanal nitrate
ETO2	CH3CH2OO	ethylperoxy radical
ETP	CH3CH2OOH	ethylhydroperoxide
GLYC	HOCH2CHO	glycoaldehyde (hydroxyacetaldehyde)
GLYX	CHOCHO	glyoxal
H2	H2	hydrogen atom
H2O	H2O	water vapor
H2O2	H2O2	hydrogen peroxide
HAC	HOCH2C(O)CH3	hydroxyacetone
HCOOH	HCOOH	formic acid
HC5	HOCH2CH=C(CH3)CHO	Hydroxycarbonyl with 5C
HC5OO		Peroxy radical from HC5 (old IAO2?)
HNO2	HONO	nitrous acid
HNO3	HNO3	nitric acid
HNO4	HNO4	pernitric acid
HO2	HO2	hydroperoxyl radical
IALD	HOCH2C(CH3)=CHCHO	hydroxy carbonyl alkenes from isoprene
IAP	HOCH2C(CH3)(OOH)CH(OH)CHO	peroxide from IAO2
IEPOX		Isoprene epoxide
IEPOXOO		RO2 from IEPOX
INO2	O2NOCH2C(OO)(CH3)CH=CH2	RO2 from ISOP+NO3
INPN	O2NOCH2C(OOH)(CH3)CH=CH2	peroxide from INO2
ISN1		nighttime isoprene nitrate
ISNOOA		peroxy radical from ISN1
ISNOOB		peroxy radical from ISN1

ISNOHOO		peroxy radical from ISN1
ISNP	HOCH2C(OOH)(CH3)CH(ONO2)CH2OH	peroxide from ISOPNBO2 and ISOPNDO2
ISOP	CH2=C(CH3)CH=CH2	isoprene
ISOPNB	C5H9NO4	Isoprene nitrate Beta
ISOPND	C5H9NO4	Isoprene nitrate Delta
KO2	RO2 from >3 ketones	RO2 from >3 ketones
M		for three body reactions
MACR	CH2=C(CH3)CHO	methacrolein
MACRN	HOCH2C(ONO2)(CH3)CHO	Nitrate from MVK
MAN2	HOCH2C(ONO2)(CH3)CHO	RO2 from MACR+NO3
MAO3	CH2=C(CH3)C(O)OO	peroxyacyl from MVK and MACR
MAOP	CH2=C(CH3)C(O)OOH	peroxide from MAO3
MAOPO2	CH2OH-CHOO*CH3C(O)OOH	Peroxy radical from MAOP (addition on the double bond)
MAP	CH3C(O)OOH	peroxyacetic acid
MCO3	CH3C(O)OO	peroxyacetyl radical
MEK	RC(O)R	>3 ketones
MGLY	CH3COCHO	methylglyoxal
MNO3	CH3ONO2	methylnitrate
MOBA	HOC(=O)C(CH3)=CHCHO	5C acid from isoprene
MOBAOO		RO2 from MOBA
MO2	CH3O2	methylperoxy radical
MOH	CH3OH	methanol
MP	CH3OOH	methylhydroperoxide
MRO2	HOCH2C(OO)(CH3)CHO	RO2 from MACR+OH
MRP	HOCH2C(OOH)(CH3)CHO	peroxide from MRO2
MVK	CH2=CHC(=O)CH3	methylvinylketone
MVKN	HOCH2CH(ONO2)C(=O)CH3	Nitrate from MACR
N2	N2	nitrogen
N2O	N2O	nitrous oxide
N2O5	N2O5	dinitrogen pentoxide
NH2	NH2	ammonia radical
NH3	NH3	ammonia
NO	NO	nitric oxide
NO2	NO2	nitrogen dioxide
NO3	NO3	nitrate radical
O2	O2	molecular oxygen
O2CH2OH	O2CH2OH	produced by CH2O+HO2
O3	O3	ozone
OH	OH	hydroxyl radical
PAN	CH3C(O)OONO2	peroxyacetylnitrate
PMN	CH2=C(CH3)C(O)OONO2	peroxymethacryloyl nitrate (MPAN)

PO2	HOCH2CH(OO)CH3	RO2 from isoprene
PP	HOCH2CH(OOH)CH3	peroxide from PO2
PPN	CH3CH2C(O)OONO2	peroxypropionylnitrate
PRN1	O2NOCH2CH(OO)CH3	RO2 from propene + NO3
PRPE	C3H6	≥C4 alkenes
PRPN	O2NOCH2CH(OOH)CH3	peroxide from PRN1
PROPNN	CH3C(=O)CH2ONO2	Propanone nitrate
PYAC	CH3COCOOH	Pyruvic acid
R4N1	RO2 from R4N2	RO2 from R4N2
R4N2	RO2NO	≥C4 alkylnitrates
R4O2	RO2 from ALK4	RO2 from ALK4
R4P	CH3CH2CH2CH2OOH	peroxide from R4O2
RA3P	CH3CH2CH2OOH	peroxide from A3O2
RB3P	CH3CH(OOH)CH3	peroxide from B3O2
RCHO	CH3CH2CHO	>C2 aldehydes
RCO3	CH3CH2C(O)OO	peroxypropionyl radical
RCOOH	C2H5C(O)OH	>C2 organic acids
RIO1	HOCH2C(OO)(CH3)CH=CHOH	RO2 from isoprene oxidation products
RIO2	HOCH2C(OO)(CH3)CH=CH2	RO2 from isoprene (named as ISOPO2 in the literature)
RIP	HOCH2C(OOH)(CH3)CH=CH2	peroxide from RIO2 (named as ISOPOOH in the literature)
ROH	C3H7OH	>C2 alcohols
RP	CH3CH2C(O)OOH	peroxide from RCO3
VRO2	HOCH2CH(OO)C(O)CH3	RO2 from MVK+OH
VRP	HOCH2CH(OOH)C(O)CH3	peroxide from VRO2
DMS	(CH3)2S	dimethylsulfide
SO2	SO2	sulfur dioxide
SO4	SO4	sulfate radical
MSA	CH4SO3	methanesulfonic acid
DRYDEP		generic entry for dry dep
DRYPMNN		Dry deposition for the different species
DRYALPH		
DRYLIMO		
DRYISOPND		
DRYISOPNB		
DRYRIP		
DRYIEPOX		
DRYMACRN		
DRYMVKN		
DRYPROPNN		
DRYHCOOH		
DRYACTA		

EMISSION		generic entry to do emissions

--Bob Y. 13:46, 12 May 2014 (EDT)

Species emitted and deposited

Species emitted	Species deposited
NO	NO2
NO2	O3
CO	PAN
ALK4	HNO3
ISOP	CH2O
ACET	N2O5
PRPE	H2O2
C3H8	PMN
C2H6	PPN
MEK	R4N2
ALD2	
CH2O	PMNN
HNO3	IEPOX
O3	RIP
	ISOPND
	ISOPNB
	PROPNN
	MACRN
	MVKN
	HCOOH
	ACTA
	HAC
	ALD2

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Henry's law constant

This is effective Henry's law constant for water near neutral pH, mainly from Wesley et al. (1989). So the value would be different when you put in wetscav_mod.F.

Species	H*(moles L-1 atm-1)	ΔH/R (K)	Reactivity factor (f0)	Reference
NO2	0.01		0.1	
Ox	0.01		1.0	
PAN	3.6		1.0	
HNO3	1.0d+14		0.0	
H2O2	1.0d+5		1.0	
PMN	as PAN			

PPN	as PAN			
R4N2	as PAN			
CH2O	6.0e+3		1.0	Karl et al., 2010
GLYX	360000	-7200	1.0	Schweitzer et al., 1998
MGLY	3700	-7500	1.0	Ito et al., 2007
GLYC	41000	-4600	1.0	Ito et al., 2007
MPAN	as PAN			
N2O5	as HNO3			
HCOOH	1.67d+5	-6100	1.0	Ito et al., 2007
ACTA	1.14d+4	-6300	1.0	Ito et al., 2007
ISOPND	1.7d+4	-9200	1.0	Ito et al., 2007
ISOPNB	1.7d+4	-9200	1.0	Ito et al., 2007
MVKN+MACRN	1.7d+4	-9200	1.0	Ito et al., 2007
PROPNN	1.0d+3		1.0	NITROOXYACETONE IN SANDER TABLE
RIP	1.7e6		1.0	Marais et al., 2012
IEPOX	1.3e8		1.0	Marais et al., 2012
MAP	8.4d+2	-5300	1.0	R. Sander
MVK	4.4d1		1.0	from R.Sander
MACR	6.5d0		1.0	from R.Sander
MOBA	23000	-6300	1.0	Ito et al., 2007
HAC	2.9e3		1.0	Ito et al., 2007
ALD2	1.5e1		1.0	R. Sander
SO2	1.0d+5		0.0	

Karl, T., Harley, P., Emmons, L., Thornton, B., Guenther, A., Basu, C., Turnipseed, A., and Jardine, K.: Efficient Atmospheric Cleansing of Oxidized Organic Trace Gases by Vegetation, Science, 330, 816-819, 10.1126/science.1192534, 2010.

Reactions

The following tables list information about new reactions in the Paulot isoprene chemistry mechanism:

New reactions

No	Reaction	Rate Constant	Reference	Note
	Reactions with OH			
	ISOP + OH = RIO2	3.1E-11exp(350/T)	Sander et al. 2012	from JPL
	MACR + OH = 0.53MAO3 +0.47MRO2	8.0E-12exp(380/T)	Paulot 2009a	MAO3(=MCO3 in the paper); MRO2(=MACROO in the paper)
	MVK+OH = VRO2	2.6E-12exp(610/T)		
	PMN + OH = HAC + CO + NO2	2.90E-11	MCM v3.2	rates and products all from MCM, originally from Orlando et al. (2002)
	GLYC + OH = 0.732CH2O +0.361CO2 + 0.505CO + 0.227OH + 0.773HO2 + 0.134GLYX + 0.134HCOOH	FRAC=1-11.0729*exp(-1/73T) Rate=8.00E-	Paulot 2009a	Butkovskaya 2006 companion paper and Paulot 2009

Reaction	Rate	Reference	Notes
	12*FRAC		
GLYC + OH = HCOOH + OH + CO	FRAC=1-11.0729*exp(-1/73T) Rate=8.00E-12*(1-FRAC)	Paulot 2009a	Butkovskaya 2006 companion paper and Paulot 2009
GLYX+ OH = HO2+2CO	3.1E-12exp(340/T)	IUPAC2008	JMAO
HAC + OH = MGLY +HO2	FRAC=1-23.7*exp(1/60T) Rate=2.15E-12exp(305/T)*FRAC	Paulot 2009a	Butkovskaya JPC A (a,b)2006 and Paulot 2009a
HAC + OH = 0.5HCOOH + OH +0.5ACTA +0.5CO2 + 0.5CO + 0.5MO2	FRAC=1-23.7*exp(1/60T) Rate=2.15E-12exp(305/T)*(1-FRAC)	Paulot 2009a	Butkovskaya JPC A (a,b)2006 and Paulot 2009a
PRPN + OH =0.209PRN1+0.791OH+0.791PROPNN	8.78E-12exp(200/T)		Branching ratio is determined by alpha and beta Hydrogen position (Kwok et al., 1995).
ETP + OH =0.64OH+0.36ETO2+0.60ALD2	5.18E-12exp(200/T)		Branching ratio is determined by alpha and beta Hydrogen position (Kwok et al., 1995).
RA3P + OH =0.64OH+0.36A3O2+0.64RCHO	5.18E-12exp(200/T)		Branching ratio is determined by alpha and beta Hydrogen position (Kwok et al., 1995).
RB3P + OH =0.791OH+0.209B3O2+0.791ACET	8.78E-12exp(200/T)		Branching ratio is determined by alpha and beta Hydrogen position (Kwok et al., 1995).
R4P + OH =0.791OH+0.209R4O2+0.791RCHO	8.78E-12exp(200/T)		Branching ratio is determined by alpha and beta Hydrogen position (Kwok et al., 1995).
RP + OH = RCO3	6.13E-13exp(200/T)	same as MAP+OH	
PP + OH =0.791OH+0.209PO2+0.791HAC	8.78E-12exp(200/T)		Branching ratio is determined by alpha and beta Hydrogen position (Kwok et al., 1995).
RIP + OH = 0.387RIO2 + 0.613OH + 0.613HC5	4.75E-12exp(200/T)	Paulot 2009b	branching ratio is derived below
RIP + OH = OH + IEPOX	1.9E-11exp(390/T)	Paulot 2009b	the yield of IEPOX is > 70% assumed to be 100%
IEPOX + OH = IEPOXOO	5.78e-11exp(-400/T)	Paulot 2009b	
IAP + OH = 0.654OH + 0.654DHMOB + 0.346HC5OO	5.31E-12 exp(200/T)		
VRP + OH =0.791OH+0.791MEK+0.209VRO2	8.78E-12exp(200/T)		
MRP + OH = MRO2	1.84E-12exp(200/T)		This channel is for the abstraction of peroxide H (OOH), which is slow and ignored in MCM v3.2
MRP + OH = CO2 + HAC + OH	4.40E-12exp(380/T)		This second channel is for the abstraction of aldehydic H, much faster! The rate is from MACR + OH.
MAOP + OH = MAO3	6.13E-13exp(200/T)		same as MAP+OH
MAOP + OH = MAOPO2	3.60E-12exp(380/T)		
OH + MAP = 1.0MCO3	6.13E-13exp(200/T)		From J. Orlando (unpublished results), how confident is this temperature dependence?

HC5 + OH =HC5OO	3.35E-11exp(380/T)	Paulot 2009a	
ISOPND + OH =ISOPNDO2	2.64E-11exp(380/T)	Paulot 2009a	
ISOPNB + OH =ISOPNBO2	3.61E-12exp(380/T)	Paulot 2009a	
ISNP + OH =0.612OH+0.612R4N1++0.193ISOPNBO2+0.193ISOPNDO2	4.75E-12exp(200/T)		replace the old ISNP+OH
MVKN + OH = 0.650HCOOH+NO3+0.650MGLY+0.350CH2O+0.350PYAC	1.5E-12exp(380/T)	Paulot 2009a	
MACRN + OH = 1.0MACRNO2	1.39E-11exp(380/T)		
DHMOB + OH = 1.5CO + 1.0HO2 + 0.5HAC + 0.5MEK	2.52E-11exp(410/T)		
MOBA + OH =MOBAOO	2.79E-11exp(380/T)		
ETHLN + OH =CH2O +CO2+NO2	1.00E-11		
PROPNN+ OH =NO2+MGLY	1.00E-15	Paulot 2009a	IUPAC says < 1e-12;Experiment suggests it is slower than than 1e-13-1e-15
ATOOH + OH = ATO2 + H2O	2.66E-12exp(200/T)	Vaghjiani and Ravishankara (1989)	Abstraction of peroxide H, follow MP + OH
ATOOH + OH = MGLY + OH +H2O	1.14E-12exp(200/T)	Vaghjiani and Ravishankara (1989)	Abstraction of alpha H, follow MP + OH
R4N2+OH = R4N1+H2O	1.6E-12	IUPAC06	JMAO: use the one from HO + 1-C4H9ONO2 → products
RO2 + NO reactions			
RIO2 + NO = 0.883NO2 + 0.783HO2 + 0.660CH2O + 0.400MVK + 0.260MACR + 0.070ISOPND + 0.047ISOPNB + 0.123HC5 + 0.1DIBOO	2.7E-12 exp(350/T)	Paulot 2009a	HNO3 channel deleted since nitrate is treated explicitly;paulothn2009;neglect methylfuran formation (increase the yield of other products)
VRO2 + NO = 0.88NO2 + 0.35HO2 + 0.35CH2O + 0.53MCO3 + 0.53GLYC + 0.35MGLY + 0.12MVKN	2.7E-12 exp(350/T)	Paulot 2009a	
MRO2 + NO = 0.85NO2 + 0.85HO2 + 0.122MGLY + 0.728HAC + 0.728CO + 0.122CH2O + 0.15MACRN	2.7E-12 exp(350/T)	Paulot 2009a	This is modified based on Chuong et al. (2004).It was equally yield for MGLY and HAC in Paulot 2009 ACP, according to Peeters decomposition scheme.
MAN2 + NO = 1.5NO2 + 0.5CH2O + 0.5MGLY + 0.5PROPNN + 0.5CO + 0.5OH	2.7E-12 exp(350/T)		Tyndall ETO2+NO
IEPOXOO + NO = 0.725HAC+0.275GLYC+0.275GLYX +0.275MGLY +0.125OH +0.825HO2+0.200CO2+0.375CH2O +0.074HCOOH +0.251CO +NO2	2.7E-12exp(350/T)		FP: No peroxide was observed
MAOPO2 + NO = 1.0HAC+1.0CO2+1.0OH+1.0NO2	K* (1-YN) where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E00)		
MAOPO2 + NO = 1.0HNO3	K* YN where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E00)		Not treated explicitly
HC5OO + NO = NO2 + 0.216GLYX + 0.234MGLY +	K* (1-YN) where YN is returned from		

Reaction	Rate	Reference	Notes
0.234GLYC + 0.216HAC + 0.290DHMOB + 0.170MOBA + 0.090RCHO + HO2 + 0.090CO	fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E00)		
HC5OO +NO=HNO3	K* YN where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=5.00E00)		
ISOPNDO2 + NO = 0.070MACRN + 0.310HCOOH + 0.440HAC + 0.130ETHLN + 0.650CH2O + 1.340NO2 + 0.150GLYC + 0.310NO3 + 0.150PROPNN + 0.340MEK + 0.350HO2	K* (1-YN) where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E00)	Paulot 2009a	
ISOPNDO2+NO=HNO3	K* YN where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=5.00E00)		Nitrates from ISOPND could not be observed in this experiment
ISOPNBO2 + NO = 0.6GLYC + 0.6HAC + 0.4CH2O + 1.6NO2 + 0.26MACRN + 0.4HO2 + 0.14MVKN	K* (1-YN) where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E00)	Paulot 2009a	
ISOPNBO2 + NO = HNO3	K* YN where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=5.00E00)		Nitrates from ISOPND could not be observed in this experiment
MACRNO2 + NO = 0.08ACTA + 0.08CH2O + 0.15NO3 + 0.07HCOOH + 0.070MGLY + 0.850HAC + 0.85NO2 + 0.93CO2 + 1.0NO2	2.7E-12exp(350/T)		no nitrate yield (acyl)
DIBOO + NO =HO2+NO2+0.520GLYC +0.520MGLY +0.480HAC+0.480GLYX	K* (1-YN) where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E00)		Dibble, 2004 Note that the yield of DIBOO Is likely overestimate (~30%)
DIBOO + NO =HNO3	K* YN where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=5.00E00)		
MOBAOO + NO =RCHO+CO2+HO2+NO2	K* (1-YN) where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E00)		
MOBAOO + NO =HNO3	K* YN where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=5.00E00)		
MAN2 + NO = 1.5NO2 + 0.5CH2O + 0.5MGLY + 0.5PROPNN + 0.5CO + 0.5OH	2.7E-12 exp(350/T)		
MCO3+NO = MO2 + NO2 + CO2	8.10E-12 exp(270/T)	JPL06	
RCO3+NO = NO2+ETO2	6.70E-12 exp(340/T)	IUPAC06	Products follow C2H5CO3+NO
MAO3 + NO = NO2 + 0.5CH2O + 0.5CO + CO2 + 0.5MO2 + 0.5MCO3	6.70E-12 exp(340/T)		
ATO2+NO = 0.96NO2 + 0.960CH2O +0.960MCO3 +			

0.04R4N2	2.80E-12 exp(300/T)		
RO2 + HO2 reactions			
RIO2 + HO2= 0.88RIP + 0.12OH + 0.047MACR + 0.073MVK + 0.12HO2 + 0.12CH2O	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=5	Paulot 2009b	Rate is from Saunders et al. (2003)
VRO2 + HO2 = 0.1VRP + 0.68OH + 0.578GLYC + 0.578MCO3 + 0.187MEK + 0.102HO2 + 0.102CH2O + 0.102MGLY + 0.033RCHO	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=4	???	crounse2010
MRO2 + HO2 = 1.0MRP	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=4		isomerization of MRO2 is included in another reaction.
MAN2 + HO2 = 0.075PROPNN + 0.075CO + 0.075HO2 + 0.075MGLY + 0.075CH2O + 0.075NO2 + 0.15OH + 0.85ISNP	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)],n=4		assume 15% recycling of OH, the rest goes to ISNP
IEPOXOO + HO2 = 0.725HAC + 0.275GLYC + 0.275GLYX + 0.275MGLY + 1.125OH + 0.825HO2 + 0.200CO2 + 0.375CH2O + 0.074HCOOH + 0.251CO	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=5	Paulot 2009b	
DIBOO + HO2 = 0.15HO2 + 0.15OH + 0.078GLYC + 0.078MGLY + 0.072HAC + 0.072GLYX + 0.85R4P	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=5		assume 15% recycling of OH, rest goes to R4P
MAOPO2 + HO2 = 1.0HAC+1.0CO2+2.0OH	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=4		
HC5OO + HO2 = 0.1IAP + 0.9OH + 0.9MGLY + 0.9GLYC + 0.9HO2	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=5		90% recycling, no experimental data. Somewhat based upon the high recycling rate observed for MVK/MACR
ISOPNDO2 + HO2 = 0.035MACRN + 0.155HCOOH + 0.22HAC + 0.065ETHLN + 0.325CH2O + 0.170NO2 + 0.075GLYC + 0.155NO3 + 0.075PROPNN + 0.170MEK + 0.175HO2 + 0.5OH + 0.5ISNP	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=5		Assume 50% recycling from HO2+RO2 (no experimental data - check Ng et al. for better estimates)
ISOPNBO2 + HO2 = 0.3GLYC + 0.3HAC + 0.2CH2O + 0.13MACRN + 0.07MVKN + 0.3NO2 + 0.2HO2 + 0.5OH + 0.5ISNP	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=5		Assume 50% recycling from HO2+RO2 (no experimental data - check Ng et al. for better estimates)
MACRNO2 + HO2 = 0.08ACTA + 0.08CH2O + 0.15NO3 + 0.07HCOOH + 0.07MGLY + 0.85HAC + 0.85NO2 + 0.93CO2 + 1.0OH	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=4		Assume 100% recycling. No experiment data. Inferred from the very high recycling observed for MAO2+HO2
MOBAOO + HO2=0.15OH + 0.15HO2 + 0.15RCHO + 0.15CO2 + 0.85R4P	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=5	Paulot 2009a	assume 15% recycling of OH, rest goes to R4P
MCO3 + HO2 = 0.15 ACTA + 0.15 O3 + 0.44 OH + 0.44 MO2 + 0.41 MAP	5.2e-13exp(980/T)	IUPAC(Feb2009)	
RCO3 + HO2 = 0.410RP + 0.150RCOOH + 0.150O3 + 0.440OH + 0.440ETO2	4.3E-13exp(1040/T)	MCM v3.2	Branching ratio is from MCMv3.2
ATO2 + HO2 = 0.15MCO3 + 0.15OH + 0.15CH2O + 0.85ATOOH	8.60E-13 exp(700/T)	Dillon et al. (2008)	Tyndall, Dillon et al. (ACP 2008) cycling 15%,reduce the recyling by 5% compared to previous version to be fully consistent with Dillon et al.
KO2 + HO2 = 0.15OH + 0.15ALD2 + 0.15 MCO3 + 0.85ATOOH	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=4	MCM	assuming 15% recycling of OH
MAO3 + HO2 = 0.44OH +0.15O3 + 0.59CH2O + 0.39MO2 +	4.3E-13exp(1040/T)		use MCM, 44% OH channel, 15% O3 channel, 41% peroxide

0.41MAOP + 0.39CO			channel.
RO2 + MO2/RO2 reactions			
RIO2 + MO2 = 1.1HO2 + 1.22CH2O + 0.280MVK + 0.180MACR + 0.3HC5 + 0.24MOH + 0.24ROH	8.37E-14		
HC5OO + MO2 = 0.50HO2 + 0.33CO + 0.09H2 + 0.18HAC + 0.13GLYC + 0.29MGLY + 0.25MEK + 0.95CH2O + 0.25MOH + 0.25ROH + 0.5HO2	8.37E-14		Tyndall MO2+MO2 Atkinson97 RO2+RO2; HC5OO=old IAO2
MRO2 + MO2 = 0.595HAC + 0.255MGLY + 0.595CO + 1.255CH2O + 1.7HO2 + 0.150ROH	8.37E-14		
VRO2 + MO2 = 0.14HO2 + 0.14CH2O + 0.36MCO3 + 0.36GLYC + 0.14MGLY + 0.25MEK + 0.75CH2O +0.25MOH + 0.25ROH + 0.5HO2	8.37E-14		
MAN2 + MO2 = 0.375PROPNN + 0.375CO + 0.375HO2 + 0.375MGLY + 0.375CH2O + 0.375NO2 + 0.250CH2O + 0.250R4N2	8.37E-14		
MAOPO2 + MO2 = 0.7HAC +0.7CO2+0.7OH+1.0CH2O+0.7HO2+0.3ROH	8.37E-14		
RIO2 + RIO2 = 1.28HO2 + 0.92CH2O + 0.56MVK + 0.36MACR + 0.48ROH + 0.5HC5	1.54E-13		
MAOPO2 + MAOPO2 = 2.0HAC+2.0CO2+2.0OH	8.37E-14		
MCO3 + MO2 = CH2O + MO2 + HO2	1.80E-12 exp(500/T)		
MCO3 + MO2 = ACTA + CH2O	2.00E-13 exp(500/T)		
RCO3 + MO2 = CH2O+HO2 + ETO2	1.68E-12 exp(500/T)		
RCO3 + MO2 = RCOOH + CH2O	1.87E-13 exp(500/T)		
MAO3 + MO2 = CH2O + HO2 + CH2O + MCO3	1.68E-12 exp(500/T)		
MAO3 + MO2 = RCOOH + CH2O	1.87E-13 exp(500/T)		
RO2 + MCO3 reactions			
MAOPO2 + MCO3 = 1.0HAC + 2.0CO2 + OH + MO2	1.68E-12exp(500/T)		
MAOPO2 + MCO3 = 1.0ACTA+1.0MEK	1.87E-13 exp(500/T)		
R4O2 + MCO3 = MO2 + 0.32ACET + 0.19MEK + 0.27HO2 + 0.32ALD2 + 0.13RCHO + 0.05A3O2 + 0.18B3O2 + 0.32ETO2	1.68E-12 exp(500/T)		
R4O2 + MCO3 = 1.0ACTA+1.0MEK	1.87E-13 exp(500/T)		
ATO2 + MCO3 = MCO3 + CH2O + MO2	1.68E-12 exp(500/T)	IUPAC06	
ATO2 + MCO3 = MGLY+ACTA	1.87E-13exp(500/T)	IUPAC06	replace MEK with MGLY
HC5OO + MCO3 = 0.216GLYX + 0.234MGLY + 0.234GLYC + 0.216HAC + 0.29DHMOB + 0.17MOBA + 0.09RCHO + HO2 + 0.09CO + MO2	1.68E-12 exp(500/T)		HC5OO=old IAO2, this radical channel use the same as HC5OO+NO without NO2 yield.
HC5OO + MCO3 = MEK +ACTA	1.87E-13 exp(500/T)		
VRO2 + MCO3 = 0.4HO2 + 0.4CH2O + 0.6MCO3 + 0.6GLYC + 0.4MGLY + 1.0MO2	1.68E-12 exp(500/T)		this radical channel use the same as VRO2+NO without NO2 and MVKN yield. And carbon balance.
VRO2 + MCO3 = MEK +ACTA	1.87E-13 exp(500/T)		
MRO2 + MCO3 = 0.850HO2 + 0.143MGLY + 0.857HAC + 0.857CO + 0.143CH2O +1.0MO2	1.68E-12 exp(500/T)		this radical channel use the same as MRO2+NO without NO2 and MACRN yield.
MRO2 + MCO3 = MEK +ACTA	1.87E-13 exp(500/T)		

Reaction	Rate	Reference	Notes
MAN2 + MCO3 = 0.5PROPNN + 0.5CO + 0.5HO2 + 0.5MGLY + 0.5CH2O + 0.5NO2 + CO2 + MO2	1.68E-12 exp(500/T)		
MAN2 + MCO3 = RCHO + ACTA + NO2	1.87E-13 exp(500/T)		
RIO2 + MCO3 = 0.887HO2 + 0.747CH2O + 0.453MVK + 0.294MACR + 0.140HC5 + 0.113DIBOO + CO2 + MO2	1.68E-12 exp(500/T)		Follow RIO2+NO without the yield of nitrate and NO2 and then rescale it.
RIO2 + MCO3 = MEK +ACTA	1.87E-13 exp(500/T)		
MCO3 + MCO3 = 2MO2	2.50E-12 exp(500/T)	Tyndall2001	
RCO3 + MCO3 = MO2 + ETO2	2.50E-12 exp(500/T)	Tyndall2001	
MAO3 + MCO3 = MO2 + MCO3 + CH2O	2.50E-12 exp(500/T)	Tyndall2001	
RO2 + NO2 equilibrium			
MCO3+NO2+M = PAN	LPL: 9.70E-29(300/T)^5.6; HPL:9.3E-12(300/T)^1.5; Fc: 0.6	JPL06	
PAN = MCO3+NO2	9.30E-29 exp(14000/T)	IUPAC06	equilibrium with the one above
RCO3+NO2 = PPN	LPL: 9.00E-28(300/T)^8.9; HPL:7.70E-12(300/T)^0.2; Fc: 0.6	JPL06	
PPN = RCO3+NO2	9e-29*exp(14000/T)	JPL06	
MAO3+NO2 = PMN	LPL: 9.00E-28(300/T)^8.9; HPL:7.70E-12(300/T)^0.2; Fc: 0.6	JPL06	
PMN = MAO3+NO2	9e-29*exp(14000/T)	JPL06	
MACRNO2+NO2= PMNN	LPL: 9.00E-28(300/T)^8.9 HPL:7.70E-12(300/T)^0.2 Fc: 0.6		
PMNN =MACRNO2 + NO2	9e-29*exp(14000/T)		
Reactions with O3			
ISOP + O3 = 0.244MVK + 0.325MACR + 0.845CH2O + 0.110H2O2 + 0.522CO + 0.204HCOOH + 0.199MCO3 + 0.026HO2 + 0.270OH + 0.128PRPE + 0.051MO2	1.00E-14 *EXP(-1970/T)	MCM v3.2	rate is from JPL 11, products from MCM, assuming CH2OO is dominated by reactions with H2O. ISOP + O3 in standard chem is not carbon-balanced.
MVK + O3 = 0.202OH + 0.202HO2 + 0.352HCOOH + 0.535CO + 0.050ALD2 + 0.950MGLY + 0.050CH2O	8.5 E-16exp(-1520/T)	MCM?	Rate is from IUPAC06
MACR + O3 = 0.261OH + 0.202HO2 + 0.326HCOOH + 0.569CO + 0.880MGLY + 0.120CH2O	1.4 E-15exp(-2100/T)	MCM?	
HC5 + O3 = 0.6MGLY + 0.1OH + 0.12CH2O + 0.28GLYC + 0.3O3 + 0.4CO + 0.2H2 + 0.2HAC + 0.2HCOOH	6.16E-15 exp(-1814/T)		HC5=old IALD??
ISOPNB + O3 = 0.610MVKN + 0.390MACRN + 0.27OH + CH2O	1.06E-16	Lockwood et al., 2010 ACP	use 1,2 for beta channel
ISOPND + O3 = 0.5PROPNN + 0.5ETHLN + 0.27OH + 0.5GLYC + 0.5HAC	5.3E-17	Lockwood et al., 2010 ACP	use 1,4 for delta channel
MOBA + O3 =OH +HO2+CO2+MEK	2.00E-17	Paulot 2009a	Weak constraint on the rate constant - no constraint on the

			products
PMN + O3 = NO2 + 0.6CH2O + HO2	8.20E-18	?	
Isomerization reactions			
RIO2 = 2.0HO2 + 1.0CH2O + 0.5MGLY + 0.5GLYC + 0.5GLYX + 0.5GLYX + 0.500HAC + 1.0OH	4.07E+08 exp(-7694/T)	Peeters et al. (2009, 2010)	Isomerization rate is adjusted according to Crounse et al. (2010), products follow Stavrakou et al. (2010).
MRO2 = 1.0CO + 1.0HAC + 1.0OH	2.90E+07 exp(-5297/T)	Crounse et al. (2012)	1,4-H-shift isomerization rate dominates over 1,5-H-shift.
Nighttime isoprene chemistry			
ISOP + NO3 = INO2	3.3E-12exp(-450/T)	Sander et al. 2012	from JPL
MACR + NO3 = MAN2	2.30E-15	IUPAC06	
MACR + NO3 = MAO3 + HNO3	1.10E-15	IUPAC06	IUPAC06 total rate is 3.4E-15, so use the ratio from Lurmann et al.,1986
INO2 + NO = 0.70ISN1 + 0.035MVK + 0.035MACR + 0.07*CH2O + 0.80HO2 + 1.3NO2 + 0.23HC5	2.7E-12 exp(350/T)	Rollins et al. (2009)	ISN1 is the NIT1 in Rollins et al. (2009)
INO2 + NO3 = 0.70ISN1 + 0.035MVK + 0.035MACR + 0.07CH2O + 0.80HO2 + 1.3NO2 + 0.23*HC5	2.3-12		
INO2 + HO2 = INPN	2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)], n=5	Xie et al. (2012)	
INPN + OH = 1.0OH + 1.0NO2 + 1.0MEK	1.9E-11exp(390/T)		
INPN + OH = 0.36INO2 + 0.64R4N2 + 0.64OH	5.18E-12exp(200/T)		
INO2 + MO2=0.35*ISN1 + 0.0175*MVK + 0.0175*MACR + 0.15*NO2 + 0.40*HO2 + 0.035*HCHO + 0.115*HC5 + 0.25*ISN1 + 0.25*ISOPND + 0.5*HCHO + 0.5*HO2 + 0.25*HCHO + 0.25*MEOH	1.30E-12		
INO2 + MCO3 = MO2 + 0.70ISN1 + 0.035MVK + 0.035MACR + 0.07CH2O + 0.80HO2 + 0.3NO2 + 0.23HC5	1.68E-12 exp(500/T)		
INO2 + MCO3 = RCHO + ACTA + NO2	1.87E-13 exp(500/T)		
INO2 + INO2 = 0.3NO2 + 0.70ISN1 + 0.035MVK + 0.035MACR + 0.07CH2O + 0.8 HO2 + 0.23HC5 + 0.5ISN1 + 0.5ISOPND	1.20E-12		
ISN1 + NO3 = 0.6*ISNOOA + 0.4* ISNOOB + 0.6*HNO3	3.15E-13*exp(-448/T)	Xie et al. (2012)	ISNOOA and ISNOOB correspond to NIT1NO3OOA and NIT1NO3OOB in Xie et al. (2012)
ISNOOA + NO3 = NO2 + R4N2 + CO +HO2	4.00E-12		
ISNOOA + NO = NO2 + R4N2 + CO +HO2	6.70E-12*exp(340/T)		
ISNOOA + HO2 = 0.75RP + 0.25RCOOH + 0.25O3	5.20E-13*exp(980/T)		
ISNOOA + NO2 = MPAN	LPL: 9.00E-28(300/T)^8.9; HPL:7.70E-12(300/T)^0.2; Fc: 0.6		
ISNOOB + NO3=R4N2 + GLYX + NO2 + NO2	2.30E-12		
ISNOOB + NO = 0.94R4N2 + 0.94GLYX + 0.94 NO2 + 0.94 NO2	2.60E-12*exp(380/T)		

Reaction	Rate	Source	Notes
ISNOOB + HO2 = INPN	2.06E-13*exp(1300/T)		
ISNOOB + MO2 = 0.7R4N2 + 0.7GLYX + 0.7NO2 + 0.25HCHO + 0.25MOH + 0.5HO2 + 0.5HCHO	2.0E-13		
ISN1 + O3 = 0.3R4N2 + 0.45CO + 0.15OH + 0.45 HO2 + 0.7 GLYX + 0.7 OH + 0.7NO2 + 0.7MGLY	4.15E-15*exp(-1520/T)		
ISN1 + OH = 0.345ISNOOA + 0.655ISNOHOO	7.48E-12*exp(410/T)		ISNOHOO is NIT1OHOO in Xie et al. (2012).
ISNOHOO + NO = 0.934R4N2 + 0.934HO2 + 0.919GLYX	2.60E-12*exp(380/T)		
ISNOHOO + HO2 = INPN	2.06E-13*exp(1300/T)		
ISNOHOO + MO2 = 0.7R4N2 + 0.7 GLYX + 0.7HO2 + 0.25 HCHO + 0.25MOH + 0.5 CH2O + 0.5 HO2	2.0E-13		
Photolysis reactions			
O3 + H2O = 2.0OH	JO1D	JPL2011	Assume steady state of O1D. The rate is calculated in calcrate.F with the quenching from N2 and O2 taken into account.
NO2 = NO + O3	JNO2		
H2O2 = 2OH	JH2O2		
MP = CH2O + HO2 + OH	J_ROOH		
CH2O = HO2 + HO2 + CO			
CH2O = H2 + CO			
HNO3 = OH + NO			
HNO4 = OH + NO3	J_HO2NO2*0.05		Chemistry_Issues#near-IR_photolysis_of_HNO4
HNO4 = HO2 + NO2	J_HO2NO2*0.95		Chemistry_Issues#near-IR_photolysis_of_HNO4
NO3 = NO2 + O3			
NO3 = NO + O2			
N2O5 = NO3 + NO2			
N2O5 = NO3 + NO + O3	0		turned off
ALD2 = MO2 + HO2 + CO			
ALD2 = CH4 + CO			
PAN = 0.6MCO3 + 0.6NO2 + 0.4MO2			
RCHO = ETO2 + HO2 + CO			
ACET = MCO3 + MO2			
ACET = 2.0MO2 + CO			
MEK = 0.85MCO3 + 0.85ETO2 + 0.15MO2 + 0.15RCO3			
GLYC = CH2O + 2.0HO2 + CO			
GLYX = 0.5H2 + CO + 0.5CH2O + 0.5CO			
GLYX = 2.0CO + 2.0HO2			
MGLY = MCO3 + CO +HO2	J_MGLY		
MGLY = ALD2 + CO	0		turned off
MVK = PRPE + CO	J_MVK*0.6		

MVK = MCO3 + CH2O + CO + HO2	J_MVK*0.2		
MVK = MO2 + MAO3	J_MVK*0.2		
MACR = MAO3 + HO2	J_MACR*0.5		
MACR = CO + HO2 + CH2O + MCO3	J_MACR*0.5		
HAC = MCO3 + CH2O + HO2			
INPN = OH + HO2 + RCHO + NO2	J_ROOH		
PRPN = OH + HO2 + RCHO + NO2	J_ROOH		
ETP = OH + HO2 + ALD2	J_ROOH		
RA3P = OH + HO2 + RCHO	J_ROOH		
RB3P = OH + HO2 + ACET	J_ROOH		
R4P = OH + HO2 + RCHO	J_ROOH		
PP = OH + HO2 + ALD2 + CH2O	J_ROOH		
RP = OH + HO2 + ALD2	J_ROOH		
RIP = OH + HO2 + 0.710CH2O + 0.425MVK + 0.285MACR + 0.29HC5	J_ROOH		
IAP = OH + HO2 + 0.67CO + 0.190H2 + 0.36HAC + 0.26GLYC + 0.580MGLY	J_ROOH		
ISNP = OH + HO2 + RCHO + NO2	J_ROOH		
VRP = OH + 0.3HO2 + 0.3CH2O + 0.7MCO3 + 0.7GLYC + 0.3MGLY	J_ROOH		
MRP = OH + HO2 + HAC + CO + CH2O	J_ROOH		
MAOP = OH + CH2O + MCO3	J_ROOH		
R4N2 = NO2 + 0.320ACET + 0.190MEK + 0.180MO2 + 0.270HO2 + 0.320ALD2 + 0.130RCHO + 0.050A3O2 + 0.180B3O2 + 0.320ETO2	J_MeNO3		
MAP = OH + MO2	J_ROOH		
MACRN = NO2 + HAC + MGLY + 0.5CH2O + HO2 + 0.5CO	J_ONIT1		
MVKN = GLYC + NO2 + MCO3	J_ONIT1		
ISOPNB = HC5 + NO2 + HO2	J_ONIT1		
ISOPND = HC5 + NO2 + HO2	J_ONIT1		
PROPNN = CH2O + NO2 + CO + MO2	J_ONIT1		
ATOOH = OH + CH2O +MCO3	J_ROOH		

--Bob Y. 13:48, 12 May 2014 (EDT)

RIP+OH

Follow SAR rules assuming a C(OOH) = 2* C(OH) = 7 (for the abstraction of the H alpha of the peroxide group). (see Kwok 1995 paper)

Assume that the abstraction of the peroxide H has a constant rate @298K of 3.6e-12

This gives for RIP:

```
43% 3.6e-12 (1,2)
28% 3.6e-12+7*1.94e-12 (4,3)
29% 3.6e-12+7*0.937e-12 (1,4)+(4,1) (I neglected 3,4 and 2,1)
9.3e-12@298K (4.75e-12*exp(200/T))
0.387 not recycling
```

Therefore 0.387=3.6/9.3. RIP + OH = 0.387RIO2 + 0.613OH + 0.613HC5.

Updates to the Paulot isoprene scheme

NO3 aerosol reactive uptake coefficient

This update was tested in the 1-month benchmark simulation v9-02g and approved on 24 Mar 2013.

The NO3 aerosol reactive uptake coefficient (gamma) has been increased from 1.0E-04 (Jacob et al., 2000) to 0.1 following Mao et al. (2013, submitted). In globchem.dat, we now have:

```
A  415 6.20E+01  1.0E-01    0 0 K   0.00    0.   0.
      NO3         +
=1.000HNO3         +              +              +
+                  +              +              +
+                  +              +              +
+                  +              +              +
```

--Melissa Sulprizio 12:44, 11 July 2013 (EDT)

There are two reasons for this modification.

1. First, a few recent papers show potential high gamma(NO3) on all types of aerosols.
2. Second, gamma(NO3) is supposed to increase at lower temperature (driven by its Henry's law constant), while most laboratory measurements are conducted at 298 K.

From the tests I have done so far, ozone seems to be insensitive to gamma(NO3) in the range of 0.0001-0.1.

--Jmao 13:11, 11 July 2013 (EDT)

Update One - RO2+HO2 Reaction Rate

This update was tested in the 1-month benchmark simulation v9-02g and approved on 24 Mar 2013.

Update applied to all >C2 RO2 species reaction with HO2. These include, in the standard scheme, R4O2, R4N1, KO2, RIO2, RIO1, IAO2,ISN1, VRO2, MRO2, MVN2, MAN2, B3O2, INO2, PRN1, A3O2, PO2.

Old RO2+HO2 reaction rate: `k = 7.40E-13*EXP(700/T)`

New RO2+HO2 reaction rate: `k = 2.91E-13*EXP(1300/T)[1-EXP(-0.245*n)]`, where n=no. of carbon atoms

Comparison of new and old RO2+HO2 reaction rates for C4 RO2 and C5 RO2:
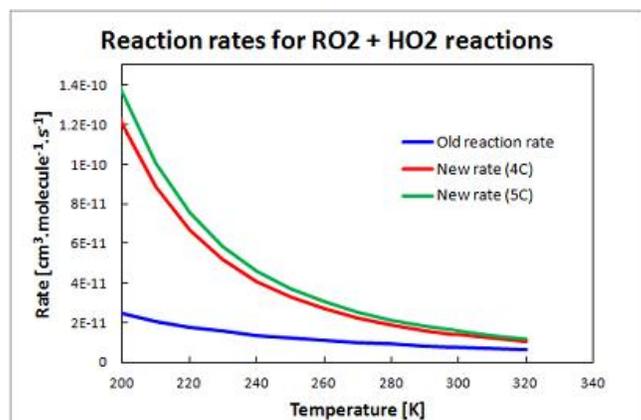
Benchmarking for this update can be viewed at: (Benchmarking results for RO2+HO2 reaction (ftp://ftp.as.harvard.edu/pub/exchange/eloise/IsopChemUpdate/RO2+HO2/))

Note: this is applied to RIO2, VRO2, MRO2, MAN2, INO2, HC5OO, ISOPNBO2, ISOPNDO2, MACRNO2, DIBOO, MOBAOO in the new isoprene chemistry, but not MAO3, MCO3, RCO3 radicals (acetyl peroxy type radicals.

--Bob Y. 13:49, 12 May 2014 (EDT)

Update Two - Transport of RIP

RIP = isoprene peroxide species formed at low-NOx (i.e. via the RO2+HO2 pathway)

This benchmark is done to understand the muted influence of the increased rate of the RO2+HO2 reaction on CH2O. Is this because the ultimate yield of CH2O is similar for all levels of NOx and RIP is not transported, leading to the realization of the ultimate yield of CH2O in the same grid box as its emission source?

Both schemes are run with initial concentrations of species set to zero. As RIP is added as an additional transported species this was viewed as the most effective way of comparing the two model runs.

Benchmarking for this update can be viewed at: (Benchmarking results for transporting RIP (ftp://ftp.as.harvard.edu/pub/exchange/eloise/IsopChemUpdate/RIPTransport/))

--Bob Y. 13:50, 12 May 2014 (EDT)

Updates 02/04/2013

These reactions are updated from the beta-version of Paulot scheme.

Old reaction	Old rate	New reaction	New rate	Note
KO2+HO2 =OH +ALD2 +MCO3	7.40E-13 exp(700/T)	KO2 + HO2 = 0.15OH +0.15ALD2 +0.15 MCO3 + 0.85 ATOOH	2.91E-13*EXP(1300/T) [1-EXP(-0.245*n)], n=4	Assuming 15% recycling of OH, consistent with MCM. Rate is also from Saunders et al. (2003).
MRO2 +HO2 =0.020MRP+0.980OH +0.980HO2+0.294CH2O+0.686HAC +0.294MGLY +0.686CO	7.40E-13 exp(700/T)	MRO2 + HO2 = 1.0MRP	2.91E-13*EXP(1300/T) [1-EXP(-0.245*n)], n=4	Isomerization of MRO2 is already taken into account in another reaction.
MAN2 + HO2 = 0.5PROPNN + 0.5CO + 0.5HO2 + 0.5MGLY + 0.5CH2O + 0.5NO2 + OH	7.40E-13 exp(700/T)	MAN2 + HO2 = 0.075PROPNN + 0.075CO + 0.075HO2 + 0.075MGLY + 0.075CH2O + 0.075NO2 + 0.15OH + 0.85ISNP	2.91E-13*EXP(1300/T) [1-EXP(-0.245*n)], n=4	assuming 15% recycling
INO2 + HO2 = 0.5INPN + 0.5ISOPND + 0.5OH + 0.5HO2	7.40E-13 exp(700/T)	INO2 + HO2 = INPN	2.91E-13*EXP(1300/T) [1-EXP(-0.245*n)], n=5	See nighttime chemistry
MAO3 + HO2 = 0.87OH +0.03O3 + 0.435CH2O + 0.435MO2 + 0.1MAOP + 0.030RCOOH + 0.283HAC + 0.152ATO2 + 0.870CO2 + 0.435CO	4.3E-13exp(1040/T)	MAO3 + HO2 = 0.44OH +0.15O3 + 0.59CH2O + 0.39MO2 + 0.41MAOP + 0.39CO	4.3E-13exp(1040/T)	use MCM, 44% OH channel, 15% O3 channel, 41% peroxide channel.
PMN + OH = 1.000PMNO2	3.20E-11	PMN + OH = HAC + CO + NO2	2.90E-11	from MCM
PMNO2 + NO = 0.6CO2 + 0.6HAC + 0.6NO3 + 0.4CH2O + 0.4HO2 + 0.4PYPAN + 0.900NO2	K* (1-YN) where YN isreturned from fyrno3.f; K=2.7E-12 exp(350/T) (Xcarbn=4.0E00)			we now remove all reactions from PMN following MCM.
PMNO2 + NO=PMNN	K* YN where YN is returned from fyrno3.f ; K=2.7E-12 exp(350/T) (Xcarbn=4.0E00)			
PMNO2 + HO2 = 0.6CO2 + 0.6HAC +	7.4E-			

0.6NO3 + 0.4CH2O + 0.4HO2 + 0.4PYPAN + 0.5R4P + 0.5OH	13exp(700/T)			
PYPO2 + NO2 + M = PYPAN	LPL: 9.0E-28(300/T)^8.9 HPL:7.70E-12(300/T)^0.2 Fc: 0.6			
PYPAN =PYPO2 +NO2	9.0E-29exp(14000/T)			
PYPO2 + NO = CO2+MCO3 +NO2	2.7E-12 exp(350/T)			
PYPO2 + HO2 = CO2+MCO3 +OH	7.40E-13 exp(700/T)			
PYPAN = 0.300NO3+0.700NO2+MCO3 +CO2	photolysis			
PYPAN = NO3 + MCO3 + CO2	photolysis			
PP+OH=0.791OH+0.209PO2+0.791RCHO	8.78E-12exp(200/T)	PP+OH=0.791OH+0.209PO2+0.791HAC		
DIBOO+HO2 = HO2 + OH + 0.52GLYC + 0.52MGLY + 0.48HAC + 0.48GLYX	7.4E-13exp(700/T)	DIBOO + HO2 = 0.15HO2 + 0.15OH + 0.078GLYC + 0.078MGLY + 0.072HAC + 0.072GLYX + 0.85R4P	2.91E-13*EXP(1300/T) [1-EXP(-0.245*n)], n=5	assume 15% recycling of OH, rest goes to R4P
MOBAOO + HO2 = 0.5OH + 0.5HO2 + 0.5RCHO + 0.5CO2 + 0.5R4P	7.4E-13exp(700/T)	MOBAOO + HO2=0.15OH + 0.15HO2 + 0.15RCHO + 0.15CO2 + 0.85R4P	2.91E-13*EXP(1300/T) [1-EXP(-0.245*n)], n=5	assume 15% recycling of OH, rest goes to R4P
IEPOXOO + HO2 =	7.4E-13exp(700/T)		2.91E-13*EXP(1300/T) [1-EXP(-0.245*n)], n=5	
MAOPO2 + HO2 =	7.4E-13exp(700/T)		2.91E-13*EXP(1300/T) [1-EXP(-0.245*n)], n=4	
HC5OO + HO2 =	7.4E-13exp(700/T)		2.91E-13*EXP(1300/T) [1-EXP(-0.245*n)], n=5	
ISOPNDO2 + HO2 =	7.4E-13exp(700/T)		2.91E-13*EXP(1300/T) [1-EXP(-0.245*n)], n=5	
ISOPNBO2 + HO2 =	7.4E-13exp(700/T)		2.91E-13*EXP(1300/T) [1-EXP(-0.245*n)], n=5	
MACRNO2 + HO2 =	7.4E-13exp(700/T)		2.91E-13*EXP(1300/T) [1-EXP(-0.245*n)], n=4	

--Bob Y. 13:50, 12 May 2014 (EDT)

Updates to be implemented

The following updates have not yet been added to GEOS-Chem as of this writing (May 2013):

Remove duplicate GLYX product from RIO2 reaction

This update was validated in the 1-month benchmark simulation v10-01d and approved on 03 Jun 2014.

Ploy Achakulwisut found a typo in this reaction for `RIO2` (in file `globchem.dat`). The product `0.5GLYX` was listed twice but should have been listed just once. The fix is as described below.

Old reaction	Old rate	New reaction	New rate	Note
RIO2 = 2.0HO2 + 1.0CH2O + 0.5MGLY + 0.5GLYC + **0.5GLYX** + **0.5GLYX** + 0.500HAC + 1.0OH	4.07E+08 exp(-7694/T)	RIO2 = 2.0HO2 + 1.0CH2O + 0.5MGLY + 0.5GLYC + **0.5GLYX** + 0.500HAC + 1.0OH	same	To balance carbon

--Bob Y. 13:53, 12 May 2014 (EDT)

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--Bob Y. 13:55, 12 May 2014 (EDT)