

The Chemical Mechanism of SCAV

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<http://www.geosci-model-dev-discuss.net>

Table 1: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
H1000f	TrAraSc	$O_2 \rightarrow O_2(aq)$	$k_{\text{exf}}(KPP_O2)$	see note
H1000b	TrAraSc	$O_2(aq) \rightarrow O_2$	$k_{\text{exb}}(KPP_O2)$	see note
H1001f	TrAraMblScScm	$O_3 \rightarrow O_3(aq)$	$k_{\text{exf}}(KPP_O3)$	see note
H1001b	TrAraMblScScm	$O_3(aq) \rightarrow O_3$	$k_{\text{exb}}(KPP_O3)$	see note
H2100f	TrAraSc	$OH \rightarrow OH(aq)$	$k_{\text{exf}}(KPP_OH)$	see note
H2100b	TrAraSc	$OH(aq) \rightarrow OH$	$k_{\text{exb}}(KPP_OH)$	see note
H2101f	TrAraSc	$HO_2 \rightarrow HO_2(aq)$	$k_{\text{exf}}(KPP_HO2)$	see note
H2101b	TrAraSc	$HO_2(aq) \rightarrow HO_2$	$k_{\text{exb}}(KPP_HO2)$	see note
H2102f	TrAraMblScScm	$H_2O_2 \rightarrow H_2O_2(aq)$	$k_{\text{exf}}(KPP_H2O2)$	see note
H2102b	TrAraMblScScm	$H_2O_2(aq) \rightarrow H_2O_2$	$k_{\text{exb}}(KPP_H2O2)$	see note
H3100f	TrAraNSc	$NO \rightarrow NO(aq)$	$k_{\text{exf}}(KPP_NO)$	see note
H3100b	TrAraNSc	$NO(aq) \rightarrow NO$	$k_{\text{exb}}(KPP_NO)$	see note
H3101f	TrAraNSc	$NO_2 \rightarrow NO_2(aq)$	$k_{\text{exf}}(KPP_NO2)$	see note
H3101b	TrAraNSc	$NO_2(aq) \rightarrow NO_2$	$k_{\text{exb}}(KPP_NO2)$	see note
H3102f	TrAraNSc	$NO_3 \rightarrow NO_3(aq)$	$k_{\text{exf}}(KPP_NO3)$	see note
H3102b	TrAraNSc	$NO_3(aq) \rightarrow NO_3$	$k_{\text{exb}}(KPP_NO3)$	see note
H3200f	TrAraNMblScScm	$NH_3 \rightarrow NH_3(aq)$	$k_{\text{exf}}(KPP_NH3)$	see note
H3200b	TrAraNMblScScm	$NH_3(aq) \rightarrow NH_3$	$k_{\text{exb}}(KPP_NH3)$	see note
H3201	TrAraMblNScScm	$N_2O_5 \rightarrow HNO_3(aq) + HNO_3(aq)$	$k_{\text{exf}}_N2O5* C(KPP_H2O_1)$	Behnke et al. (1994), Behnke et al. (1997)
H3202f	TrAraNSc	$HONO \rightarrow HONO(aq)$	$k_{\text{exf}}(KPP_HONO)$	see note
H3202b	TrAraNSc	$HONO(aq) \rightarrow HONO$	$k_{\text{exb}}(KPP_HONO)$	see note
H3203f	TrAraMblNScScm	$HNO_3 \rightarrow HNO_3(aq)$	$k_{\text{exf}}(KPP_HNO3)$	see note
H3203b	TrAraMblNScScm	$HNO_3(aq) \rightarrow HNO_3$	$k_{\text{exb}}(KPP_HNO3)$	see note
H3204f	TrAraNSc	$HNO_4 \rightarrow HNO_4(aq)$	$k_{\text{exf}}(KPP_HNO4)$	see note
H3204b	TrAraNSc	$HNO_4(aq) \rightarrow HNO_4$	$k_{\text{exb}}(KPP_HNO4)$	see note
H4100f	TrAraMblScScm	$CO_2 \rightarrow CO_2(aq)$	$k_{\text{exf}}(KPP_CO2)$	see note
H4100b	TrAraMblScScm	$CO_2(aq) \rightarrow CO_2$	$k_{\text{exb}}(KPP_CO2)$	see note
H4101f	TrAraScScm	$HCHO \rightarrow HCHO(aq)$	$k_{\text{exf}}(KPP_HCHO)$	see note
H4101b	TrAraScScm	$HCHO(aq) \rightarrow HCHO$	$k_{\text{exb}}(KPP_HCHO)$	see note
H4102f	TrAraSc	$CH_3O_2 \rightarrow CH_3OO(aq)$	$k_{\text{exf}}(KPP_CH3O2)$	see note
H4102b	TrAraSc	$CH_3OO(aq) \rightarrow CH_3O_2$	$k_{\text{exb}}(KPP_CH3O2)$	see note
H4103f	TrAraScScm	$HCOOH \rightarrow HCOOH(aq)$	$k_{\text{exf}}(KPP_HCOOH)$	see note
H4103b	TrAraScScm	$HCOOH(aq) \rightarrow HCOOH$	$k_{\text{exb}}(KPP_HCOOH)$	see note
H4104f	TrAraScScm	$CH_3OOH \rightarrow CH_3OOH(aq)$	$k_{\text{exf}}(KPP_CH3OOH)$	see note

Table 1: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
H4104b	TrAraScScm	$\text{CH}_3\text{OOH}(\text{aq}) \rightarrow \text{CH}_3\text{OOH}$	$k_{\text{exb}}(\text{KPP_CH3OOH})$	see note
H4105f	TrAraSc	$\text{CH}_3\text{OH} \rightarrow \text{CH}_3\text{OH}(\text{aq})$	$k_{\text{exf}}(\text{KPP_CH3OH})$	see note
H4105b	TrAraSc	$\text{CH}_3\text{OH}(\text{aq}) \rightarrow \text{CH}_3\text{OH}$	$k_{\text{exb}}(\text{KPP_CH3OH})$	see note
H4200f	TrAraCScScm	$\text{CH}_3\text{COOH} \rightarrow \text{CH}_3\text{COOH}(\text{aq})$	$k_{\text{exf}}(\text{KPP_CH3CO2H})$	see note
H4200b	TrAraCScScm	$\text{CH}_3\text{COOH}(\text{aq}) \rightarrow \text{CH}_3\text{COOH}$	$k_{\text{exb}}(\text{KPP_CH3CO2H})$	see note
H4201f	TrAraCSc	$\text{CH}_3\text{CHO} \rightarrow \text{CH}_3\text{CHO}(\text{aq})$	$k_{\text{exf}}(\text{KPP_CH3CHO})$	see note
H4201b	TrAraCSc	$\text{CH}_3\text{CHO}(\text{aq}) \rightarrow \text{CH}_3\text{CHO}$	$k_{\text{exb}}(\text{KPP_CH3CHO})$	see note
H4202f	TrAraCSc	$\text{PAN} \rightarrow \text{PAN}(\text{aq})$	$k_{\text{exf}}(\text{KPP_PAN})$	see note
H4202b	TrAraCSc	$\text{PAN}(\text{aq}) \rightarrow \text{PAN}$	$k_{\text{exb}}(\text{KPP_PAN})$	see note
H4300f	TrAraCSc	$\text{CH}_3\text{COCH}_3 \rightarrow \text{CH}_3\text{COCH}_3(\text{aq})$	$k_{\text{exf}}(\text{KPP_CH3COCH3})$	see note
H4300b	TrAraCSc	$\text{CH}_3\text{COCH}_3(\text{aq}) \rightarrow \text{CH}_3\text{COCH}_3$	$k_{\text{exb}}(\text{KPP_CH3COCH3})$	see note
H6000f	TrAraClMblSc	$\text{Cl}_2 \rightarrow \text{Cl}_2(\text{aq})$	$k_{\text{exf}}(\text{KPP_Cl2})$	see note
H6000b	TrAraClMblSc	$\text{Cl}_2(\text{aq}) \rightarrow \text{Cl}_2$	$k_{\text{exb}}(\text{KPP_Cl2})$	see note
H6200f	TrAraClMblScScm	$\text{HCl} \rightarrow \text{HCl}(\text{aq})$	$k_{\text{exf}}(\text{KPP_HCl})$	see note
H6200b	TrAraClMblScScm	$\text{HCl}(\text{aq}) \rightarrow \text{HCl}$	$k_{\text{exb}}(\text{KPP_HCl})$	see note
H6201f	TrAraClMblSc	$\text{HOCl} \rightarrow \text{HOCl}(\text{aq})$	$k_{\text{exf}}(\text{KPP_HOCl})$	see note
H6201b	TrAraClMblSc	$\text{HOCl}(\text{aq}) \rightarrow \text{HOCl}$	$k_{\text{exb}}(\text{KPP_HOCl})$	see note
H7000f	TrAraBrMblSc	$\text{Br}_2 \rightarrow \text{Br}_2(\text{aq})$	$k_{\text{exf}}(\text{KPP_Br2})$	see note
H7000b	TrAraBrMblSc	$\text{Br}_2(\text{aq}) \rightarrow \text{Br}_2$	$k_{\text{exb}}(\text{KPP_Br2})$	see note
H7200f	TrAraBrMblScScm	$\text{HBr} \rightarrow \text{HBr}(\text{aq})$	$k_{\text{exf}}(\text{KPP_HBr})$	see note
H7200b	TrAraBrMblScScm	$\text{HBr}(\text{aq}) \rightarrow \text{HBr}$	$k_{\text{exb}}(\text{KPP_HBr})$	see note
H7201f	TrAraBrMblSc	$\text{HOBr} \rightarrow \text{HOBr}(\text{aq})$	$k_{\text{exf}}(\text{KPP_HOBr})$	see note
H7201b	TrAraBrMblSc	$\text{HOBr}(\text{aq}) \rightarrow \text{HOBr}$	$k_{\text{exb}}(\text{KPP_HOBr})$	see note
H7600f	TrAraClBrMblSc	$\text{BrCl} \rightarrow \text{BrCl}(\text{aq})$	$k_{\text{exf}}(\text{KPP_BrCl})$	see note
H7600b	TrAraClBrMblSc	$\text{BrCl}(\text{aq}) \rightarrow \text{BrCl}$	$k_{\text{exb}}(\text{KPP_BrCl})$	see note
H9100f	TrAraSMblScScm	$\text{SO}_2 \rightarrow \text{SO}_2(\text{aq})$	$k_{\text{exf}}(\text{KPP_SO2})$	see note
H9100b	TrAraSMblScScm	$\text{SO}_2(\text{aq}) \rightarrow \text{SO}_2$	$k_{\text{exb}}(\text{KPP_SO2})$	see note
H9200	TrAraSMblScScm	$\text{H}_2\text{SO}_4 \rightarrow \text{H}_2\text{SO}_4(\text{aq})$	$k_{\text{exf}}(\text{KPP_H2SO4})$	see note
H9400f	TrAraSSc	$\text{DMSO} \rightarrow \text{DMSO}(\text{aq})$	$k_{\text{exf}}(\text{KPP_DMSO})$	see note
H9400b	TrAraSSc	$\text{DMSO}(\text{aq}) \rightarrow \text{DMSO}$	$k_{\text{exb}}(\text{KPP_DMSO})$	see note
H9401	TrAraSMblSc	$\text{CH}_3\text{SO}_3\text{H} \rightarrow \text{CH}_3\text{SO}_3^-(\text{aq}) + \text{H}^+(\text{aq})$	$k_{\text{exf}}(\text{KPP_CH3SO3H})$	see note
H9400f	TrAraSMblScScm	$\text{SO}_2\text{t} \rightarrow \text{SO}_2\text{t}$	$k_{\text{exf}}(\text{KPP_SO2t})$	see note
H9400b	TrAraSMblScScm	$\text{SO}_2\text{t} \rightarrow \text{SO}_2\text{t}$	$k_{\text{exb}}(\text{KPP_SO2t})$	see note
H9450f	TrAraSMblScScm	$\text{NH}_5\text{OW} \rightarrow \text{NH}_5\text{OW}$	$k_{\text{exf}}(\text{KPP_NH5OW})$	see note
H9450b	TrAraSMblScScm	$\text{NH}_5\text{OW} \rightarrow \text{NH}_5\text{OW}$	$k_{\text{exb}}(\text{KPP_NH5OW})$	see note

*Notes:

The forward (**k_exf**) and backward (**k_exb**) rate coefficients are calculated in the file **messy_scarb_base.f90** using the accommodation coefficients in subroutine **scav_alpha** and Henry's law constants in subroutine **scav_henry**.

k_{mt} = mass transfer coefficient

lwc = liquid water content of aerosol mode

$f_{het}(X, Y) = k_{mt}(X) \times lwc \times f(Y)[Y]/Het_T$, with $f(H_2O) = 1$, $f(Cl^-) = 5.0E2$, and $f(Br^-) = 3.0E5$, $[Y]$ = concentration of Y; $Het_T = [H_2O] + f(Cl^-)[Cl^-] + f(Br^-)[Br^-]$

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).

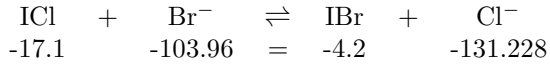
H7301, H7302, H7602: The total uptake is determined by $k_{mt}(BrNO_3)$. The relative rates are assumed to be the same as for N_2O_5 (H3201, H6300, H7300).

Table 2: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
EQ20	TrAraSc	$\text{HO}_2 \rightleftharpoons \text{O}_2^- + \text{H}^+$	1.6E-5		Weinstein-Lloyd and Schwartz (1991)
EQ21	TrAraMblScScm	$\text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{OH}^-$	1.0E-16	-6716	Chameides (1984)
EQ30	TrAraMblNScScm	$\text{NH}_4^+ \rightleftharpoons \text{H}^+ + \text{NH}_3$	5.88E-10	-2391	Chameides (1984)
EQ31	TrAraNSc	$\text{HONO} \rightleftharpoons \text{H}^+ + \text{NO}_2^-$	5.1E-4	-1260	Schwartz and White (1981)
EQ32	TrAraMblNScScm	$\text{HNO}_3 \rightleftharpoons \text{H}^+ + \text{NO}_3^-$	15	8700	Davis and de Bruin (1964)
EQ33	TrAraNSc	$\text{HNO}_4 \rightleftharpoons \text{NO}_4^- + \text{H}^+$	1.E-5		Warneck (1999)
EQ40	TrAraMblScScm	$\text{CO}_2 \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$	4.3E-7	-913	Chameides (1984)
EQ41	TrAraScScm	$\text{HCOOH} \rightleftharpoons \text{H}^+ + \text{HCOO}^-$	1.8E-4		Weast (1980)
EQ42	TrAraCScScm	$\text{CH}_3\text{COOH} \rightleftharpoons \text{H}^+ + \text{CH}_3\text{COO}^-$	1.75E-5	-46	see note
EQ61	TrAraClMblScScm	$\text{HCl} \rightleftharpoons \text{H}^+ + \text{Cl}^-$	1.7E6	6896	Marsh and McElroy (1985)
EQ62	TrAraClSc	$\text{HOCl} \rightleftharpoons \text{H}^+ + \text{ClO}^-$	3.2E-8		Lax (1969)
EQ71	TrAraBrMblScScm	$\text{HBr} \rightleftharpoons \text{H}^+ + \text{Br}^-$	1.0E9		Lax (1969)
EQ72	TrAraBrSc	$\text{HOBr} \rightleftharpoons \text{H}^+ + \text{BrO}^-$	2.3E-9	-3091	Kelley and Tartar (1956)
EQ90	TrAraSMblScScm	$\text{SO}_2 \rightleftharpoons \text{H}^+ + \text{HSO}_3^-$	1.7E-2	2090	Chameides (1984)
EQ91	TrAraSMblScScm	$\text{HSO}_3^- \rightleftharpoons \text{H}^+ + \text{SO}_3^{2-}$	6.0E-8	1120	Chameides (1984)
EQ92	TrAraSMblScScm	$\text{HSO}_4^- \rightleftharpoons \text{H}^+ + \text{SO}_4^{2-}$	1.2E-2	2720	Seinfeld and Pandis (1998)
EQ93	TrAraSMblScScm	$\text{H}_2\text{SO}_4 \rightleftharpoons \text{H}^+ + \text{HSO}_4^-$	1.0E3		Seinfeld and Pandis (1998)

*Notes:

EQ82 and EQ83: Thermodynamic calculations on the IBr/ICl equilibrium according to the data tables from Wagman et al. (1982):



$$\frac{\Delta G}{[\text{kJ/mol}]} = -4.2 - 131.228 - (-17.1 - 103.96) = -14.368$$

$$K = \frac{[\text{IBr}] \times [\text{Cl}^-]}{[\text{ICl}] \times [\text{Br}^-]} = \exp\left(\frac{-\Delta G}{RT}\right) = \exp\left(\frac{14368}{8.314 \times 298}\right) = 330$$

This means we have equal amounts of IBr and ICl when the $[\text{Cl}^-]/[\text{Br}^-]$ ratio equals 330.

Table 3: Aqueous phase reactions

#	labels	reaction	k_0 [$M^{1-n}s^{-1}$]	$-E_a/R[K]$	reference
A1000	TrAraSc	$O_3 + O_2^- \rightarrow OH + OH^-$	1.5E9		Sehested et al. (1983)
A2100	TrAraSc	$OH + O_2^- \rightarrow OH^-$	1.0E10		Sehested et al. (1968)
A2101	TrAraSc	$OH + OH \rightarrow H_2O_2$	5.5E9		Buxton et al. (1988)
A2102	TrAraSc	$HO_2 + O_2^- \rightarrow H_2O_2 + OH^-$	1.0E8	-900	Christensen and Sehested (1988)
A2103	TrAraSc	$HO_2 + OH \rightarrow H_2O$	7.1E9		Sehested et al. (1968)
A2104	TrAraSc	$HO_2 + HO_2 \rightarrow H_2O_2$	9.7E5	-2500	Christensen and Sehested (1988)
A2105	TrAraSc	$H_2O_2 + OH \rightarrow HO_2$	2.7E7	-1684	Christensen et al. (1982)
A3100	TrAraNSc	$NO_2^- + O_3 \rightarrow NO_3^-$	5.0E5	-6950	Damschen and Martin (1983)
A3101	TrAraNSc	$NO_2 + NO_2 \rightarrow HNO_3 + HONO$	1.0E8		Lee and Schwartz (1981)
A3102	TrAraNSc	$NO_4^- \rightarrow NO_2^-$	8.0E1		Warneck (1999)
A3200	TrAraNSc	$NO_2 + HO_2 \rightarrow HNO_4$	1.8E9		Warneck (1999)
A3201	TrAraNSc	$NO_2^- + OH \rightarrow NO_2 + OH^-$	1.0E10		Wingenter et al. (1999)
A3202	TrAraNSc	$NO_3 + OH^- \rightarrow NO_3^- + OH$	8.2E7	-2700	Exner et al. (1992)
A3203	TrAraNSc	$HONO + OH \rightarrow NO_2$	1.0E10		Barker et al. (1970)
A3204	TrAraNSc	$HONO + H_2O_2 \rightarrow HNO_3$	4.6E3	-6800	Damschen and Martin (1983)
A4100	TrAraSc	$CO_3^- + O_2^- \rightarrow HCO_3^- + OH^-$	6.5E8		Ross et al. (1992)
A4101	TrAraSc	$CO_3^- + H_2O_2 \rightarrow HCO_3^- + HO_2$	4.3E5		Ross et al. (1992)
A4102	TrAraSc	$HCOO^- + CO_3^- \rightarrow 2 HCO_3^- + HO_2$	1.5E5		Ross et al. (1992)
A4103	TrAraSc	$HCOO^- + OH \rightarrow OH^- + HO_2 + CO_2$	3.1E9	-1240	Chin and Wine (1994)
A4104	TrAraSc	$HCO_3^- + OH \rightarrow CO_3^-$	8.5E6		Ross et al. (1992)
A4105	TrAraSc	$HCHO + OH \rightarrow HCOOH + HO_2$	7.7E8	-1020	Chin and Wine (1994)
A4106	TrAraSc	$HCOOH + OH \rightarrow HO_2 + CO_2$	1.1E8	-991	Chin and Wine (1994)
A4107	TrAraSc	$CH_3OO + O_2^- \rightarrow CH_3OOH + OH^-$	5.0E7		Jacob (1986)
A4108	TrAraSc	$CH_3OO + HO_2 \rightarrow CH_3OOH$	4.3E5		Jacob (1986)
A4109	TrAraSc	$CH_3OH + OH \rightarrow HCHO + HO_2$	9.7E8		Buxton et al. (1988)
A4110a	TrAraSc	$CH_3OOH + OH \rightarrow CH_3OO$	2.7E7	-1715	Jacob (1986)
A4110b	TrAraSc	$CH_3OOH + OH \rightarrow HCHO + OH$	1.1E7	-1715	Jacob (1986)
A9100	TrAraSSc	$SO_3^- + O_2 \rightarrow SO_5^-$	1.5E9		Huie and Neta (1987)
A9101	TrAraSMblScScm	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-}$	1.5E9	-5300	Hoffmann (1986)
A9102	TrAraSSc	$SO_4^- + O_2^- \rightarrow SO_4^{2-}$	3.5E9		Jiang et al. (1992)
A9103	TrAraSSc	$SO_4^- + SO_3^{2-} \rightarrow SO_3^- + SO_4^{2-}$	4.6E8		Huie and Neta (1987)
A9104	TrAraSSc	$SO_5^- + O_2^- \rightarrow HSO_5^- + OH^-$	2.3E8		Buxton et al. (1996)
A9200	TrAraSSc	$SO_3^{2-} + OH \rightarrow SO_3^- + OH^-$	5.5E9		Buxton et al. (1988)
A9201	TrAraSSc	$SO_4^- + OH \rightarrow HSO_5^-$	1.0E9		Jiang et al. (1992)

Table 3: Aqueous phase reactions (...continued)

#	labels	reaction	k_0 [$M^{1-n}s^{-1}$]	$-E_a/R[K]$	reference
A9202	TrAraSSc	$SO_4^{2-} + HO_2 \rightarrow SO_4^{2-} + H^+$	3.5E9		Jiang et al. (1992)
A9203	TrAraSSc	$SO_4^{2-} + H_2O \rightarrow SO_4^{2-} + H^+ + OH$	1.1E1	-1110	Herrmann et al. (1995)
A9204	TrAraSSc	$SO_4^{2-} + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2$	1.2E7		Wine et al. (1989)
A9205	TrAraSSc	$HSO_3^- + O_2^- \rightarrow SO_4^{2-} + OH$	3.0E3		see note
A9206	TrAraSMblScScm	$HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+$	3.7E5	-5500	Hoffmann (1986)
A9207	TrAraSSc	$HSO_3^- + OH \rightarrow SO_3^-$	4.5E9		Buxton et al. (1988)
A9208	TrAraSSc	$HSO_3^- + HO_2 \rightarrow SO_4^{2-} + OH + H^+$	3.0E3		see note
A9209	TrAraSMblScScm	$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$	5.2E6	-3650	Martin and Damschen (1981)
A9210	TrAraSSc	$HSO_3^- + SO_4^{2-} \rightarrow SO_3^- + SO_4^{2-} + H^+$	8.0E8		Huie and Neta (1987)
A9212	TrAraSSc	$HSO_3^- + HSO_5^- \rightarrow 2 SO_4^{2-} + 2 H^+$	7.1E6		Betterton and Hoffmann (1988)
A9300	TrAraSSc	$SO_3^{2-} + NO_2 \rightarrow SO_4^{2-} + 2 HONO - NO_2$	2.0E7		Clifton et al. (1988)
A9301	TrAraSSc	$SO_4^{2-} + NO_3^- \rightarrow SO_4^{2-} + NO_3$	5.0E4		Exner et al. (1992)
A9302	TrAraSSc	$SO_4^{2-} + NO_3 \rightarrow NO_3^- + SO_4^{2-}$	1.0E5		Logager et al. (1993)
A9303	TrAraSSc	$HSO_3^- + NO_2 \rightarrow HSO_4^- + 2 HONO - NO_2$	2.0E7		Clifton et al. (1988)
A9304	TrAraSSc	$HSO_3^- + NO_3 \rightarrow SO_3^- + NO_3^- + H^+$	1.4E9	-2000	Exner et al. (1992)
A9305	TrAraSSc	$HSO_3^- + HNO_4 \rightarrow HSO_4^- + NO_3^- + H^+$	3.1E5		Warneck (1999)
A9400	TrAraSSc	$SO_3^{2-} + HCHO \rightarrow CH_2OH SO_3^- + OH^-$	1.4E4		Boyce and Hoffmann (1984)
A9401	TrAraSSc	$SO_3^{2-} + CH_3OOH \rightarrow SO_4^{2-} + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A9402	TrAraSSc	$HSO_3^- + HCHO \rightarrow CH_2OH SO_3^-$	4.3E-1		Boyce and Hoffmann (1984)
A9403	TrAraSSc	$HSO_3^- + CH_3OOH \rightarrow SO_4^{2-} + H^+ + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A9404	TrAraSSc	$CH_2OH SO_3^- + OH^- \rightarrow SO_3^{2-} + HCHO$	3.6E3		Seinfeld and Pandis (1998)

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 $Br_2^- + H_2O_2$.

A9106: see also: (Huie and Neta, 1987; Warneck, 1991). If this reaction produces a lot of SO_4^{2-} , it will have an effect. However, we currently assume only the stable $S_2O_8^{2-}$ as product.

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

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

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).

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

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

Table 4: Photolysis reactions

#	labels	reaction	rate coefficient	reference
PH2100	TrAraScJ	$\text{H}_2\text{O}_2 + h\nu \rightarrow 2 \text{ OH}$	$\text{JX}(\text{ip_H202}) * 2.33$	see note

*Notes: J-values are calculated with an external module and then supplied to the SCAV chemistry

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