Kinetic data for MANIC

June 26, 2009

supplemental material to:

D. Lowe, D. Topping, and G. McFiggans

Modelling multi-phase halogen chemistry in the remote marine boundary layer: investigation of the influence of aerosol size resolution on predicted gas- and condensed-phase chemistry.

Atmos. Chem. Phys., 2009

1 Model Runs

Included here is a listing of all testcases examined in the paper (Table 1), with a summary of the main conclusions to be drawn. Each testcase consists of a set of model runs, one for each combination of model settings listed; e.g. the Base testcase consists of 15 model runs (5 different size resolutions multiplied by 3 different size distribution initialisation schemes for the seasalt mode). See main text for explanations of the different model settings.

Table 1: Model testcase details

Testcases	Number of size bins	Size distribution initialisation	Aerosol turnover schemes	Accommodation coeff. schemes	Main Conclusions
Base	ss: 1, 2, 4, 8, 16 nss: 1	ss: N/S, N/V, S/V nss: S/V	fixed	Base	Gas-phase chemistry influenced by choice of aerosol initialisation. If the S/V initialisation is used then the aerosol size-resolution is unimportant.
NSS	ss: 1 nss: 1, 2, 4, 8, 16	ss: S/V nss: N/S, N/V, S/V	fixed	Base	Gas-phase chemistry is unaffected by choice of initialisation or size-resolution of nss mode.
Size Dep. Turnover	ss: 1, 2, 4, 8, 16 nss: 1	ss: S/V, N/V nss: S/V	ss: size dependent nss: fixed	Base	Size-dependence of ss turnover rates are important to gas-phase chemistry.
Acc. Coeff.	ss: 16 nss: 1	ss: S/V nss: S/V	ss: size dependent nss: fixed	Base Toyota Low	Reducing accommodation coefficients of halogen species reduces the influence of the HOX and XO destruction cycles, and increases the influence of the $XONO_2$ cycles.

ss: seasalt mode
nss: non-seasalt mode
N/S: Number & Surface Area
N/V: Number & Volume
S/V: Surface Area & Volume

2 Chemistry Scheme

This collection comprises a complete listing of all gas and aqueous phase species (Table 2), gas phase (Table 3) and aqueous phase (Table 4) reaction rates, as well as rates for the heterogeneous (particle surface) reactions (Table 5), aqueous phase equilibrium constants (Table 6), Henry constants and accommodation coefficients (Table 7). Unless otherwise indicated, the chemical rate constants are taken from Pechtl et al. (2006).

Table 2: Species

Gas phase
O^1D, O_2, O_3, OH, HO_2, H_2O_2, H_2O
NO, NO_2, NO_3, N_2O_5, HONO, HNO_3, HNO_4, PAN, NH_3
CO, CO_2, CH_4, C_2H_6, C_2H_4, HCHO, HCOOH, ALD, $HOCH_2O_2$, CH_3CO_3, CH_3O_2, $C_2H_5O_2$, EO_2, ROOH
SO_2, SO_3, $HOSO_2$, H_2SO_4, DMS, CH_3SCH_2OO, DMSO, $DMSO_2$, CH_3S, CH_3SO, CH_3SO_2, CH_3SO_3, CH_3SO_2H, CH_3SO_3H
Cl, ClO, OClO, HCl, HOCl, Cl_2, Cl_2O_2, $ClNO_2$, $ClONO_2$
Br, BrO, HBr, HOBr, Br_2, $BrNO_2$, $BrONO_2$, BrCl
I, IO, OIO, HI, HOI, INO_2, $IONO_2$, I_2, ICl, IBr, HIO_3, CH_3I, C_2H_5I, C_3H_7I, CH_3ClI, CH_2BrI, CH_2I_2
Liquid phase (neutral)
O_2, O_3, OH, HO_2, H_2O_2, H_2O
NO, NO_2, NO_3, HONO, HNO_3, HNO_4, NH_3
CO_2, HCHO, HCOOH, CH_3OH, CH_3OO, CH_3OOH, DOM, ROOH
SO_2, H_2SO_4, DMS, DMSO, $DMSO_2$, CH_3SO_2H, CH_3SO_3H
Cl, HCl, HOCl, Cl_2
Br, HBr, HOBr, Br_2, BrCl
IO, HI, HOI, I_2, ICl, IBr
Liquid phase (ions)
H^+, OH^-, O_2^-, HO_2^-
NO_2^-, NO_3^-, NO_4^-, NH_4^+
HCO_3^-, CO_3^-, $HCOO^-$
HSO_3^-, SO_3^{2-}, HSO_4^-, SO_4^{2-}, HSO_5^-, SO_3^-, SO_4^-, SO_5^-, $CH_3SO_3^-$, $CH_2OHSO_2^-$, $CH_2OHSO_3^-$
Cl^-, Cl_2^-, ClO^-, $ClOH^-$
Br^-, Br_2^-, BrO^-, $BrCl_2^-$, Br_2Cl^-, $BrOH^-$
I^-, IO_2^-, IO_3^-, ICl_2^-, IBr_2^-, $IClBr^-$

Table 3: Gas phase reactions.

no	reaction	n	$A\,[(cm^{-3})^{1-n}s^{-1}]$	$-E_a/R\,[K]$	reference
O 1	$O^1D + O_2 \longrightarrow O_3$	2	3.2×10^{-11}	70	
O 2	$O^1D + N_2 \longrightarrow O_3$	2	1.8×10^{-11}	110	
O 3	$O^1D + H_2O \longrightarrow 2\,OH$	2	2.2×10^{-10}		
O 4	$OH + O_3 \longrightarrow HO_2 + O_2$	2	1.7×10^{-12}	-940	
O 5	$OH + HO_2 \longrightarrow H_2O + O_2$	2	4.8×10^{-11}	250	
O 6	$OH + H_2O_2 \longrightarrow HO_2 + H_2O$	2	2.9×10^{-12}	-160	
O 7	$HO_2 + O_3 \longrightarrow OH + 2\,O_2$	2	1.0×10^{-14}	-490	
O 8	$HO_2 + HO_2 \longrightarrow H_2O_2 + O_2$	2	2.3×10^{-13}	600	
O 9	$O_3 + hv \longrightarrow O_2 + O^1D$	1	[1]		
O 10	$H_2O_2 + hv \longrightarrow 2\,OH$	1	[1]		
N 1	$NO + OH \xrightarrow{M} HONO$	3	[2]		Sander et al. (2006)
N 2	$NO + HO_2 \longrightarrow NO_2 + OH$	2	3.5×10^{-12}	250	
N 3	$NO + O_3 \longrightarrow NO_2 + O_2$	2	3.0×10^{-12}	-1500	
N 4	$NO + NO_3 \longrightarrow 2\,NO_2$	2	1.5×10^{-11}	170	
N 5	$NO_2 + OH \xrightarrow{M} HNO_3$	3	[2]		Sander et al. (2006)
N 6	$NO_2 + HO_2 \xrightarrow{M} HNO_4$	3	[2]		Sander et al. (2006)
N 7	$NO_2 + O_3 \longrightarrow NO_3 + O_2$	2	1.2×10^{-13}	-2450	
N 8	$NO_2 + hv \longrightarrow NO + O_3$	1	[1]		
N 9	$NO_2 + NO_3 \xrightarrow{M} N_2O_5$	3	[2]		Sander et al. (2006)
N 10	$NO_3 + hv \longrightarrow NO + O_3$	1	[1]		
N 11	$NO_3 + HO_2 \longrightarrow 0.3\,HNO_3 + 0.7\,OH + 0.7\,NO_2 + O_2$	2	4.0×10^{-12}		
N 12	$NO_3 + NO_3 \longrightarrow NO_2 + NO_2 + O_2$	2	8.5×10^{-13}	-2450	
N 13	$NO_3 + hv \longrightarrow NO_2 + O_3$	1	[1]		
N 14	$N_2O_5 \xrightarrow{M} NO_2 + NO_3$	2	[2]		Sander et al. (2006), see note
N 15	$N_2O_5 + H_2O \longrightarrow 2\,HNO_3$	2	2.6×10^{-22}		
N 16	$N_2O_5 + hv \longrightarrow NO_2 + NO_3$	1	[1]		
N 17	$HONO + OH \longrightarrow NO_2$	2	1.8×10^{-11}	-390	
N 18	$HONO + hv \longrightarrow NO + OH$	1	[1]		
N 19	$HNO_3 + hv \longrightarrow NO_2 + OH$	1	[1]		

Table 3: Continued

no	reaction	n	$A\,[(cm^{-3})^{1-n}s^{-1}]$	$-E_a/R\,[K]$	reference
N 20	$HNO_3 + OH \longrightarrow NO_3 + H_2O$	2	[2]		Sander et al. (2006)
N 21	$HNO_4 \xrightarrow{M} NO_2 + HO_2$	2	[2]		Sander et al. (2006), see note
N 22	$HNO_4 + OH \longrightarrow NO_2 + H_2O + O_2$	2	1.3×10^{-12}	380	
N 23	$HNO_4 + hv \longrightarrow NO_2 + HO_2$	1	[1]		
N 24	$HNO_4 + hv \longrightarrow OH + NO_3$	1	[1]		
C 1	$CO + OH \xrightarrow{O_2} HO_2 + CO_2$	2	[2]		Sander et al. (2006)
C 2	$CH_4 + OH \xrightarrow{O_2} CH_3OO + H_2O$	2	2.4×10^{-12}	-1175	
C 3	$C_2H_6 + OH \longrightarrow C_2H_5O_2 + H_2O$	2	1.7×10^{-11}	-1232	
C 4	$C_2H_4 + OH \longrightarrow EO_2$	2	1.66×10^{-12}	474	
C 5	$C_2H_4 + O_3 \longrightarrow HCHO + 0.4\,HCOOH + 0.12\,HO_2$ $+0.42\,CO + 0.06\,CH_4$	2	1.2×10^{-14}	-2633	
C 6	$HO_2 + CH_3OO \longrightarrow ROOH + O_2$	2	4.1×10^{-13}	750	
C 7	$HO_2 + C_2H_5O_2 \longrightarrow ROOH + O_2$	2	7.5×10^{-13}	700	
C 8	$HO_2 + CH_3CO_3 \longrightarrow ROOH + O_2$	2	4.5×10^{-13}	1000	
C 9	$CH_3OO + CH_3OO \longrightarrow 1.4\,HCHO + 0.8\,HO_2 + O_2$	2	1.5×10^{-13}	220	
C 10	$C_2H_5O_2 + NO \longrightarrow ALD + HO_2 + NO_2$	2	4.2×10^{-12}	180	
C 11	$2\,C_2H_5O_2 \longrightarrow 1.6\,ALD + 1.2\,HO_2$	2	5.00×10^{-14}		
C 12	$EO_2 + NO \longrightarrow NO_2 + 2\,HCHO + O_2$	2	4.2×10^{-12}	180	
C 13	$EO_2 + EO_2 \longrightarrow 2.4\,HCHO + 1.2\,HO_2 + 0.4\,ALD$	2	5.00×10^{-14}		
C 14	$HO_2 + EO_2 \longrightarrow ROOH + O_2$	2	3.00×10^{-12}		
C 15	$HCHO + hv \longrightarrow 2\,HO_2 + CO$	1	[1]		
C 16	$HCHO + hv \longrightarrow CO + H_2$	1	[1]		
C 17	$HCHO + OH \xrightarrow{O_2} HO_2 + CO + H_2O$	2	1.00×10^{-11}		
C 18	$HCHO + HO_2 \longrightarrow HOCH_2O_2$	2	6.7×10^{-15}	600	
C 19	$HCHO + NO_3 \xrightarrow{O_2} HNO_3 + HO_2 + CO$	2	5.8×10^{-16}		
C 20	$ALD + OH \longrightarrow CH_3CO_3 + H_2O$	2	6.9×10^{-12}	250	
C 21	$ALD + NO_3 \longrightarrow HNO_3 + CH_3CO_3$	2	1.40×10^{-15}		
C 22	$ALD + hv \longrightarrow CH_3OO + HO_2 + CO$	1	[1]		
C 23	$ALD + hv \longrightarrow CH_4 + CO$	1	[1]		

Table 3: Continued

no	reaction	n	$A\,[(cm^{-3})^{1-n}s^{-1}]$	$-E_a/R\,[K]$	reference
C 24	$HOCH_2O_2 + NO \longrightarrow HCOOH + HO_2 + NO_2$	2	4.2×10^{-12}	180	
C 25	$HOCH_2O_2 + HO_2 \longrightarrow HCOOH + H_2O + O_2$	2	2.00×10^{-12}		
C 26	$2\,HOCH_2O_2 \longrightarrow 2\,HCOOH + HO_2 + 2\,O_2$	2	1.00×10^{-13}		
C 27	$HCOOH + OH \xrightarrow{O_2} HO_2 + H_2O + CO_2$	2	4.0×10^{-13}		
C 28	$CH_3CO_3 + NO_2 \longrightarrow PAN$	2	4.70×10^{-12}		
C 29	$PAN \longrightarrow CH_3CO_3 + NO_2$	1	1.9×10^{16}	-13543	
C 30	$CH_3CO_3 + NO \longrightarrow CH_3OO + NO_2 + CO_2$	2	4.2×10^{-12}	180	
C 31	$CH_3OO + NO \xrightarrow{O_2} HCHO + NO_2 + HO_2$	2	3.0×10^{-12}	280	
C 32	$ROOH + OH \longrightarrow 0.7\,CH_3OO + 0.3\,HCHO + 0.3\,OH$	2	3.8×10^{-12}	200	
C 33	$ROOH + hv \longrightarrow HCHO + OH + HO_2$	1	[1]		
S 1	$SO_2 + OH \xrightarrow{M} HOSO_2$	3	[2]		Atkison et al. (2006)
S 2	$HOSO_2 + O_2 \longrightarrow HO_2 + SO_3$	2	1.3×10^{-12}	330	
S 3	$SO_3 \xrightarrow{H_2O} H_2SO_4$	1	$3.9 \times 10^{-41} \times [H_2O]^2$	6830.6	Jayne et al. (1997)
S 4	$CH_3SCH_3 + OH \longrightarrow CH_3SCH_2OO + H_2O$	2	1.12×10^{-11}	-250	Atkison et al. (2006), see note
S 5	$CH_3SCH_3 + OH \xrightarrow{O_2} CH_3SOCH_3 + HO_2$	3	[2]		Atkison et al. (2006)
S 6	$CH_3SCH_3 + NO_3 \xrightarrow{O_2} CH_3SCH_2OO + HNO_3$	2	1.9×10^{-13}	520	
S 7	$CH_3SCH_3 + Cl \xrightarrow{O_2} CH_3SCH_2OO + HCl$	2	3.3×10^{-10}		
S 8	$CH_3SCH_3 + Br \xrightarrow{O_2} CH_3SCH_2OO + HBr$	2	9.0×10^{-11}	-2386	
S 9	$CH_3SCH_3 + BrO \longrightarrow CH_3SOCH_3 + Br$	2	2.54×10^{-14}	850	
S 10	$CH_3SCH_3 + ClO \longrightarrow CH_3SOCH_3 + Cl$	2	9.5×10^{-15}		
S 11	$CH_3SCH_3 + IO \longrightarrow CH_3SOCH_3 + I$	2	1.4×10^{-14}		
S 12	$CH_3SCH_2OO + NO \longrightarrow HCHO + CH_3S + NO_2$	2	4.9×10^{-12}	263	
S 13	$CH_3SCH_2OO + CH_3SCH_2OO \xrightarrow{O_2} 2\,HCHO + 2\,CH_3S$	2	1.0×10^{-11}		
S 14	$CH_3S + O_3 \longrightarrow CH_3SO + O_2$	2	1.15×10^{-12}	432	
S 15	$CH_3S + NO_2 \longrightarrow CH_3SO + NO$	2	3.0×10^{-11}	210	
S 16	$CH_3SO + NO_2 \xrightarrow{O_2} 0.82\,CH_3SO_2 + 0.18\,SO_2 + 0.18\,CH_3OO + NO$	2	1.2×10^{-11}		
S 17	$CH_3SO + O_3 \xrightarrow{O_2} CH_3SO_2$	2	6.0×10^{-13}		

Table 3: Continued

no	reaction	n	$A\,[(cm^{-3})^{1-n}s^{-1}]$	$-E_a/R\,[K]$	reference
S 18	$CH_3SO_2 \longrightarrow SO_2 + CH_3OO$	1	1.9×10^{13}	-8661	
S 19	$CH_3SO_2 + NO_2 \longrightarrow CH_3SO_3 + NO$	2	2.2×10^{-12}		
S 20	$CH_3SO_2 + O_3 \longrightarrow CH_3SO_3$	2	3×10^{-13}		
S 21	$CH_3SO_3 + HO_2 \longrightarrow CH_3SO_3H$	2	5×10^{-11}		
S 22	$CH_3SO_3 \xrightarrow{H_2O,O_2} CH_3OO + H_2SO_4$	1	1.36×10^{14}	-11071	
S 23	$CH_3SOCH_3 + OH \longrightarrow 0.95\,CH_3SO_2H + 0.95\,CH_3OO$ $+0.05\,DMSO_2$	2	8.7×10^{-11}		
S 24	$CH_3SO_2H + OH \longrightarrow 0.95\,CH_3SO_2 + 0.05\,CH_3SO_3H$ $+0.05\,HO_2 + H_2O$	2	9×10^{-11}		
S 25	$CH_3SO_2H + NO_3 \longrightarrow CH_3SO_2 + HNO_3$	2	1.0×10^{-13}		
Cl 1	$Cl + O_3 \longrightarrow ClO + O_2$	2	2.8×10^{-11}	-250	
Cl 2	$Cl + HO_2 \longrightarrow HCl + O_2$	2	1.8×10^{-11}	170	
Cl 3	$Cl + HO_2 \longrightarrow ClO + OH$	2	4.1×10^{-11}	-450	
Cl 4	$Cl + H_2O_2 \longrightarrow HCl + HO_2$	2	1.1×10^{-11}	-980	
Cl 5	$Cl + CH_3OO \longrightarrow 0.5\,ClO + 0.5\,HCHO + 0.5\,HO_2$ $+0.5\,HCl + 0.5\,CO + 0.5\,H_2O$	2	1.6×10^{-10}		
Cl 6	$Cl + CH_4 \xrightarrow{O_2} HCl + CH_3OO$	2	9.6×10^{-12}	-1360	
Cl 7	$Cl + C_2H_6 \xrightarrow{O_2} HCl + C_2H_5O_2$	2	7.7×10^{-11}	-90	
Cl 8	$Cl + C_2H_4 \xrightarrow{O_2} HCl + C_2H_5O_2$	2	1×10^{-10}		
Cl 9	$Cl + HCHO \xrightarrow{O_2} HCl + HO_2 + CO$	2	8.1×10^{-11}	-30	
Cl 10	$Cl + ROOH \longrightarrow CH_3OO + HCl$	2	5.7×10^{-11}		
Cl 11	$Cl + OClO \longrightarrow ClO + ClO$	2	3.2×10^{-11}	170	
Cl 12	$Cl + ClONO_2 \longrightarrow Cl_2 + NO_3$	2	6.5×10^{-12}	135	
Cl 13	$ClO + OH \longrightarrow Cl + HO_2$	2	7.4×10^{-12}	-270	
Cl 14	$ClO + OH \longrightarrow HCl + O_2$	2	6.0×10^{-13}	-230	
Cl 15	$ClO + HO_2 \longrightarrow HOCl + O_2$	2	2.2×10^{-12}	340	
Cl 16	$ClO + CH_3OO \longrightarrow Cl + HCHO + HO_2$	2	3.3×10^{-12}	-115	
Cl 17	$ClO + NO \longrightarrow Cl + NO_2$	2	6.2×10^{-12}	295	
Cl 18	$ClO + NO_2 \xrightarrow{M} ClONO_2$	3	[2]		M. Kanakidou, pers. comm.

Table 3: Continued

no	reaction	n	$A\,[(cm^{-3})^{1-n}s^{-1}]$	$-E_a/R\,[K]$	reference
Cl 19	$ClO + ClO \longrightarrow Cl_2O_2$	2	[2]		Atkison et al. (2006)
Cl 20	$ClO + ClO \longrightarrow Cl_2 + O_2$	2	1.0×10^{-12}	-1590	
Cl 21	$ClO + ClO \longrightarrow 2\,Cl + O_2$	2	3.0×10^{-11}	-2450	
Cl 22	$ClO + ClO \longrightarrow Cl + OClO$	2	3.5×10^{-13}	-1370	
Cl 23	$OClO + OH \longrightarrow HOCl + O_2$	2	4.5×10^{-13}	800	
Cl 24	$OClO + NO \longrightarrow ClO + NO_2$	2	1.1×10^{-13}	350	
Cl 25	$Cl_2O_2 \longrightarrow ClO + ClO$	1	[2]		M. Kanakidou, pers. comm.
Cl 26	$HOCl + OH \longrightarrow ClO + H_2O$	2	3.0×10^{-12}	-500	
Cl 27	$HCl + OH \longrightarrow H_2O + Cl$	2	1.8×10^{-12}	-240	
Cl 28	$ClNO_2 + OH \longrightarrow HOCl + NO_2$	2	2.4×10^{-12}	-1250	
Cl 29	$ClONO_2 + OH \longrightarrow 0.5\,ClO + 0.5\,HNO_3 + 0.5\,HOCl + 0.5\,NO_3$	2	1.2×10^{-12}	-330	
Cl 30	$ClONO_2 \longrightarrow ClO + NO_2$	1	[2]		M. Kanakidou, pers. comm.
Cl 31	$OClO + hv \xrightarrow{O_2,O_3} O_3 + ClO$	1	[1]		
Cl 32	$Cl_2O_2 + hv \longrightarrow Cl + Cl + O_2$	1	[1]		
Cl 33	$Cl_2 + hv \longrightarrow 2\,Cl$	1	[1]		
Cl 34	$HOCl + hv \longrightarrow Cl + OH$	1	[1]		
Cl 35	$ClNO_2 + hv \longrightarrow Cl + NO_2$	1	[1]		
Cl 36	$ClONO_2 + hv \longrightarrow Cl + NO_3$	1	[1]		
Br 1	$Br + O_3 \longrightarrow BrO + O_2$	2	1.7×10^{-11}	-800	
Br 2	$Br + HO_2 \longrightarrow HBr + O_2$	2	7.7×10^{-12}	-450	
Br 3	$Br + C_2H_4 \xrightarrow{O_2} HBr + C_2H_5O_2$	2	5×10^{-14}		
Br 4	$Br + HCHO \xrightarrow{O_2} HBr + CO + HO_2$	2	1.7×10^{-11}	-800	
Br 5	$Br + ROOH \longrightarrow CH_3OO + HBr$	2	2.66×10^{-12}	-1610	
Br 6	$Br + NO_2 \xrightarrow{M} BrNO_2$	3	[2]		Sander et al. (2006)
Br 7	$Br + BrONO_2 \longrightarrow Br_2 + NO_3$	2	4.9×10^{-11}		
Br 8	$BrO + OH \longrightarrow Br + HO_2$	2	1.8×10^{-11}	250	
Br 9	$BrO + HO_2 \longrightarrow HOBr + O_2$	2	4.5×10^{-12}	500	
Br 10	$BrO + CH_3OO \longrightarrow HOBr + HCHO$	2	4.1×10^{-12}		
Br 11	$BrO + CH_3OO \longrightarrow Br + HCHO + HO_2$	2	1.6×10^{-12}		

Table 3: Continued

no	reaction	n	$A\,[(cm^{-3})^{1-n}s^{-1}]$	$-E_a/R\,[K]$	reference
Br 12	$BrO + HCHO \xrightarrow{O_2} HOBr + CO + HO_2$	2	1.5×10^{-14}		
Br 13	$BrO + NO \longrightarrow Br + NO_2$	2	8.7×10^{-12}	260	
Br 14	$BrO + NO_2 \xrightarrow{M} BrONO_2$	3	[2]		Sander et al. (2006)
Br 15	$BrO + BrO \longrightarrow 2\,Br + O_2$	2	2.4×10^{-12}	40	
Br 16	$BrO + BrO \longrightarrow Br_2 + O_2$	2	2.9×10^{-14}	860	
Br 17	$HBr + OH \longrightarrow Br + H_2O$	2	5.5×10^{-12}	205	
Br 18	$BrONO_2 \longrightarrow BrO + NO_2$	1	[2]		M. Kanakidou, pers. comm.
Br 19	$BrO + hv \xrightarrow{O_2} Br + O_3$	1	[1]		
Br 20	$Br_2 + hv \longrightarrow 2\,Br$	1	[1]		
Br 21	$HOBr + hv \longrightarrow Br + OH$	1	[1]		
Br 22	$BrNO_2 + hv \longrightarrow Br + NO_2$	1	[1]		
Br 23	$BrONO_2 + hv \longrightarrow Br + NO_3$	1	[1]		
I 1	$I + O_3 \longrightarrow IO + O_2$	2	1.9×10^{-11}	-830	
I 2	$I + HO_2 \longrightarrow HI + O_2$	2	1.5×10^{-11}	-1090	
I 3	$I + NO_2 \xrightarrow{M} INO_2$	3	[2]		M. Kanakidou, pers. comm.
I 4	$I + NO_3 \longrightarrow IO + NO_2$	2	4.5×10^{-10}		
I 5	$I + I \longrightarrow I_2$	2	2.99×10^{-11}		
I 6	$IO + HO_2 \longrightarrow HOI + O_2$	2	1.4×10^{-11}	540	
I 7	$IO + NO \longrightarrow I + NO_2$	2	7.15×10^{-12}	300	
I 8	$IO + NO_2 \xrightarrow{M} IONO_2$	3	[2]		M. Kanakidou, pers. comm.
I 9	$IO + IO \longrightarrow OIO + I$	2	5.4×10^{-11}	180	
I 10	$OIO + OH \longrightarrow 0.5\,HOIO_2 + 0.5\,HOI$	2	2.0×10^{-10}		
I 11	$OIO + NO \longrightarrow NO_2 + IO$	2	5.1×10^{-13}	712	
I 12	$HI + OH \longrightarrow I + H_2O$	2	1.6×10^{-11}	440	
I 13	$HI + NO_3 \longrightarrow I + HNO_3$	2	1.3×10^{-12}	-1830	
I 14	$INO_2 \xrightarrow{M} I + NO_2$	2	2.4		
I 15	$IONO_2 \xrightarrow{M} IO + NO_2$	2	1.1×10^{15}	-12060	
I 16	$I_2 + OH \longrightarrow I + HOI$	2	2.1×10^{-10}		
I 17	$I_2 + NO_3 \longrightarrow I + IONO_2$	2	1.5×10^{-12}		

Table 3: Continued

no	reaction	n	$A\,[(cm^{-3})^{1-n}s^{-1}]$	$-E_a/R\,[K]$	reference
I 18	$CH_3I + OH \longrightarrow HCHO + I$	2	4.3×10^{-12}	-1120	
I 19	$C_3H_7I + OH \longrightarrow CH_3OO + I$	2	1.2×10^{-12}		
I 20	$IO + hv \xrightarrow{O_2} I + O_3$	1	[1]		
I 21	$OIO + hv \longrightarrow I + O_2$	1	0		Pechtl et al. (2006)
I 22	$HOI + hv \longrightarrow I + OH$	1	[1]		
I 23	$INO_2 + hv \longrightarrow I + NO_2$	1	[1]		
I 24	$IONO_2 + hv \longrightarrow I + NO_3$	1	[1]		$= BrONO_2$
I 25	$I_2 + hv \longrightarrow 2\,I$	1	[1]		
I 26	$CH_3I + hv \longrightarrow I + CH_3OO$	1	[1]		
I 27	$C_2H_5I + hv \longrightarrow I + ROOH$	1	[1]		$= CH_3I$
I 28	$C_3H_7I + hv \longrightarrow I + ROOH$	1	[1]		
I 29	$CH_2ClI + hv \longrightarrow I + Cl + 2\,HO_2 + CO$	1	[1]		
I 30	$CH_2BrI + hv \longrightarrow I + Br + 2\,HO_2 + CO$	1	[1]		
I 31	$CH_2I_2 + hv \longrightarrow I + IO + HCHO$	1	[1]		
Hx 1	$Cl + CH_3I \longrightarrow HCl + HCHO + I$	2	2.9×10^{-11}	-1000	
Hx 2	$Cl + BrCl \longrightarrow Br + Cl_2$	2	1.5×10^{-11}		
Hx 3	$Cl + Br_2 \longrightarrow BrCl + Br$	2	1.2×10^{-10}		
Hx 4	$I_2 + Cl \longrightarrow I + ICl$	2	2.09×10^{-10}		
Hx 5	$Br + OClO \longrightarrow BrO + ClO$	2	2.6×10^{-11}	-1300	
Hx 6	$Br + Cl_2 \longrightarrow BrCl + Cl$	2	1.1×10^{-15}		
Hx 7	$Br + BrCl \longrightarrow Br_2 + Cl$	2	3.3×10^{-15}		
Hx 8	$I_2 + Br \longrightarrow I + IBr$	2	1.2×10^{-10}		
Hx 9	$I + BrO \longrightarrow IO + Br$	2	1.2×10^{-11}		
Hx 10	$BrO + ClO \longrightarrow Br + OClO$	2	1.6×10^{-12}	430	
Hx 11	$BrO + ClO \longrightarrow Br + Cl + O_2$	2	2.9×10^{-12}	220	
Hx 12	$BrO + ClO \longrightarrow BrCl + O_2$	2	5.8×10^{-13}	170	
Hx 13	$IO + ClO \longrightarrow 0.8\,I + 0.55\,OClO + 0.45\,O_2 + 0.25\,Cl + 0.2\,ICl$	2	4.7×10^{-12}	280	
Hx 14	$IO + BrO \longrightarrow Br + 0.8\,OIO + 0.2\,I + 0.2\,O_2$	2	1.5×10^{-11}	510	
Hx 15	$BrCl + hv \longrightarrow Br + Cl$	1	[1]		
Hx 16	$ICl + hv \longrightarrow I + Cl$	1	[1]		

Table 3: Continued

no	reaction	n	$A\,[(cm^{-3})^{1-n}s^{-1}]$	$-E_a/R\,[K]$	reference
Hx 17	$IBr + hv \longrightarrow I + Br$	1	[1]		

n is the order of the reaction. [1] Photolysis rates are calculated for summer mid-day, in the mid-latitudes, using the PAPER model (Brühl and Crutzen, 1989; Landgraf and Crutzen, 1998), this maximum rate is then sinusiodally scaled using the in-built subroutine from KPP (Damian et al., 2002). [2] Special rate functions (pressure and/or humidity dependent). Notes: Self dissociation rates of N_2O_5 and HNO_4 are calculated by dividing their formation rates (reactions N9 and N6 respectively) by the equilibrium constants given in Sander et al. (2006). CH_3SCH_3 reacts with OH and O_2 to form CH_3SCH_2OO, however the second step of this process (that involving O_2) is extremely rapid, so it is assumed that the process is controlled only by the first reaction rate. The temperature dependence is $k = A \times \exp\left(\frac{-E_a}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right)$, where $T_0 = 298\,K$.

Table 4: Aqueous phase reactions

no	reaction	n	$k_0\,[(M^{1-n})s^{-1}]$	$-E_a/R\,[K]$	reference
O 1	$O_3 + OH \longrightarrow HO_2$	2	1.1×10^8		
O 2	$O_3 + O_2^- \longrightarrow OH + OH^-$	2	1.5×10^9		
O 3	$OH + OH \longrightarrow H_2O_2$	2	5.5×10^9		
O 4	$OH + HO_2 \longrightarrow H_2O$	2	7.1×10^9		
O 5	$OH + O_2^- \longrightarrow OH^-$	2	1.0×10^{10}		
O 6	$OH + H_2O_2 \longrightarrow HO_2$	2	2.7×10^7	-1684	
O 7	$HO_2 + HO_2 \longrightarrow H_2O_2$	2	9.7×10^5	-2500	
O 8	$HO_2 + O_2^- \xrightarrow{H^+} H_2O_2$	2	1.0×10^8	-900	
N 1	$HONO + OH \longrightarrow NO_2$	2	1.0×10^{10}		$=$ N7
N 2	$HONO + H_2O_2 \xrightarrow{H^+} HNO_3 + H^+$	3	4.6×10^3	-6800	
N 3	$NO_3 + OH^- \longrightarrow NO_3^- + OH$	2	8.2×10^7	-2700	
N 4	$NO_2 + NO_2 \longrightarrow HNO_3 + HONO$	2	1.0×10^8		
N 5	$NO_2 + HO_2 \longrightarrow HNO_4$	2	1.8×10^9		
N 6	$NO_2^- + O_3 \longrightarrow NO_3^- + O_2$	2	5.0×10^5	-6950	
N 7	$NO_2^- + OH \longrightarrow NO_2 + OH^-$	2	1.0×10^{10}		
N 8	$NO_4^- \longrightarrow NO_2^- + O_2$	1	8.0×10^{-1}		
C 1	$HCHO + OH \longrightarrow HCOOH + HO_2$	2	7.7×10^8	-1020	
C 2	$HCOOH + OH \longrightarrow HO_2 + CO_2$	2	1.1×10^8	-991	
C 3	$HCOO^- + OH \longrightarrow OH^- + HO_2 + CO_2$	2	3.1×10^9	-1240	
C 4	$CH_3OO + HO_2 \longrightarrow CH_3OOH$	2	4.3×10^5		
C 5	$CH_3OO + O_2^- \longrightarrow CH_3OOH + OH^-$	2	5.0×10^7		
C 6	$CH_3OH + OH \longrightarrow HCHO + HO_2$	2	9.7×10^8		
C 7	$CH_3OOH + OH \longrightarrow CH_3OO$	2	2.7×10^7	-1715	
C 8	$CH_3OOH + OH \longrightarrow HCHO + OH$	2	1.1×10^7	-1715	
C 9	$CO_3^- + O_2^- \longrightarrow HCO_3^- + OH^-$	2	6.5×10^8		
C 10	$CO_3^- + H_2O_2 \longrightarrow HCO_3^- + HO_2$	2	4.3×10^5		
C 11	$CO_3^- + HCOO^- \longrightarrow 2\,HCO_3^- + HO_2$	2	1.5×10^5		
C 12	$HCO_3^- + OH \longrightarrow CO_3^-$	2	8.5×10^6		
C 13	$DOM + OH \longrightarrow HO_2$	2	5.0×10^9		

Table 4: Continued

no	reaction	n	$k_0\,[(M^{1-n})s^{-1}]$	$-E_a/R\,[K]$	reference
S 1	$SO_3^- + O_2 \longrightarrow SO_5^-$	2	1.5×10^9		
S 2	$HSO_3^- + O_3 \longrightarrow SO_4^{2-} + H^+ + O_2$	2	3.7×10^5	-5500	
S 3	$SO_3^{2-} + O_3 \longrightarrow SO_4^{2-} + O_2$	2	1.5×10^9	-5300	
S 4	$HSO_3^- + OH \longrightarrow SO_3^-$	2	4.5×10^9		
S 5	$SO_3^{2-} + OH \longrightarrow SO_3^- + OH^-$	2	5.5×10^9		
S 6	$HSO_3^- + HO_2 \longrightarrow SO_4^{2-} + OH + H^+$	2	3.0×10^3		
S 7	$HSO_3^- + O_2^- \longrightarrow SO_4^{2-} + OH$	2	3.0×10^3		
S 8	$HSO_3^- + H_2O_2 \longrightarrow SO_4^{2-} + H^+$	2	$5.2\times10^6 \times \frac{[H^+]}{[H^+]+0.1M}$	-3650	
S 9	$HSO_3^- + NO_2 \xrightarrow{NO_2} HSO_4^- + HONO + HONO$	2	2.0×10^7		
S 10	$SO_3^{2-} + NO_2 \xrightarrow{NO_2} SO_4^{2-} + HONO + HONO$	2	2.0×10^7		
S 11	$HSO_3^- + NO_3 \longrightarrow SO_3^- + NO_3^- + H^+$	2	1.4×10^9	-2000	
S 12	$HSO_3^- + HNO_4 \longrightarrow HSO_4^- + NO_3^- + H^+$	2	3.1×10^5		
S 13	$HSO_3^- + CH_3OOH \xrightarrow{H^+} SO_4^{2-} + H^+ + CH_3OH$	3	1.6×10^7	-3800	
S 14	$SO_3^{2-} + CH_3OOH \xrightarrow{H^+} SO_4^{2-} + CH_3OH$	3	1.6×10^7	-3800	
S 15	$HSO_3^- + HCHO \longrightarrow CH_2OHSO_3^-$	2	4.3×10^{-1}		
S 16	$SO_3^{2-} + HCHO \xrightarrow{H^+} CH_2OHSO_3^-$	2	1.4×10^4		
S 17	$CH_2OHSO_3^- + OH^- \longrightarrow SO_3^{2-} + HCHO$	2	3.6×10^3		
S 18	$HSO_3^- + HSO_5^- \xrightarrow{H^+} SO_4^{2-} + SO_4^{2-} + H^+ + H^+$	2	7.1×10^6		
S 19	$SO_4^- + OH \longrightarrow HSO_5^-$	2	1.0×10^9		
S 20	$SO_4^- + HO_2 \longrightarrow SO_4^{2-} + H^+$	2	3.5×10^9		
S 21	$SO_4^- + O_2^- \longrightarrow SO_4^{2-}$	2	3.5×10^9		= S20
S 22	$SO_4^- + H_2O \longrightarrow SO_4^{2-} + H^+ + OH$	2	1.1×10^1	-1110	
S 23	$SO_4^- + H_2O_2 \longrightarrow SO_4^{2-} + H^+ + HO_2$	2	1.2×10^7		
S 24	$SO_4^- + NO_3^- \longrightarrow SO_4^{2-} + NO_3$	2	5.0×10^4		
S 25	$SO_4^- + HSO_3^- \longrightarrow SO_3^- + SO_4^{2-} + H^+$	2	8.0×10^8		
S 26	$SO_4^- + SO_3^{2-} \longrightarrow SO_3^- + SO_4^{2-}$	2	4.6×10^8		
S 27	$SO_4^{2-} + NO_3 \longrightarrow NO_3^- + SO_4^-$	2	1.0×10^5		
S 28	$SO_5^- + HSO_3^- \longrightarrow SO_4^- + SO_4^{2-} + H^+$	2	7.5×10^4		

Table 4: Continued

no	reaction	n	$k_0\,[(M^{1-n})s^{-1}]$	$-E_a/R\,[K]$	reference
S 29	$SO_5^- + SO_3^{2-} \longrightarrow SO_4^- + SO_4^{2-}$	2	9.4×10^6		
S 30	$SO_5^- + HSO_3^- \longrightarrow SO_3^- + HSO_5^-$	2	2.5×10^4		
S 31	$SO_5^- + SO_3^{2-} \xrightarrow{H^+} SO_3^- + HSO_5^-$	2	3.6×10^6		
S 32	$SO_5^- + O_2^- \xrightarrow{H^+} HSO_5^- + O_2$	2	2.3×10^8		
S 33	$SO_5^- + SO_5^- \longrightarrow 2\,SO_4^-$	2	1.0×10^8		
S 34	$DMS + O_3 \longrightarrow O_2 + DMSO$	2	8.6×10^8	-2600	
S 35	$DMS + OH \longrightarrow 0.5\,CH_3SO_3^- + 0.5\,CH_3OO$ $+0.5\,HSO_4^- + HCHO + H^+$	2	1.9×10^{10}		
S 36	$DMSO + OH \longrightarrow CH_3SO_2^- + CH_3OO + H^+$	2	4.5×10^9		
S 37	$CH_3SO_2^- + OH \longrightarrow CH_3SO_3^- + H_2O + O_2$	2	1.2×10^{10}		
S 38	$CH_3SO_3^- + OH \longrightarrow SO_4^{2-} + H^+ + CH_3OO$	2	1.2×10^7		
Cl 1	$Cl + H_2O_2 \longrightarrow HO_2 + Cl^- + H^+$	2	2.0×10^9		
Cl 2	$Cl + H_2O \longrightarrow H^+ + ClOH^-$	2	1.8×10^5		
Cl 3	$Cl + NO_3^- \longrightarrow NO_3 + Cl^-$	2	1.0×10^8		
Cl 4	$Cl + DOM \longrightarrow Cl^- + HO_2$	2	5.0×10^9		
Cl 5	$Cl + SO_4^{2-} \longrightarrow SO_4^- + Cl^-$	2	2.1×10^8		
Cl 6	$Cl + Cl \longrightarrow Cl_2$	2	8.8×10^7		
Cl 7	$Cl^- + OH \longrightarrow ClOH^-$	2	4.2×10^9		
Cl 8	$Cl^- + O_3 \longrightarrow ClO^- + O_2$	2	3.0×10^{-3}		
Cl 9	$Cl^- + NO_3 \longrightarrow NO_3^- + Cl$	2	9.3×10^6	-4330	
Cl 10	$Cl^- + SO_4^- \longrightarrow SO_4^{2-} + Cl$	2	2.5×10^8		
Cl 11	$Cl^- + HSO_5^- \longrightarrow HOCl + SO_4^{2-}$	2	1.8×10^{-3}	-7352	
Cl 12	$Cl^- + HOCl + H^+ \longrightarrow Cl_2$	3	2.2×10^4	-3508	
Cl 13	$Cl_2 \longrightarrow Cl^- + HOCl + H^+$	1	2.2×10^1	-8012	
Cl 14	$Cl_2^- + OH \longrightarrow HOCl + Cl^-$	2	1.0×10^9		
Cl 15	$Cl_2^- + OH^- \longrightarrow Cl^- + Cl^- + OH$	2	4.0×10^6		
Cl 16	$Cl_2^- + HO_2 \longrightarrow Cl^- + Cl^- + H^+ + O_2$	2	3.1×10^9		
Cl 17	$Cl_2^- + O_2^- \longrightarrow Cl^- + Cl^- + O_2$	2	6.0×10^9		
Cl 18	$Cl_2^- + H_2O_2 \longrightarrow Cl^- + Cl^- + H^+ + HO_2$	2	7.0×10^5	-3340	
Cl 19	$Cl_2^- + NO_2^- \longrightarrow Cl^- + Cl^- + NO_2$	2	6.0×10^7		

Table 4: Continued

no	reaction	n	$k_0\,[(M^{1-n})s^{-1}]$	$-E_a/R\,[K]$	reference
Cl 20	$Cl_2^- + CH_3OOH \longrightarrow Cl^- + Cl^- + H^+ + CH_3OO$	2	7.0×10^5	-3340	
Cl 21	$Cl_2^- + DOM \longrightarrow Cl^- + Cl^- + HO_2$	2	1.0×10^6		
Cl 22	$Cl_2^- + HSO_3^- \longrightarrow SO_3^- + Cl^- + Cl^- + H^+$	2	4.7×10^8	-1082	
Cl 23	$Cl_2^- + SO_3^{2-} \longrightarrow SO_3^- + Cl^- + Cl^-$	2	6.2×10^7		
Cl 24	$Cl_2^- + Cl_2^- \longrightarrow Cl_2 + 2\,Cl^-$	2	6.2×10^9		
Cl 25	$Cl_2^- + Cl \longrightarrow Cl^- + Cl_2$	2	2.7×10^9		
Cl 26	$Cl_2^- + DMS \longrightarrow 0.5\,CH_3SO_3^- + 0.5\,CH_3OO + 0.5\,HSO_4^-$ $+HCHO + 2\,Cl^- + 2\,H^+$	2	3.0×10^9		
Cl 27	$ClOH^- \longrightarrow Cl^- + OH$	1	6.0×10^9		
Cl 28	$ClOH^- + H^+ \longrightarrow Cl$	2	4.0×10^{10}		
Cl 29	$HOCl + HO_2 \longrightarrow Cl + O_2$	2	7.5×10^6		$=$ Cl30
Cl 30	$HOCl + O_2^- \longrightarrow Cl + OH^- + O_2$	2	7.5×10^6		
Cl 31	$HOCl + SO_3^{2-} \longrightarrow Cl^- + HSO_4^-$	2	7.6×10^8		
Cl 32	$HOCl + HSO_3^- \longrightarrow Cl^- + HSO_4^- + H^+$	2	7.6×10^8		$=$ Cl31
Cl 33	$Cl_2 + HO_2 \longrightarrow Cl_2^- + H^+ + O_2$	2	1.0×10^9		
Cl 34	$Cl_2 + O_2^- \longrightarrow Cl_2^- + O_2$	2	1.0×10^9		$=$ Cl33
Br 1	$Br + OH^- \longrightarrow BrOH^-$	2	1.3×10^{10}		
Br 2	$Br + DOM \longrightarrow Br^- + HO_2$	2	2.0×10^8		
Br 3	$Br^- + OH \longrightarrow BrOH^-$	2	1.1×10^{10}		
Br 4	$Br^- + O_3 \longrightarrow BrO^-$	2	2.1×10^2	-4450	
Br 5	$Br^- + NO_3 \longrightarrow Br + NO_3^-$	2	3.8×10^9		
Br 6	$Br^- + SO_4^- \longrightarrow Br + SO_4^{2-}$	2	2.1×10^9		
Br 7	$Br^- + HSO_5^- \longrightarrow HOBr + SO_4^{2-}$	2	1.0	-5338	
Br 8	$Br^- + HOBr + H^+ \longrightarrow Br_2$	3	1.6×10^{10}		
Br 9	$Br_2 \longrightarrow Br^- + HOBr + H^+$	1	9.7×10^1	7457	
Br 10	$Br_2^- + O_2^- \longrightarrow Br^- + Br^-$	2	1.7×10^8		
Br 11	$Br_2^- + HO_2 \longrightarrow Br_2 + H_2O_2 - H^+$	2	4.4×10^9		
Br 12	$Br_2^- + H_2O_2 \longrightarrow Br^- + Br^- + H^+ + HO_2$	2	5.0×10^2		
Br 13	$Br_2^- + Br_2^- \longrightarrow Br^- + Br^- + Br_2$	1	1.9×10^9		
Br 14	$Br_2^- + CH_3OOH \longrightarrow Br^- + Br^- + H^+ + CH_3OO$	2	1.0×10^5		

Table 4: Continued

no	reaction	n	$k_0\,[(M^{1-n})s^{-1}]$	$-E_a/R\,[K]$	reference
Br 15	$Br_2^- + DOM \longrightarrow Br^- + Br^- + HO_2$	2	1.0×10^5		
Br 16	$Br_2^- + NO_2^- \longrightarrow Br^- + Br^- + NO_2$	2	1.7×10^7	-1720	
Br 17	$Br_2^- + HSO_3^- \longrightarrow Br^- + Br^- + H^+ + SO_3^-$	2	6.3×10^7	-782	
Br 18	$Br_2^- + SO_3^{2-} \longrightarrow Br^- + Br^- + SO_3^-$	2	2.2×10^8	-650	
Br 19	$Br_2^- + DMS \longrightarrow 0.5\,CH_3SO_3^- + 0.5\,CH_3OO + 0.5\,HSO_4^- + HCHO + 2\,Br^- + 2\,H^+$	2	3.2×10^9		
Br 20	$BrOH^- \longrightarrow Br^- + OH$	1	3.3×10^7		
Br 21	$BrOH^- \longrightarrow Br + OH^-$	1	4.2×10^6		
Br 22	$BrOH^- + H^+ \longrightarrow Br$	2	4.4×10^{10}		
Br 23	$BrOH^- + Br^- \longrightarrow Br_2^- + OH^-$	2	1.9×10^8		
Br 24	$BrO^- + SO_3^{2-} \longrightarrow Br^- + SO_4^{2-}$	2	1.0×10^8		
Br 25	$HOBr + HO_2 \longrightarrow Br + O_2$	2	1.0×10^9		
Br 26	$HOBr + O_2^- \longrightarrow Br + OH^- + O_2$	2	3.5×10^9		
Br 27	$HOBr + H_2O_2 \longrightarrow Br^- + H^+ + O_2$	2	1.2×10^6		
Br 28	$HOBr + SO_3^{2-} \longrightarrow Br^- + HSO_4^-$	2	5.0×10^9		
Br 29	$HOBr + HSO_3^- \longrightarrow Br^- + HSO_4^- + H^+$	2	5.0×10^9		$=$ Br28
Br 30	$Br_2 + HO_2 \longrightarrow Br_2^- + H^+ + O_2$	2	1.1×10^8		
Br 31	$Br_2 + O_2^- \longrightarrow Br_2^- + O_2$	2	5.6×10^9		
I 1	$HOI + I^- + H^+ \longrightarrow I_2$	3	4.4×10^{12}		
I 2	$HOI + Cl^- + H^+ \longrightarrow ICl$	3	2.9×10^{10}		
I 3	$ICl \longrightarrow HOI + Cl^- + H^+$	1	2.4×10^6		
I 4	$HOI + Br^- + H^+ \longrightarrow IBr$	3	3.3×10^{12}		
I 5	$IBr \longrightarrow HOI + H^+ + Br^-$	1	8.0×10^5		
I 6	$HOCl + I^- + H^+ \longrightarrow ICl$	3	3.5×10^{11}		
I 7	$HOBr + I^- \longrightarrow IBr + OH^-$	2	5.0×10^9		
I 8	$IO_2^- + H_2O_2 \longrightarrow IO_3^-$	2	6.0×10^1		
I 9	$IO + IO \longrightarrow HOI + IO_2^- + H^+$	2	1.5×10^9		
I 10	$I^- + O_3 \xrightarrow{H^+} HOI$	2	4.2×10^9	-9311	
I 11	$HOI + Cl_2 \longrightarrow IO_2^- + 2\,Cl^- + 3\,H^+$	2	1.0×10^6		
I 12	$HOI + HOCl \longrightarrow IO_2^- + Cl^- + 2\,H^+$	2	5.0×10^5		

Table 4: Continued

no	reaction	n	$k_0\,[(M^{1-n})s^{-1}]$	$-E_a/R\,[K]$	reference
I 13	$HOI + HOBr \longrightarrow IO_2^- + Br^- + 2\,H^+$	2	1.0×10^6		
I 14	$IO_2^- + HOCl \longrightarrow IO_3^- + Cl^- + H^+$	2	1.5×10^3		
I 15	$IO_2^- + HOBr \longrightarrow IO_3^- + Br^- + H^+$	2	1.0×10^6		
I 16	$IO_2^- + HOI \longrightarrow IO_3^- + I^- + H^+$	2	6.0×10^2		
I 17	$I_2 + HSO_3^- \longrightarrow 2\,I^- + HSO_4^- + 2\,H^+$	2	1.0×10^6		
Hx 1	$Br^- + HOCl + H^+ \longrightarrow BrCl$	3	1.3×10^6		
Hx 2	$Cl^- + HOBr + H^+ \longrightarrow BrCl$	3	2.3×10^{10}		
Hx 3	$BrCl \longrightarrow Cl^- + HOBr + H^+$	1	3.0×10^6		
Hx 4	$Br^- + ClO^- + H^+ \longrightarrow BrCl + OH^-$	3	3.7×10^{10}		
Hx 5	$Cl_2 + Br^- \longrightarrow BrCl_2^-$	2	7.7×10^9		
Hx 6	$BrCl_2^- \longrightarrow Cl_2 + Br^-$	1	1.83×10^3		
hv 1	$O_3 + hv \longrightarrow OH + OH + O_2$	1	[1]		assumed 2× gas phase
hv 2	$H_2O_2 + hv \longrightarrow OH + OH$	1	[1]		assumed 2× gas phase
hv 3	$NO_3^- + hv \xrightarrow{H^+} NO_2 + OH$	1	[1]		
hv 4	$NO_2^- + hv \xrightarrow{H^+} NO + OH$	1	[1]		
hv 5	$HOCl + hv \longrightarrow OH + Cl$	1	[1]		assumed 2× gas phase
hv 6	$Cl_2 + hv \longrightarrow Cl + Cl$	1	[1]		assumed 2× gas phase
hv 7	$HOBr + hv \longrightarrow OH + Br$	1	[1]		assumed 2× gas phase
hv 8	$Br_2 + hv \longrightarrow Br + Br$	1	[1]		assumed 2× gas phase
hv 9	$BrCl + hv \longrightarrow Cl + Br$	1	[1]		assumed 2× gas phase

n is the order of the reaction. The temperature dependence is $k = k_0 \times \exp\left(\frac{-E_a}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right)$, where $T_0 = 298\,\mathrm{K}$.

Table 5: Heterogeneous reactions

no	reaction	k	reference
H 1	$N_2O_5 \xrightarrow{H_2O} HNO_{3aq} + HNO_{3aq}$	$\overline{k_t}(N_2O_5)w_{l,i}[H_2O]/\mathrm{Het}_T$	
H 2	$N_2O_5 \xrightarrow{Cl^-} ClNO_2 + NO_3^-$	$\overline{k_t}(N_2O_5)w_{l,i}f(Cl^-)[Cl^-]/\mathrm{Het}_T$	
H 3	$N_2O_5 \xrightarrow{Br^-} BrNO_2 + NO_3^-$	$\overline{k_t}(N_2O_5)w_{l,i}f(Br^-)[Br^-]/\mathrm{Het}_T$	
H 4	$ClONO_2 \xrightarrow{H_2O} HOCl_{aq} + HNO_{3aq}$	$\overline{k_t}(ClONO_2)w_{l,i}[H_2O]/\mathrm{Het}_T$	see note
H 5	$ClONO_2 \xrightarrow{Cl^-} Cl_{2aq} + NO_3^-$	$\overline{k_t}(ClONO_2)w_{l,i}(Cl^-)[Cl^-]/\mathrm{Het}_T$	see note
H 6	$ClONO_2 \xrightarrow{Br^-} BrCl_{aq} + NO_3^-$	$\overline{k_t}(ClONO_2)w_{l,i}(Br^-)[Br^-]/\mathrm{Het}_T$	see note
H 7	$BrONO_2 \xrightarrow{H_2O} HOBr_{aq} + HNO_{3aq}$	$\overline{k_t}(BrONO_2)w_{l,i}[H_2O]/\mathrm{Het}_T$	see note
H 8	$BrONO_2 \xrightarrow{Cl^-} BrCl_{aq} + NO_3^-$	$\overline{k_t}(BrONO_2)w_{l,i}(Cl^-)[Cl^-]/\mathrm{Het}_T$	see note
H 9	$BrONO_2 \xrightarrow{Br^-} Br_{2aq} + NO_3^-$	$\overline{k_t}(BrONO_2)w_{l,i}(Br^-)[Br^-]/\mathrm{Het}_T$	see note
H 10	$IONO_2 \xrightarrow{H_2O} HOI_{aq} + HNO_{3aq}$	$\overline{k_t}(IONO_2)w_{l,i}$	
H 11	$HI \xrightarrow{H_2O} H^+ + I^-$	$\overline{k_t}(HI)w_{l,i}$	
H 12	$INO_2 \xrightarrow{H_2O} HOI_{aq} + HONO_{aq}$	$\overline{k_t}(INO_2)w_{l,i}$	
H 13	$OIO \xrightarrow{H_2O} HOI_{aq} + HO_{2aq}$	$\overline{k_t}(H_2O)w_{l,i}$	
H 14	$HIO_3 \xrightarrow{H_2O} IO_3^- + H^+$	$\overline{k_t}(HIO_3)w_{l,i}$	

For a definition of $\overline{k_t}$ and $w_{l,i}$ see Sander (1999). $\mathrm{Het}_T = [H_2O] + f(Cl^-)[Cl^-] + f(Br^-)[Br^-]$, with $f(Cl^-) = 5.0 \times 10^2$ and $f(Br^-) = 3.0 \times 10^5$. H4–H9: the total rate is determined by $\overline{k_t}$, the distribution among the different reaction paths was assumed to be the same as for reactions H1–H3.

Table 6: Aqueous phase equilibrium constants

no	reaction	m	n	$K_0\,[\mathrm{M^{n-m}}]$	$-\Delta H/R[\mathrm{K}]$	reference
EQ 1	$\mathrm{CO_{2aq} \rightleftharpoons H^+ + HCO_3^-}$	1	2	4.3×10^{-7}	-913	
EQ 2	$\mathrm{NH_{3aq} \rightleftharpoons OH^- + NH_4^+}$	1	2	1.7×10^{-5}	-4325	
EQ 3	$\mathrm{H_2O_{aq} \rightleftharpoons H^+ + OH^-}$	1	2	1.0×10^{-14}	-6716	
EQ 4	$\mathrm{HCOOH_{aq} \rightleftharpoons H^+ + HCOO^-}$	1	2	1.8×10^{-4}		
EQ 5	$\mathrm{HSO_3^- \rightleftharpoons H^+ + SO_3^{2-}}$	1	2	6.0×10^{-8}	1120	
EQ 6	$\mathrm{H_2SO_{4aq} \rightleftharpoons H^+ + HSO_4^-}$	1	2	1.0×10^{3}		
EQ 7	$\mathrm{HSO_4^- \rightleftharpoons H^+ + SO_4^{2-}}$	1	2	1.2×10^{-2}	1120	
EQ 8	$\mathrm{HO_{2aq} \rightleftharpoons O_2^- + H^+}$	1	2	1.6×10^{-5}		
EQ 9	$\mathrm{SO_{2aq} \rightleftharpoons H^+ + HSO_3^-}$	1	2	1.7×10^{-2}	2090	
EQ 10	$\mathrm{Cl_2^- \rightleftharpoons Cl_{aq} + Cl^+}$	1	2	5.2×10^{-6}		
EQ 11	$\mathrm{HOCl_{aq} \rightleftharpoons H^+ + ClO^-}$	1	2	3.2×10^{-8}		
EQ 12	$\mathrm{HBr_{aq} \rightleftharpoons H^+ + Br^-}$	1	2	1.0×10^{9}		
EQ 13	$\mathrm{Br_2^- \rightleftharpoons Br_{aq} + Br^-}$	1	2	9.1×10^{-6}		
EQ 14	$\mathrm{HOBr_{aq} \rightleftharpoons H^+ + BrO^-}$	1	2	2.3×10^{-9}	-3091	
EQ 15	$\mathrm{BrCl_{aq} + Cl^- \rightleftharpoons BrCl_2^-}$	2	1	3.8	1143	
EQ 16	$\mathrm{BrCl_{aq} + Br^- \rightleftharpoons Br_2Cl^-}$	2	1	1.8×10^{4}		
EQ 17	$\mathrm{Br_{2aq} + Cl^- \rightleftharpoons Br_2Cl^-}$	2	1	1.3		
EQ 18	$\mathrm{HNO_{3aq} \rightleftharpoons H^+ + NO_3^-}$	1	2	1.5×10^{1}		
EQ 19	$\mathrm{HCl_{aq} \rightleftharpoons H^+ + Cl^-}$	1	2	1.7×10^{6}		
EQ 20	$\mathrm{HONO_{aq} \rightleftharpoons H^+ + NO_2^-}$	1	2	5.1×10^{-4}	-1260	
EQ 21	$\mathrm{HNO_{4aq} \rightleftharpoons NO_4^- + H^+}$	1	2	1.0×10^{-5}	8700	
EQ 22	$\mathrm{ICl_{aq} + Cl^- \rightleftharpoons ICl_2^-}$	2	1	7.7×10^{1}		
EQ 23	$\mathrm{IBr_{aq} + Br^- \rightleftharpoons IBr_2^-}$	2	1	2.9×10^{2}		
EQ 24	$\mathrm{ICl_{aq} + Br^- \rightleftharpoons IClBr^-}$	2	1	1.8×10^{4}		assumed = EQ 16
EQ 25	$\mathrm{IBr_{aq} + Cl^- \rightleftharpoons IClBr^-}$	2	1	1.3		assumed = EQ 17

The temperature dependence is $K = K_0 \times \exp\left(\frac{-E_a}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right)$, where $T_0 = 298\,\mathrm{K}$.

Table 7: Henry Law coefficients

species	K_H^0[M/atm]	$-\Delta_{soln}H/R$[K]	reference	α^0	reference
O_3	1.2×10^{-2}	2560		0.002	
O_2	1.3×10^{-3}	1500		0.01	estimated by Pechtl et al. (2006)
OH	3.0×10^{1}	4300		0.01	
HO_2	3.9×10^{3}	5900		0.2	
H_2O_2	1.0×10^{5}	6338		0.077	
NO_2	6.4×10^{-3}	2500		0.0015	
NO_3	2.0	2000		0.04	
N_2O_5	∞	—		0.03	Behnke et al. (1997), see note
				0.003	estimated by Allan et al. (1999), see note
HONO	4.9×10^{1}	4780		0.04	
HNO_3	1.7×10^{5}	8694		0.5	
HNO_4	1.2×10^{4}	6900		0.1	
NH_3	5.8×10^{1}	4085		0.06	
CH_3OO	6.0	$= HO_2$		0.01	estimated by Pechtl et al. (2006)
ROOH	3.0×10^{2}	5322		0.0046	
HCHO	7.0×10^{3}	6425		0.04	
HCOOH	3.7×10^{3}	5700		0.014	
CO_2	3.1×10^{-2}	2423		0.01	estimated by Pechtl et al. (2006)
HCl	1.2	9001		0.074	
HOCl	6.7×10^{2}	5862		= HOBr	estimated by Pechtl et al. (2006)
$ClONO_2$	∞	—		0.1	
Cl_2	9.1×10^{-2}	2500		0.038	
HBr	1.3	10239		0.031	
HOBr	9.3×10^{1}	= HOCl		0.5	
$BrONO_2$	∞	—		0.8	
Br_2	7.6×10^{-1}	4094		0.038	
BrCl	9.4×10^{-1}	5600		$= Cl_2$	estimated by Pechtl et al. (2006)
DMSO	5.0×10^{4}	= HCHO		0.048	
$DMSO_2$	∞	—	assumed by Pechtl et al. (2006)	0.03	
SO_2	1.2	3120		0.11	

Table 7: Continued

species	K_H^0[M/atm]	$-\Delta_{soln}H/R$[K]	reference	α^0	reference
H_2SO_4	∞	—		0.65	
CH_3SO_2H	∞	—	assumed by Pechtl et al. (2006)	0.0002	
CH_3SO_3H	∞	—	assumed by Pechtl et al. (2006)	0.076	
HI	∞	—		0.036	
IO	4.5×10^2	= HOI		0.5	
HOI	4.5×10^2	= HOCl		HOBr	estimated by Pechtl et al. (2006)
INO_2	∞	—		0.2	
$IONO_2$	∞	—		0.2	
I_2	3.0	4431		0.01	
ICl	1.1×10^2	= BrCl		0.01	
IBr	2.4×10^1	= BrCl		0.01	
OIO	∞	—		1	estimated by Pechtl et al. (2006)
HIO_3	∞	—		0.01	estimated by Pechtl et al. (2006)

The temperature dependence for the Henry Law constants is $K_H = K_H^0 \times \exp\left(\frac{-\Delta_{soln}H}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right)$, where $T_0 = 298\,\mathrm{K}$.

No temperature dependence is considered for accommodation coefficients. Notes: The accommodation coefficient for N_2O_5 is determined based on the composition of the condensed-phase. For the seasalt mode a value of 0.03 is used (Behnke et al., 1997), while the lower value of 0.003 is used for the non-seasalt mode (after estimations made by Allan et al., 1999).

References

Allan, B. J., Carslaw, N., Coe, H., Burgess, R. A., and Plane, J. M. C.: Observations of the Nitrate Radical in the Marine Boundary Layer, Journal of Atmospheric Chemistry, 33, 129–154, 1999.

Atkison, R., Cox, R. A., Crowley, J. N., R. F. Hampson, J., Hynes, R. G., Jenkin, M. E., Kerr, J. A., Rossi, M. J., and Troe, J.: Summary of Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry, URL `http://www.iupac-kinetic.ch.cam.ac.uk`, 2006.

Behnke, W., George, C., Scheer, V., and Zetzsch, C.: Production and decay of $ClNO_2$ from the reaction of gaseous N_2O_5 with $NaCl$ solution: Bulk and aerosol experiments, Journal of Geophysical Research, 102, 3795–3804, 1997.

Brühl, C. and Crutzen, P. J.: On the disproportionate role of tropospheric ozone as a filter against solar UV-B radiation, Geophysical Research Letters, 16, 703–706, 1989.

Damian, V., Sandu, A., Damian, M., Potra, F., and Carmichael, G. R.: The Kinetic PreProcessor KPP — A Software Environment for Solving Chemical Kinetics, Computers and Chemical Engineering, 26, 1567–1579, 2002.

Jayne, J. T., Pöschl, U., min Chen, Y., Dai, D., Molina, L. T., Worsnop, D. R., Kolb, C. E., and Molina, M. J.: Pressure and Temperature Dependence of the Gas-Phase Reaction of SO_3 with H_2O and the Heterogeneous Reaction of SO_2 with H_2O/H_2SO_4 Surfaces, Journal of Physical Chemistry A., 101, 10 000–10 011, 1997.

Landgraf, J. and Crutzen, P. J.: An efficient method for online calculations of photolysis and heating rates, Journal of Atmospheric Science, 55, 863–878, 1998.

Pechtl, S., Lovejoy, E. R., Burkholder, J. B., and von Glasow, R.: Modeling the possible role of iodine oxides in atmospheric new particle formations, Atmospheric Chemistry and Physics, 6, 505–523, 2006.

Sander, R.: Modeling atmospheric chemistry: interactions between gas-phase species and liquid cloud/aerosol particles, Surveys in Geophysics, 20, 1–31, 1999.

Sander, S. P., Friedl, R. R., Ravishankara, A. R., Golden, D. M., Kolb, C. E., Kurylo, M. J., Molina, M. J., Moortgat, G. K., Keller-Rudek, H., Finlayson-Pitts, B. J., Wine, P. H., Huie, R. E., and Orkin, V. L.: Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Evaluation number 15, JPL Publication 06-02, Pasadena, 2006.