The Chemical Mechanism of MECCA

KPP version: `2.2.3_rs3`

MECCA version: `4.4.0.m1`

Date: June 10, 2024

Batch file: `stratsulf_oracle.bat`

Integrator: `rosenbrock_mz`

Gas equation file: `gas.eqn`

Replacement file: `stratsulf_oracle`

Selected reactions:

“`(((Tr && (G || Het) && !I) || St || (Tr && D && !Cl && !Br && !I && !Hg)) && !Hg)`”

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase:	119
Aqueous phase:	0
All species:	119

Number of reactions in selected mechanism:

Gas phase (Gnnn):	224
Aqueous phase (Annn):	0
Henry (Hnnn):	0
Photolysis (Jnnn):	72
Aqueous phase photolysis (PHnnn):	0
Heterogeneous (HETnnn):	12
Equilibria (EQnn):	0
Isotope exchange (IEXnnn):	0
Tagging equations (TAGnnn):	0
Dummy (Dnn):	0
All equations:	308

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	UpStTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	`3.3E-11*EXP(55./temp)`	Burkholder et al. (2015)
G1001	UpStTrG	$O_2 + O(^3P) \rightarrow O_3$	`6.0E-34*((temp/300.)**(-2.4)) *cair`	Burkholder et al. (2015)
G1002a	UpStG	$O_3 + O(^1D) \rightarrow 2\ O_2$	`1.2E-10`	Burkholder et al. (2015)*
G1003	UpStG	$O_3 + O(^3P) \rightarrow 2\ O_2$	`8.0E-12*EXP(-2060./temp)`	Burkholder et al. (2015)
G2100	UpStTrG	$H + O_2 \rightarrow HO_2$	`k_3rd(temp,cair,4.4E-32,1.3, 7.5E-11,-0.2,0.6)`	Burkholder et al. (2015)
G2101	UpStG	$H + O_3 \rightarrow OH + O_2$	`1.4E-10*EXP(-470./temp)`	Burkholder et al. (2015)
G2102	UpStG	$H_2 + O(^1D) \rightarrow H + OH$	`1.2E-10`	Burkholder et al. (2015)
G2103	UpStG	$OH + O(^3P) \rightarrow H + O_2$	`1.8E-11*EXP(180./temp)`	Burkholder et al. (2015)
G2104	UpStTrG	$OH + O_3 \rightarrow HO_2 + O_2$	`1.7E-12*EXP(-940./temp)`	Burkholder et al. (2015)
G2105	UpStTrG	$OH + H_2 \rightarrow H_2O + H$	`2.8E-12*EXP(-1800./temp)`	Burkholder et al. (2015)
G2106	UpStG	$HO_2 + O(^3P) \rightarrow OH + O_2$	`3.E-11*EXP(200./temp)`	Burkholder et al. (2015)
G2107	UpStTrG	$HO_2 + O_3 \rightarrow OH + 2\ O_2$	`1.E-14*EXP(-490./temp)`	Burkholder et al. (2015)
G2108a	UpStG	$HO_2 + H \rightarrow 2\ OH$	`7.2E-11`	Burkholder et al. (2015)
G2108b	UpStG	$HO_2 + H \rightarrow H_2 + O_2$	`6.9E-12`	Burkholder et al. (2015)
G2108c	UpStG	$HO_2 + H \rightarrow O(^3P) + H_2O$	`1.6E-12`	Burkholder et al. (2015)
G2109	UpStTrG	$HO_2 + OH \rightarrow H_2O + O_2$	`4.8E-11*EXP(250./temp)`	Burkholder et al. (2015)
G2110	UpStTrG	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	`k_HO2_HO2`	Burkholder et al. (2015)*
G2111	UpStTrG	$H_2O + O(^1D) \rightarrow 2\ OH$	`1.63E-10*EXP(60./temp)`	Burkholder et al. (2015)
G2112	UpStTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	`1.8E-12`	Burkholder et al. (2015)
G3100	UpStGN	$N + O_2 \rightarrow NO + O(^3P)$	`1.5E-11*EXP(-3600./temp)`	Burkholder et al. (2015)
G3101	UpStTrGN	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	`2.15E-11*EXP(110./temp)`	Burkholder et al. (2015)
G3102a	UpStGN	$N_2O + O(^1D) \rightarrow 2\ NO$	`7.259E-11*EXP(20./temp)`	Burkholder et al. (2015)
G3102b	StGN	$N_2O + O(^1D) \rightarrow N_2 + O_2$	`4.641E-11*EXP(20./temp)`	Burkholder et al. (2015)
G3103	UpStTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	`3.0E-12*EXP(-1500./temp)`	Burkholder et al. (2015)
G3104	UpStGN	$NO + N \rightarrow O(^3P) + N_2$	`2.1E-11*EXP(100./temp)`	Burkholder et al. (2015)
G3105	UpStGN	$NO_2 + O(^3P) \rightarrow NO + O_2$	`5.1E-12*EXP(210./temp)`	Burkholder et al. (2015)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	`1.2E-13*EXP(-2450./temp)`	Burkholder et al. (2015)
G3107	UpStGN	$NO_2 + N \rightarrow N_2O + O(^3P)$	`5.8E-12*EXP(220./temp)`	Burkholder et al. (2015)
G3108	StTrGN	$NO_3 + NO \rightarrow 2\ NO_2$	`1.5E-11*EXP(170./temp)`	Burkholder et al. (2015)
G3109	UpStTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	`k_NO3_NO2`	Burkholder et al. (2015)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	`k_NO3_NO2/(5.8E-27*EXP(10840./ temp))`	Burkholder et al. (2015)*

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G3200	TrGN	$NO + OH \rightarrow HONO$	k_3rd(temp,cair,7.0E-31,2.6, 3.6E-11,0.1,0.6)	Burkholder et al. (2015)
G3201	UpStTrGN	$NO + HO_2 \rightarrow NO_2 + OH$	3.3E-12*EXP(270./temp)	Burkholder et al. (2015)
G3202	UpStTrGN	$NO_2 + OH \rightarrow HNO_3$	k_3rd(temp,cair,1.8E-30,3.0, 2.8E-11,0.,0.6)	Burkholder et al. (2015)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	k_NO2_HO2	Burkholder et al. (2015)*
G3204	TrGN	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	3.5E-12	Burkholder et al. (2015)
G3205	TrGN	$HONO + OH \rightarrow NO_2 + H_2O$	1.8E-11*EXP(-390./temp)	Burkholder et al. (2015)
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3$	k_HNO3_OH	Dulitz et al. (2018)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	k_NO2_HO2/(2.1E-27*EXP(10900./ temp))	Burkholder et al. (2015)*
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	1.3E-12*EXP(380./temp)	Burkholder et al. (2015)
G3209	TrGN	$NH_3 + OH \rightarrow NH_2 + H_2O$	1.7E-12*EXP(-710./temp)	Kohlmann and Poppe (1999)
G3210	TrGN	$NH_2 + O_3 \rightarrow NH_2O + O_2$	4.3E-12*EXP(-930./temp)	Kohlmann and Poppe (1999)
G3211	TrGN	$NH_2 + HO_2 \rightarrow NH_2O + OH$	4.8E-07*EXP(-628./temp)*(temp) **(-1.32)	Kohlmann and Poppe (1999)
G3212	TrGN	$NH_2 + HO_2 \rightarrow HNO + H_2O$	9.4E-09*EXP(-356./temp)*(temp) **(-1.12)	Kohlmann and Poppe (1999)
G3213	TrGN	$NH_2 + NO \rightarrow HO_2 + OH + N_2$	1.92E-12*((temp/298.)**(-1.5))	Kohlmann and Poppe (1999)
G3214	TrGN	$NH_2 + NO \rightarrow N_2 + H_2O$	1.41E-11*((temp/298.)**(-1.5))	Kohlmann and Poppe (1999)
G3215	TrGN	$NH_2 + NO_2 \rightarrow N_2O + H_2O$	1.2E-11*((temp/298.)**(-2.0))	Kohlmann and Poppe (1999)
G3216	TrGN	$NH_2 + NO_2 \rightarrow NH_2O + NO$	0.8E-11*((temp/298.)**(-2.0))	Kohlmann and Poppe (1999)
G3217	TrGN	$NH_2O + O_3 \rightarrow NH_2 + O_2$	1.2E-14	Kohlmann and Poppe (1999)
G3218	TrGN	$NH_2O \rightarrow NHOH$	1.3E3	Kohlmann and Poppe (1999)
G3219	TrGN	$HNO + OH \rightarrow NO + H_2O$	8.0E-11*EXP(-500./temp)	Kohlmann and Poppe (1999)
G3220	TrGN	$HNO + NHOH \rightarrow NH_2OH + NO$	1.66E-12*EXP(-1500./temp)	Kohlmann and Poppe (1999)
G3221	TrGN	$HNO + NO_2 \rightarrow HONO + NO$	1.0E-12*EXP(-1000./temp)	Kohlmann and Poppe (1999)
G3222	TrGN	$NHOH + OH \rightarrow HNO + H_2O$	1.66E-12	Kohlmann and Poppe (1999)
G3223	TrGN	$NH_2OH + OH \rightarrow NHOH + H_2O$	4.13E-11*EXP(-2138./temp)	Kohlmann and Poppe (1999)
G3224	TrGN	$HNO + O_2 \rightarrow HO_2 + NO$	3.65E-14*EXP(-4600./temp)	Kohlmann and Poppe (1999)
G4100	UpStG	$CH_4 + O(^1D) \rightarrow .75\ CH_3O_2 + .75\ OH + .25\ HCHO + .4\ H + .05\ H_2$	1.75E-10	Sander et al. (2011)
G4101	StTrG	$CH_4 + OH \rightarrow CH_3O_2 + H_2O$	1.85E-20*EXP(2.82*LOG(temp) -987./temp)	Atkinson (2003)
G4102	TrG	$CH_3OH + OH \rightarrow HCHO + HO_2$	2.9E-12*EXP(-345./temp)	Sander et al. (2011)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4103	StTrG	$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$	`4.1E-13*EXP(750./temp)`	Sander et al. (2011)*
G4104	UpStTrGN	$CH_3O_2 + NO \rightarrow HCHO + NO_2 + HO_2$	`2.8E-12*EXP(300./temp)`	Sander et al. (2011)
G4105	TrGN	$CH_3O_2 + NO_3 \rightarrow HCHO + HO_2 + NO_2$	`1.3E-12`	Atkinson et al. (2006)
G4106a	StTrG	$CH_3O_2 + CH_3O_2 \rightarrow 2\ HCHO + 2\ HO_2$	`9.5E-14*EXP(390./temp)/(1.+1./26.2*EXP(1130./temp))`	Sander et al. (2011)
G4106b	StTrG	$CH_3O_2 + CH_3O_2 \rightarrow HCHO + CH_3OH + O_2$	`9.5E-14*EXP(390./temp)/(1.+26.2*EXP(-1130./temp))`	Sander et al. (2011)
G4107	StTrG	$CH_3OOH + OH \rightarrow .7\ CH_3O_2 + .3\ HCHO + .3\ OH + H_2O$	`k_CH3OOH_OH`	Wallington et al. (2018)
G4108	StTrG	$HCHO + OH \rightarrow CO + H_2O + HO_2$	`9.52E-18*EXP(2.03*LOG(temp)+636./temp)`	Sivakumaran et al. (2003)
G4109	TrGN	$HCHO + NO_3 \rightarrow HNO_3 + CO + HO_2$	`3.4E-13*EXP(-1900./temp)`	Sander et al. (2011)*
G4110	UpStTrG	$CO + OH \rightarrow H + CO_2$	`(1.57E-13+cair*3.54E-33)`	McCabe et al. (2001)
G4111	TrG	$HCOOH + OH \rightarrow CO_2 + HO_2 + H_2O$	`4.0E-13`	Sander et al. (2011)
G4200	TrGC	$C_2H_6 + OH \rightarrow C_2H_5O_2 + H_2O$	`1.49E-17*temp*temp*EXP(-499./temp)`	Atkinson (2003)
G4201	TrGC	$C_2H_4 + O_3 \rightarrow HCHO + .63\ CO + .13\ HO_2 + 0.23125\ HCOOH + 0.13875\ HCHO + 0.13875\ H_2O_2 + .13\ OH$	`1.2E-14*EXP(-2630./temp)`	Sander et al. (2011)*
G4202	TrGC	$C_2H_4 + OH \rightarrow .6666667\ CH_3CH(O_2)CH_2OH$	`k_3rd(temp,cair,1.0E-28,4.5,7.5E-12,0.85,0.6)`	Sander et al. (2011)
G4203	TrGC	$C_2H_5O_2 + HO_2 \rightarrow C_2H_5OOH$	`7.5E-13*EXP(700./temp)`	Sander et al. (2011)
G4204	TrGCN	$C_2H_5O_2 + NO \rightarrow CH_3CHO + HO_2 + NO_2$	`2.6E-12*EXP(365./temp)`	Sander et al. (2011)
G4205	TrGCN	$C_2H_5O_2 + NO_3 \rightarrow CH_3CHO + HO_2 + NO_2$	`2.3E-12`	Wallington et al. (2018)
G4206	TrGC	$C_2H_5O_2 + CH_3O_2 \rightarrow .75\ HCHO + HO_2 + .75\ CH_3CHO + .25\ CH_3OH$	`1.6E-13*EXP(195./temp)`	see note*
G4207	TrGC	$C_2H_5OOH + OH \rightarrow .3\ C_2H_5O_2 + .7\ CH_3CHO + .7\ OH$	`k_CH3OOH_OH`	see note*
G4208	TrGC	$CH_3CHO + OH \rightarrow CH_3C(O)OO + H_2O$	`4.4E-12*EXP(365./temp)`	Atkinson et al. (2006)
G4209	TrGCN	$CH_3CHO + NO_3 \rightarrow CH_3C(O)OO + HNO_3$	`1.4E-12*EXP(-1900./temp)`	Sander et al. (2011)
G4210	TrGC	$CH_3COOH + OH \rightarrow CH_3O_2 + CO_2 + H_2O$	`4.2E-14*EXP(855./temp)`	Atkinson et al. (2006)
G4211a	TrGC	$CH_3C(O)OO + HO_2 \rightarrow CH_3C(O)OOH$	`4.3E-13*EXP(1040./temp)/(1.+1./37.*EXP(660./temp))`	Tyndall et al. (2001)
G4211b	TrGC	$CH_3C(O)OO + HO_2 \rightarrow CH_3COOH + O_3$	`4.3E-13*EXP(1040./temp)/(1.+37.*EXP(-660./temp))`	Tyndall et al. (2001)
G4212	TrGCN	$CH_3C(O)OO + NO \rightarrow CH_3O_2 + CO_2 + NO_2$	`8.1E-12*EXP(270./temp)`	Tyndall et al. (2001)
G4213	TrGCN	$CH_3C(O)OO + NO_2 \rightarrow PAN$	`k_CH3CO3_NO2`	Sander et al. (2011)*
G4214	TrGCN	$CH_3C(O)OO + NO_3 \rightarrow CH_3O_2 + NO_2 + CO_2$	`4.E-12`	Canosa-Mas et al. (1996)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4215a	TrGC	$CH_3C(O)OO + CH_3O_2 \rightarrow HCHO + HO_2 + CH_3O_2 + CO_2$	`0.9*2.0E-12*EXP(500./temp)`	Sander et al. (2011)
G4215b	TrGC	$CH_3C(O)OO + CH_3O_2 \rightarrow CH_3COOH + HCHO$	`0.1*2.0E-12*EXP(500./temp)`	Sander et al. (2011)
G4216	TrGC	$CH_3C(O)OO + C_2H_5O_2 \rightarrow .82\ CH_3O_2 + CH_3CHO + .82\ HO_2 + .18\ CH_3COOH$	`4.9E-12*EXP(211./temp)`	Wallington et al. (2018), Kirchner and Stockwell (1996)
G4217	TrGC	$CH_3C(O)OO + CH_3C(O)OO \rightarrow 2\ CH_3O_2 + 2\ CO_2 + O_2$	`2.5E-12*EXP(500./temp)`	Tyndall et al. (2001)
G4218	TrGC	$CH_3C(O)OOH + OH \rightarrow CH_3C(O)OO + H_2O$	`0.6*k_CH3OOH_OH`	Rickard and Pascoe (2009)
G4219	TrGCN	$NACA + OH \rightarrow NO_2 + HCHO + CO$	`5.6E-12*EXP(270./temp)`	Pöschl et al. (2000)
G4220	TrGCN	$PAN + OH \rightarrow HCHO + CO + NO_2 + H_2O$	`9.50E-13*EXP(-650./temp)`	Rickard and Pascoe (2009)
G4221	TrGCN	$PAN \rightarrow CH_3C(O)OO + NO_2$	`k_PAN_M`	Sander et al. (2011)*
G4300	TrGC	$C_3H_8 + OH \rightarrow .82\ iC_3H_7O_2 + .18\ C_2H_5O_2 + H_2O$	`1.65E-17*temp*temp*EXP(-87./temp)`	Atkinson (2003)
G4301	TrGC	$C_3H_6 + O_3 \rightarrow .57\ HCHO + .47\ CH_3CHO + .33\ OH + .26\ HO_2 + .07\ CH_3O_2 + .06\ C_2H_5O_2 + .23\ CH_3C(O)OO + .04\ MGLYOX + .06\ CH_4 + .31\ CO + .22\ HCOOH + .03\ CH_3OH$	`6.5E-15*EXP(-1900./temp)`	Sander et al. (2011)
G4302	TrGC	$C_3H_6 + OH \rightarrow CH_3CH(O_2)CH_2OH$	`k_3rd(temp,cair,8.E-27,3.5, 3.E-11,0.,0.5)`	Wallington et al. (2018)
G4303	TrGCN	$C_3H_6 + NO_3 \rightarrow LC4H9NO3$	`4.6E-13*EXP(-1155./temp)`	Wallington et al. (2018)
G4304	TrGC	$iC_3H_7O_2 + HO_2 \rightarrow iC_3H_7OOH$	`k_PrO2_HO2`	Atkinson (1997)
G4305	TrGCN	$iC_3H_7O_2 + NO \rightarrow .96\ CH_3COCH_3 + .96\ HO_2 + .96\ NO_2 + .04\ iC_3H_7ONO_2$	`k_PrO2_NO`	Wallington et al. (2018)
G4306	TrGC	$iC_3H_7O_2 + CH_3O_2 \rightarrow CH_3COCH_3 + .8\ HCHO + .8\ HO_2 + .2\ CH_3OH$	`k_PrO2_CH3O2`	Kirchner and Stockwell (1996)
G4307	TrGC	$iC_3H_7OOH + OH \rightarrow .3\ iC_3H_7O_2 + .7\ CH_3COCH_3 + .7\ OH$	`k_CH3OOH_OH`	see note*
G4308	TrGC	$CH_3CH(O_2)CH_2OH + HO_2 \rightarrow CH_3CH(OOH)CH_2OH$	`6.5E-13*EXP(650./temp)`	Müller and Brasseur (1995)
G4309	TrGCN	$CH_3CH(O_2)CH_2OH + NO \rightarrow .98\ CH_3CHO + .98\ HCHO + .98\ HO_2 + .98\ NO_2 + .02\ LC4H9NO3$	`4.2E-12*EXP(180./temp)`	Müller and Brasseur (1995)
G4310	TrGC	$CH_3CH(OOH)CH_2OH + OH \rightarrow .5\ CH_3CH(O_2)CH_2OH + .5\ CH_3COCH_2OH + .5\ OH + H_2O$	`3.8E-12*EXP(200./temp)`	Müller and Brasseur (1995)
G4311	TrGC	$CH_3COCH_3 + OH \rightarrow CH_3COCH_2O_2 + H_2O$	`1.33E-13+3.82E-11*EXP(-2000./ temp)`	Sander et al. (2011)
G4312	TrGC	$CH_3COCH_2O_2 + HO_2 \rightarrow CH_3COCH_2O_2H$	`8.6E-13*EXP(700./temp)`	Tyndall et al. (2001)
G4313	TrGCN	$CH_3COCH_2O_2 + NO \rightarrow CH_3C(O)OO + HCHO + NO_2$	`2.9E-12*EXP(300./temp)`	Sander et al. (2011)
G4314	TrGC	$CH_3COCH_2O_2 + CH_3O_2 \rightarrow .5\ MGLYOX + .5\ CH_3OH + .3\ CH_3C(O)OO + .8\ HCHO + .3\ HO_2 + .2\ CH_3COCH_2OH$	`7.5E-13*EXP(500./temp)`	Tyndall et al. (2001)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4315	TrGC	$CH_3COCH_2O_2H$ + OH → .3 $CH_3COCH_2O_2$ + .7 MGLYOX + .7 OH	`k_CH3OOH_OH`	see note*
G4316	TrGC	CH_3COCH_2OH + OH → MGLYOX + HO_2	`2.15E-12*EXP(305./temp)`	Dillon et al. (2006)
G4317	TrGC	MGLYOX + OH → $CH_3C(O)OO$ + CO	`8.4E-13*EXP(830./temp)`	Tyndall et al. (1995)
G4320	TrGCN	$iC_3H_7ONO_2$ + OH → CH_3COCH_3 + NO_2	`6.2E-13*EXP(-230./temp)`	Wallington et al. (2018)
G4400	TrGC	C_4H_{10} + OH → $LC_4H_9O_2$ + H_2O	`1.81E-17*temp*temp*EXP(114./temp)`	Atkinson (2003)
G4401	TrGC	$LC_4H_9O_2$ + CH_3O_2 → .88 MEK + .68 HCHO + 1.23 HO_2 + .12 CH_3CHO + .12 $C_2H_5O_2$ + .18 CH_3OH	`k_PrO2_CH3O2`	see note*
G4402	TrGC	$LC_4H_9O_2$ + HO_2 → LC_4H_9OOH	`k_PrO2_HO2`	see note*
G4403	TrGCN	$LC_4H_9O_2$ + NO → .84 NO_2 + .56 MEK + .56 HO_2 + .28 $C_2H_5O_2$ + .28 CH_3CHO + .16 LC4H9NO3	`k_PrO2_NO`	see note*
G4404	TrGC	LC_4H_9OOH + OH → .15 $LC_4H_9O_2$ + .85 MEK + .85 OH + .85 H_2O	`k_CH3OOH_OH`	see note*
G4405	TrGC	MVK + O_3 → .45 HCOOH + .9 MGLYOX + .1 $CH_3C(O)OO$ + .19 OH + .22 CO + .32 HO_2	`.5*(1.36E-15*EXP(-2112./temp) +7.51E-16*EXP(-1521./temp))`	Pöschl et al. (2000)
G4406	TrGC	MVK + OH → MVKO2	`.5*(4.1E-12*EXP(452./temp) +1.9E-11*EXP(175./temp))`	Pöschl et al. (2000)
G4407	TrGC	MVKO2 + HO_2 → MVKOOH	`1.82E-13*EXP(1300./temp)`	Pöschl et al. (2000)
G4408	TrGCN	MVKO2 + NO → NO_2 + .25 $CH_3C(O)OO$ + .25 CH_3COCH_2OH + .75 HCHO + .25 CO + .75 HO_2 + .5 MGLYOX	`2.54E-12*EXP(360./temp)`	Pöschl et al. (2000)
G4409	TrGCN	MVKO2 + NO_2 → MPAN	`.25*k_3rd(temp,cair,9.7E-29,5.6, 9.3E-12,1.5,0.6)`	Pöschl et al. (2000)
G4410	TrGC	MVKO2 + CH_3O_2 → .5 MGLYOX + .375 CH_3COCH_2OH + .125 $CH_3C(O)OO$ + 1.125 HCHO + .875 HO_2 + .125 CO + .25 CH_3OH	`2.E-12`	von Kuhlmann (2001)
G4411	TrGC	MVKO2 + MVKO2 → CH_3COCH_2OH + MGLYOX + .5 CO + .5 HCHO + HO_2	`2.E-12`	Pöschl et al. (2000)
G4412	TrGC	MVKOOH + OH → MVKO2	`3.E-11`	Pöschl et al. (2000)
G4413	TrGC	MEK + OH → LMEKO2	`1.3E-12*EXP(-25./temp)`	Wallington et al. (2018)
G4414	TrGC	LMEKO2 + HO_2 → LMEKOOH	`k_PrO2_HO2`	see note*
G4415	TrGCN	LMEKO2 + NO → .985 CH_3CHO + .985 $CH_3C(O)OO$ + .985 NO_2 + .015 LC4H9NO3	`k_PrO2_NO`	see note*
G4416	TrGC	LMEKOOH + OH → .8 BIACET + .8 OH + .2 LMEKO2	`k_CH3OOH_OH`	see note*
G4417	TrGCN	LC4H9NO3 + OH → MEK + NO_2 + H_2O	`1.7E-12`	Wallington et al. (2018)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4418	TrGCN	MPAN + OH → CH_3COCH_2OH + NO_2	3.2E-11	Orlando et al. (2002)
G4419	TrGCN	MPAN → MVKO2 + NO_2	k_PAN_M	see note*
G4500	TrGC	C_5H_8 + O_3 → .28 HCOOH + .65 MVK + .1 MVKO2 + .1 $CH_3C(O)OO$ + .14 CO + .58 HCHO + .09 H_2O_2 + .08 CH_3O_2 + .25 OH + .25 HO_2	7.86E-15*EXP(-1913./temp)	Pöschl et al. (2000)
G4501	TrGC	C_5H_8 + OH → ISO2	2.54E-11*EXP(410./temp)	Pöschl et al. (2000)
G4502	TrGCN	C_5H_8 + NO_3 → ISON	3.03E-12*EXP(-446./temp)	Pöschl et al. (2000)
G4503	TrGC	ISO2 + HO_2 → ISOOH	2.22E-13*EXP(1300./temp)	Boyd et al. (2003)
G4504	TrGCN	ISO2 + NO → .956 NO_2 + .956 MVK + .956 HCHO + .956 HO_2 + .044 ISON	2.54E-12*EXP(360./temp)	Pöschl et al. (2000)
G4505	TrGC	ISO2 + CH_3O_2 → .5 MVK + 1.25 HCHO + HO_2 + .25 MGLYOX + .25 CH_3COCH_2OH + .25 CH_3OH	2.E-12	von Kuhlmann (2001)
G4506	TrGC	ISO2 + ISO2 → 2 MVK + HCHO + HO_2	2.E-12	Pöschl et al. (2000)
G4507	TrGC	ISOOH + OH → MVK + OH	1.E-10	Pöschl et al. (2000)
G4508	TrGCN	ISON + OH → CH_3COCH_2OH + NACA	1.3E-11	Pöschl et al. (2000)
G6100	UpStTrGCl	Cl + O_3 → ClO + O_2	2.8E-11*EXP(-250./temp)	Atkinson et al. (2007)
G6101	UpStGCl	ClO + $O(^3P)$ → Cl + O_2	2.5E-11*EXP(110./temp)	Atkinson et al. (2007)
G6102a	StTrGCl	ClO + ClO → Cl_2 + O_2	1.0E-12*EXP(-1590./temp)	Atkinson et al. (2007)
G6102b	StTrGCl	ClO + ClO → 2 Cl + O_2	3.0E-11*EXP(-2450./temp)	Atkinson et al. (2007)
G6102c	StTrGCl	ClO + ClO → Cl + OClO	3.5E-13*EXP(-1370./temp)	Atkinson et al. (2007)
G6102d	StTrGCl	ClO + ClO → Cl_2O_2	k_ClO_ClO	Burkholder et al. (2015)
G6103	StTrGCl	Cl_2O_2 → ClO + ClO	k_ClO_ClO/(2.16E-27*EXP(8537./temp))	Burkholder et al. (2015)*
G6200	StGCl	Cl + H_2 → HCl + H	3.9E-11*EXP(-2310./temp)	Atkinson et al. (2007)
G6201a	StGCl	Cl + HO_2 → HCl + O_2	4.4E-11-7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6201b	StGCl	Cl + HO_2 → ClO + OH	7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6202	StTrGCl	Cl + H_2O_2 → HCl + HO_2	1.1E-11*EXP(-980./temp)	Atkinson et al. (2007)
G6203	StGCl	ClO + OH → .94 Cl + .94 HO_2 + .06 HCl + .06 O_2	7.3E-12*EXP(300./temp)	Atkinson et al. (2007)
G6204	StTrGCl	ClO + HO_2 → HOCl + O_2	2.2E-12*EXP(340./temp)	Atkinson et al. (2007)*
G6205	StTrGCl	HCl + OH → Cl + H_2O	1.7E-12*EXP(-230./temp)	Atkinson et al. (2007)
G6206	StGCl	HOCl + OH → ClO + H_2O	3.0E-12*EXP(-500./temp)	Burkholder et al. (2015)
G6300	UpStTrGClN	ClO + NO → NO_2 + Cl	6.2E-12*EXP(295./temp)	Atkinson et al. (2007)
G6301	StTrGClN	ClO + NO_2 → $ClNO_3$	k_3rd_iupac(temp,cair,1.6E-31,3.4,7.E-11,0.,0.4)	Atkinson et al. (2007)
G6302	TrGClN	$ClNO_3$ → ClO + NO_2	6.918E-7*EXP(-10909./temp)*cair	Anderson and Fahey (1990)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G6303	StGClN	$ClNO_3 + O(^3P) \rightarrow ClO + NO_3$	4.5E-12*EXP(-900./temp)	Atkinson et al. (2007)
G6304	StTrGClN	$ClNO_3 + Cl \rightarrow Cl_2 + NO_3$	6.2E-12*EXP(145./temp)	Atkinson et al. (2007)
G6400	StTrGCl	$Cl + CH_4 \rightarrow HCl + CH_3O_2$	6.6E-12*EXP(-1240./temp)	Atkinson et al. (2006)
G6401	StTrGCl	$Cl + HCHO \rightarrow HCl + CO + HO_2$	8.1E-11*EXP(-34./temp)	Atkinson et al. (2006)
G6402	StTrGCl	$Cl + CH_3OOH \rightarrow HCHO + HCl + OH$	5.9E-11	Atkinson et al. (2006)*
G6403	StTrGCl	$ClO + CH_3O_2 \rightarrow HO_2 + Cl + HCHO$	1.8E-12*EXP(-600./temp)	Burkholder et al. (2015)
G6404	StGCl	$CCl_4 + O(^1D) \rightarrow$ LCARBON + ClO + 3 Cl	3.3E-10	Burkholder et al. (2015)
G6405	StGCl	$CH_3Cl + O(^1D) \rightarrow OH + Cl$	1.65E-10	see note*
G6406	StGCl	$CH_3Cl + OH \rightarrow$ LCARBON + H_2O + Cl	1.96E-12*EXP(-1200./temp)	Burkholder et al. (2015)
G6407	StGCCl	$CH_3CCl_3 + O(^1D) \rightarrow$ 2 LCARBON + OH + 3 Cl	3.25E-10	Burkholder et al. (2015)
G6408	StTrGCCl	$CH_3CCl_3 + OH \rightarrow$ 2 LCARBON + H_2O + 3 Cl	1.64E-12*EXP(-1520./temp)	Burkholder et al. (2015)
G6409	TrGCCl	$Cl + C_2H_4 \rightarrow .6666667\ CH_3CH(O_2)CH_2OH + HCl$	k_3rd_iupac(temp,cair,1.85E-29, 3.3,6.0E-10,0.0,0.4)	Atkinson et al. (2006)
G6410	TrGCCl	$Cl + CH_3CHO \rightarrow HCl + CH_3C(O)OO$	8.0e-11	Atkinson et al. (2006)
G6500	StGClF	$CF_2Cl_2 + O(^1D) \rightarrow$ LCARBON + 2 LFLUORINE + ClO + Cl	1.4E-10	Burkholder et al. (2015)
G6501	StGClF	$CFCl_3 + O(^1D) \rightarrow$ LCARBON + LFLUORINE + ClO + 2 Cl	2.3E-10	Burkholder et al. (2015)
G7100	StTrGBr	$Br + O_3 \rightarrow BrO + O_2$	1.7E-11*EXP(-800./temp)	Atkinson et al. (2007)
G7101	StGBr	$BrO + O(^3P) \rightarrow Br + O_2$	1.9E-11*EXP(230./temp)	Atkinson et al. (2007)
G7102a	StTrGBr	$BrO + BrO \rightarrow 2\ Br + O_2$	2.7E-12	Atkinson et al. (2007)
G7102b	StTrGBr	$BrO + BrO \rightarrow Br_2 + O_2$	2.9E-14*EXP(840./temp)	Atkinson et al. (2007)
G7200	StTrGBr	$Br + HO_2 \rightarrow HBr + O_2$	7.7E-12*EXP(-450./temp)	Atkinson et al. (2007)
G7201	StTrGBr	$BrO + HO_2 \rightarrow HOBr + O_2$	4.5E-12*EXP(500./temp)	Atkinson et al. (2007)
G7202	StTrGBr	$HBr + OH \rightarrow Br + H_2O$	6.7E-12*EXP(155./temp)	Atkinson et al. (2007)
G7203	StGBr	$HOBr + O(^3P) \rightarrow OH + BrO$	1.2E-10*EXP(-430./temp)	Atkinson et al. (2007)
G7204	StTrGBr	$Br_2 + OH \rightarrow HOBr + Br$	2.0E-11*EXP(240./temp)	Atkinson et al. (2007)
G7300	TrGBrN	$Br + BrNO_3 \rightarrow Br_2 + NO_3$	4.9E-11	Orlando and Tyndall (1996)
G7301	StTrGBrN	$BrO + NO \rightarrow Br + NO_2$	8.7E-12*EXP(260./temp)	Atkinson et al. (2007)
G7302	StTrGBrN	$BrO + NO_2 \rightarrow BrNO_3$	k_BrO_NO2	Atkinson et al. (2007)*
G7303	TrGBrN	$BrNO_3 \rightarrow BrO + NO_2$	k_BrO_NO2/(5.44E-9*EXP(14192./ temp)*1.E6*R_gas*temp/(atm2Pa*N_ A))	Orlando and Tyndall (1996), Atkinson et al. (2007)*
G7400	StTrGBr	$Br + HCHO \rightarrow HBr + CO + HO_2$	7.7E-12*EXP(-580./temp)	Atkinson et al. (2006)
G7401	TrGBr	$Br + CH_3OOH \rightarrow CH_3O_2 + HBr$	2.6E-12*EXP(-1600./temp)	Kondo and Benson (1984)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G7402a	TrGBr	$BrO + CH_3O_2 \rightarrow HOBr + HCHO$	`f_BrO_CH3O2*5.7E-12`	Aranda et al. (1997)
G7402b	TrGBr	$BrO + CH_3O_2 \rightarrow Br + HCHO + HO_2$	`(1.-f_BrO_CH3O2)*5.7E-12`	Aranda et al. (1997)
G7403	StTrGBr	$CH_3Br + OH \rightarrow LCARBON + H_2O + Br$	`1.42E-12*EXP(-1150./temp)`	Burkholder et al. (2015)
G7404	TrGBrC	$Br + C_2H_4 \rightarrow .6666667\ CH_3CH(O_2)CH_2OH + HBr$	`2.8E-13*EXP(224./temp)/(1.+ 1.13E24*EXP(-3200./temp) /C(ind_O2))`	Atkinson et al. (2006)
G7405	TrGBrC	$Br + CH_3CHO \rightarrow HBr + CH_3C(O)OO$	`1.8e-11*EXP(-460./temp)`	Atkinson et al. (2006)
G7407	TrGBr	$CHBr_3 + OH \rightarrow LCARBON + H_2O + 3\ Br$	`9.0E-13*EXP(-360./temp)`	Burkholder et al. (2015)*
G7408	TrGBr	$CH_2Br_2 + OH \rightarrow LCARBON + H_2O + 2\ Br$	`2.0E-12*EXP(-840./temp)`	Burkholder et al. (2015)*
G7600	TrGBrCl	$Br + BrCl \rightarrow Br_2 + Cl$	`3.32E-15`	Manion et al. (2015)
G7601	TrGBrCl	$Br + Cl_2 \rightarrow BrCl + Cl$	`1.10E-15`	Dolson and Leone (1987)
G7602	TrGBrCl	$Br_2 + Cl \rightarrow BrCl + Br$	`2.3E-10*EXP(135./temp)`	Bedjanian et al. (1998)
G7603a	StTrGBrCl	$BrO + ClO \rightarrow Br + OClO$	`1.6E-12*EXP(430./temp)`	Atkinson et al. (2007)
G7603b	StTrGBrCl	$BrO + ClO \rightarrow Br + Cl + O_2$	`2.9E-12*EXP(220./temp)`	Atkinson et al. (2007)
G7603c	StTrGBrCl	$BrO + ClO \rightarrow BrCl + O_2$	`5.8E-13*EXP(170./temp)`	Atkinson et al. (2007)
G7604	TrGBrCl	$BrCl + Cl \rightarrow Br + Cl_2$	`1.45E-11`	Clyne and Cruse (1972)
G7605	TrGBrCl	$CHCl_2Br + OH \rightarrow LCARBON + 2\ Cl + H_2O + Br$	`2.0E-12*EXP(-840./temp)`	see note*
G7606	TrGBrCl	$CHClBr_2 + OH \rightarrow LCARBON + Cl + H_2O + 2\ Br$	`2.0E-12*EXP(-840./temp)`	see note*
G7607	TrGBrCl	$CH_2ClBr + OH \rightarrow LCARBON + Cl + H_2O + Br$	`2.1E-12*EXP(-880./temp)`	Burkholder et al. (2015)*
G9200a	StTrGS	$SO_2 + OH \rightarrow SO_3 + HO_2$	`k_3rd(temp,cair,3.3E-31,4.3, 1.6E-12,0.,0.6)`	Sander et al. (2011)
G9400a	TrGCS	$DMS + OH \rightarrow CH_3SO_2 + HCHO$	`1.13E-11*EXP(-253./temp)`	Atkinson et al. (2004)*
G9400b	TrGCS	$DMS + OH \rightarrow DMSO + HO_2$	`k_DMS_OH`	Atkinson et al. (2004)*
G9401	TrGCNS	$DMS + NO_3 \rightarrow CH_3SO_2 + HNO_3 + HCHO$	`1.9E-13*EXP(520./temp)`	Atkinson et al. (2004)
G9402	TrGCS	$DMSO + OH \rightarrow .6\ SO_2 + HCHO + .6\ CH_3O_2 + .4\ HO_2 + .4\ CH_3SO_3H$	`1.E-10`	Hynes and Wine (1996)
G9403	TrGS	$CH_3SO_2 \rightarrow SO_2 + CH_3O_2$	`1.8E13*EXP(-8661./temp)`	Barone et al. (1995)
G9404	TrGS	$CH_3SO_2 + O_3 \rightarrow CH_3SO_3$	`3.E-13`	Barone et al. (1995)
G9405	TrGS	$CH_3SO_3 + HO_2 \rightarrow CH_3SO_3H$	`5.E-11`	Barone et al. (1995)
G9600	TrGCClS	$DMS + Cl \rightarrow CH_3SO_2 + HCl + HCHO$	`3.3E-10`	Atkinson et al. (2004)
G9700	TrGBrCS	$DMS + Br \rightarrow CH_3SO_2 + HBr + HCHO$	`9.E-11*EXP(-2386./temp)`	Jefferson et al. (1994)
G9701	TrGBrCS	$DMS + BrO \rightarrow DMSO + Br$	`4.4E-13`	Ingham et al. (1999)
G9100	TrStGS	$SO + O_2 \rightarrow SO_2 + O(^3P)$	`1.25e-13*exp(-2190/temp)`	Sander et al. (2011)
G9101	TrStGS	$SO + O_3 \rightarrow SO_2 + O_2$	`3.4e-12*exp(-1100/temp)`	Sander et al. (2011)
G9102	TrStGS	$S + O_2 \rightarrow SO + O(^3P)$	`2.3e-12`	Sander et al. (2011)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G9201	TrStGS	$SH + O_2 \rightarrow OH + SO$	4.e-19	Sander et al. (2011)
G9202	TrStGS	$SO_3 + H_2O \rightarrow H_2SO_4$	8.5e-41*exp(6540./temp)*C(ind_H2O)	Sander et al. (2003)
G9406	TrStGS	$OCS + OH \rightarrow SH + CO_2$	1.1e-13*exp(-1200./temp)	Sander et al. (2011)
G9407	TrStGS	$OCS + O(^3P) \rightarrow CO + SO$	2.1e-11*exp(-2200./temp)	Sander et al. (2011)

General notes

Three-body reactions

Rate coefficients for three-body reactions are defined via the function `k_3rd`(T, M, k_0^{300}, n, k_{inf}^{300}, m, f_c). In the code, the temperature T is called `temp` and the concentration of "air molecules" M is called `cair`. Using the auxiliary variables $k_0(T)$, $k_{\mathrm{inf}}(T)$, and k_{ratio}, `k_3rd` is defined as:

$$k_0(T) = k_0^{300} \times \left(\frac{300\mathrm{K}}{T}\right)^n \tag{1}$$

$$k_{\mathrm{inf}}(T) = k_{\mathrm{inf}}^{300} \times \left(\frac{300\mathrm{K}}{T}\right)^m \tag{2}$$

$$k_{\mathrm{ratio}} = \frac{k_0(T)M}{k_{\mathrm{inf}}(T)} \tag{3}$$

$$\texttt{k\_3rd} = \frac{k_0(T)M}{1+k_{\mathrm{ratio}}} \times f_\mathrm{c}^{\left(\frac{1}{1+(\log_{10}(k_{\mathrm{ratio}}))^2}\right)} \tag{4}$$

A similar function, called `k_3rd_iupac` here, is used by Wallington et al. (2018) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined as:

$$k_0(T) = k_0^{300} \times \left(\frac{300\mathrm{K}}{T}\right)^n \tag{5}$$

$$k_{\mathrm{inf}}(T) = k_{\mathrm{inf}}^{300} \times \left(\frac{300\mathrm{K}}{T}\right)^m \tag{6}$$

$$k_{\mathrm{ratio}} = \frac{k_0(T)M}{k_{\mathrm{inf}}(T)} \tag{7}$$

$$N = 0.75 - 1.27 \times \log_{10}(f_\mathrm{c}) \tag{8}$$

$$\texttt{k\_3rd\_iupac} = \frac{k_0(T)M}{1+k_{\mathrm{ratio}}} \times f_\mathrm{c}^{\left(\frac{1}{1+(\log_{10}(k_{\mathrm{ratio}})/N)^2}\right)} \tag{9}$$

Structure-Activity Relationships (SAR)

Some unmeasured rate coefficients are estimated with structure-activity relationships, using the following parameters and substituent factors:

k for H-abstraction by OH in $\mathrm{cm}^{-3}\mathrm{s}^{-1}$	
`k_p`	$4.49 \times 10^{-18} \times (T/\mathrm{K})^2 \exp(-320\,\mathrm{K}/T)$
`k_s`	$4.50 \times 10^{-18} \times (T/\mathrm{K})^2 \exp(253\,\mathrm{K}/T)$
`k_t`	$2.12 \times 10^{-18} \times (T/\mathrm{K})^2 \exp(696\,\mathrm{K}/T)$
`k_ROHRO`	$2.1 \times 10^{-18} \times (T/\mathrm{K})^2 \exp(-85\,\mathrm{K}/T)$
`k_CO2H`	$0.7 \times k_{\mathrm{CH_3CO_2H+OH}}$
`k_ROOHRO`	$0.6 \times k_{\mathrm{CH_3OOH+OH}}$
`f_alk`	1.23
`f_sOH`	3.44
`f_tOH`	2.68
`f_sOOH`	8.
`f_tOOH`	8.
`f_ONO2`	0.04
`f_CH2ONO2`	0.20
`f_cpan`	0.25
`f_allyl`	3.6
`f_CHO`	0.55
`f_CO2H`	1.67
`f_CO`	0.73
`f_O`	8.15
`f_pCH2OH`	1.29
`f_tCH2OH`	0.53

k for OH-addition to double bonds in $\mathrm{cm}^{-3}\mathrm{s}^{-1}$	
`k_adp`	$4.5 \times 10^{-12} \times (T/300\,\mathrm{K})^{-0.85}$
`k_ads`	$1/4 \times (1.1 \times 10^{-11} \times \exp(485\,\mathrm{K}/T) +$ $1.0 \times 10^{-11} \times \exp(553\,\mathrm{K}/T))$
`k_adt`	$1.922 \times 10^{-11} \times \exp(450\,\mathrm{K}/T) - k_{\mathrm{ads}}$
`k_adsecprim`	3.0×10^{-11}
`k_adtertprim`	5.7×10^{-11}
`a_PAN`	0.56
`a_CHO`	0.31
`a_COCH3`	0.76
`a_CH2OH`	1.7
`a_CH2OOH`	1.7
`a_COH`	2.2
`a_COOH`	2.2
`a_CO2H`	0.25
`a_CH2ONO2`	0.64

RO_2 self and cross reactions

The self and cross reactions of organic peroxy radicals are treated according to the permutation reaction formalism as implemented in the MCM (Rickard and Pascoe, 2009), as decribed by Jenkin et al. (1997). Every organic peroxy radical reacts in a pseudo-first-order reaction with a rate constant that is expressed as $k^{\mathrm{1st}} = 2 \times \sqrt{k_{\mathrm{self}} \times \texttt{k\_CH3O2}} \times [\mathrm{RO_2}]$ where k_{self} = second-order rate coefficient of the self reaction of the organic peroxy radical, `k_CH3O2` = second-order rate coefficient of the self reaction of CH_3O_2, and $[RO_2]$ = sum of the concentrations of all organic peroxy radicals.

Specific notes

`G1002a`: The path leading to 2 $O(^3P) + O_2$ results in a null cycle regarding odd oxygen and is neglected.

`G2110`: The rate coefficient is: `k_HO2_HO2` = `(3.0E-13*EXP(460./temp)+2.1E-33*EXP(920./temp)*cair)*(1.+1.4E-21*EXP(2200./temp)*C(ind_H2O))`.

`G3109`: The rate coefficient is: `k_NO3_NO2` = `k_3rd(temp,cair,2.4E-30,3.0,1.6E-12,-0.1,0.6)`.

`G3110`: The rate coefficient is defined as backward reaction divided by equilibrium constant.

`G3203`: The rate coefficient is: `k_NO2_HO2` = `k_3rd(temp,cair,1.9E-31,3.4,4.0E-12,0.3,0.6)`.

`G3206`: The rate coefficient is: `k_HNO3_OH` = `1.32E-14 * EXP(527/temp) + 1 / ( 1 / (7.39E-32 * EXP(453/temp)*cair) + 1 / (9.73E-17 * EXP(1910/temp)) )`

`G3207`: The rate coefficient is defined as backward reaction divided by equilibrium constant.

`G4103`: Sander et al. (2006) recommend a zero product yield for HCHO.

`G4109`: The same temperature dependence assumed as for $CH_3CHO+NO_3$. At 298 K, $k = 5.8 \times 10^{-16}$.

`G4201`: The product distribution is from Rickard and Pascoe (2009), after substitution of the Criegee intermediate by its decomposition products.

`G4206`: The product C_2H_5OH, which reacts only with OH, is substituted by its degradation products $\approx$ 0.1 $HOCH_2CH_2O_2$ + 0.9 CH_3CHO + 0.9 HO_2.

`G4207`: Same value as for G4107

`G4213`: The rate coefficient is: `k_CH3CO3_NO2` = `k_3rd(temp,cair,9.7E-29,5.6,9.3E-12,1.5,0.6)`.

`G4221`: The rate coefficient is`k_PAN_M` = `k_CH3CO3_NO2/9.E-29*EXP(-14000./temp)`, i.e. the rate coefficient is defined as backward reaction divided by equilibrium constant.

`G4307`: Same value as for G4107

`G4315`: Same value as for G4107

`G4401`: Same value as for G4306

`G4402`: Same value as for G4304

`G4403`: Same value as for G4305

`G4404`: Same value as for G4107

`G4414`: Same value as for G4304

`G4415`: Same value as for G4305

`G4416`: Same value as for G4107

`G4419`: Same value as for G4221

`G6103`: The rate coefficient is defined as backward reaction divided by equilibrium constant.

`G6204`: At low temperatures, there may be a minor reaction channel leading to O_3+HCl. See Finkbeiner et al. (1995) for details. It is neglected here.

`G6402`: The initial products are probably HCl and CH_2OOH (Atkinson et al., 2006). It is assumed that CH_2OOH dissociates into HCHO and OH.

`G6405`: Sander et al. (2006), but simplified shortcut to release all Cl

`G7302`: The rate coefficient is: `k_BrO_NO2` = `k_3rd(temp,cair,5.2E-31,3.2,6.9E-12,2.9,0.6)`.

`G7303`: The rate coefficient is defined as backward reaction (Atkinson et al., 2007) divided by equilibrium constant (Orlando and Tyndall, 1996).

`G7407`: It is assumed that the reaction liberates all Br atoms. The fate of the carbon atom is currently not considered.

`G7408`: It is assumed that the reaction liberates all Br atoms. The fate of the carbon atom is currently not considered.

`G7605`: Same value as for G7408: CH_2Br_2+OH assumed. It is assumed that the reaction liberates all Br and all Cl. The fate of the carbon atom is currently not considered.

`G7606`: Same value as for G7408: CH_2Br_2+OH assumed. It is assumed that the reaction liberates all Br atoms and also Cl. The fate of the carbon atom is currently not considered.

`G7607`: It is assumed that the reaction liberates all Br atoms and also Cl. The fate of the carbon atom is currently not considered.

`G9400a`: For the abstraction path, the assumed reaction sequence (omitting H_2O and O_2 as products) according to Yin et al. (1990) is:

$$\begin{array}{rcl}
\mathrm{DMS} + \mathrm{OH} & \rightarrow & \mathrm{CH_3SCH_2} \\
\mathrm{CH_3SCH_2} + \mathrm{O_2} & \rightarrow & \mathrm{CH_3SCH_2OO} \\
\mathrm{CH_3SCH_2OO} + \mathrm{NO} & \rightarrow & \mathrm{CH_3SCH_2O} + \mathrm{NO_2} \\
\mathrm{CH_3SCH_2O} & \rightarrow & \mathrm{CH_3S} + \mathrm{HCHO} \\
\mathrm{CH_3S} + \mathrm{O_3} & \rightarrow & \mathrm{CH_3SO} \\
\mathrm{CH_3SO} + \mathrm{O_3} & \rightarrow & \mathrm{CH_3SO_2} \\
\hline
\mathrm{DMS} + \mathrm{OH} + \mathrm{NO} + 2\mathrm{O_3} & \rightarrow & \mathrm{CH_3SO_2} + \mathrm{HCHO} + \mathrm{NO_2}
\end{array}$$

Neglecting the effect on O_3 and NO_x, the remaining reaction is:

$$\mathrm{DMS} + \mathrm{OH} + \mathrm{O_3} \rightarrow \mathrm{CH_3SO_2} + \mathrm{HCHO}$$

.

`G9400b`: For the addition path, the rate coefficient is: `k_DMS_OH` = `1.0E-39*EXP(5820./temp)*C(ind_O2) / (1.+5.0E-30*EXP(6280./temp)*C(ind_O2))`.

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J (gas)				
J1000a	UpStTrGJ	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$	`jx(ip_O2)`	Sander et al. (2014)
J1001a	UpStTrGJ	$O_3 + h\nu \rightarrow O(^1D) + O_2$	`jx(ip_O1D)`	Sander et al. (2014)
J1001b	UpStTrGJ	$O_3 + h\nu \rightarrow O(^3P) + O_2$	`jx(ip_O3P)`	Sander et al. (2014)
J2100a	UpStGJ	$H_2O + h\nu \rightarrow H + OH$	`jx(ip_H2O)`	Sander et al. (2014)
J2101	UpStTrGJ	$H_2O_2 + h\nu \rightarrow 2\ OH$	`jx(ip_H2O2)`	Sander et al. (2014)
J3100	UpStGJN	$N_2O + h\nu \rightarrow O(^1D) + N_2$	`jx(ip_N2O)`	Sander et al. (2014)
J3101	UpStTrGJN	$NO_2 + h\nu \rightarrow NO + O(^3P)$	`jx(ip_NO2)`	Sander et al. (2014)
J3102a	UpStGJN	$NO + h\nu \rightarrow N + O(^3P)$	`jx(ip_NO)`	Sander et al. (2014)
J3103a	UpStTrGJN	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	`jx(ip_NO2O)`	Sander et al. (2014)
J3103b	UpStTrGJN	$NO_3 + h\nu \rightarrow NO + O_2$	`jx(ip_NOO2)`	Sander et al. (2014)
J3104	StTrGJN	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	`jx(ip_N2O5)`	Sander et al. (2014)
J3200	TrGJN	$HONO + h\nu \rightarrow NO + OH$	`jx(ip_HONO)`	Sander et al. (2014)
J3201	StTrGJN	$HNO_3 + h\nu \rightarrow NO_2 + OH$	`jx(ip_HNO3)`	Sander et al. (2014)
J3202	StTrGJN	$HNO_4 + h\nu \rightarrow .667\ NO_2 + .667\ HO_2 + .333\ NO_3 + .333\ OH$	`jx(ip_HNO4)`	Sander et al. (2014)
J4100	StTrGJ	$CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$	`jx(ip_CH3OOH)`	Sander et al. (2014)
J4101a	StTrGJ	$HCHO + h\nu \rightarrow H_2 + CO$	`jx(ip_COH2)`	Sander et al. (2014)
J4101b	StTrGJ	$HCHO + h\nu \rightarrow H + CO + HO_2$	`jx(ip_CHOH)`	Sander et al. (2014)
J4102	StGJ	$CO_2 + h\nu \rightarrow CO + O(^3P)$	`jx(ip_CO2)`	Sander et al. (2014)
J4103	StGJ	$CH_4 + h\nu \rightarrow CO + 0.31\ H + 0.69\ H_2 + 1.155\ H_2O$	`jx(ip_CH4)`	Sander et al. (2014)
J4200	TrGJC	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	`jx(ip_CH3OOH)`	von Kuhlmann (2001)
J4201	TrGJC	$CH_3CHO + h\nu \rightarrow CH_3O_2 + HO_2 + CO$	`jx(ip_CH3CHO)`	Sander et al. (2014)
J4202	TrGJC	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH + CO_2$	`jx(ip_CH3CO3H)`	Sander et al. (2014)
J4203	TrGJCN	$NACA + h\nu \rightarrow NO_2 + HCHO + CO$	`0.19*jx(ip_CHOH)`	von Kuhlmann (2001)
J4204	TrGJCN	$PAN + h\nu \rightarrow CH_3C(O)OO + NO_2$	`jx(ip_PAN)`	Sander et al. (2014)
J4300	TrGJC	$iC_3H_7OOH + h\nu \rightarrow CH_3COCH_3 + HO_2 + OH$	`jx(ip_CH3OOH)`	von Kuhlmann (2001)
J4301	TrGJC	$CH_3COCH_3 + h\nu \rightarrow CH_3C(O)OO + CH_3O_2$	`jx(ip_CH3COCH3)`	Sander et al. (2014)
J4302	TrGJC	$CH_3COCH_2OH + h\nu \rightarrow CH_3C(O)OO + HCHO + HO_2$	`0.074*jx(ip_CHOH)`	see note*
J4303	TrGJC	$MGLYOX + h\nu \rightarrow CH_3C(O)OO + CO + HO_2$	`jx(ip_MGLYOX)`	Sander et al. (2014)
J4304	TrGJC	$CH_3COCH_2O_2H + h\nu \rightarrow CH_3C(O)OO + HCHO + OH$	`jx(ip_CH3OOH)`	see note*
J4306	TrGJCN	$iC_3H_7ONO_2 + h\nu \rightarrow CH_3COCH_3 + NO_2 + HO_2$	`3.7*jx(ip_PAN)`	von Kuhlmann et al. (2003)*
J4400	TrGJC	$LC_4H_9OOH + h\nu \rightarrow OH + .67\ MEK + .67\ HO_2 + .33\ C_2H_5O_2 + .33\ CH_3CHO$	`jx(ip_CH3OOH)`	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4401	TrGJC	MVK + hν $\rightarrow$ $CH_3C(O)OO$ + HCHO + CO + HO_2	`0.019*jx(ip_COH2)+.015*jx(ip_MGLYOX)`	Sander et al. (2014)
J4402	TrGJC	MVKOOH + hν $\rightarrow$ OH + .5 MGLYOX + .25 CH_3COCH_2OH + .75 HCHO + .75 HO_2 + .25 $CH_3C(O)OO$ + .25 CO	`jx(ip_CH3OOH)`	see note*
J4403	TrGJC	MEK + hν $\rightarrow$ $CH_3C(O)OO$ + $C_2H_5O_2$	`0.42*jx(ip_CHOH)`	von Kuhlmann et al. (2003)
J4404	TrGJC	LMEKOOH + hν $\rightarrow$ $CH_3C(O)OO$ + CH_3CHO + OH	`jx(ip_CH3OOH)`	Rickard and Pascoe (2009)
J4405	TrGJC	BIACET + hν $\rightarrow$ 2 $CH_3C(O)OO$	`2.15*jx(ip_MGLYOX)`	see note*
J4406	TrGJCN	LC4H9NO3 + hν $\rightarrow$ NO_2 + .67 MEK + .67 HO_2 + .33 $C_2H_5O_2$ + .33 CH_3CHO	`3.7*jx(ip_PAN)`	von Kuhlmann (2001)
J4407	TrGJCN	MPAN + hν $\rightarrow$ CH_3COCH_2OH + NO_2	`jx(ip_PAN)`	see note*
J4500	TrGJC	ISOOH + hν $\rightarrow$ MVK + HCHO + HO_2 + OH	`jx(ip_CH3OOH)`	see note*
J4501	TrGJCN	ISON + hν $\rightarrow$ MVK + HCHO + NO_2 + HO_2	`3.7*jx(ip_PAN)`	von Kuhlmann (2001)
J6000	StTrGJCl	Cl_2 + hν $\rightarrow$ Cl + Cl	`jx(ip_Cl2)`	Sander et al. (2014)
J6100	StTrGJCl	Cl_2O_2 + hν $\rightarrow$ 2 Cl	`jx(ip_Cl2O2)`	Sander et al. (2014)
J6101	StTrGJCl	OClO + hν $\rightarrow$ ClO + O(^{3}P)	`jx(ip_OClO)`	Sander et al. (2014)
J6200	StGJCl	HCl + hν $\rightarrow$ Cl + H	`jx(ip_HCl)`	Sander et al. (2014)
J6201	StTrGJCl	HOCl + hν $\rightarrow$ OH + Cl	`jx(ip_HOCl)`	Sander et al. (2014)
J6300	TrGJClN	$ClNO_2$ + hν $\rightarrow$ Cl + NO_2	`jx(ip_ClNO2)`	Sander et al. (2014)
J6301a	StTrGJClN	$ClNO_3$ + hν $\rightarrow$ Cl + NO_3	`jx(ip_ClNO3)`	Sander et al. (2014)
J6301b	StTrGJClN	$ClNO_3$ + hν $\rightarrow$ ClO + NO_2	`jx(ip_ClONO2)`	Sander et al. (2014)
J6400	StGJCl	CH_3Cl + hν $\rightarrow$ Cl + CH_3O_2	`jx(ip_CH3Cl)`	Sander et al. (2014)
J6401	StGJCl	CCl_4 + hν $\rightarrow$ LCARBON + 4 Cl	`jx(ip_CCl4)`	Sander et al. (2014)
J6402	StGJCCl	CH_3CCl_3 + hν $\rightarrow$ 2 LCARBON + 3 Cl	`jx(ip_CH3CCl3)`	Sander et al. (2014)
J6500	StGJClF	$CFCl_3$ + hν $\rightarrow$ 3 Cl + LCARBON + LFLUORINE	`jx(ip_CFCl3)`	Sander et al. (2014)
J6501	StGJClF	CF_2Cl_2 + hν $\rightarrow$ 2 Cl + LCARBON + 2 LFLUORINE	`jx(ip_CF2Cl2)`	Sander et al. (2014)
J7000	StTrGJBr	Br_2 + hν $\rightarrow$ Br + Br	`jx(ip_Br2)`	Sander et al. (2014)
J7100	StTrGJBr	BrO + hν $\rightarrow$ Br + O(^{3}P)	`jx(ip_BrO)`	Sander et al. (2014)
J7200	StTrGJBr	HOBr + hν $\rightarrow$ Br + OH	`jx(ip_HOBr)`	Sander et al. (2014)
J7300	TrGJBrN	$BrNO_2$ + hν $\rightarrow$ Br + NO_2	`jx(ip_BrNO2)`	Sander et al. (2014)
J7301	StTrGJBrN	$BrNO_3$ + hν $\rightarrow$ .85 Br + .85 NO_3 + .15 BrO + .15 NO_2	`jx(ip_BrNO3)`	Sander et al. (2014)*
J7400	StGJBr	CH_3Br + hν $\rightarrow$ Br + CH_3O_2	`jx(ip_CH3Br)`	Sander et al. (2014)
J7401	TrGJBr	CH_2Br_2 + hν $\rightarrow$ LCARBON + 2 Br	`jx(ip_CH2Br2)`	Sander et al. (2014)
J7402	TrGJBr	$CHBr_3$ + hν $\rightarrow$ LCARBON + 3 Br	`jx(ip_CHBr3)`	Sander et al. (2014)
J7500	StGJBrF	CF_3Br + hν $\rightarrow$ LCARBON + 3 LFLUORINE + Br	`jx(ip_CF3Br)`	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J7600	StTrGJBrCl	$BrCl + h\nu \rightarrow Br + Cl$	`jx(ip_BrCl)`	Sander et al. (2014)
J7601	StGJBrClF	$CF_2ClBr + h\nu \rightarrow LCARBON + 2\ LFLUORINE + Br + Cl$	`jx(ip_CF2ClBr)`	Sander et al. (2014)
J7602	TrGJBrCl	$CH_2ClBr + h\nu \rightarrow LCARBON + Br + Cl$	`jx(ip_CH2ClBr)`	Sander et al. (2014)
J7603	TrGJBrCl	$CHCl_2Br + h\nu \rightarrow LCARBON + Br + 2\ Cl$	`jx(ip_CHCl2Br)`	Sander et al. (2014)
J7604	TrGJBrCl	$CHClBr_2 + h\nu \rightarrow LCARBON + 2\ Br + Cl$	`jx(ip_CHClBr2)`	Sander et al. (2014)
J8401a	StTrGJI	$CH_3I + h\nu \rightarrow CH_3O_2$	`JX(ip_CH3I)`	Sander et al. (2014)
J9000	TrStGJS	$OCS + h\nu \rightarrow CO + S$	`JX(ip_OCS)`	[redacted]
J9001	TrStGJS	$SO_2 + h\nu \rightarrow SO + O(^3P)$	`60.*JX(ip_OCS)`	[redacted]
J9002	TrStGJS	$SO_3 + h\nu \rightarrow SO_2 + O(^3P)$	`JX(ip_SO3)`	[redacted]
J9003	TrStGJS	$H_2SO_4 + h\nu \rightarrow SO_3 + H_2O$	`JX(ip_H2SO4)`	[redacted]
PH (aqueous)				

General notes

j-values are calculated with an external module (e.g., JVAL) and then supplied to the MECCA chemistry.

Values that originate from the Master Chemical Mechanism (MCM) by Rickard and Pascoe (2009) are translated according in the following way:
j(11) → `jx(ip_COH2)`
j(12) → `jx(ip_CHOH)`
j(15) → `jx(ip_HOCH2CHO)`
j(18) → `jx(ip_MACR)`
j(22) → `jx(ip_ACETOL)`
j(23)+j(24) → `jx(ip_MVK)`
j(31)+j(32)+j(33) → `jx(ip_GLYOX)`
j(34) → `jx(ip_MGLYOX)`
j(41) → `jx(ip_CH3OOH)`
j(53) → j(isopropyl nitrate)
j(54) → j(isopropyl nitrate)
j(55) → j(isopropyl nitrate)
j(56)+j(57) → `jx(ip_NOA)`

Specific notes

J4302: It is assumed that J(CH_3COCH_2OH) is 0.074 times that of J4101b.

J4304: It is assumed that J($CH_3COCH_2O_2H$) is the same as J(CH_3OOH).

J4306: Following von Kuhlmann et al. (2003), we use J($iC_3H_7ONO_2$) = `3.7*jx(ip_PAN)`.

J4402: It is assumed that J(MVKOOH) is the same as J(CH_3OOH).

J4405: It is assumed that J(BIACET) is 2.15 times larger than J(MGLYOX), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J4407: It is assumed that J(MPAN) is the same as J(PAN).

J4500: It is assumed that J(ISOOH) is the same as J(CH_3OOH).

J7301: The quantum yields are recommended by Burkholder et al. (2015) for $\lambda > 300$nm and used here for the entire spectrum.

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

#	labels	reaction	rate coefficient	reference

General notes

The forward (`k_exf`) and backward (`k_exb`) rate coefficients are calculated in subroutine `mecca_aero_calc_k_ex` in the file `messy_mecca_aero.f90` using accommodation coefficients and Henry's law constants from chemprop (see `chemprop.pdf`).

For uptake of X (X = N_2O_5, $ClNO_3$, or $BrNO_3$) and subsequent reaction with H_2O, Cl^-, and Br^- in H3201, H6300, H6301, H6302, H7300, H7301, H7302, H7601, and H7602, we define:

$$k_{\mathrm{exf}}(\mathrm{X}) = \frac{k_{\mathrm{mt}}(\mathrm{X}) \times \mathrm{LWC}}{[\mathrm{H_2O}] + 5 \times 10^2[\mathrm{Cl^-}] + 3 \times 10^5[\mathrm{Br^-}]}$$

Here, k_{mt} = mass transfer coefficient, and LWC = liquid water content of the aerosol. The total uptake rate of X is only determined by k_{mt}. The factors only affect the branching between hydrolysis and the halide reactions. The factor 5×10^2 was chosen such that the chloride reaction dominates over hydrolysis at about $[Cl^-]$ > 0.1 M (see Fig. 3 in Behnke et al. (1997)), i.e. when the ratio $[H_2O]/[Cl^-]$ is less than 5×10^2. The ratio $5\times10^2/3\times10^5$ was chosen such that the reactions with chloride and bromide are roughly equal for sea water composition (Behnke et al., 1994). These ratios were measured for uptake of N_2O_5. Here, they are also used for $ClNO_3$ and $BrNO_3$.

Table 4: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
HET200	StHetN	$N_2O_5 + H_2O \rightarrow 2\ HNO_3$	`khet_St(ihs_N2O5_H2O)`	see general notes*
HET201	TrHetN	$N_2O_5 \rightarrow 2\ NO_3^-(cs) + 2\ H^+(cs)$	`khet_Tr(iht_N2O5)`	see general notes*
HET410	StHetCl	$HOCl + HCl \rightarrow Cl_2 + H_2O$	`khet_St(ihs_HOCl_HCl)`	see general notes*
HET420	StHetClN	$ClNO_3 + HCl \rightarrow Cl_2 + HNO_3$	`khet_St(ihs_ClNO3_HCl)`	see general notes*
HET421	StHetClN	$ClNO_3 + H_2O \rightarrow HOCl + HNO_3$	`khet_St(ihs_ClNO3_H2O)`	see general notes*
HET422	StHetClN	$N_2O_5 + HCl \rightarrow ClNO_2 + HNO_3$	`khet_St(ihs_N2O5_HCl)`	see general notes*
HET510	StHetBr	$HOBr + HBr \rightarrow Br_2 + H_2O$	`khet_St(ihs_HOBr_HBr)`	see general notes*
HET520	StHetBrN	$BrNO_3 + H_2O \rightarrow HOBr + HNO_3$	`khet_St(ihs_BrNO3_H2O)`	see general notes*
HET540	StHetBrClN	$ClNO_3 + HBr \rightarrow BrCl + HNO_3$	`khet_St(ihs_ClNO3_HBr)`	see general notes*
HET541	StHetBrClN	$BrNO_3 + HCl \rightarrow BrCl + HNO_3$	`khet_St(ihs_BrNO3_HCl)`	see general notes*
HET542	StHetBrCl	$HOCl + HBr \rightarrow BrCl + H_2O$	`khet_St(ihs_HOCl_HBr)`	see general notes*
HET543	StHetBrCl	$HOBr + HCl \rightarrow BrCl + H_2O$	`khet_St(ihs_HOBr_HCl)`	see general notes*

General notes

Heterogeneous reaction rates are calculated with an external module (e.g., MECCA_KHET) and then supplied to the MECCA chemistry (see `www.messy-interface.org` for details)

Table 5: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	-$\Delta H/R[K]$	reference

Specific notes

Table 6: Aqueous phase reactions

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference

Specific notes

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