The Chemical Mechanism of SCAV

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“The 1-way on-line coupled model system MECO(n) – Part 4: Chemical evaluation (based on MESSy v2.52)”
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Table 1: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
H1000f	TrAraSc	$O_2 \rightarrow O_2(aq)$	`k_exf(KPP_O2)`	see note
H1000b	TrAraSc	$O_2(aq) \rightarrow O_2$	`k_exb(KPP_O2)`	see note
H1001f	TrAraMblScScm	$O_3 \rightarrow O_3(aq)$	`k_exf(KPP_O3)`	see note
H1001b	TrAraMblScScm	$O_3(aq) \rightarrow O_3$	`k_exb(KPP_O3)`	see note
H2100f	TrAraSc	$OH \rightarrow OH(aq)$	`k_exf(KPP_OH)`	see note
H2100b	TrAraSc	$OH(aq) \rightarrow OH$	`k_exb(KPP_OH)`	see note
H2101f	TrAraSc	$HO_2 \rightarrow HO_2(aq)$	`k_exf(KPP_HO2)`	see note
H2101b	TrAraSc	$HO_2(aq) \rightarrow HO_2$	`k_exb(KPP_HO2)`	see note
H2102f	TrAraMblScScm	$H_2O_2 \rightarrow H_2O_2(aq)$	`k_exf(KPP_H2O2)`	see note
H2102b	TrAraMblScScm	$H_2O_2(aq) \rightarrow H_2O_2$	`k_exb(KPP_H2O2)`	see note
H3100f	TrAraNSc	$NO \rightarrow NO(aq)$	`k_exf(KPP_NO)`	see note
H3100b	TrAraNSc	$NO(aq) \rightarrow NO$	`k_exb(KPP_NO)`	see note
H3101f	TrAraNSc	$NO_2 \rightarrow NO_2(aq)$	`k_exf(KPP_NO2)`	see note
H3101b	TrAraNSc	$NO_2(aq) \rightarrow NO_2$	`k_exb(KPP_NO2)`	see note
H3102f	TrAraNSc	$NO_3 \rightarrow NO_3(aq)$	`k_exf(KPP_NO3)`	see note
H3102b	TrAraNSc	$NO_3(aq) \rightarrow NO_3$	`k_exb(KPP_NO3)`	see note
H3200f	TrAraNMblScScm	$NH_3 \rightarrow NH_3(aq)$	`k_exf(KPP_NH3)`	see note
H3200b	TrAraNMblScScm	$NH_3(aq) \rightarrow NH_3$	`k_exb(KPP_NH3)`	see note
H3201	TrAraMblNScScm	$N_2O_5 \rightarrow HNO_3(aq) + HNO_3(aq)$	`k_exf_N2O5*C(KPP_H2O_l)`	Behnke et al. (1994), Behnke et al. (1997)
H3202f	TrAraNSc	$HONO \rightarrow HONO(aq)$	`k_exf(KPP_HONO)`	see note
H3202b	TrAraNSc	$HONO(aq) \rightarrow HONO$	`k_exb(KPP_HONO)`	see note
H3203f	TrAraMblNScScm	$HNO_3 \rightarrow HNO_3(aq)$	`k_exf(KPP_HNO3)`	see note

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#	labels	reaction	rate coefficient	reference
H3203b	TrAraMblNScScm	$HNO_3(aq) \rightarrow HNO_3$	`k_exb(KPP_HNO3)`	see note
H3204f	TrAraNSc	$HNO_4 \rightarrow HNO_4(aq)$	`k_exf(KPP_HNO4)`	see note
H3204b	TrAraNSc	$HNO_4(aq) \rightarrow HNO_4$	`k_exb(KPP_HNO4)`	see note
H4100f	TrAraMblScScm	$CO_2 \rightarrow CO_2(aq)$	`k_exf(KPP_CO2)`	see note
H4100b	TrAraMblScScm	$CO_2(aq) \rightarrow CO_2$	`k_exb(KPP_CO2)`	see note
H4101f	TrAraScScm	$HCHO \rightarrow HCHO(aq)$	`k_exf(KPP_HCHO)`	see note
H4101b	TrAraScScm	$HCHO(aq) \rightarrow HCHO$	`k_exb(KPP_HCHO)`	see note
H4102f	TrAraSc	$CH_3O_2 \rightarrow CH_3OO(aq)$	`k_exf(KPP_CH3O2)`	see note
H4102b	TrAraSc	$CH_3OO(aq) \rightarrow CH_3O_2$	`k_exb(KPP_CH3O2)`	see note
H4103f	TrAraScScm	$HCOOH \rightarrow HCOOH(aq)$	`k_exf(KPP_HCOOH)`	see note
H4103b	TrAraScScm	$HCOOH(aq) \rightarrow HCOOH$	`k_exb(KPP_HCOOH)`	see note
H4104f	TrAraScScm	$CH_3OOH \rightarrow CH_3OOH(aq)$	`k_exf(KPP_CH3OOH)`	see note
H4104b	TrAraScScm	$CH_3OOH(aq) \rightarrow CH_3OOH$	`k_exb(KPP_CH3OOH)`	see note
H4105f	TrAraSc	$CH_3OH \rightarrow CH_3OH(aq)$	`k_exf(KPP_CH3OH)`	see note
H4105b	TrAraSc	$CH_3OH(aq) \rightarrow CH_3OH$	`k_exb(KPP_CH3OH)`	see note
H4200f	TrAraCScScm	$CH_3COOH \rightarrow CH_3COOH(aq)$	`k_exf(KPP_CH3CO2H)`	see note
H4200b	TrAraCScScm	$CH_3COOH(aq) \rightarrow CH_3COOH$	`k_exb(KPP_CH3CO2H)`	see note
H4201f	TrAraCSc	$CH_3CHO \rightarrow CH_3CHO(aq)$	`k_exf(KPP_CH3CHO)`	see note
H4201b	TrAraCSc	$CH_3CHO(aq) \rightarrow CH_3CHO$	`k_exb(KPP_CH3CHO)`	see note
H4202f	TrAraCSc	$PAN \rightarrow PAN(aq)$	`k_exf(KPP_PAN)`	see note
H4202b	TrAraCSc	$PAN(aq) \rightarrow PAN$	`k_exb(KPP_PAN)`	see note
H4300f	TrAraCSc	$CH_3COCH_3 \rightarrow CH_3COCH_3(aq)$	`k_exf(KPP_CH3COCH3)`	see note
H4300f	TrAraCSc	$CH_3COCH_3(aq) \rightarrow CH_3COCH_3$	`k_exb(KPP_CH3COCH3)`	see note
H6000f	TrAraClMblSc	$Cl_2 \rightarrow Cl_2(aq)$	`k_exf(KPP_Cl2)`	see note
H6000b	TrAraClMblSc	$Cl_2(aq) \rightarrow Cl_2$	`k_exb(KPP_Cl2)`	see note
H6200f	TrAraClMblScScm	$HCl \rightarrow HCl(aq)$	`k_exf(KPP_HCl)`	see note
H6200b	TrAraClMblScScm	$HCl(aq) \rightarrow HCl$	`k_exb(KPP_HCl)`	see note
H6201f	TrAraClMblSc	$HOCl \rightarrow HOCl(aq)$	`k_exf(KPP_HOCl)`	see note
H6201b	TrAraClMblSc	$HOCl(aq) \rightarrow HOCl$	`k_exb(KPP_HOCl)`	see note
H7000f	TrAraBrMblSc	$Br_2 \rightarrow Br_2(aq)$	`k_exf(KPP_Br2)`	see note
H7000b	TrAraBrMblSc	$Br_2(aq) \rightarrow Br_2$	`k_exb(KPP_Br2)`	see note
H7200f	TrAraBrMblScScm	$HBr \rightarrow HBr(aq)$	`k_exf(KPP_HBr)`	see note
H7200b	TrAraBrMblScScm	$HBr(aq) \rightarrow HBr$	`k_exb(KPP_HBr)`	see note
H7201f	TrAraBrMblSc	$HOBr \rightarrow HOBr(aq)$	`k_exf(KPP_HOBr)`	see note
H7201b	TrAraBrMblSc	$HOBr(aq) \rightarrow HOBr$	`k_exb(KPP_HOBr)`	see note

Table 1: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
H7600f	TrAraClBrMblSc	$BrCl \rightarrow BrCl(aq)$	`k_exf(KPP_BrCl)`	see note
H7600b	TrAraClBrMblSc	$BrCl(aq) \rightarrow BrCl$	`k_exb(KPP_BrCl)`	see note
H9100f	TrAraSMblScScm	$SO_2 \rightarrow SO_2(aq)$	`k_exf(KPP_SO2)`	see note
H9100b	TrAraSMblScScm	$SO_2(aq) \rightarrow SO_2$	`k_exb(KPP_SO2)`	see note
H9200	TrAraSMblScScm	$H_2SO_4 \rightarrow H_2SO_4(aq)$	`k_exf(KPP_H2SO4)`	see note
H9400f	TrAraSSc	$DMSO \rightarrow DMSO(aq)$	`k_exf(KPP_DMSO)`	see note
H9400b	TrAraSSc	$DMSO(aq) \rightarrow DMSO$	`k_exb(KPP_DMSO)`	see note
H9401	TrAraSMblSc	$CH_3SO_3H \rightarrow CH_3SO_3^-(aq) + H^+(aq)$	`k_exf(KPP_CH3SO3H)`	see note
H9400f	TrAraSMblScScm	SO2t → SO2t	`k_exf(KPP_SO2t)`	see note
H9400b	TrAraSMblScScm	SO2t → SO2t	`k_exb(KPP_SO2t)`	see note
H9450f	TrAraSMblScScm	NH50W → NH50W	`k_exf(KPP_NH50W)`	see note
H9450b	TrAraSMblScScm	NH50W → NH50W	`k_exb(KPP_NH50W)`	see note

*Notes:

The forward (`k_exf`) and backward (`k_exb`) rate coefficients are calculated in the file `messy_scav_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

$fhet(X,Y) = k_{mt}(X) \times lwc \times f(Y)[Y]/Het_T$, 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 eqilibria

#	labels	reaction	$K_0[M^{m-n}]$	-$\Delta H/R[K]$	reference
EQ20	TrAraSc	$HO_2 \rightleftharpoons O_2^- + H^+$	1.6E-5		Weinstein-Lloyd and Schwartz (1991)
EQ21	TrAraMblScScm	$H_2O \rightleftharpoons H^+ + OH^-$	1.0E-16	-6716	Chameides (1984)
EQ30	TrAraMblNScScm	$NH_4^+ \rightleftharpoons H^+ + NH_3$	5.88E-10	-2391	Chameides (1984)
EQ31	TrAraNSc	$HONO \rightleftharpoons H^+ + NO_2^-$	5.1E-4	-1260	Schwartz and White (1981)
EQ32	TrAraMblNScScm	$HNO_3 \rightleftharpoons H^+ + NO_3^-$	15	8700	Davis and de Bruin (1964)
EQ33	TrAraNSc	$HNO_4 \rightleftharpoons NO_4^- + H^+$	1.E-5		Warneck (1999)
EQ40	TrAraMblScScm	$CO_2 \rightleftharpoons H^+ + HCO_3^-$	4.3E-7	-913	Chameides (1984)
EQ41	TrAraScScm	$HCOOH \rightleftharpoons H^+ + HCOO^-$	1.8E-4		Weast (1980)
EQ42	TrAraCScScm	$CH_3COOH \rightleftharpoons H^+ + CH_3COO^-$	1.75E-5	-46	see note
EQ61	TrAraClMblScScm	$HCl \rightleftharpoons H^+ + Cl^-$	1.7E6	6896	Marsh and McElroy (1985)
EQ62	TrAraClSc	$HOCl \rightleftharpoons H^+ + ClO^-$	3.2E-8		Lax (1969)
EQ71	TrAraBrMblScScm	$HBr \rightleftharpoons H^+ + Br^-$	1.0E9		Lax (1969)
EQ72	TrAraBrSc	$HOBr \rightleftharpoons H^+ + BrO^-$	2.3E-9	-3091	Kelley and Tartar (1956)
EQ90	TrAraSMblScScm	$SO_2 \rightleftharpoons H^+ + HSO_3^-$	1.7E-2	2090	Chameides (1984)
EQ91	TrAraSMblScScm	$HSO_3^- \rightleftharpoons H^+ + SO_3^{2-}$	6.0E-8	1120	Chameides (1984)
EQ92	TrAraSMblScScm	$HSO_4^- \rightleftharpoons H^+ + SO_4^{2-}$	1.2E-2	2720	Seinfeld and Pandis (1998)
EQ93	TrAraSMblScScm	$H_2SO_4 \rightleftharpoons H^+ + HSO_4^-$	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):

ICl	+	Br^-	$\rightleftharpoons$	IBr	+	Cl^-
-17.1		-103.96	=	-4.2		-131.228

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

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

This means we have equal amounts of IBr and ICl when the $[Cl^-]/[Br^-]$ 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	$SO_4^- + HO_2 \rightarrow SO_4^{2-} + H^+$	3.5E9		Jiang et al. (1992)
A9203	TrAraSSc	$SO_4^- + H_2O \rightarrow SO_4^{2-} + H^+ + OH$	1.1E1	-1110	Herrmann et al. (1995)
A9204	TrAraSSc	$SO_4^- + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2$	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	$HSO_3^- + SO_4^- \rightarrow SO_3^- + SO_4^{2-} + H^+$	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	$SO_4^- + NO_3^- \rightarrow SO_4^{2-} + NO_3$	5.0E4		Exner et al. (1992)
A9302	TrAraSSc	$SO_4^{2-} + NO_3 \rightarrow NO_3^- + SO_4^-$	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	$SO_3^{2-} + HCHO \rightarrow CH_2OHSO_3^- + OH^-$	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	$HSO_3^- + HCHO \rightarrow CH_2OHSO_3^-$	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	$CH_2OHSO_3^- + OH^- \rightarrow SO_3^{2-} + HCHO$	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^-, 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	$H_2O_2 + h\nu \rightarrow 2\ OH$	`JX(ip_H2O2)*2.33`	see note

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

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