Figure S1a. Sampling gear deployed above the navigation bridge on the ship.

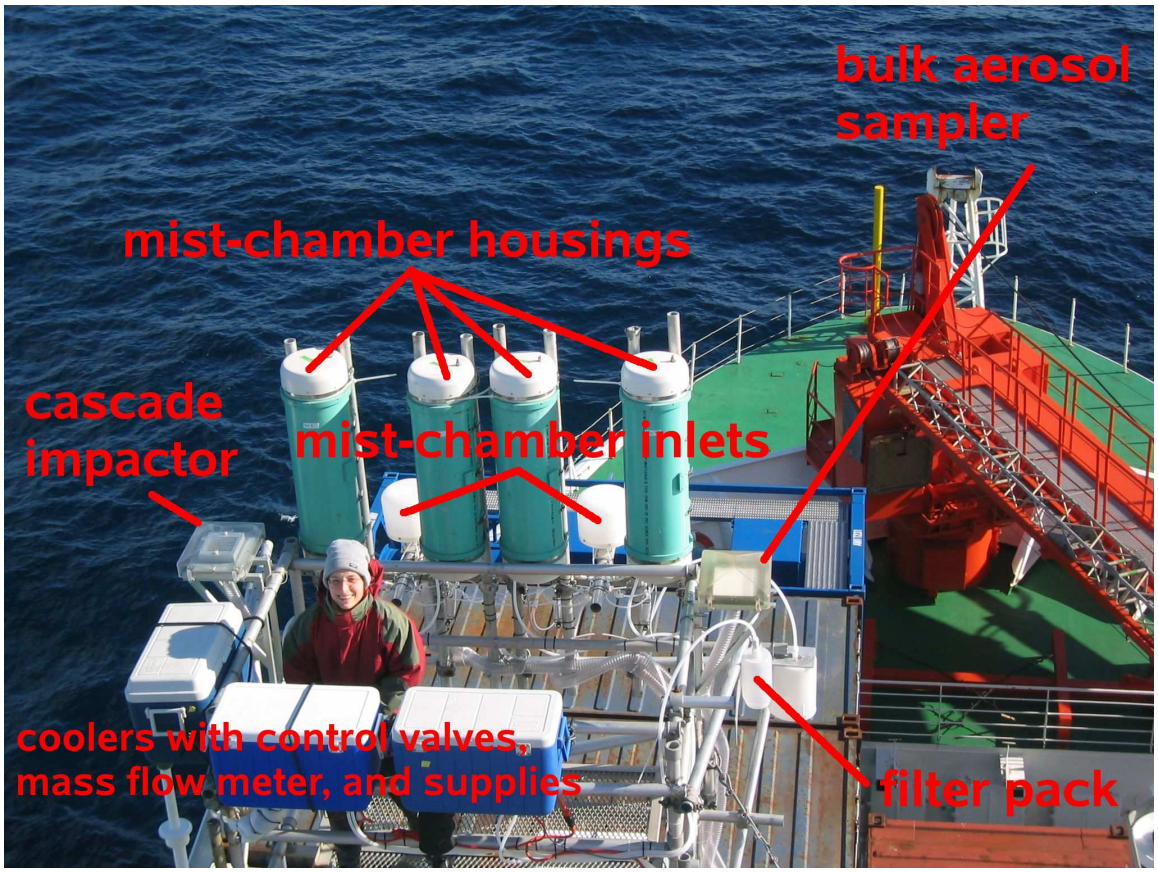

Figure S1b. Arrangement of sampling gear installed on the aluminum scaffold.

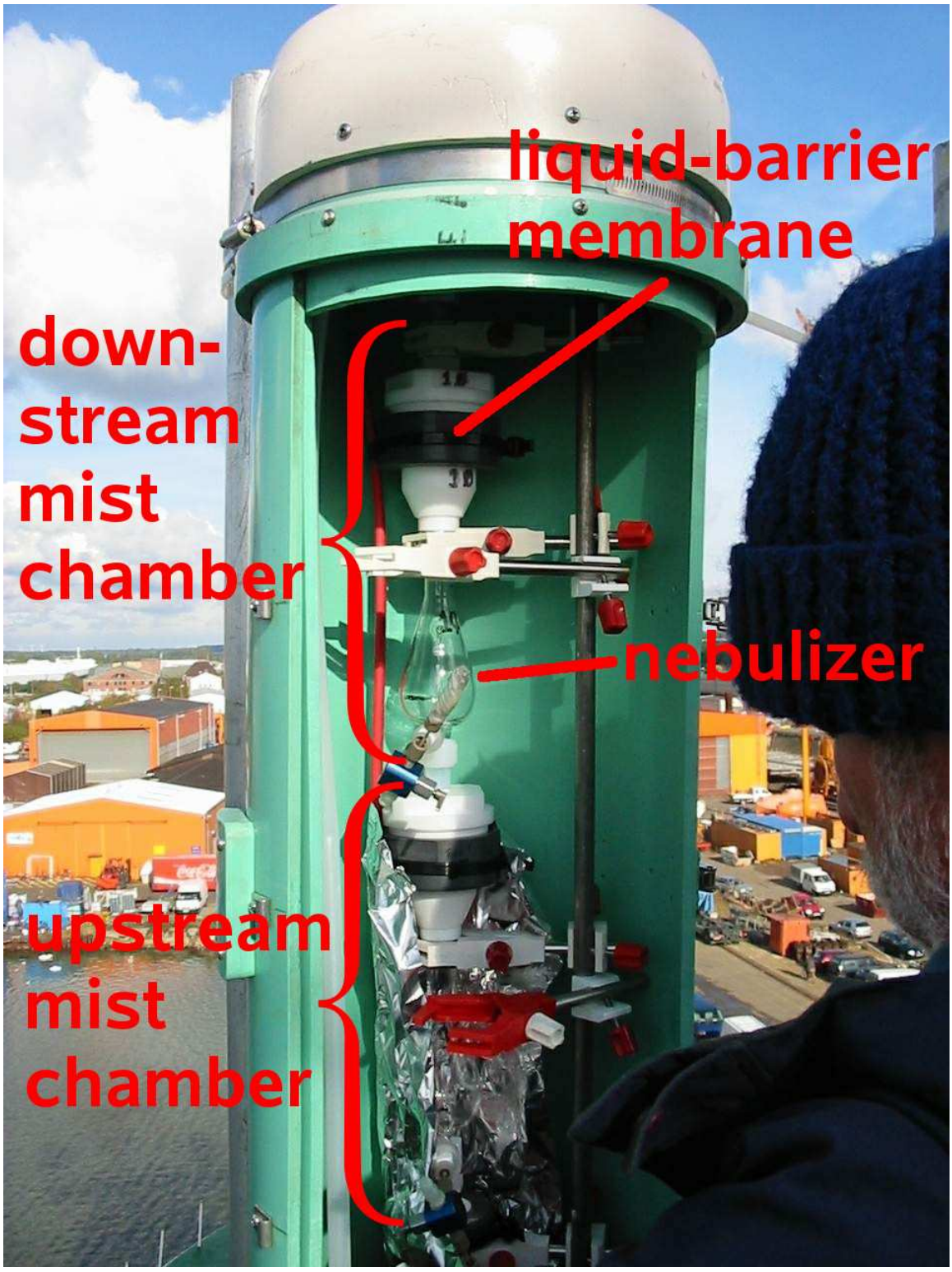

Figure S1c. Tandem mist chamber samplers mounted within housing.

The Chemical Mechanism of MECCA

KPP version: `2.2.1_rs3`

MECCA version: `2.5d`

Date: August 21, 2009.

Selected reactions:
"`Tr && (G || Aa) && !C && !I && ! Hg`"

Number of aerosol phases: 1

Number of species in selected mechanism:

Gas phase:	57
Aqueous phase:	62
All species:	119

Number of reactions in selected mechanism:

Gas phase (Gnnn):	93
Aqueous phase (Annn):	115
Henry (Hnnn):	61
Photolysis (Jnnn):	32
Heterogeneous (HETnnn):	0
Equilibria (EQnn):	44
Dummy (Dnn):	1
All equations:	346

The following describes the full chemical mechanism and relevant parameters as used for the simulations reported in this publication. Reactions labeled with "a01" correspond to a specific aerosol size bin. Since the reaction mechanisms were identical for each size bin, the chemical mechanism for only one of the eight bins is described here. Further information can be found in the article "Technical Note: The new comprehensive atmospheric chemistry module MECCA" by R. Sander et al. (Atmos. Chem. Phys. **5**, 445-450, 2005), available at `http://www.atmos-chem-phys.net/5/445`.

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	StTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	3.3E-11*EXP(55./temp)	Sander et al. (2006)
G1001	StTrG	$O_2 + O(^3P) \rightarrow O_3$	6.E-34*((temp/300.)**(-2.4))*cair	Sander et al. (2006)
G2100	StTrG	$H + O_2 \rightarrow HO_2$	k_3rd(temp,cair,4.4E-32,1.3, 4.7E-11,0.2,0.6)	Sander et al. (2006)
G2104	StTrG	$OH + O_3 \rightarrow HO_2 + O_2$	1.7E-12*EXP(-940./temp)	Sander et al. (2006)
G2105	StTrG	$OH + H_2 \rightarrow H_2O + H$	2.8E-12*EXP(-1800./temp)	Sander et al. (2006)
G2107	StTrG	$HO_2 + O_3 \rightarrow OH + 2\ O_2$	1.E-14*EXP(-490./temp)	Sander et al. (2006)
G2109	StTrG	$HO_2 + OH \rightarrow H_2O + O_2$	4.8E-11*EXP(250./temp)	Sander et al. (2006)
G2110	StTrG	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	k_HO2_HO2	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	StTrG	$H_2O + O(^1D) \rightarrow 2\ OH$	1.63E-10*EXP(60./temp)	Sander et al. (2006)
G2112	StTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	1.8E-12	Sander et al. (2006)
G3101	StTrG	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	2.15E-11*EXP(110./temp)	Sander et al. (2006)
G3103	StTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	3.E-12*EXP(-1500./temp)	Sander et al. (2006)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	1.2E-13*EXP(-2450./temp)	Sander et al. (2006)
G3108	StTrGN	$NO_3 + NO \rightarrow 2\ NO_2$	1.5E-11*EXP(170./temp)	Sander et al. (2006)
G3109	StTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	k_NO3_NO2	Sander et al. (2006)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	k_NO3_NO2/(2.7E-27*EXP(11000./ temp))	Sander et al. (2006)*
G3200	TrG	$NO + OH \rightarrow HONO$	k_3rd(temp,cair,7.0E-31,2.6, 3.6E-11,0.1,0.6)	Sander et al. (2006)
G3201	StTrGN	$NO + HO_2 \rightarrow NO_2 + OH$	3.5E-12*EXP(250./temp)	Sander et al. (2006)
G3202	StTrGN	$NO_2 + OH \rightarrow HNO_3$	k_3rd(temp,cair,1.8E-30,3.0, 2.8E-11,0.,0.6)	Sander et al. (2006)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	k_NO2_HO2	Sander et al. (2006)*
G3204	TrGN	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	3.5E-12	Sander et al. (2006)
G3205	TrG	$HONO + OH \rightarrow NO_2 + H_2O$	1.8E-11*EXP(-390./temp)	Sander et al. (2006)
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3$	k_HNO3_OH	Sander et al. (2006)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	k_NO2_HO2/(2.1E-27*EXP(10900./ temp))	Sander et al. (2006)*

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

#	labels	reaction	rate coefficient	reference
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	1.3E-12*EXP(380./temp)	Sander et al. (2006)
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. (2006)
G4103	StTrG	$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$	4.1E-13*EXP(750./temp)	Sander et al. (2006)*
G4104	StTrGN	$CH_3O_2 + NO \rightarrow HCHO + NO_2 + HO_2$	2.8E-12*EXP(300./temp)	Sander et al. (2006)
G4105	TrGN	$CH_3O_2 + NO_3 \rightarrow HCHO + HO_2 + NO_2$	1.3E-12	Atkinson et al. (1999)
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. (2006)
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. (2006)
G4107	StTrG	$CH_3OOH + OH \rightarrow .7\ CH_3O_2 + .3\ HCHO + .3\ OH + H_2O$	k_CH3OOH_OH	Sander et al. (2006)*
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. (2006)*
G4110	StTrG	$CO + OH \rightarrow H + CO_2$	1.57E-13 + cair*3.54E-33	McCabe et al. (2001)
G4111	TrG	$HCOOH + OH \rightarrow HO_2$	4.0E-13	Sander et al. (2006)
G6100	StTrGCl	$Cl + O_3 \rightarrow ClO + O_2$	2.8E-11*EXP(-250./temp)	Atkinson et al. (2007)
G6102a	StTrGCl	$ClO + ClO \rightarrow Cl_2 + O_2$	1.0E-12*EXP(-1590./temp)	Atkinson et al. (2007)
G6102b	StTrGCl	$ClO + ClO \rightarrow 2\ Cl + O_2$	3.0E-11*EXP(-2450./temp)	Atkinson et al. (2007)
G6102c	StTrGCl	$ClO + ClO \rightarrow Cl + OClO$	3.5E-13*EXP(-1370./temp)	Atkinson et al. (2007)
G6102d	StTrGCl	$ClO + ClO \rightarrow Cl_2O_2$	k_ClO_ClO	Atkinson et al. (2007)
G6103	StTrGCl	$Cl_2O_2 \rightarrow ClO + ClO$	k_ClO_ClO/(9.3E-28*EXP(8835./ temp))	Atkinson et al. (2007), Sander et al. (2006)*
G6202	StTrGCl	$Cl + H_2O_2 \rightarrow HCl + HO_2$	1.1E-11*EXP(-980./temp)	Atkinson et al. (2007)
G6204	StTrGCl	$ClO + HO_2 \rightarrow HOCl$	2.2E-12*EXP(340./temp)	Atkinson et al. (2007)
G6205	StTrGCl	$HCl + OH \rightarrow Cl + H_2O$	1.7E-12*EXP(-230./temp)	Atkinson et al. (2007)
G6300	StTrGNCl	$ClO + NO \rightarrow NO_2 + Cl$	6.2E-12*EXP(295./temp)	Atkinson et al. (2007)

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

#	labels	reaction	rate coefficient	reference
G6301	StTrGNCl	$ClO + NO_2 \rightarrow ClNO_3$	k_3rd_iupac(temp,cair,1.6E-31, 3.4,7.E-11,0.,0.4)	Atkinson et al. (2007)
G6302	TrGCl	$ClNO_3 \rightarrow ClO + NO_2$	6.918E-7*exp(-10909./temp)*cair	Anderson and Fahey (1990)
G6304	StTrGNCl	$ClNO_3 + Cl \rightarrow Cl_2 + NO_3$	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	$ClO + CH_3O_2 \rightarrow HO_2 + Cl + HCHO$	3.3E-12*EXP(-115./temp)	Sander et al. (2006)
G7100	StTrGBr	$Br + O_3 \rightarrow BrO + O_2$	1.7E-11*EXP(-800./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)
G7204	StTrGBr	$Br_2 + OH \rightarrow HOBr + Br$	2.0E-11*EXP(240./temp)	Atkinson et al. (2007)
G7300	TrGBr	$Br + BrNO_3 \rightarrow Br_2 + NO_3$	4.9E-11	Orlando and Tyndall (1996)
G7301	StTrGNBr	$BrO + NO \rightarrow Br + NO_2$	8.7E-12*EXP(260./temp)	Atkinson et al. (2007)
G7302	StTrGNBr	$BrO + NO_2 \rightarrow BrNO_3$	k_BrO_NO2	Atkinson et al. (2007)*
G7303	TrGBr	$BrNO_3 \rightarrow BrO + NO_2$	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	$Br + CH_3OOH \rightarrow CH_3O_2 + HBr$	2.66E-12*EXP(-1610./temp)	Mallard et al. (1993)
G7402a	TrGBr	$BrO + CH_3O_2 \rightarrow HOBr + HCHO$	0.8/1.1*5.7E-12	Aranda et al. (1997)
G7402b	TrGBr	$BrO + CH_3O_2 \rightarrow Br + HCHO + HO_2$	0.3/1.1*5.7E-12	Aranda et al. (1997)
G7403	StTrGBr	$CH_3Br + OH \rightarrow H_2O + Br$	2.35E-12*EXP(-1300./temp)	Sander et al. (2006)
G7407	TrGBr	$CHBr_3 + OH \rightarrow H_2O + 3\ Br$	1.35E-12*EXP(-600./temp)	Sander et al. (2006)*
G7408	TrGBr	$CH_2Br_2 + OH \rightarrow H_2O + 2\ Br$	2.0E-12*EXP(-840./temp)	Sander et al. (2006)*
G7600	TrGBrCl	$Br + BrCl \rightarrow Br_2 + Cl$	3.3E-15	Mallard et al. (1993)
G7601	TrGClBr	$Br + Cl_2 \rightarrow BrCl + Cl$	1.1E-15	Mallard et al. (1993)

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

#	labels	reaction	rate coefficient	reference
G7602	TrGClBr	$Br_2 + Cl \rightarrow BrCl + Br$	1.2E-10	Mallard et al. (1993)
G7603a	StTrGClBr	$BrO + ClO \rightarrow Br + OClO$	1.6E-12*EXP(430./temp)	Atkinson et al. (2007)
G7603b	StTrGClBr	$BrO + ClO \rightarrow Br + Cl + O_2$	2.9E-12*EXP(220./temp)	Atkinson et al. (2007)
G7603c	StTrGClBr	$BrO + ClO \rightarrow BrCl + O_2$	5.8E-13*EXP(170./temp)	Atkinson et al. (2007)
G7604	TrGClBr	$BrCl + Cl \rightarrow Br + Cl_2$	1.5E-11	Mallard et al. (1993)
G7605	TrGBr	$CHCl_2Br + OH \rightarrow H_2O + Br$	2.0E-12*EXP(-840./temp)	see note
G7606	TrGBr	$CHClBr_2 + OH \rightarrow H_2O + 2\ Br$	2.0E-12*EXP(-840./temp)	see note
G7607	TrGBr	$CH_2ClBr + OH \rightarrow H_2O + Br$	2.4E-12*EXP(-920./temp)	Sander et al. (2006)*
G9200	StTrGS	$SO_2 + OH \rightarrow H_2SO_4 + HO_2$	k_3rd(temp,cair,3.3E-31,4.3, 1.6E-12,0.,0.6)	Sander et al. (2006)
G9400a	TrGS	$DMS + OH \rightarrow CH_3SO_2 + HCHO$	1.13E-11*EXP(-253./temp)	Atkinson et al. (2004)*
G9400b	TrGS	$DMS + OH \rightarrow DMSO + HO_2$	k_DMS_OH	Atkinson et al. (2004)*
G9401	TrGNS	$DMS + NO_3 \rightarrow CH_3SO_2 + HNO_3 + HCHO$	1.9E-13*EXP(520./temp)	Atkinson et al. (2004)
G9402	TrGS	$DMSO + OH \rightarrow .6\ SO_2 + HCHO + .6\ CH_3O_2 + .4\ HO_2 + .4\ CH_3SO_3H$	1.E-10	Hynes and Wine (1996)
G9403	TrGS	$CH_3SO_2 \rightarrow SO_2 + CH_3O_2$	1.9E13*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	TrGSCl	$DMS + Cl \rightarrow CH_3SO_2 + HCl + HCHO$	3.3E-10	Atkinson et al. (2004)
G9700	TrGSBr	$DMS + Br \rightarrow CH_3SO_2 + HBr + HCHO$	9.E-11*EXP(-2386./temp)	Jefferson et al. (1994)
G9701	TrGSBr	$DMS + BrO \rightarrow DMSO + Br$	2.54E-14*EXP(850./temp)	Ingham et al. (1999)

*Notes:

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

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

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

$$k_{\rm ratio} = \frac{k_0(T)M}{k_{\rm inf}(T)} \quad (3)$$

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

A similar function, called `k_3rd_iupac` here, is used by Atkinson et al. (2005) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined as:

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

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

$$k_{\rm ratio} = \frac{k_0(T)M}{k_{\rm inf}(T)} \quad (7)$$

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

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

G2110: The rate coefficient is: `k_HO2_HO2 = (1.5E-12*EXP(19./temp)+1.7E-33*EXP(1000./temp)*cair)* (1.+1.4E-21*EXP(2200./temp)*C(ind_H2O))`. The value for the first (pressure-independent) part is from Christensen et al. (2002), the water term from Kircher and Sander (1984).

G3109: The rate coefficient is: `k_NO3_NO2 = k_3rd(temp,cair,2.E-30,4.4,1.4E-12,0.7,0.6)`.

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,1.8E-31,3.2,4.7E-12,1.4,0.6)`.

G3206: The rate coefficient is: `k_HNO3_OH = 2.4E-14 * EXP(460./temp) + 1./ ( 1./(6.5E-34 * EXP(1335./temp)*cair) + 1./(2.7E-17 * EXP(2199./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.

G4107: The rate coefficient is: `k_CH3OOH_OH = 3.8E-12*EXP(200./temp)`.

G4109: The same temperature dependence assumed as for $CH_3CHO+NO_3$.

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

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.

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 atoms but not 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 but not Cl. The fate of the carbon atom is currently not considered.

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

G9400: 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
J1000	StTrGJ	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$	jx(ip_O2)	see note
J1001a	StTrGJ	$O_3 + h\nu \rightarrow O(^1D)$	jx(ip_O1D)	see note
J1001b	StTrGJ	$O_3 + h\nu \rightarrow O(^3P)$	jx(ip_O3P)	see note
J2101	StTrGJ	$H_2O_2 + h\nu \rightarrow 2\ OH$	jx(ip_H2O2)	see note
J3101	StTrGNJ	$NO_2 + h\nu \rightarrow NO + O(^3P)$	jx(ip_NO2)	see note
J3103a	StTrGNJ	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	jx(ip_NO2O)	see note
J3103b	StTrGNJ	$NO_3 + h\nu \rightarrow NO$	jx(ip_NOO2)	see note
J3104a	StTrGNJ	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	jx(ip_N2O5)	see note
J3200	TrGJ	$HONO + h\nu \rightarrow NO + OH$	jx(ip_HONO)	see note
J3201	StTrGNJ	$HNO_3 + h\nu \rightarrow NO_2 + OH$	jx(ip_HNO3)	see note
J3202	StTrGNJ	$HNO_4 + h\nu \rightarrow .667\ NO_2 + .667\ HO_2 + .333\ NO_3 + .333\ OH$	jx(ip_HNO4)	see note
J4100	StTrGJ	$CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$	jx(ip_CH3OOH)	see note
J4101a	StTrGJ	$HCHO + h\nu \rightarrow H_2 + CO$	jx(ip_COH2)	see note
J4101b	StTrGJ	$HCHO + h\nu \rightarrow H + CO + HO_2$	jx(ip_CHOH)	see note
J6000	StTrGClJ	$Cl_2 + h\nu \rightarrow Cl + Cl$	jx(ip_Cl2)	see note
J6100	StTrGClJ	$Cl_2O_2 + h\nu \rightarrow 2\ Cl$	1.4*jx(ip_Cl2O2)	see note
J6101	StTrGClJ	$OClO + h\nu \rightarrow ClO + O(^3P)$	jx(ip_OClO)	see note
J6201	StTrGClJ	$HOCl + h\nu \rightarrow OH + Cl$	jx(ip_HOCl)	see note
J6300	TrGNClJ	$ClNO_2 + h\nu \rightarrow Cl + NO_2$	jx(ip_ClNO2)	see note
J6301a	StTrGNClJ	$ClNO_3 + h\nu \rightarrow Cl + NO_3$	jx(ip_ClNO3)	see note
J6301b	StTrGNClJ	$ClNO_3 + h\nu \rightarrow ClO + NO_2$	jx(ip_ClONO2)	see note
J7000	StTrGBrJ	$Br_2 + h\nu \rightarrow Br + Br$	jx(ip_Br2)	see note
J7100	TrGBrJ	$BrO + h\nu \rightarrow Br + O(^3P)$	jx(ip_BrO)	see note
J7200	StTrGBrJ	$HOBr + h\nu \rightarrow Br + OH$	jx(ip_HOBr)	see note
J7300	TrGNBrJ	$BrNO_2 + h\nu \rightarrow Br + NO_2$	jx(ip_BrNO2)	see note
J7301	StTrGNBrJ	$BrNO_3 + h\nu \rightarrow 0.29\ Br + 0.29\ NO_3 + 0.71\ BrO + 0.71\ NO_2$	jx(ip_BrNO3)	see note
J7401	TrGBrJ	$CH_2Br_2 + h\nu \rightarrow 2\ Br$	jx(ip_CH2Br2)	see note
J7402	TrGBrJ	$CHBr_3 + h\nu \rightarrow 3\ Br$	jx(ip_CHBr3)	see note
J7600	StTrGClBrJ	$BrCl + h\nu \rightarrow Br + Cl$	jx(ip_BrCl)	see note
J7602	TrGClBrJ	$CH_2ClBr + h\nu \rightarrow Br + Cl$	jx(ip_CH2ClBr)	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J7603	TrGClBrJ	$CHCl_2Br + h\nu \rightarrow Br + 2\ Cl$	jx(ip_CHCl2Br)	see note
J7604	TrGClBrJ	$CHClBr_2 + h\nu \rightarrow 2\ Br + Cl$	jx(ip_CHClBr2)	see note

*Notes:

J-values are calculated with an external module and then supplied to the MECCA chemistry

J6100: Stimpfle et al. (2004) claim that the combination of absorption cross sections from Burkholder et al. (1990) and the Cl_2O_2 formation rate coefficient by Sander et al. (2003) can approximately reproduce the observed Cl_2O_2/ClO ratios and ozone depletion. They give an almost zenith-angle independent ratio of 1.4 for Burkholder et al. (1990) to Sander et al. (2003) J-values. The IUPAC recommendation for the Cl_2O_2 formation rate is about 5 to 15 % less than the value by Sander et al. (2003) but more than 20 % larger than the value by Sander et al. (2000). The J-values by Burkholder et al. (1990) are within the uncertainty range of the IUPAC recommendation.

J7301: The quantum yields are from Sander et al. (2003).

Table 3: Henry's law coefficients

substance	$\frac{k_{\mathrm{H}}^{\ominus}}{\mathrm{M/atm}}$	$\frac{-\Delta_{\mathrm{soln}}H/R}{\mathrm{K}}$	reference
O_2	1.3×10^{-3}	1500.	Wilhelm et al. (1977)
O_3	1.2×10^{-2}	2560.	Chameides (1984)
OH	3.0×10^{1}	4300.	Hanson et al. (1992)
HO_2	3.9×10^{3}	5900.	Hanson et al. (1992)
H_2O_2	$1.\times10^{5}$	6338.	Lind and Kok (1994)
NH_3	58.	4085.	Chameides (1984)
NO	1.9×10^{-3}	1480.	Schwartz and White (1981)
NO_2	7.0×10^{-3}	2500.	Lee and Schwartz (1981)*
NO_3	2.	2000.	Thomas et al. (1993)
HONO	4.9×10^{1}	4780.	Schwartz and White (1981)
HNO_3	$2.45\times10^{6}/1.5\times10^{1}$	8694.	Brimblecombe and Clegg (1989)*
HNO_4	1.2×10^{4}	6900.	Régimbal and Mozurkewich (1997)
CH_3O_2	6.	5600.	Jacob (1986)*
CH_3OOH	3.0×10^{2}	5322.	Lind and Kok (1994)
HCHO	7.0×10^{3}	6425.	Chameides (1984)
HCOOH	3.7×10^{3}	5700.	Chameides (1984)
CO_2	3.1×10^{-2}	2423.	Chameides (1984)
Cl_2	9.2×10^{-2}	2081.	Bartlett and Margerum (1999)
HCl	2./1.7	9001.	Brimblecombe and Clegg (1989)
HOCl	6.7×10^{2}	5862.	Huthwelker et al. (1995)
Br_2	7.7×10^{-1}	3837.	Bartlett and Margerum (1999)
HBr	1.3	10239.	Brimblecombe and Clegg (1989)*
HOBr	9.3×10^{1}	5862.	Vogt et al. (1996)*
BrCl	9.4×10^{-1}	5600.	Bartlett and Margerum (1999)
SO_2	1.2	3120.	Chameides (1984)
H_2SO_4	$1.\times10^{11}$	0.	see note
DMSO	$5.\times10^{4}$	6425.	De Bruyn et al. (1994)*

*Notes:

The temperature dependence of the Henry constants is:

$$K_{\mathrm{H}} = K_{\mathrm{H}}^{\ominus} \times \exp\left(\frac{-\Delta_{\mathrm{soln}}H}{R}\left(\frac{1}{T} - \frac{1}{T^{\ominus}}\right)\right)$$

where $\Delta_{\mathrm{soln}}H$ = molar enthalpy of dissolution [J/mol] and $R = 8.314$ J/(mol K).

NO_2: The temperature dependence is from Chameides (1984).

HNO_3: Calculated using the acidity constant from Davis and de Bruin (1964).

CH_3O_2: This value was estimated by Jacob (1986).

HBr: Calculated using the acidity constant from Lax (1969).

HOBr: This value was estimated by Vogt et al. (1996).

H_2SO_4: To account for the very high Henry's law coefficient of H_2SO_4, a very high value was chosen arbitrarily.

DMSO: Lower limit cited from another reference.

Table 4: Accommodation coefficients

substance	$\alpha^{\ominus}$	$\frac{-\Delta_{\mathrm{obs}}H/R}{\mathrm{K}}$	reference
O_2	0.01	2000.	see note
O_3	0.002	0.	DeMore et al. (1997)*
OH	0.01	0.	Takami et al. (1998)*
HO_2	0.5	0.	Thornton and Abbatt (2005)
H_2O_2	0.077	3127.	Worsnop et al. (1989)
NH_3	0.06	0.	DeMore et al. (1997)*
NO	5.0×10^{-5}	0.	Saastad et al. (1993)*
NO_2	0.0015	0.	Ponche et al. (1993)*
NO_3	0.04	0.	Rudich et al. (1996)*
N_2O_5	0.1	0.	DeMore et al. (1997)*
HONO	0.04	0.	DeMore et al. (1997)*
HNO_3	0.5	0.	Abbatt and Waschewsky (1998)*
HNO_4	0.1	0.	DeMore et al. (1997)*
CH_3O_2	0.01	2000.	see note
CH_3OOH	0.0046	3273.	Magi et al. (1997)
HCHO	0.04	0.	DeMore et al. (1997)*
HCOOH	0.014	3978.	DeMore et al. (1997)
CO_2	0.01	2000.	see note
Cl_2	0.038	6546.	Hu et al. (1995)
HCl	0.074	3072.	Schweitzer et al. (2000)*
HOCl	0.5	0.	see note
$ClNO_3$	0.108	0.	Deiber et al. (2004)*
Br_2	0.038	6546.	Hu et al. (1995)
HBr	0.032	3940.	Schweitzer et al. (2000)*
HOBr	0.5	0.	Abbatt and Waschewsky (1998)*
$BrNO_3$	0.063	0.	Deiber et al. (2004)*
BrCl	0.38	6546.	see note
SO_2	0.11	0.	DeMore et al. (1997)
H_2SO_4	0.65	0.	Pöschl et al. (1998)*

Table 4: Accommodation coefficients (... continued)

substance	$\alpha^{\ominus}$	$\frac{-\Delta_{\rm obs}H/R}{\rm K}$	reference
CH_3SO_3H	0.076	1762.	De Bruyn et al. (1994)
DMSO	0.048	2578.	De Bruyn et al. (1994)

*Notes:

The temperature dependence of the accommodation coefficients is given by (Jayne et al., 1991):

$$\frac{\alpha}{1-\alpha} = \exp\left(\frac{-\Delta_{\rm obs}G}{RT}\right) = \exp\left(\frac{-\Delta_{\rm obs}H}{RT}+\frac{\Delta_{\rm obs}S}{R}\right)$$

where $\Delta_{\rm obs}G$ is the Gibbs free energy barrier of the transition state toward solution (Jayne et al., 1991), and $\Delta_{\rm obs}H$ and $\Delta_{\rm obs}S$ are the corresponding enthalpy and entropy, respectively. The equation can be rearranged to:

$$\ln\left(\frac{\alpha}{1-\alpha}\right) = \frac{-\Delta_{\rm obs}H}{R}\times\frac{1}{T}+\frac{-\Delta_{\rm obs}S}{R}$$

and further:

$$\mathrm{d}\ln\left(\frac{\alpha}{1-\alpha}\right)\Big/\mathrm{d}\left(\frac{1}{T}\right) = \frac{-\Delta_{\rm obs}H}{R}$$

If no data were available, a value of $\alpha = 0.01$, $\alpha = 0.1$, or $\alpha = 0.5$, and a temperature dependence of $-\Delta_{\rm obs}H/R = 2000$ K has been assumed.

O_2: Estimate.

O_3: Value measured at 292 K.

OH: Value measured at 293 K.

NH_3: Value measured at 295 K.

NO: Value measured between 193 and 243 K.

NO_2: Value measured at 298 K.

NO_3: Value is a lower limit, measured at 273 K.

N_2O_5: Value for sulfuric acid, measured between 195 and 300 K.

HONO: Value measured between 247 and 297 K.

HNO_3: Value measured at room temperature. Abbatt and Waschewsky (1998) say $\gamma > 0.2$. Here $\alpha = 0.5$ is used.

HNO_4: Value measured at 200 K for water ice.

CH_3O_2: Estimate.

HCHO: Value measured between 260 and 270 K.

CO_2: Estimate.

HCl: Temperature dependence derived from published data at 2 different temperatures

HOCl: Assumed to be the same as α(HOBr).

$ClNO_3$: Value measured at 274.5 K.

HBr: Temperature dependence derived from published data at 2 different temperatures

HOBr: Value measured at room temperature. Abbatt and Waschewsky (1998) say $\gamma > 0.2$. Here $\alpha = 0.5$ is used.

$BrNO_3$: Value measured at 273 K.

BrCl: Assumed to be the same as $\alpha(Cl_2)$.

H_2SO_4: Value measured at 303 K.

Table 5: Reversible (Henry's law) transfer and irreversible ("heterogenous") uptake

#	labels	reaction	rate coefficient	reference
H1000f_a01	TrAa01Sc	$O_2 \rightarrow O_2(aq)$	k_exf(01,ind_O2)	see note
H1000b_a01	TrAa01Sc	$O_2(aq) \rightarrow O_2$	k_exb(01,ind_O2)	see note
H1001f_a01	TrAa01MblScScm	$O_3 \rightarrow O_3(aq)$	k_exf(01,ind_O3)	see note
H1001b_a01	TrAa01MblScScm	$O_3(aq) \rightarrow O_3$	k_exb(01,ind_O3)	see note
H2100f_a01	TrAa01Sc	$OH \rightarrow OH(aq)$	k_exf(01,ind_OH)	see note
H2100b_a01	TrAa01Sc	$OH(aq) \rightarrow OH$	k_exb(01,ind_OH)	see note
H2101f_a01	TrAa01Sc	$HO_2 \rightarrow HO_2(aq)$	k_exf(01,ind_HO2)	see note
H2101b_a01	TrAa01Sc	$HO_2(aq) \rightarrow HO_2$	k_exb(01,ind_HO2)	see note
H2102f_a01	TrAa01MblScScm	$H_2O_2 \rightarrow H_2O_2(aq)$	k_exf(01,ind_H2O2)	see note
H2102b_a01	TrAa01MblScScm	$H_2O_2(aq) \rightarrow H_2O_2$	k_exb(01,ind_H2O2)	see note
H3101f_a01	TrAa01NSc	$NO_2 \rightarrow NO_2(aq)$	k_exf(01,ind_NO2)	see note
H3101b_a01	TrAa01NSc	$NO_2(aq) \rightarrow NO_2$	k_exb(01,ind_NO2)	see note
H3102f_a01	TrAa01NSc	$NO_3 \rightarrow NO_3(aq)$	k_exf(01,ind_NO3)	see note
H3102b_a01	TrAa01NSc	$NO_3(aq) \rightarrow NO_3$	k_exb(01,ind_NO3)	see note
H3200f_a01	TrAa01NMblScScm	$NH_3 \rightarrow NH_3(aq)$	k_exf(01,ind_NH3)	see note
H3200b_a01	TrAa01NMblScScm	$NH_3(aq) \rightarrow NH_3$	k_exb(01,ind_NH3)	see note
H3201_a01	TrAa01MblNScScm	$N_2O_5 \rightarrow HNO_3(aq) + HNO_3(aq)$	k_exf_N2O5(01)*C(ind_H2O_a01)	Behnke et al. (1994), Behnke et al. (1997)*
H3202f_a01	TrAa01NSc	$HONO \rightarrow HONO(aq)$	k_exf(01,ind_HONO)	see note
H3202b_a01	TrAa01NSc	$HONO(aq) \rightarrow HONO$	k_exb(01,ind_HONO)	see note
H3203f_a01	TrAa01MblNScScm	$HNO_3 \rightarrow HNO_3(aq)$	k_exf(01,ind_HNO3)	see note
H3203b_a01	TrAa01MblNScScm	$HNO_3(aq) \rightarrow HNO_3$	k_exb(01,ind_HNO3)	see note
H3204f_a01	TrAa01NSc	$HNO_4 \rightarrow HNO_4(aq)$	k_exf(01,ind_HNO4)	see note
H3204b_a01	TrAa01NSc	$HNO_4(aq) \rightarrow HNO_4$	k_exb(01,ind_HNO4)	see note
H4100f_a01	TrAa01MblScScm	$CO_2 \rightarrow CO_2(aq)$	k_exf(01,ind_CO2)	see note
H4100b_a01	TrAa01MblScScm	$CO_2(aq) \rightarrow CO_2$	k_exb(01,ind_CO2)	see note
H4101f_a01	TrAa01ScScm	$HCHO \rightarrow HCHO(aq)$	k_exf(01,ind_HCHO)	see note
H4101b_a01	TrAa01ScScm	$HCHO(aq) \rightarrow HCHO$	k_exb(01,ind_HCHO)	see note
H4102f_a01	TrAa01Sc	$CH_3O_2 \rightarrow CH_3OO(aq)$	k_exf(01,ind_CH3O2)	see note
H4102b_a01	TrAa01Sc	$CH_3OO(aq) \rightarrow CH_3O_2$	k_exb(01,ind_CH3O2)	see note

Table 5: Reversible (Henry's law) transfer and irreversible ("heterogenous") uptake

#	labels	reaction	rate coefficient	reference
H4103f_a01	TrAa01ScScm	$HCOOH \rightarrow HCOOH(aq)$	k_exf(01,ind_HCOOH)	see note
H4103b_a01	TrAa01ScScm	$HCOOH(aq) \rightarrow HCOOH$	k_exb(01,ind_HCOOH)	see note
H4104f_a01	TrAa01ScScm	$CH_3OOH \rightarrow CH_3OOH(aq)$	k_exf(01,ind_CH3OOH)	see note
H4104b_a01	TrAa01ScScm	$CH_3OOH(aq) \rightarrow CH_3OOH$	k_exb(01,ind_CH3OOH)	see note
H6000f_a01	TrAa01ClMblSc	$Cl_2 \rightarrow Cl_2(aq)$	k_exf(01,ind_Cl2)	see note
H6000b_a01	TrAa01ClMblSc	$Cl_2(aq) \rightarrow Cl_2$	k_exb(01,ind_Cl2)	see note
H6200f_a01	TrAa01ClMblScScm	$HCl \rightarrow HCl(aq)$	k_exf(01,ind_HCl)	see note
H6200b_a01	TrAa01ClMblScScm	$HCl(aq) \rightarrow HCl$	k_exb(01,ind_HCl)	see note
H6201f_a01	TrAa01ClMblSc	$HOCl \rightarrow HOCl(aq)$	k_exf(01,ind_HOCl)	see note
H6201b_a01	TrAa01ClMblSc	$HOCl(aq) \rightarrow HOCl$	k_exb(01,ind_HOCl)	see note
H6300_a01	TrAa01ClMblN	$N_2O_5 + Cl^-(aq) \rightarrow ClNO_2 + NO_3^-(aq)$	k_exf_N2O5(01) * 5.E2	Behnke et al. (1994), Behnke et al. (1997)*
H6301_a01	TrAa01ClMblN	$ClNO_3 \rightarrow HOCl(aq) + HNO_3(aq)$	k_exf_ClNO3(01) * C(ind_H2O_a01)	see note
H6302_a01	TrAa01ClMblN	$ClNO_3 + Cl^-(aq) \rightarrow Cl_2(aq) + NO_3^-(aq)$	k_exf_ClNO3(01) * 5.E2	see note
H7000f_a01	TrAa01BrMblSc	$Br_2 \rightarrow Br_2(aq)$	k_exf(01,ind_Br2)	see note
H7000b_a01	TrAa01BrMblSc	$Br_2(aq) \rightarrow Br_2$	k_exb(01,ind_Br2)	see note
H7200f_a01	TrAa01BrMblScScm	$HBr \rightarrow HBr(aq)$	k_exf(01,ind_HBr)	see note
H7200b_a01	TrAa01BrMblScScm	$HBr(aq) \rightarrow HBr$	k_exb(01,ind_HBr)	see note
H7201f_a01	TrAa01BrMblSc	$HOBr \rightarrow HOBr(aq)$	k_exf(01,ind_HOBr)	see note
H7201b_a01	TrAa01BrMblSc	$HOBr(aq) \rightarrow HOBr$	k_exb(01,ind_HOBr)	see note
H7300_a01	TrAa01BrMblN	$N_2O_5 + Br^-(aq) \rightarrow BrNO_2 + NO_3^-(aq)$	k_exf_N2O5(01) * 3.E5	Behnke et al. (1994), Behnke et al. (1997)*
H7301_a01	TrAa01BrMblN	$BrNO_3 \rightarrow HOBr(aq) + HNO_3(aq)$	k_exf_BrNO3(01) * C(ind_H2O_a01)	see note
H7302_a01	TrAa01BrMblN	$BrNO_3 + Br^-(aq) \rightarrow Br_2(aq) + NO_3^-(aq)$	k_exf_BrNO3(01) * 3.E5	see note
H7600f_a01	TrAa01ClBrMblSc	$BrCl \rightarrow BrCl(aq)$	k_exf(01,ind_BrCl)	see note
H7600b_a01	TrAa01ClBrMblSc	$BrCl(aq) \rightarrow BrCl$	k_exb(01,ind_BrCl)	see note
H7601_a01	TrAa01ClBrMblN	$ClNO_3 + Br^-(aq) \rightarrow BrCl(aq) + NO_3^-(aq)$	k_exf_ClNO3(01) * 3.E5	see note

Table 5: Reversible (Henry's law) transfer and irreversible ("heterogenous") uptake

#	labels	reaction	rate coefficient	reference
H7602_a01	TrAa01ClBrMblN	$BrNO_3 + Cl^-(aq) \rightarrow BrCl(aq) + NO_3^-(aq)$	k_exf_BrNO3(01) * 5.E2	see note
H9100f_a01	TrAa01SMblScScm	$SO_2 \rightarrow SO_2(aq)$	k_exf(01,ind_SO2)	see note
H9100b_a01	TrAa01SMblScScm	$SO_2(aq) \rightarrow SO_2$	k_exb(01,ind_SO2)	see note
H9200_a01	TrAa01SMblScScm	$H_2SO_4 \rightarrow H_2SO_4(aq)$	xnom7sulf*k_exf(01,ind_H2SO4)	see note
H9400f_a01	TrAa01S	$DMSO \rightarrow DMSO(aq)$	k_exf(01,ind_DMSO)	see note
H9400b_a01	TrAa01S	$DMSO(aq) \rightarrow DMSO$	k_exb(01,ind_DMSO)	see note
H9401_a01	TrAa01SMbl	$CH_3SO_3H \rightarrow CH_3SO_3^-(aq) + H^+(aq)$	k_exf(01,ind_CH3SO3H)	see note

*Notes:

The forward (k_exf) and backward (k_exb) rate coefficients are calculated in the file messy_mecca_aero.f90 using the accommodation coefficients in subroutine mecca_aero_alpha and Henry's law constants in subroutine mecca_aero_henry.

k_{mt} = mass transfer coefficient

lwc = liquid water content of aerosol mode

H3201, H6300, H6301, H6302, H7300, H7301, H7302, H7601, H7602: For uptake of X (= N_2O_5, $ClNO_3$, $BrNO_3$) and subsequent reaction with H_2O, Cl^-, and Br^-, we define $k_{exf}(X) = k_{mt}(X) \times lwc/([H_2O] + 5.0E2[Cl^-] + 3.0E5[Br^-])$.

H6301, H6302, H7601: The total uptake is determined by $k_{mt}(ClNO_3)$. The relative rates are assumed to be the same as for N_2O_5 (H3201, H6300, H7300).

H7301, H7302, H7602: The total uptake is determined by $k_{mt}(BrNO_3)$. The relative rates are assumed to be the same as for N_2O_5 (H3201, H6300, H7300).

Table 6: Acid-base and other eqilibria

#	labels	reaction	$K_0[M^{m-n}]$	- $\Delta H/R[K]$	reference
EQ20_a01	TrAa01Sc	$HO_2 \rightleftharpoons O_2^- + H^+$	1.6E-5		Weinstein-Lloyd and Schwartz (1991)
EQ21_a01	TrAa01MblScScm	$H_2O \rightleftharpoons H^+ + OH^-$	1.0E-16	-6716	Chameides (1984)
EQ30_a01	TrAa01MblNScScm	$NH_4^+ \rightleftharpoons H^+ + NH_3$	5.88E-10	-2391	Chameides (1984)
EQ31_a01	TrAa01NSc	$HONO \rightleftharpoons H^+ + NO_2^-$	5.1E-4	-1260	Schwartz and White (1981)
EQ32_a01	TrAa01MblNScScm	$HNO_3 \rightleftharpoons H^+ + NO_3^-$	15	8700	Davis and de Bruin (1964)
EQ33_a01	TrAa01NSc	$HNO_4 \rightleftharpoons NO_4^- + H^+$	1.E-5		Warneck (1999)
EQ40_a01	TrAa01MblScScm	$CO_2 \rightleftharpoons H^+ + HCO_3^-$	4.3E-7	-913	Chameides (1984)*
EQ41_a01	TrAa01ScScm	$HCOOH \rightleftharpoons H^+ + HCOO^-$	1.8E-4		Weast (1980)
EQ60_a01	TrAa01Cl	$Cl_2^- \rightleftharpoons Cl + Cl^-$	7.3E-6		Yu (2004)
EQ61_a01	TrAa01ClMblScScm	$HCl \rightleftharpoons H^+ + Cl^-$	1.7E6	6896	Marsh and McElroy (1985)
EQ62_a01	TrAa01ClSc	$HOCl \rightleftharpoons H^+ + ClO^-$	3.2E-8		Lax (1969)
EQ70_a01	TrAa01Br	$Br_2^- \rightleftharpoons Br + Br^-$	2.54E-6	-2256	Liu et al. (2002)
EQ71_a01	TrAa01BrMblScScm	$HBr \rightleftharpoons H^+ + Br^-$	1.0E9		Lax (1969)
EQ72_a01	TrAa01BrSc	$HOBr \rightleftharpoons H^+ + BrO^-$	2.3E-9	-3091	Kelley and Tartar (1956)*
EQ73_a01	TrAa01ClBrMbl	$BrCl + Cl^- \rightleftharpoons BrCl_2^-$	3.8	1191	Wang et al. (1994)
EQ74_a01	TrAa01ClBrMbl	$BrCl + Br^- \rightleftharpoons Br_2Cl^-$	1.8E4	7457	Wang et al. (1994)
EQ75_a01	TrAa01ClBrMbl	$Br_2 + Cl^- \rightleftharpoons Br_2Cl^-$	1.3	0	Wang et al. (1994)
EQ76_a01	TrAa01ClBrMbl	$Br^- + Cl_2 \rightleftharpoons BrCl_2^-$	4.2E6	14072	Wang et al. (1994)
EQ90_a01	TrAa01SMblScScm	$SO_2 \rightleftharpoons H^+ + HSO_3^-$	1.7E-2	2090	Chameides (1984)
EQ91_a01	TrAa01SMblScScm	$HSO_3^- \rightleftharpoons H^+ + SO_3^{2-}$	6.0E-8	1120	Chameides (1984)
EQ92_a01	TrAa01SMblScScm	$HSO_4^- \rightleftharpoons H^+ + SO_4^{2-}$	1.2E-2	2720	Seinfeld and Pandis (1998)
EQ93_a01	TrAa01SMblScScm	$H_2SO_4 \rightleftharpoons H^+ + HSO_4^-$	1.0E3		Seinfeld and Pandis (1998)

*Notes:

EQ40: For $pK_a(CO_2)$, see also Dickson and Millero (1987).

EQ72: For pK_a(HOBr), see also Keller-Rudek et al. (1992).

Table 7: Aqueous phase reactions

#	labels	reaction	$k_0\ [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A1000_a01	TrAa01Sc	$O_3 + O_2^- \rightarrow OH + OH^-$	1.5E9		Sehested et al. (1983)
A2100_a01	TrAa01Sc	$OH + O_2^- \rightarrow OH^-$	1.0E10		Sehested et al. (1968)
A2101_a01	TrAa01Sc	$OH + OH \rightarrow H_2O_2$	5.5E9		Buxton et al. (1988)
A2102_a01	TrAa01Sc	$HO_2 + O_2^- \rightarrow H_2O_2 + OH^-$	1.0E8	-900	Christensen and Sehested (1988)
A2103_a01	TrAa01Sc	$HO_2 + OH \rightarrow H_2O$	7.1E9		Sehested et al. (1968)
A2104_a01	TrAa01Sc	$HO_2 + HO_2 \rightarrow H_2O_2$	9.7E5	-2500	Christensen and Sehested (1988)
A2105_a01	TrAa01Sc	$H_2O_2 + OH \rightarrow HO_2$	2.7E7	-1684	Christensen et al. (1982)
A3100_a01	TrAa01NSc	$NO_2^- + O_3 \rightarrow NO_3^-$	5.0E5	-6950	Damschen and Martin (1983)
A3101_a01	TrAa01NSc	$NO_2 + NO_2 \rightarrow HNO_3 + HONO$	1.0E8		Lee and Schwartz (1981)
A3102_a01	TrAa01NSc	$NO_4^- \rightarrow NO_2^-$	8.0E1		Warneck (1999)
A3200_a01	TrAa01NSc	$NO_2 + HO_2 \rightarrow HNO_4$	1.8E9		Warneck (1999)
A3201_a01	TrAa01NSc	$NO_2^- + OH \rightarrow NO_2 + OH^-$	1.0E10		Wingenter et al. (1999)
A3202_a01	TrAa01NSc	$NO_3 + OH^- \rightarrow NO_3^- + OH$	8.2E7	-2700	Exner et al. (1992)
A3203_a01	TrAa01NSc	$HONO + OH \rightarrow NO_2$	1.0E10		Barker et al. (1970)
A3204_a01	TrAa01NSc	$HONO + H_2O_2 + H^+ \rightarrow HNO_3 + H^+$	4.6E3	-6800	Damschen and Martin (1983)
A4100_a01	TrAa01Sc	$CO_3^- + O_2^- \rightarrow HCO_3^- + OH^-$	6.5E8		Ross et al. (1992)
A4101_a01	TrAa01Sc	$CO_3^- + H_2O_2 \rightarrow HCO_3^- + HO_2$	4.3E5		Ross et al. (1992)
A4102_a01	TrAa01Sc	$HCOO^- + CO_3^- \rightarrow 2\ HCO_3^- + HO_2$	1.5E5		Ross et al. (1992)
A4103_a01	TrAa01Sc	$HCOO^- + OH \rightarrow OH^- + HO_2 + CO_2$	3.1E9	-1240	Chin and Wine (1994)
A4104_a01	TrAa01Sc	$HCO_3^- + OH \rightarrow CO_3^-$	8.5E6		Ross et al. (1992)
A4105_a01	TrAa01Sc	$HCHO + OH \rightarrow HCOOH + HO_2$	7.7E8	-1020	Chin and Wine (1994)
A4106_a01	TrAa01Sc	$HCOOH + OH \rightarrow HO_2 + CO_2$	1.1E8	-991	Chin and Wine (1994)
A4107_a01	TrAa01Sc	$CH_3OO + O_2^- \rightarrow CH_3OOH + OH^-$	5.0E7		Jacob (1986)
A4108_a01	TrAa01Sc	$CH_3OO + HO_2 \rightarrow CH_3OOH$	4.3E5		Jacob (1986)
A4109_a01	TrAa01Sc	$CH_3OH + OH \rightarrow HCHO + HO_2$	9.7E8		Buxton et al. (1988)

Table 7: Aqueous phase reactions (...continued)

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A4110a_a01	TrAa01Sc	$CH_3OOH + OH \rightarrow CH_3OO$	2.7E7	-1715	Jacob (1986)
A4110b_a01	TrAa01Sc	$CH_3OOH + OH \rightarrow HCHO + OH$	1.1E7	-1715	Jacob (1986)
A6000_a01	TrAa01Cl	$Cl + Cl \rightarrow Cl_2$	8.8E7		Wu et al. (1980)
A6001_a01	TrAa01Cl	$Cl_2^- + Cl_2^- \rightarrow Cl_2 + 2\ Cl^-$	3.5E9		Yu (2004)
A6100_a01	TrAa01Cl	$Cl^- + O_3 \rightarrow ClO^-$	3.0E-3		Hoigné et al. (1985)
A6101_a01	TrAa01Cl	$Cl_2 + O_2^- \rightarrow Cl_2^-$	1.0E9		Bjergbakke et al. (1981)
A6102_a01	TrAa01Cl	$Cl_2^- + O_2^- \rightarrow 2\ Cl^-$	1.0E9		Jacobi (1996)*
A6200_a01	TrAa01Cl	$Cl \rightarrow H^+ + ClOH^-$	1.8E5		Yu (2004)
A6201_a01	TrAa01Cl	$Cl + H_2O_2 \rightarrow HO_2 + Cl^- + H^+$	2.7E7	-1684	Christensen et al. (1982)
A6202_a01	TrAa01Cl	$Cl^- + OH \rightarrow ClOH^-$	4.2E9		Yu (2004)
A6203_a01	TrAa01Cl	$Cl_2 + HO_2 \rightarrow Cl_2^- + H^+$	1.0E9		Bjergbakke et al. (1981)
A6204_a01	TrAa01ClMbl	$Cl_2 \rightarrow Cl^- + HOCl + H^+$	21.8	-8012	Wang and Margerum (1994)
A6205_a01	TrAa01Cl	$Cl_2^- + HO_2 \rightarrow 2\ Cl^- + H^+$	1.3E10		Jacobi (1996)
A6206_a01	TrAa01Cl	$HOCl + O_2^- \rightarrow Cl + OH^-$	7.5E6		Long and Bielski (1980)
A6207_a01	TrAa01Cl	$HOCl + HO_2 \rightarrow Cl$	7.5E6		Long and Bielski (1980)
A6208_a01	TrAa01ClMbl	$HOCl + Cl^- + H^+ \rightarrow Cl_2$	2.2E4	-3508	Wang and Margerum (1994)
A6209_a01	TrAa01Cl	$ClOH^- \rightarrow Cl^- + OH$	6.0E9		Yu (2004)
A6210_a01	TrAa01Cl	$ClOH^- + H^+ \rightarrow Cl$	2.4E10		Yu (2004)
A6300_a01	TrAa01Cl	$Cl + NO_3^- \rightarrow NO_3 + Cl^-$	1.0E8		Buxton et al. (1999b)
A6301_a01	TrAa01Cl	$Cl^- + NO_3 \rightarrow NO_3^- + Cl$	3.4E8		Buxton et al. (1999b)*
A6302_a01	TrAa01Cl	$Cl_2^- + NO_2^- \rightarrow 2\ Cl^- + NO_2$	6.0E7		Jacobi et al. (1996)
A6400_a01	TrAa01Cl	$Cl_2^- + CH_3OOH \rightarrow 2\ Cl^- + H^+ + CH_3OO$	5.0E4		Jacobi et al. (1996)
A7000_a01	TrAa01Br	$Br_2^- + Br_2^- \rightarrow 2\ Br^- + Br_2$	1.9E9		Ross et al. (1992)
A7100_a01	TrAa01Br	$Br^- + O_3 \rightarrow BrO^-$	2.1E2	-4450	Haag and Hoigné (1983)
A7101_a01	TrAa01Br	$Br_2 + O_2^- \rightarrow Br_2^-$	5.6E9		Sutton and Downes (1972)
A7102_a01	TrAa01Br	$Br_2^- + O_2^- \rightarrow 2\ Br^-$	1.7E8		Wagner and Strehlow (1987)
A7200_a01	TrAa01Br	$Br^- + OH \rightarrow BrOH^-$	1.1E10		Zehavi and Rabani (1972)

Table 7: Aqueous phase reactions (...continued)

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A7201_a01	TrAa01Br	$Br_2 + HO_2 \rightarrow Br_2^- + H^+$	1.1E8		Sutton and Downes (1972)
A7202_a01	TrAa01BrMbl	$Br_2 \rightarrow Br^- + HOBr + H^+$	9.7E1	-7457	Beckwith et al. (1996)
A7203_a01	TrAa01Br	$Br_2^- + HO_2 \rightarrow Br_2 + H_2O_2 + OH^-$	4.4E9		Matthew et al. (2003)
A7204_a01	TrAa01Br	$Br_2^- + H_2O_2 \rightarrow 2\ Br^- + H^+ + HO_2$	1.0E5		Jacobi (1996)
A7205_a01	TrAa01Br	$HOBr + O_2^- \rightarrow Br + OH^-$	3.5E9		Schwarz and Bielski (1986)
A7206_a01	TrAa01Br	$HOBr + HO_2 \rightarrow Br$	1.0E9		Herrmann et al. (1999)
A7207_a01	TrAa01Br	$HOBr + H_2O_2 \rightarrow Br^- + H^+$	1.2E6		Bichsel and von Gunten (1999)
A7208_a01	TrAa01BrMbl	$HOBr + Br^- + H^+ \rightarrow Br_2$	1.6E10		Beckwith et al. (1996)
A7209a_a01	TrAa01Br	$BrOH^- \rightarrow Br^- + OH$	3.3E7		Zehavi and Rabani (1972)
A7209b_a01	TrAa01Br	$BrOH^- \rightarrow Br + OH^-$	4.2E6		Zehavi and Rabani (1972)
A7210_a01	TrAa01Br	$BrOH^- + H^+ \rightarrow Br$	4.4E10		Zehavi and Rabani (1972)
A7300_a01	TrAa01Br	$Br^- + NO_3 \rightarrow Br + NO_3^-$	4.0E9		Neta and Huie (1986)
A7301_a01	TrAa01Br	$Br_2^- + NO_2^- \rightarrow 2\ Br^- + NO_2$	1.7E7	-1720	Shoute et al. (1991)
A7400_a01	TrAa01Br	$Br_2^- + CH_3OOH \rightarrow 2\ Br^- + H^+ + CH_3OO$	1.0E5		Jacobi (1996)*
A7601_a01	TrAa01Br	$Br^- + ClO^- + H^+ \rightarrow BrCl + OH^-$	3.7E10		Kumar and Margerum (1987)
A7602_a01	TrAa01ClBrMbl	$Br^- + HOCl + H^+ \rightarrow BrCl$	1.32E6		Kumar and Margerum (1987)
A7603_a01	TrAa01ClBrMbl	$HOBr + Cl^- + H^+ \rightarrow BrCl$	2.3E10		see note
A7604_a01	TrAa01ClBrMbl	$BrCl \rightarrow Cl^- + HOBr + H^+$	3.0E6		Liu and Margerum (2001)
A9100_a01	TrAa01SSc	$SO_3^- + O_2 \rightarrow SO_5^-$	1.5E9		Huie and Neta (1987)
A9101_a01	TrAa01SMblScScm	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-}$	1.5E9	-5300	Hoffmann (1986)
A9102_a01	TrAa01SSc	$SO_4^- + O_2^- \rightarrow SO_4^{2-}$	3.5E9		Jiang et al. (1992)
A9103_a01	TrAa01SSc	$SO_4^- + SO_3^{2-} \rightarrow SO_3^- + SO_4^{2-}$	4.6E8		Huie and Neta (1987)
A9104_a01	TrAa01SSc	$SO_5^- + O_2^- \rightarrow HSO_5^- + OH^-$	2.3E8		Buxton et al. (1996)
A9105_a01	TrAa01S	$SO_5^- + SO_3^{2-} \rightarrow .72\ SO_4^- + .72\ SO_4^{2-} + .28\ SO_3^- + .28\ HSO_5^- + .28\ OH^-$	1.3E7		Huie and Neta (1987), Deister and Warneck (1990)*

Table 7: Aqueous phase reactions (...continued)

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A9106_a01	TrAa01S	$SO_5^- + SO_5^- \rightarrow O_2 + SO_4^{2-}$	1.0E8		Ross et al. (1992)*
A9200_a01	TrAa01SSc	$SO_3^{2-} + OH \rightarrow SO_3^- + OH^-$	5.5E9		Buxton et al. (1988)
A9201_a01	TrAa01SSc	$SO_4^- + OH \rightarrow HSO_5^-$	1.0E9		Jiang et al. (1992)
A9202_a01	TrAa01SSc	$SO_4^- + HO_2 \rightarrow SO_4^{2-} + H^+$	3.5E9		Jiang et al. (1992)
A9203_a01	TrAa01SSc	$SO_4^- + H_2O \rightarrow SO_4^{2-} + H^+ + OH$	1.1E1	-1110	Herrmann et al. (1995)
A9204_a01	TrAa01SSc	$SO_4^- + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2$	1.2E7		Wine et al. (1989)
A9205_a01	TrAa01SSc	$HSO_3^- + O_2^- \rightarrow SO_4^{2-} + OH$	3.0E3		see note
A9206_a01	TrAa01SMblScScm	$HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+$	3.7E5	-5500	Hoffmann (1986)
A9207_a01	TrAa01SSc	$HSO_3^- + OH \rightarrow SO_3^-$	4.5E9		Buxton et al. (1988)
A9208_a01	TrAa01SSc	$HSO_3^- + HO_2 \rightarrow SO_4^{2-} + OH + H^+$	3.0E3		see note
A9209_a01	TrAa01SMblScScm	$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$	5.2E6	-3650	Martin and Damschen (1981)
A9210_a01	TrAa01SSc	$HSO_3^- + SO_4^- \rightarrow SO_3^- + SO_4^{2-} + H^+$	8.0E8		Huie and Neta (1987)
A9211_a01	TrAa01S	$HSO_3^- + SO_5^- \rightarrow .75\ SO_4^- + .75\ SO_4^{2-} + .75\ H^+ + .25\ SO_3^- + .25\ HSO_5^-$	1.0E5		Huie and Neta (1987)
A9212_a01	TrAa01SSc	$HSO_3^- + HSO_5^- + H^+ \rightarrow 2\ HSO_4^- + H^+$	7.1E6		Betterton and Hoffmann (1988)
A9300_a01	TrAa01SSc	$SO_3^{2-} + NO_2 \rightarrow SO_4^{2-} + 2\ HONO - NO_2$	2.0E7		Clifton et al. (1988)
A9301_a01	TrAa01SSc	$SO_4^- + NO_3^- \rightarrow SO_4^{2-} + NO_3$	5.0E4		Exner et al. (1992)
A9302_a01	TrAa01SSc	$SO_4^{2-} + NO_3 \rightarrow NO_3^- + SO_4^-$	1.0E5		Logager et al. (1993)
A9303_a01	TrAa01SSc	$HSO_3^- + NO_2 \rightarrow HSO_4^- + 2\ HONO - NO_2$	2.0E7		Clifton et al. (1988)
A9304_a01	TrAa01SSc	$HSO_3^- + NO_3 \rightarrow SO_3^- + NO_3^- + H^+$	1.4E9	-2000	Exner et al. (1992)
A9305_a01	TrAa01SSc	$HSO_3^- + HNO_4 \rightarrow HSO_4^- + NO_3^- + H^+$	3.1E5		Warneck (1999)
A9400_a01	TrAa01SSc	$SO_3^{2-} + HCHO \rightarrow CH_2OHSO_3^- + OH^-$	1.4E4		Boyce and Hoffmann (1984)
A9401_a01	TrAa01SSc	$SO_3^{2-} + CH_3OOH + H^+ \rightarrow SO_4^{2-} + H^+ + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A9402_a01	TrAa01SSc	$HSO_3^- + HCHO \rightarrow CH_2OHSO_3^-$	4.3E-1		Boyce and Hoffmann (1984)
A9403_a01	TrAa01SSc	$HSO_3^- + CH_3OOH + H^+ \rightarrow HSO_4^- + H^+ + CH_3OH$	1.6E7	-3800	Lind et al. (1987)

Table 7: Aqueous phase reactions (...continued)

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A9404_a01	TrAa01SSc	$CH_2OHSO_3^- + OH^- \rightarrow SO_3^{2-} + HCHO$	3.6E3		Seinfeld and Pandis (1998)
A9600_a01	TrAa01SCl	$SO_3^{2-} + Cl_2^- \rightarrow SO_3^- + 2\ Cl^-$	6.2E7		Jacobi et al. (1996)
A9601_a01	TrAa01SClMbl	$SO_3^{2-} + HOCl \rightarrow Cl^- + HSO_4^-$	7.6E8		Fogelman et al. (1989)
A9602_a01	TrAa01SCl	$SO_4^- + Cl^- \rightarrow SO_4^{2-} + Cl$	2.5E8		Buxton et al. (1999a)
A9603_a01	TrAa01SCl	$SO_4^{2-} + Cl \rightarrow SO_4^- + Cl^-$	2.1E8		Buxton et al. (1999a)
A9604_a01	TrAa01SCl	$HSO_3^- + Cl_2^- \rightarrow SO_3^- + 2\ Cl^- + H^+$	4.7E8	-1082	Shoute et al. (1991)
A9605_a01	TrAa01SClMbl	$HSO_3^- + HOCl \rightarrow Cl^- + HSO_4^- + H^+$	7.6E8		see note
A9606_a01	TrAa01SCl	$HSO_5^- + Cl^- \rightarrow HOCl + SO_4^{2-}$	1.8E-3	-7352	Fortnum et al. (1960)
A9700_a01	TrAa01SBr	$SO_3^{2-} + Br_2^- \rightarrow 2\ Br^- + SO_3^-$	2.2E8	-649	Shoute et al. (1991)
A9701_a01	TrAa01SBr	$SO_3^{2-} + BrO^- \rightarrow Br^- + SO_4^{2-}$	1.0E8		Troy and Margerum (1991)
A9702_a01	TrAa01SBrMbl	$SO_3^{2-} + HOBr \rightarrow Br^- + HSO_4^-$	5.0E9		Troy and Margerum (1991)
A9703_a01	TrAa01SBr	$SO_4^- + Br^- \rightarrow Br + SO_4^{2-}$	2.1E9		Jacobi (1996)
A9704_a01	TrAa01SBr	$HSO_3^- + Br_2^- \rightarrow 2\ Br^- + H^+ + SO_3^-$	6.3E7	-782	Shoute et al. (1991)
A9705_a01	TrAa01SBrMbl	$HSO_3^- + HOBr \rightarrow Br^- + HSO_4^- + H^+$	5.0E9		see note
A9706_a01	TrAa01SBr	$HSO_5^- + Br^- \rightarrow HOBr + SO_4^{2-}$	1.0E0	-5338	Fogelman et al. (1989)

*Notes:

A6102: Jacobi (1996) found an upper limit of 6E9 and cite an upper limit from another study of 2E9. Here, we set the rate coefficient to 1E9.

A6301: There is also an earlier study by Exner et al. (1992) which found a smaller rate coefficient but did not consider the back reaction.

A7400: Assumed to be the same as for $Br_2^- + H_2O_2$.

A9105: The rate coefficient for the sum of the paths (leading to either HSO_5^- or SO_4^{2-}) is from Huie and Neta (1987), the ratio 0.28/0.72 is from Deister and Warneck (1990).

A9106: See also: (Huie and Neta, 1987; Warneck, 1991). If this reaction produces a lot of SO_4^-, it will have an effect. However, we currently assume only the stable $S_2O_8^{2-}$ as product. Since $S_2O_8^{2-}$ is not treated explicitly in the mechanism, we use SO_4^{2-} as a proxy. Note that this destroys the mass consistency for sulfur species.

A9205: D. Sedlak, pers. comm. (1993).

A9208: D. Sedlak, pers. comm. (1993).

A9605: assumed to be the same as for $SO_3^{2-} + HOCl$.

A9705: assumed to be the same as for $SO_3^{2-} + HOBr$.

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