

# The Chemical Mechanism of SCAV

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Table 1: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
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
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
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)
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
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
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
H4104b	TrAraScScm	$CH_3OOH(aq) \rightarrow CH_3OOH$	$k_{\text{exb}}(KPP\_CH3OOH)$	see note
H4200f	TrAraCScScm	$CH_3COOH \rightarrow CH_3COOH(aq)$	$k_{\text{exf}}(KPP\_CH3COOH)$	see note
H4200b	TrAraCScScm	$CH_3COOH(aq) \rightarrow CH_3COOH$	$k_{\text{exb}}(KPP\_CH3COOH)$	see note
H6200f	TrAraClMblScScm	$HCl \rightarrow HCl(aq)$	$k_{\text{exf}}(KPP\_HCl)$	see note
H6200b	TrAraClMblScScm	$HCl(aq) \rightarrow HCl$	$k_{\text{exb}}(KPP\_HCl)$	see note
H7200f	TrAraBrMblScScm	$HBr \rightarrow HBr(aq)$	$k_{\text{exf}}(KPP\_HBr)$	see note
H7200b	TrAraBrMblScScm	$HBr(aq) \rightarrow HBr$	$k_{\text{exb}}(KPP\_HBr)$	see note
H9100f	TrAraSMblScScm	$SO_2 \rightarrow SO_2(aq)$	$k_{\text{exf}}(KPP\_SO2)$	see note
H9100b	TrAraSMblScScm	$SO_2(aq) \rightarrow SO_2$	$k_{\text{exb}}(KPP\_SO2)$	see note
H9200	TrAraSMblScScm	$H_2SO_4 \rightarrow H_2SO_4(aq)$	$k_{\text{exf}}(KPP\_H2SO4)$	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`. The rate coefficients are determined with the help of  $k_{\text{mt}}$ , the mass transfer coefficient, the Henry coefficient and the LWC (liquid water content) of the droplets, both in clouds and precipitation.

Table 2: Acid-base and other equilibria

#	labels	reaction	$K_0 [M^{m-n}]$	$-\Delta H/R[K]$	reference
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)
EQ32	TrAraMblNScScm	$\text{HNO}_3 \rightleftharpoons \text{H}^+ + \text{NO}_3^-$	15	8700	Davis and de Bruin (1964)
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)
EQ71	TrAraBrMblScScm	$\text{HBr} \rightleftharpoons \text{H}^+ + \text{Br}^-$	1.0E9		Lax (1969)
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)

Table 3: Aqueous phase reactions

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A9101	TrAraSMblScScm	$\text{SO}_3^{2-} + \text{O}_3 \rightarrow \text{SO}_4^{2-}$	1.5E9	-5300	Hoffmann (1986)
A9206	TrAraSMblScScm	$\text{HSO}_3^- + \text{O}_3 \rightarrow \text{SO}_4^{2-} + \text{H}^+$	3.7E5	-5500	Hoffmann (1986)
A9209	TrAraSMblScScm	$\text{HSO}_3^- + \text{H}_2\text{O}_2 \rightarrow \text{SO}_4^{2-} + \text{H}^+$	5.2E6	-3650	Martin and Damschen (1981)

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