ELECTRONIC SUPPLEMENT FOR
Modeling chemistry in and above snow at Summit, Greenland
Part 1: Model description and results

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SUPPLEMENT INCLUDES:
Gas and aqueous species included in the model, henry constants, accommodation coefficients, gas phase reaction rates, and aqueous phase reaction rates, and sensitivity run plots.

Table 1: A complete list of all gas and aqueous phase species included in the MISTRA-SNOW model.

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 (i.e., CH_3CHO), CH_2O_2, $HOCH_2O_2$, CH_3CO_3, CH_3O_2, $C_2H_5O_2$, CH_3O_2, EO_2 (i.e., $H_2C(OH)CH_2OO$), CH_2O_2, ROOH (i.e., alkylhydroperoxides)
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 $ClNO_2$, $ClNO_3$
Br, BrO, HBr, HOBr, Br_2, $BrNO_2$, $BrNO_3$, BrCl
Liquid phase (neutrals)
$O(^3P)$, 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
SO_2, H_2SO_4, DMSO, $DMSO_2$, CH_3SO_2H, CH_3SO_3H
Cl, HCl, HOCl, Cl_2
Br, HBr, HOBr, Br_2, BrCl
Liquid phase (ions)
H^+, OH^-, O_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^-, $BrOH^-$

Table 2: Henry constants and accommodation coefficients.[‡]

species	K_H^0 [M/atm]	$-\Delta_{soln}H/R$ [K]	reference	α^0	$-\Delta_{obs}H/R$ [K]	reference
O_3	1.2×10^{-2}	2560	Chameides (1984)	0.04	(water ice at 195-262 K)	Sander et al. (2006)
O_2	1.3×10^{-3}	1500	Wilhelm et al. (1977)	0.01	2000	estimated
OH	3.0×10^{1}	4300	Hanson et al. (1992)	0.1	(water ice at 205-253 K)	Sander et al. (2006)
HO_2	3.9×10^{3}	5900	Hanson et al. (1992)	0.02	(at 275 K)	Sander et al. (2006)
H_2O_2	1.0×10^{5}	6338	Lind and Kok (1994)	0.077	2769	Worsnop et al. (1989)
NO	1.9×10^{-3}	1480	Schwartz and White (1981)	5×10^{-5}	0	Saastad et al. (1993)
NO_2	6.4×10^{-3}	2500	Lelieveld and Crutzen (1991)	0.0001	(water ice at 195 K)	Sander et al. (2006)
NO_3	2.0	2000	Thomas et al. (1993)	0.04	(at 273 K)	Rudich et al. (1996)
N_2O_5	∞	—		0.1	(at 195-300 K)	DeMore et al. (1997)
HONO	4.9×10^{1}	4780	Schwartz and White (1981)	0.001	(water ice at 180-200 K)	Sander et al. (2006)
HNO_3	$2.5 \times 10^{6}/K_A$	8694	Brimblecombe and Clegg (1989)	0.003	(water ice at 220 K)	Sander et al. (2006)
HNO_4	1.2×10^{4}	6900	Régimbal and Mozurkewich (1997)	0.1	(at 200 K)	DeMore et al. (1997)
NH_3	5.8×10^{1}	4085	Chameides (1984)	0.06	(at 295 K)	DeMore et al. (1997)
CH3OO	6.0	$=HO_2$	Pandis and Seinfeld (1989)	0.01	2000	estimated
ROOH	3.0×10^{2}	5322	Lind and Kok (1994)	0.0046	3273	Magi et al. (1997)
HCHO	7.0×10^{3}	6425	Chameides (1984)	0.04	(at 260-270 K)	DeMore et al. (1997)
HCOOH	3.7×10^{3}	5700	Chameides (1984)	0.014	3978	DeMore et al. (1997)
CO_2	3.1×10^{-2}	2423	Chameides (1984)	0.01	2000	estimated
HCl	1.2	9001	Brimblecombe and Clegg (1989)	0.3	water ice (191 211 K) α = 0.18 for liquid water at 273 K	Sander et al. (2006)
HOCl	6.7×10^{2}	5862	Huthwelker et al. (1995)	=HOBr	=HOBr	estimated
$ClNO_3$	∞	—		0.1	(at RT)	Koch and Rossi (1998)
Cl_2	9.1×10^{-2}	2500	Wilhelm et al. (1977)	0.0001	(water ice at 200 K)	Sander et al. (2006)
HBr	1.3	10239	Brimblecombe and Clegg (1989)	0.2	(water ice at 200 K)	Sander et al. (2006)
HOBr	9.3×10^{1}	=HOCl	Vogt et al. (1996)	0.003	(water ice at 223-239 K)	Sander et al. (2006)
$BrNO_3$	∞	—		0.8	0	Hanson et al. (1996)
Br_2	7.6×10^{-1}	4094	Dean (1992)	0.038	6546	Hu et al. (1995)
BrCl	9.4×10^{-1}	5600	Bartlett and Margerum (1999)	0.15	(at 270-285 K)	Sander et al. (2006)

[‡] For ROOH the values of CH_3OOH have been assumed. The temperature dependence is for the Henry constants is $K_H = K_H^0 \times \exp(\frac{-\Delta_{soln}H}{R}(\frac{1}{T} - \frac{1}{T_0}))$, $T_0 = 298$ K and for the accommodation coefficients $dln(\frac{\alpha}{1-\alpha})/d(\frac{1}{T}) = \frac{-\Delta_{obs}H}{R}$. RT stands for "room temperature".

Table 2 - Henry constants and accommodation coefficients.

species	K_H^0 [M/atm]	$-\Delta_{soln}H/R$ [K]	reference	α^0	$-\Delta_{obs}H/R$ [K]	reference
DMS	4.8×10^{-1}	3100	De Bruyn et al. (1995)	0.01		assumed
DMSO	5.0×10^4	=HCHO	De Bruyn et al. (1994)	0.048	2578	De Bruyn et al. (1994)
$DMSO_2$	∞	—	assumed	0.03	5388	De Bruyn et al. (1994)
SO_2	1.2	3120	Chameides (1984)	0.11	0	DeMore et al. (1997)
H_2SO_4	∞	—		0.65	(at 303 K)	Pöschl et al. (1998)
CH_3SO_2H	∞	—	assumed	0.0002	0	Lucas and Prinn (2002)
CH_3SO_3H	∞	—	assumed	0.076	1762	De Bruyn et al. (1994)
CH_4	1.3×10^{-3}	—	Mackay and Shiu. (1981)	0.1	0	assumed

[‡]For ROOH the values of CH_3OOH have been assumed. The temperature dependence is for the Henry constants is $K_H = K_H^0 \times \exp(\frac{-\Delta_{soln}H}{R}(\frac{1}{T}-\frac{1}{T_0}))$, $T_0 = 298$ K and for the accommodation coefficients $dln(\frac{\alpha}{1-\alpha})/d(\frac{1}{T}) = \frac{-\Delta_{obs}H}{R}$. RT stands for “room temperature”.

Table 2: Gas phase reactions.

no	reaction	n	A [$(\mathrm{cm}^{-3})^{1-n}\mathrm{s}^{-1}$]	$-E_a$ / R [K]	reference
Ox and HOx reactions					
O1	$O(^1D) + O_2 \longrightarrow O_3$	2	3.2×10^{-11}	70	Atkinson et al. (2004)
O2	$O(^1D) + N_2 \longrightarrow O_3$	2	1.8×10^{-11}	110	Atkinson et al. (2004)
O3	$O(^1D) + H_2O \longrightarrow 2\,OH$	2	2.2×10^{-10}		Atkinson et al. (2004)
O4	$OH + O_3 \longrightarrow HO_2 + O_2$	2	1.7×10^{-12}	-940	Atkinson et al. (2004)
O5	$OH + HO_2 \longrightarrow H_2O + O_2$	2	4.8×10^{-11}	250	Atkinson et al. (2004)
O6	$OH + H_2O_2 \longrightarrow HO_2 + H_2O$	2	2.9×10^{-12}	-160	Atkinson et al. (2004)
O7	$HO_2 + O_3 \longrightarrow OH + 2\,O_2$	2	1.0×10^{-14}	-490	Atkinson et al. (2004)
O8	$HO_2 + HO_2 \longrightarrow H_2O_2 + O_2$	2	^{b}		Atkinson et al. (2006)
O9	$O_3 + h\nu \longrightarrow O_2 + O(^1D)$	1	^{a}		DeMore et al. (1997)
O10	$H_2O_2 + h\nu \longrightarrow 2\,OH$	1	^{a}		DeMore et al. (1997)
NOy reactions					
N1	$NO + OH \xrightarrow{M} HONO$	3	^{b}		Sander et al. (2003)
N2	$NO + HO_2 \longrightarrow NO_2 + OH$	2	3.5×10^{-12}	250	Atkinson et al. (2004)
N3	$NO + O_3 \longrightarrow NO_2 + O_2$	2	3.0×10^{-12}	-1500	Sander et al. (2003)
N4	$NO + NO_3 \longrightarrow 2\,NO_2$	2	1.5×10^{-11}	170	Sander et al. (2003)
N5	$NO_2 + OH \xrightarrow{M} HNO_3$	3	^{b}		Sander et al. (2003)
N6	$NO_2 + HO_2 \xrightarrow{M} HNO_4$	3	^{b}		Atkinson et al. (2004)
N7	$NO_2 + O_3 \longrightarrow NO_3 + O_2$	2	1.2×10^{-13}	-2450	Sander et al. (2003)
N8	$NO_2 + h\nu \longrightarrow NO + O_3$	1	^{a}		DeMore et al. (1997)
N9	$NO_2 + NO_3 \xrightarrow{M} N_2O_5$	3	^{b}		Sander et al. (2003)
N10	$NO_3 + h\nu \longrightarrow NO + O_2$	1	^{a}		Wayne et al. (1991)
N11	$NO_3 + HO_2 \longrightarrow 0.3\ HNO_3 + 0.7\ OH + 0.7\ NO_2 + O_2$	2	4.0×10^{-12}		Atkinson et al. (2004)
N12	$NO_3 + NO_3 \longrightarrow NO_2 + NO_2 + O_2$	2	8.5×10^{-13}	-2450	Sander et al. (2003)
N13	$NO_3 + h\nu \longrightarrow NO_2 + O_3$	1	^{a}		Wayne et al. (1991)
N14	$N_2O_5 \xrightarrow{M} NO_2 + NO_3$	2	^{b}		Sander et al. (2003)
N15	$N_2O_5 + H_2O \longrightarrow 2\,HNO_3$	2	2.6×10^{-22}		Atkinson et al. (2004)
N16	$N_2O_5 + h\nu \longrightarrow NO_2 + NO_3$	1	^{a}		DeMore et al. (1997)
N17	$HONO + OH \longrightarrow NO_2$	2	1.8×10^{-11}	-390	Sander et al. (2003)
N18	$HONO + h\nu \longrightarrow NO + OH$	1	^{a}		DeMore et al. (1997)
N19	$HNO_3 + h\nu \longrightarrow NO_2 + OH$	1	^{a}		DeMore et al. (1997)
N20	$HNO_3 + OH \longrightarrow NO_3 + H_2O$	2	^{b}		Atkinson et al. (2004)
N21	$HNO_4 \xrightarrow{M} NO_2 + HO_2$	2	^{b}		Sander et al. (2003)
N22	$HNO_4 + OH \longrightarrow NO_2 + H_2O + O_2$	2	1.3×10^{-12}	380	Haggerstone et al. (2005)
N23	$HNO_4 + h\nu \longrightarrow NO_2 + HO_2$	1	^{a}		DeMore et al. (1997)
N24	$HNO_4 + h\nu \longrightarrow OH + NO_3$	1	^{a}		DeMore et al. (1997)
N25	$RONO_2 + OH \longrightarrow H_2O + NO_2$	2	1.3×10^{-12}		pers. comm. with R. Sander
N26	$RONO_2 + h\nu \longrightarrow NO_2$	1	^{a}		assumed similar to HNO_3 photolysis
organic reactions					
C1	$CO + OH \xrightarrow{O_2} HO_2 + CO_2$	2	^{b}		Sander et al. (2003)
C2	$CH_4 + OH \xrightarrow{O_2} CH_3O_2 + H_2O$	2	2.4×10^{-12}	-1775	Sander et al. (2003)
C3	$C_2H_6 + OH \longrightarrow C_2H_5O_2 + H_2O$	2	1.7×10^{-11}	-1232	Lurmann et al. (1986)
C4	$C_2H_4 + OH \longrightarrow C_2H_4OHO_2$	2	1.66×10^{-12}	474	Lurmann et al. (1986), see note
C5	$C_2H_4 + O_3 \longrightarrow HCHO + 0.4\ CH_2O_2 + 0.12\ HO_2 + 0.42\ CO + 0.06CH_4$	2	1.2×10^{-14}	-2633	Lurmann et al. (1986), see note
C6	$HO_2 + CH_3O_2 \longrightarrow ROOH + O_2$	2	4.1×10^{-13}	750	Sander et al. (2003)
C7	$HO_2 + C_2H_5O_2 \longrightarrow ROOH + O_2$	2	7.5×10^{-13}	700	Sander et al. (2003)
C8	$HO_2 + CH_3CO_3 \longrightarrow ROOH + O_2$	2	4.5×10^{-13}	1000	DeMore et al. (1997)
C9	$CH_3O_2 + CH_3O_2 \longrightarrow 1.4\ HCHO + 0.8\ HO_2 + O_2$	2	1.5×10^{-13}	220	Lurmann et al. (1986)

n reaction order, ^{a} photolysis rates calculated online, ^{b} special rate functions.

Table 2 - Gas phase reactions.

no	reaction	n	$A\ [(\mathrm{cm}^{-3})^{1-n}\mathrm{s}^{-1}]$	$-E_a\ /\ R$ [K]	reference
C10	$C_2H_5O_2 + NO \longrightarrow ALD + HO_2 + NO_2$	2	4.2×10^{-12}	180	Lurmann et al. (1986)
C11	$2\,C_2H_5O_2 \longrightarrow 1.6\ ALD + 1.2\ HO_2$	2	5.0×10^{-14}		Lurmann et al. (1986)
C12	$C_2H_4OHO_2 + NO \longrightarrow NO_2 + 2\,HCHO + HO_2$	2	4.2×10^{-12}	180	Lurmann et al. (1986)
C13	$C_2H_4OHO_2 + C_2H_4OHO_2 \longrightarrow 2.4\ HCHO + 1.2\ HO_2 + 0.4\ ALD$	2	5.0×10^{-14}		Lurmann et al. (1986)
C14	$HO_2 + C_2H_4OHO_2 \longrightarrow ROOH + O_2$	2	3.0×10^{-12}		Lurmann et al. (1986)
C15	$HCHO + h\nu \longrightarrow 2\,HO_2 + CO$	1	^{a}		DeMore et al. (1997)
C16	$HCHO + h\nu \longrightarrow CO + H_2$	1	^{a}		DeMore et al. (1997)
C17	$HCHO + OH \xrightarrow{O_2} HO_2 + CO + H_2O$	2	1.0×10^{-11}		DeMore et al. (1997)
C18	$NO_3 + HCHO \xrightarrow{O_2} HNO_3 + HO_2 + CO$	2	5.8×10^{-16}		DeMore et al. (1997)
C19	$ALD + OH \longrightarrow CH_3CO_3 + H_2O$	2	6.9×10^{-12}	250	Lurmann et al. (1986)
C20	$ALD + NO_3 \longrightarrow HNO_3 + CH_3CO_3$	2	1.40×10^{-15}		DeMore et al. (1997)
C21	$ALD + h\nu \longrightarrow CH_3O_2 + HO_2 + CO$	1	^{a}		Lurmann et al. (1986)
C22	$ALD + h\nu \longrightarrow CH_4 + CO$	1	^{a}		Lurmann et al. (1986)
C23	$HOCH_2O_2 + NO \longrightarrow HCOOH + HO_2 + NO_2$	2	4.2×10^{-12}	180	Lurmann et al. (1986)
C24	$HOCH_2O_2 + HO_2 \longrightarrow HCOOH + H_2O + O_2$	2	2.00×10^{-12}		Lurmann et al. (1986)
C25	$2\,HOCH_2O_2 \longrightarrow 2\,HCOOH + 2\,HO_2 + 2\,O_2$	2	1.0×10^{-13}		Lurmann et al. (1986)
C26	$HCOOH + OH \xrightarrow{O_2} HO_2 + H_2O + CO_2$	2	4.0×10^{-13}		DeMore et al. (1997)
C27	$CH_3CO_3 + NO_2 \longrightarrow PAN$	2	4.7×10^{-12}		Lurmann et al. (1986)
C28	$PAN \longrightarrow CH_3CO_3 + NO_2$	1	1.9×10^{16}	-13543	DeMore et al. (1997)
C29	$CH_3CO_3 + NO \longrightarrow CH_3O_2 + NO_2 + CO_2$	2	4.2×10^{-12}	180	Lurmann et al. (1986)
C30	$CH_3O_2 + NO \xrightarrow{O_2} HCHO + NO_2 + HO_2$	2	3.0×10^{-12}	280	DeMore et al. (1997)
C31	$ROOH + OH \longrightarrow 0.7CH_3O_2 + 0.3HCHO + 0.3OH$	2	3.8×10^{-12}	200	DeMore et al. (1997), see note
C32	$ROOH + h\nu \longrightarrow HCHO + OH + HO_2$	1	^{a}		DeMore et al. (1997), see note
	S reactions				
S1	$SO_2 + OH \xrightarrow{M} HOSO_2$	3	^{b}		Atkinson et al. (2004)
S2	$HOSO_2 + O_2 \longrightarrow HO_2 + SO_3$	2	1.3×10^{-12}	-330	Atkinson et al. (2004)
S3	$SO_3 \xrightarrow{H_2O} H_2SO_4$	1	^{b}		Jayne et al. (1997)
S4	$DMS + OH \xrightarrow{O_2} DMOO + H_2O$	2	^{b}		Atkinson et al. (1997)
S5	$DMS + OH \xrightarrow{O_2} DMSO + HO_2$	2	^{b}		Atkinson et al. (1997)
S6	$DMS + NO_3 \xrightarrow{O_2} DMOO + HNO_3$	2	1.9×10^{-13}	520	Atkinson et al. (1999)
S7	$DMS + Cl \xrightarrow{O_2} DMOO + HCl$	2	3.3×10^{-10}		Jefferson et al. (1994)
S8	$DMS + Br \xrightarrow{O_2} DMOO + HBr$	2	9.0×10^{-11}	-2386	Ingham et al. (1999)
S9	$DMS + BrO \longrightarrow DMSO + Br$	2	2.54×10^{-14}	850	Ingham et al. (1999)
S10	$DMS + ClO \longrightarrow DMSO + Cl$	2	9.5×10^{-15}		Barnes et al. (1991)
S11	$DMOO + NO \longrightarrow HCHO + CH_3S + NO_2$	2	4.9×10^{-12}	263	Urbanski et al. (1997)
S12	$DMOO + DMOO \xrightarrow{O_2} 2\,HCHO + 2\,CH_3S$	2	1.0×10^{-11}		Urbanski et al. (1997); Atkinson et al. (2004)
S13	$CH_3S + O_3 \longrightarrow CH_3SO + O_2$	2	1.15×10^{-12}	432	Atkinson et al. (2004)
S14	$CH_3S + NO_2 \longrightarrow CH_3SO + NO$	2	3.0×10^{-11}	210	Atkinson et al. (2004)
S15	$CH_3SO + NO_2 \xrightarrow{O_2} 0.82CH_3SO_2 + 0.18SO_2 + 0.18CH_3O_2 + NO$	2	1.2×10^{-11}		Atkinson et al. (2004); Kukui et al. (2000), product ratios from van Dingenen et al. (1994)
S16	$CH_3SO + O_3 \longrightarrow CH_3SO_2 + O_2$	2	6.0×10^{-13}		Atkinson et al. (2004)
S17	$CH_3SO_2 \xrightarrow{O_2} CH_3O_2 + SO_2$	1	1.36×10^{14}	-8656	Kukui et al. (2000)
S18	$CH_3SO_2 + NO_2 \longrightarrow CH_3SO_3 + NO$	2	2.2×10^{-12}		Ray et al. (1996)
S19	$CH_3SO_2 + O_3 \longrightarrow CH_3SO_3$	2	5.0×10^{-15}		Ray et al. (1996)
S20	$CH_3SO_3 + HO_2 \longrightarrow CH_3SO_3H$	2	5.0×10^{-11}		Barone et al. (1995)
S21	$CH_3SO_3 \xrightarrow{H_2O,\ O_2} CH_3O_2 + H_2SO_4$	1	1.36×10^{14}	-11071	Barone et al. (1995)

n reaction order, ^{a} photolysis rates calculated online, ^{b} special rate functions.

Table 2 - Gas phase reactions.

no	reaction	n	A [(cm^{-3})$^{1-n}$s^{-1}]	$-E_a$ / R [K]	reference
S22	$\mathrm{DMSO} + \mathrm{OH} \longrightarrow 0.95\ \mathrm{CH_3SO_2H} + 0.95\ \mathrm{CH_3O_2} + 0.05\ \mathrm{DMSO_2}$	2	8.7×10^{-11}		Urbanski et al. (1998)
S23	$\mathrm{CH_3SO_2H} + \mathrm{OH} \longrightarrow 0.95\ \mathrm{CH_3SO_2} + 0.05\ \mathrm{CH_3SO_3H} + 0.05\ \mathrm{HO_2}$	2	$9.\times10^{-11}$		Kukui et al. (2003)
S24	$\mathrm{CH_3SO_2H} + \mathrm{NO_3} \longrightarrow \mathrm{CH_3SO_2} + \mathrm{HNO_3}$	2	1.0×10^{-13}		Yin et al. (1990)
	Cl reactions				
Cl1	$\mathrm{Cl} + \mathrm{O_3} \longrightarrow \mathrm{ClO} + \mathrm{O_2}$	2	2.8×10^{-11}	-250	Atkinson et al. (2004)
Cl2	$\mathrm{Cl} + \mathrm{HO_2} \longrightarrow \mathrm{HCl} + \mathrm{O_2}$	2	1.8×10^{-11}	170	Sander et al. (2003)
Cl3	$\mathrm{Cl} + \mathrm{HO_2} \longrightarrow \mathrm{ClO} + \mathrm{OH}$	2	4.1×10^{-11}	-450	Sander et al. (2003)
Cl4	$\mathrm{Cl} + \mathrm{H_2O_2} \longrightarrow \mathrm{HCl} + \mathrm{HO_2}$	2	1.1×10^{-11}	-980	Atkinson et al. (2004)
Cl5	$\mathrm{Cl} + \mathrm{CH_3O_2} \longrightarrow 0.5\mathrm{ClO} + 0.5\mathrm{HCHO} + 0.5\mathrm{HO_2} + 0.5\mathrm{HCl} + 0.5\mathrm{CO} + 0.5\mathrm{H_2O}$	2	1.6×10^{-10}		Sander et al. (2003)
Cl6	$\mathrm{Cl} + \mathrm{NO_3} \longrightarrow \mathrm{ClO} + \mathrm{NO_2}$	2	2.4×10^{-11}		Sander et al. (2003)
Cl7	$\mathrm{Cl} + \mathrm{CH_4} \xrightarrow{\mathrm{O_2}} \mathrm{HCl} + \mathrm{CH_3O_2}$	2	9.6×10^{-12}	-1360	Atkinson et al. (2004)
Cl8	$\mathrm{Cl} + \mathrm{C_2H_6} \xrightarrow{\mathrm{O_2}} \mathrm{HCl} + \mathrm{C_2H_5O_2}$	2	7.7×10^{-11}	-90	Sander et al. (2003)
Cl9	$\mathrm{Cl} + \mathrm{C_2H_4} \xrightarrow{\mathrm{O_2}} \mathrm{HCl} + \mathrm{C_2H_5O_2}$	2	$1.\times10^{-10}$		see note
Cl10	$\mathrm{Cl} + \mathrm{HCHO} \xrightarrow{\mathrm{O_2}} \mathrm{HCl} + \mathrm{HO_2} + \mathrm{CO}$	2	8.1×10^{-11}	-30	Sander et al. (2003)
Cl11	$\mathrm{Cl} + \mathrm{ROOH} \longrightarrow \mathrm{CH_3O_2} + \mathrm{HCl}$	2	5.7×10^{-11}		Wallington et al. (1990), see note
Cl12	$\mathrm{Cl} + \mathrm{OClO} \longrightarrow \mathrm{ClO} + \mathrm{ClO}$	2	3.2×10^{-11}	170	Atkinson et al. (2004)
Cl13	$\mathrm{Cl} + \mathrm{ClNO_3} \longrightarrow \mathrm{Cl_2} + \mathrm{NO_3}$	2	6.5×10^{-12}	135	Sander et al. (2003)
Cl14	$\mathrm{Cl} + \mathrm{PAN} \longrightarrow \mathrm{HCl} + \mathrm{HCHO} + \mathrm{NO_3}$	2	1.0×10^{-14}		Sander et al. (2003)
Cl15	$\mathrm{Cl} + \mathrm{HNO_3} \longrightarrow \mathrm{HCl} + \mathrm{NO_2}$	2	1.0×10^{-16}		Sander et al. (2003)
Cl16	$\mathrm{Cl} + \mathrm{RONO_2} \longrightarrow \mathrm{HCl} + \mathrm{NO_2}$	2	7.7×10^{-11}		Michalowski et al. (2000)
Cl17	$\mathrm{ClO} + \mathrm{OH} \longrightarrow \mathrm{Cl} + \mathrm{HO_2}$	2	7.4×10^{-12}	270	Sander et al. (2003)
Cl18	$\mathrm{ClO} + \mathrm{OH} \longrightarrow \mathrm{HCl} + \mathrm{O_2}$	2	6.0×10^{-13}	230	Sander et al. (2003)
Cl19	$\mathrm{ClO} + \mathrm{HO_2} \longrightarrow \mathrm{HOCl} + \mathrm{O_2}$	2	2.2×10^{-12}	340	Atkinson et al. (2004)
Cl20	$\mathrm{ClO} + \mathrm{CH_3O_2} \longrightarrow \mathrm{Cl} + \mathrm{HCHO} + \mathrm{HO_2}$	2	3.3×10^{-12}	-115	Sander et al. (2003)
Cl21	$\mathrm{ClO} + \mathrm{NO} \longrightarrow \mathrm{Cl} + \mathrm{NO_2}$	2	6.2×10^{-12}	295	Atkinson et al. (2004)
Cl22	$\mathrm{ClO} + \mathrm{NO_2} \xrightarrow{\mathrm{M}} \mathrm{ClNO_3}$	3	[b]		Atkinson et al. (2004)
Cl23	$\mathrm{ClO} + \mathrm{ClO} \longrightarrow \mathrm{Cl_2O_2}$	2	[b]		Atkinson et al. (2004)
Cl24	$\mathrm{ClO} + \mathrm{ClO} \longrightarrow \mathrm{Cl_2} + \mathrm{O_2}$	2	1.0×10^{-12}	-1590	Atkinson et al. (2004)
Cl25	$\mathrm{ClO} + \mathrm{ClO} \longrightarrow 2\,\mathrm{Cl} + \mathrm{O_2}$	2	3.0×10^{-11}	-2450	Atkinson et al. (2004)
Cl26	$\mathrm{ClO} + \mathrm{ClO} \longrightarrow \mathrm{Cl} + \mathrm{OClO}$	2	3.5×10^{-13}	-1370	Atkinson et al. (2004)
Cl27	$\mathrm{OClO} + \mathrm{OH} \longrightarrow \mathrm{HOCl} + \mathrm{O_2}$	2	4.5×10^{-13}	800	Atkinson et al. (2004)
Cl28	$\mathrm{OClO} + \mathrm{NO} \longrightarrow \mathrm{ClO} + \mathrm{NO_2}$	2	1.1×10^{-13}	350	Atkinson et al. (2004)
Cl29	$\mathrm{Cl_2O_2} \longrightarrow \mathrm{ClO} + \mathrm{ClO}$	1	[b]		Atkinson et al. (2004)
Cl30	$\mathrm{HOCl} + \mathrm{OH} \longrightarrow \mathrm{ClO} + \mathrm{H_2O}$	2	3.0×10^{-12}	-500	Sander et al. (2003)
Cl31	$\mathrm{HCl} + \mathrm{OH} \longrightarrow \mathrm{H_2O} + \mathrm{Cl}$	2	1.8×10^{-12}	-240	Atkinson et al. (2004)
Cl32	$\mathrm{ClNO_2} + \mathrm{OH} \longrightarrow \mathrm{HOCl} + \mathrm{NO_2}$	2	2.4×10^{-12}	-1250	Atkinson et al. (2004)
Cl33	$\mathrm{ClNO_3} + \mathrm{OH} \longrightarrow 0.5\ \mathrm{ClO} + 0.5\ \mathrm{HNO_3} + 0.5\ \mathrm{HOCl} + 0.5\ \mathrm{NO_3}$	2	1.2×10^{-12}	-330	Atkinson et al. (2004)
Cl34	$\mathrm{ClNO_3} \longrightarrow \mathrm{ClO} + \mathrm{NO_2}$	1	[b]		Anderson and Fahey (1990)
Cl35	$\mathrm{OClO} + h\nu \xrightarrow{\mathrm{O_2},\ \mathrm{O_3}} \mathrm{O_3} + \mathrm{ClO}$	1	[a]		DeMore et al. (1997)
Cl36	$\mathrm{Cl_2O_2} + h\nu \longrightarrow \mathrm{Cl} + \mathrm{Cl} + \mathrm{O_2}$	1	[a]		DeMore et al. (1997)
Cl37	$\mathrm{Cl_2} + h\nu \longrightarrow 2\,\mathrm{Cl}$	1	[a]		DeMore et al. (1997)
Cl38	$\mathrm{HOCl} + h\nu \longrightarrow \mathrm{Cl} + \mathrm{OH}$	1	[a]		DeMore et al. (1997)
Cl39	$\mathrm{ClNO_2} + h\nu \longrightarrow \mathrm{Cl} + \mathrm{NO_2}$	1	[a]		DeMore et al. (1997)
Cl40	$\mathrm{ClNO_3} + h\nu \longrightarrow \mathrm{Cl} + \mathrm{NO_3}$	1	[a]		DeMore et al. (1997)
	Br reactions				
Br1	$\mathrm{Br} + \mathrm{O_3} \longrightarrow \mathrm{BrO} + \mathrm{O_2}$	2	1.7×10^{-11}	-800	Atkinson et al. (2004)
Br2	$\mathrm{Br} + \mathrm{HO_2} \longrightarrow \mathrm{HBr} + \mathrm{O_2}$	2	7.7×10^{-12}	-450	Atkinson et al. (2004)
Br3	$\mathrm{Br} + \mathrm{C_2H_4} \xrightarrow{\mathrm{O_2}} \mathrm{HBr} + \mathrm{C_2H_5O_2}$	2	$5.\times10^{-14}$		see note
Br4	$\mathrm{Br} + \mathrm{HCHO} \xrightarrow{\mathrm{O_2}} \mathrm{HBr} + \mathrm{CO} + \mathrm{HO_2}$	2	1.7×10^{-11}	-800	Sander et al. (2003)

n reaction order, [a] photolysis rates calculated online, [b] special rate functions.

Table 2 - Gas phase reactions.

no	reaction	n	A $[(\mathrm{cm}^{-3})^{1-n}\mathrm{s}^{-1}]$	$-E_a$ / R [K]	reference
Br5	$\mathrm{Br + ROOH \longrightarrow CH_3O_2 + HBr}$	2	2.66×10^{-12}	-1610	Mallard et al. (1993), see note
Br6	$\mathrm{Br + NO_2 \longrightarrow BrNO_2}$	2	[b]		Sander et al. (2003)
Br7	$\mathrm{Br + BrNO_3 \longrightarrow Br_2 + NO_3}$	2	4.9×10^{-11}		Orlando and Tyndall (1996)
Br8	$\mathrm{BrO + OH \longrightarrow Br + HO_2}$	2	1.8×10^{-11}	250	Atkinson et al. (2004)
Br9	$\mathrm{BrO + HO_2 \longrightarrow HOBr + O_2}$	2	4.5×10^{-12}	500	Atkinson et al. (2004)
Br10	$\mathrm{BrO + CH_3O_2 \longrightarrow HOBr + HCHO}$	2	$4.1\ \times10^{-12}$		Aranda et al. (1997)
Br11	$\mathrm{BrO + CH_3O_2 \longrightarrow Br + HCHO + HO_2}$	2	$1.6\ \times10^{-12}$		Aranda et al. (1997)
Br12	$\mathrm{BrO + HCHO \xrightarrow{O_2} HOBr + CO + HO_2}$	2	1.5×10^{-14}		Hansen et al. (1999)
Br13	$\mathrm{BrO + NO \longrightarrow Br + NO_2}$	2	8.7×10^{-12}	260	Atkinson et al. (2004)
Br14	$\mathrm{BrO + NO_2 \xrightarrow{M} BrNO_3}$	3	[b]		Atkinson et al. (2004)
Br15	$\mathrm{BrO + BrO \longrightarrow 2\,Br + O_2}$	2	2.4×10^{-12}	40	Sander et al. (2003)
Br16	$\mathrm{BrO + BrO \longrightarrow Br_2 + O_2}$	2	2.9×10^{-14}	860	Sander et al. (2003)
Br17	$\mathrm{HBr + OH \longrightarrow Br + H_2O}$	2	5.5×10^{-12}	205	Atkinson et al. (2004)
Br18	$\mathrm{BrNO_3 \longrightarrow BrO + NO_2}$	2	[b]		Orlando and Tyndall (1996)
Br19	$\mathrm{BrO} + h\nu \xrightarrow{\mathrm{O_2}} \mathrm{Br + O_3}$	1	[a]		DeMore et al. (1997)
Br20	$\mathrm{Br_2} + h\nu \longrightarrow 2\,\mathrm{Br}$	1	[a]		Hubinger and Nee (1995)
Br21	$\mathrm{HOBr} + h\nu \longrightarrow \mathrm{Br + OH}$	1	[a]		Ingham et al. (1999)
Br22	$\mathrm{BrNO_2} + h\nu \longrightarrow \mathrm{Br + NO_2}$	1	[a]		Scheffler et al. (1997)
Br23	$\mathrm{BrNO_3} + h\nu \longrightarrow \mathrm{Br + NO_3}$	1	[a]		DeMore et al. (1997)
Br24	$\mathrm{Br_2 + OH \longrightarrow HOBr + Br}$	2	2.0×10^{-11}	240	Atkinson et al. (2004); Oum et al. (1998)
Br25	$\mathrm{CH_3Br + OH \longrightarrow H_2O + Br}$	2	1.7×10^{-12}	-1215	Atkinson et al. (2003)
Br26	$\mathrm{CHBr_3 + OH \longrightarrow H_2O + Br}$	2	1.35×10^{-12}	-600	Atkinson et al. (2003)
interhalogen reactions					
Hx1	$\mathrm{Cl + BrCl \longrightarrow Br + Cl_2}$	2	1.5×10^{-11}		Mallard et al. (1993)
Hx2	$\mathrm{Cl + Br_2 \longrightarrow BrCl + Br}$	2	1.2×10^{-10}		Mallard et al. (1993)
Hx3	$\mathrm{Br + OClO \longrightarrow BrO + ClO}$	2	2.6×10^{-11}	-1300	Atkinson et al. (2004)
Hx4	$\mathrm{Br + Cl_2 \longrightarrow BrCl + Cl}$	2	1.1×10^{-15}		Mallard et al. (1993)
Hx5	$\mathrm{Br + BrCl \longrightarrow Br_2 + Cl}$	2	3.3×10^{-15}		Mallard et al. (1993)
Hx6	$\mathrm{BrO + ClO \longrightarrow Br + OClO}$	2	1.6×10^{-12}	430	Atkinson et al. (2004)
Hx7	$\mathrm{BrO + ClO \longrightarrow Br + Cl + O_2}$	2	2.9×10^{-12}	220	Atkinson et al. (2004)
Hx8	$\mathrm{BrO + ClO \longrightarrow BrCl + O_2}$	2	5.8×10^{-13}	170	Atkinson et al. (2004)
Hx9	$\mathrm{BrCl} + h\nu \longrightarrow \mathrm{Br + Cl}$	1	[a]		DeMore et al. (1997)

n reaction order, [a] photolysis rates calculated online, [b] special rate functions.

Notes: The rates for ROOH were assumed as that of $\mathrm{CH_3OOH}$; $\mathrm{C_2H_4}$ is used as generic alkene as in the Lurmann et al. (1986) mechanism. The rate coefficients are calculated with $k = A \times \exp(\frac{-E_a}{RT})$.

Table 3: Aqueous phase reactions.

no	reaction	n	A [$M^{1-n}s^{-1}$]	$-E_a$ / R [K]	reference
Ox and HOx reactions					
O1	$O_3 + OH \longrightarrow HO_2$	2	1.1×10^8		Sehested et al. (1984)
O2	$O_3 + O_2^- \longrightarrow OH + OH^-$	2	1.5×10^9		Sehested et al. (1983)
O3	$OH + OH \longrightarrow H_2O_2$	2	5.5×10^9		Buxton et al. (1988)
O4	$OH + HO_2 \longrightarrow H_2O$	2	7.1×10^9		Sehested et al. (1968)
O5	$OH + O_2^- \longrightarrow OH^-$	2	1.0×10^{10}		Sehested et al. (1968)
O6	$OH + H_2O_2 \longrightarrow HO_2$	2	2.7×10^7	-1684	Christensen et al. (1982)
O7	$HO_2 + HO_2 \longrightarrow H_2O_2$	2	9.7×10^5	-2500	Christensen and Sehested (1988)
O8	$HO_2 + O_2^- \xrightarrow{H^+} H_2O_2$	2	1.0×10^8	-900	Christensen and Sehested (1988)
O9	$O(^3P) + O_2 \longrightarrow O_3$	2	4.0×10^9		Kläning et al. (1984)
NOy reactions					
N1	$HONO + OH \longrightarrow NO_2$	2	1.0×10^{10}		assumed =N7 Barker et al. (1970)
N2	$HONO + H_2O_2 \xrightarrow{H^+} HNO_3$	3	4.6×10^3	-6800	Damschen and Martin (1983)
N3	$NO_3 + OH^- \longrightarrow NO_3^- + OH$	2	8.2×10^7	-2700	Exner et al. (1992)
N4	$NO_2 + NO_2 \longrightarrow HNO_3 + HONO$	2	1.0×10^8		Lee and Schwartz (1981)
N5	$NO_2 + HO_2 \longrightarrow HNO_4$	2	1.8×10^9		Warneck (1999)
N6	$NO_2^- + O_3 \longrightarrow NO_3^- + O_2$	2	5.0×10^5	-6950	Damschen and Martin (1983)
N7	$NO_2^- + OH \longrightarrow NO_2 + OH^-$	2	1.0×10^{10}		Barker et al. (1970)
N8	$NO_4^- \longrightarrow NO_2^- + O_2$	1	8.0×10^{-1}		Warneck (1999)
N9	$O(^3P) + NO_2^- \longrightarrow NO_3^-$	2	1.48×10^9		Boxe and Saiz-Lopez (2008); Mack and Bolton (1999)
N10	$O(^3P) + NO_3^- \longrightarrow NO_2^- + O_2$	2	2.24×10^8		Boxe and Saiz-Lopez (2008); Mack and Bolton (1999)
N11	$NO_2 + NO_2 \longrightarrow NO_2^- + NO_3^- + 2\,H^+$	2	1.0×10^8		Boxe and Saiz-Lopez (2008); Mack and Bolton (1999)
N12	$NO + NO_2 \longrightarrow NO_2^- + NO_2^- + 2\,H^+$	2	2.0×10^8		Boxe and Saiz-Lopez (2008); Mack and Bolton (1999)
N13	$NO + OH \longrightarrow NO_2^- + H^+$	2	2.0×10^{10}		Boxe and Saiz-Lopez (2008); Mack and Bolton (1999)
N14	$NO_2 + OH \longrightarrow NO_3^- + H^+$	2	1.3×10^9		Boxe and Saiz-Lopez (2008); Mack and Bolton (1999)
organic reactions					
C1	$HCHO + OH \longrightarrow HCOOH + HO_2$	2	7.7×10^8	-1020	Chin and Wine (1994)
C2	$HCOOH + OH \longrightarrow HO_2 + CO_2$	2	1.1×10^8	-991	Chin and Wine (1994)
C3	$HCOO^- + OH \longrightarrow OH^- + HO_2 + CO_2$	2	3.1×10^9	-1240	Chin and Wine (1994)
C4	$CH_3O_2 + HO_2 \longrightarrow CH_3OOH$	2	4.3×10^5		estimated by Jacob (1986)
C5	$CH_3O_2 + O_2^- \longrightarrow CH_3OOH + OH^-$	2	5.0×10^7		estimated by Jacob (1986)
C6	$CH_3OH + OH \longrightarrow HCHO + HO_2$	2	9.7×10^8		Buxton et al. (1988)
C7	$CH_3OOH + OH \longrightarrow CH_3O_2$	2	2.7×10^7	-1715	estimated by Jacob (1986)
C8	$CH_3OOH + OH \longrightarrow HCHO + OH$	2	1.1×10^7	-1715	estimated by Jacob (1986)

n reaction order, ^{a} photolysis rates calculated online, ^{b} special rate functions

Table 3 - Aqueous phase reactions.

no	reaction	n	A [$M^{1-n}s^{-1}$]	$-E_a$ / R [K]	reference
C9	$CO_3^- + O_2^- \longrightarrow HCO_3^- + OH^-$	2	$6.5{\times}10^8$		Ross et al. (1992)
C10	$CO_3^- + H_2O_2 \longrightarrow HCO_3^- + HO_2$	2	$4.3{\times}10^5$		Ross et al. (1992)
C11	$CO_3^- + HCOO^- \longrightarrow HCO_3^- + HCO_3^- + HO_2$	2	$1.5{\times}10^5$		Ross et al. (1992)
C12	$HCO_3^- + OH \longrightarrow CO_3^-$	2	$8.5{\times}10^6$		Ross et al. (1992)
C13	$DOM + OH \longrightarrow HO_2$	2	$5.0{\times}10^9$		estimated by (C. Anastasio, pers. comm.) from Ross et al. (1998)
S reactions					
S1	$SO_3^- + O_2 \longrightarrow SO_5^-$	2	$1.5{\times}10^9$		Huie and Neta (1987)
S2	$HSO_3^- + O_3 \longrightarrow SO_4^{2-} + H^+ + O_2$	2	$3.7{\times}10^5$	-5500	Hoffmann (1986)
S3	$SO_3^{2-} + O_3 \longrightarrow SO_4^{2-} + O_2$	2	$1.5{\times}10^9$	-5300	Hoffmann (1986)
S4	$HSO_3^- + OH \longrightarrow SO_3^-$	2	$4.5{\times}10^9$		Buxton et al. (1988)
S5	$SO_3^{2-} + OH \longrightarrow SO_3^- + OH^-$	2	$5.5{\times}10^9$		Buxton et al. (1988)
S6	$HSO_3^- + HO_2 \longrightarrow SO_4^{2-} + OH + H^+$	2	$3.0{\times}10^3$		upper limit D. Sedlak pers. comm. with R. Sander
S7	$HSO_3^- + O_2^- \longrightarrow SO_4^{2-} + OH$	2	$3.0{\times}10^3$		upper limit D. Sedlak pers. comm. with R. Sander
S8	$HSO_3^- + H_2O_2 \longrightarrow SO_4^{2-} + H^+$	2	$5.2{\times}10^6 \times \frac{[H^+]}{[H^+]+0.1M}$	-3650	Damschen and Martin (1983)
S9	$HSO_3^- + NO_2 \xrightarrow{NO_2} HSO_4^- + 2\,HONO$	2	$2.0{\times}10^7$		Clifton et al. (1988)
S10	$SO_3^{2-} + NO_2 \xrightarrow{NO_2} SO_4^{2-} + 2\,HONO$	2	$2.0{\times}10^7$		Clifton et al. (1988)
S11	$HSO_3^- + NO_3 \longrightarrow SO_3^- + NO_3^- + H^+$	2	$1.4{\times}10^9$	-2000	Exner et al. (1992)
S12	$HSO_3^- + HNO_4 \longrightarrow HSO_4^- + NO_3^- + H^+$	2	$3.1{\times}10^5$		Warneck (1999)
S13	$HSO_3^- + CH_3OOH \xrightarrow{H^+} SO_4^{2-} + H^+ + CH_3OH$	3	$1.6{\times}10^7$	-3800	Lind et al. (1987)
S14	$SO_3^{2-} + CH_3OOH \xrightarrow{H^+} SO_4^{2-} + CH_3OH$	3	$1.6{\times}10^7$	-3800	Lind et al. (1987)
S15	$HSO_3^- + HCHO \longrightarrow CH_2OHSO_3^-$	2	$4.3{\times}10^{-1}$		Boyce and Hoffmann (1984)
S16	$SO_3^{2-} + HCHO \xrightarrow{H^+} CH_2OHSO_3^-$	2	$1.4{\times}10^4$		Boyce and Hoffmann (1984)
S17	$CH_2OHSO_3^- + OH^- \longrightarrow SO_3^{2-} + HCHO$	2	$3.6{\times}10^3$		Seinfeld and Pandis (1998)
S18	$HSO_3^- + HSO_5^- \xrightarrow{H^+} 2\,SO_4^{2-} + 2\,H^+$	3	$7.1{\times}10^6$		Betterton and Hoffmann (1988)
S19	$SO_4^- + OH \longrightarrow HSO_5^-$	2	$1.0{\times}10^9$		Jiang et al. (1992)
S20	$SO_4^- + HO_2 \longrightarrow SO_4^{2-} + H^+$	2	$3.5{\times}10^9$		Jiang et al. (1992)
S21	$SO_4^- + O_2^- \longrightarrow SO_4^{2-}$	2	$3.5{\times}10^9$		assumed =S20
S22	$SO_4^- + H_2O \longrightarrow SO_4^{2-} + H^+ + OH$	2	$1.1{\times}10^1$	-1110	Herrmann et al. (1995)
S23	$SO_4^- + H_2O_2 \longrightarrow SO_4^{2-} + H^+ + HO_2$	2	$1.2{\times}10^7$		Wine et al. (1989)
S24	$SO_4^- + NO_3^- \longrightarrow SO_4^{2-} + NO_3$	2	$5.0{\times}10^4$		Exner et al. (1992)
S25	$SO_4^- + HSO_3^- \longrightarrow SO_3^- + SO_4^{2-} + H^+$	2	$8.0{\times}10^8$		Huie and Neta (1987)
S26	$SO_4^- + SO_3^{2-} \longrightarrow SO_3^- + SO_4^{2-}$	2	$4.6{\times}10^8$		Huie and Neta (1987)
S27	$SO_4^{2-} + NO_3 \longrightarrow NO_3^- + SO_4^-$	2	$1.0{\times}10^5$		Logager et al. (1993)
S28	$SO_5^- + HSO_3^- \longrightarrow SO_4^- + SO_4^{2-} + H^+$	2	$7.5{\times}10^4$		Huie and Neta (1987)
S29	$SO_5^- + SO_3^{2-} \longrightarrow SO_4^- + SO_4^{2-}$	2	$9.4{\times}10^6$		Huie and Neta (1987)
S30	$SO_5^- + HSO_3^- \longrightarrow SO_3^- + HSO_5^-$	2	$2.5{\times}10^4$		Huie and Neta (1987); Deister and Warneck (1990)
S31	$SO_5^- + SO_3^{2-} \xrightarrow{H^+} SO_3^- + HSO_5^-$	2	$3.6{\times}10^6$		Huie and Neta (1987); Deister and Warneck (1990)
S32	$SO_5^- + O_2^- \xrightarrow{H^+} HSO_5^- + O_2$	2	$2.3{\times}10^8$		Buxton et al. (1996)
S33	$SO_5^- + SO_5^- \longrightarrow$ products	2	$1.0{\times}10^8$		Ross et al. (1992)

n reaction order, ^{a} photolysis rates calculated online, ^{b} special rate functions

Table 3 - Aqueous phase reactions.

no	reaction	n	A [$M^{1-n}s^{-1}$]	$-E_a$ / R [K]	reference
S34	$DMS + O_3 \longrightarrow O_2 + DMSO$	2	8.6×10^{8}	-2600	Gershenzon et al. (2001)
S35	$DMS + OH \longrightarrow 0.5\ CH_3SO_3^- + 0.5\ CH_3O_2 + 0.5\ HSO_4^- + HCHO + H^+$	2	1.9×10^{10}		Ross et al. (1998)
S36	$DMSO + OH \xrightarrow{O_2} CH_3SO_2^- + CH_3O_2 + H^+$	2	4.5×10^{9}		Bardouki et al. (2002)
S37	$CH_3SO_2^- + OH \xrightarrow{O_2} CH_3SO_3^- + H_2O$	2	1.2×10^{10}		Bardouki et al. (2002)
S38	$CH_3SO_3^- + OH \longrightarrow SO_4^{2-} + H^+ + CH_3O_2$	2	1.2×10^{7}		Bonsang et al. (1991)
Cl reactions					
Cl1	$Cl + H_2O_2 \longrightarrow HO_2 + Cl^- + H^+$	2	2.0×10^{9}		Yu (2001)
Cl2	$Cl + H_2O \longrightarrow H^+ + ClOH^-$	2	1.8×10^{5}		Yu (2001)
Cl3	$Cl + NO_3^- \xrightarrow{H_2O} NO_3 + Cl^-$	2	1.0×10^{8}		Buxton et al. (1999b)
Cl4	$Cl + DOM \longrightarrow Cl^- + HO_2$	2	5.0×10^{9}		estimated (C. Anastasio, pers. comm.) from Ross et al. (1998)
Cl5	$Cl + SO_4^{2-} \longrightarrow SO_4^- + Cl^-$	2	2.1×10^{8}		Buxton et al. (1999a)
Cl6	$Cl + Cl \longrightarrow Cl_2$	2	8.8×10^{7}		Wu et al. (1980)
Cl7	$Cl^- + OH \longrightarrow ClOH^-$	2	4.2×10^{9}		Yu (2001)
Cl8	$Cl^- + O_3 \longrightarrow ClO^- + O_2$	2	3.0×10^{-3}		Hoigné et al. (1985)
Cl9	$Cl^- + NO_3 \longrightarrow NO_3^- + Cl$	2	9.3×10^{6}	-4330	Exner et al. (1992)
Cl10	$Cl^- + SO_4^- \longrightarrow SO_4^{2-} + Cl$	2	2.5×10^{8}		Buxton et al. (1999a)
Cl11	$Cl^- + HSO_5^- \longrightarrow HOCl + SO_4^{2-}$	2	1.8×10^{-3}	-7352	Fortnum et al. (1960)
Cl12	$Cl^- + HOCl + H^+ \longrightarrow Cl_2$	3	2.2×10^{4}	-3508	Ayers et al. (1996)
Cl13	$Cl_2 \longrightarrow Cl^- + HOCl + H^+$	1	2.2×10^{1}	-8012	Ayers et al. (1996)
Cl14	$Cl_2^- + OH \longrightarrow HOCl + Cl^-$	2	1.0×10^{9}		Ross et al. (1998)
Cl15	$Cl_2^- + OH^- \longrightarrow Cl^- + Cl^- + OH$	2	4.0×10^{6}		Jacobi (1996)
Cl16	$Cl_2^- + HO_2 \longrightarrow Cl^- + Cl^- + H^+ + O_2$	2	3.1×10^{9}		Yu (2001)
Cl17	$Cl_2^- + O_2^- \longrightarrow Cl^- + Cl^- + O_2$		6.0×10^{9}		Jacobi (1996)
Cl18	$Cl_2^- + H_2O_2 \longrightarrow Cl^- + Cl^- + H^+ + HO_2$	2	7.0×10^{5}	-3340	Jacobi (1996)
Cl19	$Cl_2^- + NO_2^- \longrightarrow Cl^- + Cl^- + NO_2$	2	6.0×10^{7}		Jacobi (1996)
Cl20	$Cl_2^- + CH_3OOH \longrightarrow Cl^- + Cl^- + H^+ + CH_3O_2$	2	7.0×10^{5}	-3340	assumed by Jacobi (1996)
Cl21	$Cl_2^- + DOM \longrightarrow Cl^- + Cl^- + HO_2$	2	1.0×10^{6}		estimated (C. Anastasio, pers. comm.) from Ross et al. (1998)
Cl22	$Cl_2^- + HSO_3^- \longrightarrow SO_3^- + Cl^- + Cl^- + H^+$	2	4.7×10^{8}	-1082	Shoute et al. (1991)
Cl23	$Cl_2^- + SO_3^{2-} \longrightarrow SO_3^- + Cl^- + Cl^-$	2	6.2×10^{7}		Jacobi et al. (1996)
Cl24	$Cl_2^- + Cl_2^- \longrightarrow Cl_2 + 2\,Cl^-$	2	6.2×10^{9}		Yu (2001)
Cl25	$Cl_2^- + Cl \longrightarrow Cl^- + Cl_2$	2	2.7×10^{9}		Yu (2001)
Cl26	$Cl_2^- + DMS \longrightarrow 0.5CH_3SO_3^- + 0.5CH_3O_2 + 0.5HSO_4^- + HCHO + 2\,Cl^- + 2\,H^+$	2	3.0×10^{9}		rate from Ross et al. (1998)
Cl27	$ClOH^- \longrightarrow Cl^- + OH$	1	6.0×10^{9}		Yu (2001)
Cl28	$ClOH^- + H^+ \longrightarrow Cl + H_2O$	2	4.0×10^{10}		Yu (2001)
Cl29	$HOCl + HO_2 \longrightarrow Cl + O_2$	2	7.5×10^{6}		assumed = Cl30 Long and Bielski (1980)
Cl30	$HOCl + O_2^- \longrightarrow Cl + OH^- + O_2$	2	7.5×10^{6}		Long and Bielski (1980)
Cl31	$HOCl + SO_3^{2-} \longrightarrow Cl^- + HSO_4^-$	2	7.6×10^{8}		Fogelman et al. (1989)
Cl32	$HOCl + HSO_3^- \longrightarrow Cl^- + HSO_4^- + H^+$	2	7.6×10^{8}		assumed = Cl31 Fogelman et al. (1989)
Cl33	$Cl_2 + HO_2 \longrightarrow Cl_2^- + H^+ + O_2$	2	1.0×10^{9}		Bjergbakke et al. (1981)
Cl34	$Cl_2 + O_2^- \longrightarrow Cl_2^- + O_2$	2	1.0×10^{9}		assumed = Cl33 Bjergbakke et al. (1981)
Cl35	$Cl^- + HNO_4 \longrightarrow HOCl + NO_3^-$	2	1.4×10^{-2}		Evans et al. (2003)
Br reactions					
Br1	$Br + OH^- \longrightarrow BrOH^-$	2	1.3×10^{10}		Zehavi and Rabani (1972)

n reaction order, ^{a} photolysis rates calculated online, ^{b} special rate functions

Table 3 - Aqueous phase reactions.

no	reaction	n	A [$M^{1-n}s^{-1}$]	$-E_a$ / R [K]	reference
Br2	$Br + DOM \longrightarrow Br^- + HO_2$	2	2.0×10^{8}		estimated (C. Anastasio, pers. comm.) from Ross et al. (1998)
Br3	$Br^- + OH \longrightarrow BrOH^-$	2	1.1×10^{10}		Zehavi and Rabani (1972)
Br4	$Br^- + O_3 \longrightarrow BrO^- + O_2$	2	2.1×10^{2}	-4450	Haag and Hoigné (1983)
Br5	$Br^- + NO_3 \longrightarrow Br + NO_3^-$	2	3.8×10^{9}		Zellner et al. 1996 in Herrmann et al. (2000)
Br6	$Br^- + SO_4^- \longrightarrow Br + SO_4^{2-}$	2	2.1×10^{9}		Jacobi (1996)
Br7	$Br^- + HSO_5^- \longrightarrow HOBr + SO_4^{2-}$	2	1.0	-5338	Fortnum et al. (1960)
Br8	$Br^- + HOBr + H^+ \longrightarrow Br_2$	3	1.6×10^{10}		Liu and Margerum (2001)
Br9	$Br_2 \longrightarrow Br^- + HOBr + H^+$	1	9.7×10^{1}	7457	Liu and Margerum (2001)
Br10	$Br_2^- + O_2^- \longrightarrow Br^- + Br^-$	2	1.7×10^{8}		Wagner and Strehlow (1987)
Br11	$Br_2^- + HO_2 \xrightarrow{H^+} Br_2 + H_2O_2$	2	4.4×10^{9}		Matthew et al. (2003)
Br12	$Br_2^- + H_2O_2 \longrightarrow Br^- + Br^- + H^+ + HO_2$	2	5.0×10^{2}		Chameides and Stelson (1992)
Br13	$Br_2^- + Br_2^- \longrightarrow Br^- + Br^- + Br_2$	2	1.9×10^{9}		Ross et al. (1992)
Br14	$Br_2^- + CH_3OOH \longrightarrow Br^- + Br^- + H^+ + CH_3O_2$	2	1.0×10^{5}		assumed by Jacobi (1996)
Br15	$Br_2^- + DOM \longrightarrow Br^- + Br^- + HO_2$	2	1.0×10^{5}		estimated (C. Anastasio, pers. comm.) from Ross et al. (1998)
Br16	$Br_2^- + NO_2^- \longrightarrow Br^- + Br^- + NO_2$	2	1.7×10^{7}	-1720	Shoute et al. (1991)
Br17	$Br_2^- + HSO_3^- \longrightarrow Br^- + Br^- + H^+ + SO_3^-$	2	6.3×10^{7}	-782	Shoute et al. (1991)
Br18	$Br_2^- + SO_3^{2-} \longrightarrow Br^- + Br^- + SO_3^-$	2	2.2×10^{8}	-650	Shoute et al. (1991)
Br19	$Br_2^- + DMS \longrightarrow 0.5\ CH_3SO_3^- + 0.5\ CH_3O_2 + 0.5\ HSO_4^- + HCHO + 2\,Br^- + 2\,H^+$	2	3.2×10^{9}		rate from Ross et al. (1998)
Br20	$BrOH^- \longrightarrow Br^- + OH$	1	3.3×10^{7}		Zehavi and Rabani (1972)
Br21	$BrOH^- \longrightarrow Br + OH^-$	1	4.2×10^{6}		Zehavi and Rabani (1972)
Br22	$BrOH^- + H^+ \longrightarrow Br$	2	4.4×10^{10}		Zehavi and Rabani (1972)
Br23	$BrOH^- + Br^- \longrightarrow Br_2^- + OH^-$	2	1.9×10^{8}		Zehavi and Rabani (1972)
Br24	$BrO^- + SO_3^{2-} \longrightarrow Br^- + SO_4^{2-}$	2	1.0×10^{8}		Troy and Margerum (1991)
Br25	$HOBr + HO_2 \longrightarrow Br + O_2$	2	1.0×10^{9}		Herrmann et al. (1999)
Br26	$HOBr + O_2^- \longrightarrow Br + OH^- + O_2$	2	3.5×10^{9}		Schwarz and Bielski (1986)
Br27	$HOBr + H_2O_2 \longrightarrow Br^- + H^+ + O_2$	2	1.2×10^{6}		von Gunten and Oliveras (1998)
Br28	$HOBr + SO_3^{2-} \longrightarrow Br^- + HSO_4^-$	2	5.0×10^{9}		Troy and Margerum (1991)
Br29	$HOBr + HSO_3^- \longrightarrow Br^- + HSO_4^- + H^+$	2	5.0×10^{9}		assumed = Br28 Troy and Margerum (1991)
Br30	$Br_2 + HO_2 \longrightarrow Br_2^- + H^+ + O_2$	2	1.1×10^{8}		Ross et al. (1998)
Br31	$Br_2 + O_2^- \longrightarrow Br_2^- + O_2$	2	5.6×10^{9}		Ross et al. (1998)
Br32	$Br^- + HNO_4 \longrightarrow HOBr + NO_3^-$	2	5.4×10^{-1}		Evans et al. (2003)
Br33	$Br^- + O_3 + H^+ \longrightarrow HOBr + O_2$	2	11.7		Evans et al. (2003)
mixed halide reactions					
Hx1	$Br^- + HOCl + H^+ \longrightarrow BrCl$	3	1.3×10^{6}		Liu and Margerum (2001)
Hx2	$Cl^- + HOBr + H^+ \longrightarrow BrCl$	3	2.3×10^{10}		Liu and Margerum (2001)

n reaction order, ^{a} photolysis rates calculated online, ^{b} special rate functions

Table 3 - Aqueous phase reactions.

no	reaction	n	A [$M^{1-n}s^{-1}$]	$-E_a$ / R [K]	reference
Hx3	$BrCl \longrightarrow Cl^- + HOBr + H^+$	1	3.0×10^6		Liu and Margerum (2001)
Hx4	$Br^- + ClO^- + H^+ \longrightarrow BrCl + OH^-$	3	3.7×10^{10}		Kumar and Margerum (1987)
Hx5	$Cl_2 + Br^- \longrightarrow BrCl_2^-$	2	7.7×10^9		Liu and Margerum (2001)
Hx6	$BrCl_2^- \longrightarrow Cl_2 + Br^-$	1	1.83×10^3		Liu and Margerum (2001)
photolysis					
hv1	$O_3 + h\nu \longrightarrow OH + OH + O_2$		^{a}		equal to gas phase
hv2	$H_2O_2 + h\nu \longrightarrow OH + OH$		^{a}		equal to gas phase
hv3	$NO_3^- + h\nu \xrightarrow{H^+} NO_2 + OH$		^{a}		Warneck and Wurzinger (1988); Zellner et al. (1990)
hv4	$NO_2^- + h\nu \xrightarrow{H^+} NO + OH$		^{a}		Warneck and Wurzinger (1988); Zellner et al. (1990)
hv5	$HOCl + h\nu \longrightarrow OH + Cl$		^{a}		equal to gas phase
hv6	$Cl_2 + h\nu \longrightarrow Cl + Cl$		^{a}		equal to gas phase
hv7	$HOBr + h\nu \longrightarrow OH + Br$		^{a}		equal to gas phase
hv8	$Br_2 + h\nu \longrightarrow Br + Br$		^{a}		equal to gas phase
hv9	$BrCl + h\nu \longrightarrow Cl + Br$		^{a}		equal to gas phase
hv10	$NO_3^- + h\nu \longrightarrow NO_2^- + O(^3P)$		^{a}		Warneck and Wurzinger (1988); Zellner et al. (1990)
hv11	$O_3 + h\nu \longrightarrow O_2 + O(^3P)$		^{a}		equal to gas phase

n reaction order, ^{a} photolysis rates calculated online, ^{b} special rate functions

Table 4: Aqueous phase equilibrium constants.

no	reaction	n	m	$K[M^{n-m}]$	$\Delta H/R$	reference
equilibrium reactions						
Eq1	$CO_2 \longleftrightarrow H^+ + HCO_3^-$	1	2	4.3×10^{-7}	-913	Chameides (1984)
Eq2	$NH_3 \longleftrightarrow OH^- + NH_4^+$	1	2	1.7×10^{-5}	-4325	Chameides (1984)
Eq3	$H_2O \longleftrightarrow H^+ + OH^-$	1	2	1.0×10^{-14}	-6716	Chameides (1984)
Eq4	$HCOOH \longleftrightarrow H^+ + HCOO^-$	1	2	1.8×10^{-4}		Weast (1980)
Eq5	$HSO_3^- \longleftrightarrow H^+ + SO_3^{2-}$	1	2	6.0×10^{-8}	1120	Chameides (1984)
Eq6	$H_2SO_4 \longleftrightarrow H^+ + HSO_4^-$	1	2	1.0×10^{3}		Seinfeld and Pandis (1998)
Eq7	$HSO_4^- \longleftrightarrow H^+ + SO_4^{2-}$	1	2	1.2×10^{-2}	1120	Weast (1980)
Eq8	$HO_2 \longleftrightarrow O_2^- + H^+$	1	2	1.6×10^{-5}		Weinstein-Lloyd and Schwartz (1991)
Eq9	$SO_2 \longleftrightarrow H^+ + HSO_3^-$	1	2	1.7×10^{-2}	2090	Chameides (1984)
Eq10	$Cl_2^- \longleftrightarrow Cl + Cl^-$	1	2	5.2×10^{-6}		Jayson et al. (1973)
Eq11	$HOCl \longleftrightarrow H^+ + ClO^-$	1	2	3.2×10^{-8}		Lax (1969)
Eq12	$HBr \longleftrightarrow H^+ + Br^-$	1	2	1.0×10^{9}		Lax (1969)
Eq13	$Br_2^- \longleftrightarrow Br + Br^-$	1	2	9.1×10^{-6}		Mamou et al. (1977)
Eq14	$HOBr \longleftrightarrow H^+ + BrO^-$	1	2	2.3×10^{-9}	-3091	Kelley and Tartar (1956)
Eq15	$BrCl + Cl^- \longleftrightarrow BrCl_2^-$	2	1	3.8	1143	Wang et al. (1994)
Eq16	$BrCl + Br^- \longleftrightarrow Br_2Cl^-$	2	1	1.8×10^{4}		Wang et al. (1994)
Eq17	$Br_2 + Cl^- \longleftrightarrow Br_2Cl^-$	2	1	1.3		Wang et al. (1994)
Eq18	$HNO_3 \longleftrightarrow H^+ + NO_3^-$	1	2	1.5×10^{1}		Davis and de Bruin (1964)
Eq19	$HCl \longleftrightarrow H^+ + Cl^-$	1	2	1.7×10^{6}		Marsh and McElroy (1985)
Eq20	$HONO \longleftrightarrow H^+ + NO_2^-$	1	2	5.1×10^{-4}	-1260	Schwartz and White (1981)
Eq21	$HNO_4 \longleftrightarrow NO_4^- + H^+$	1	2	1.0×10^{-5}	8700	Warneck (1999)

The temperature dependence is $K = K_0 \times \exp(\frac{-\Delta H}{R}(\frac{1}{T} - \frac{1}{T_0})), T_0 = 298K$.

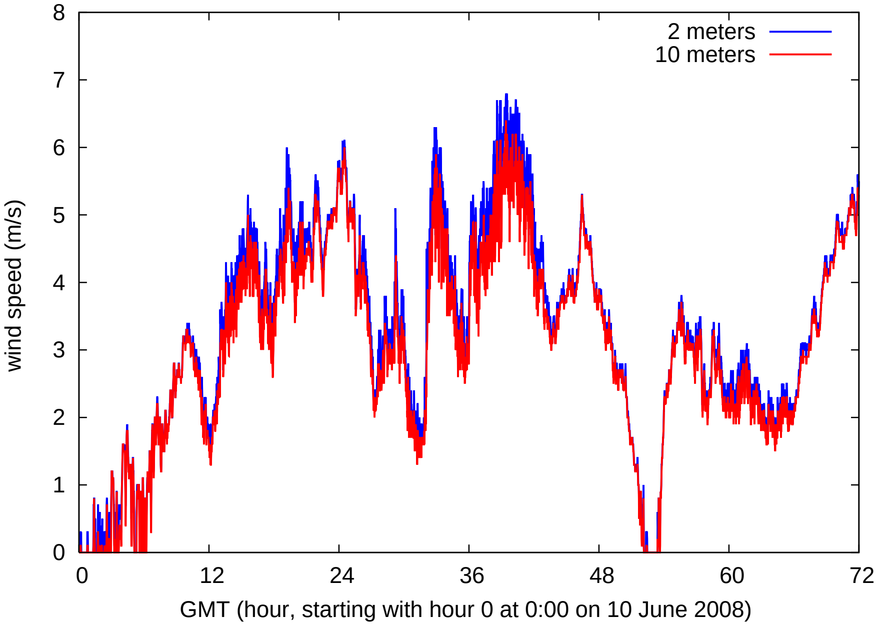

Figure 1: Measured 2 m and 10 m wind speeds at Summit on June 10, 2008-June13, 2008.

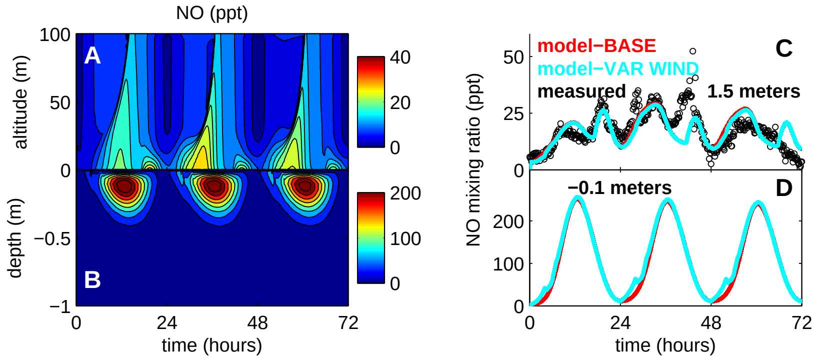

Figure 2: Wind Speed Sensitivity Run: Modeled NO mixing ratios using hourly binned measured wind speed (in cyan) during June 10, 2008-June 13, 2008 (instead of a constant 3 m/s 10 meter wind speed, in red) in the atmosphere (A) and interstitial (B) air. Modeled mixing ratios in the atmosphere at an altitude of 1.5 m above the snowpack are compared with measurements in panel C. Predicted interstitial air mixing ratios 10 cm below the snow surface are shown in panel D.

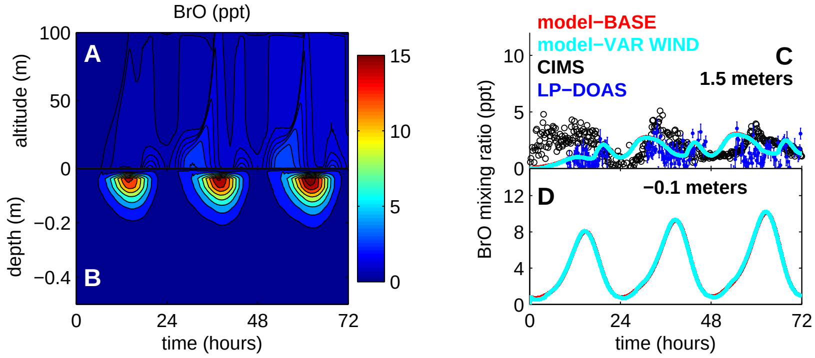

Figure 3: Wind Speed Sensitivity Run: Modeled BrO mixing ratios using hourly binned measured wind speed (in cyan) during June 10, 2008-June 13, 2008 (instead of a constant 3 m/s 10 meter wind speed, in red) in the atmosphere (A) and interstitial (B) air. Modeled mixing ratios in the atmosphere at an altitude of 1.5 m above the snowpack are compared with measurements in panel C. Predicted interstitial air mixing ratios 10 cm below the snow surface are shown in panel D.

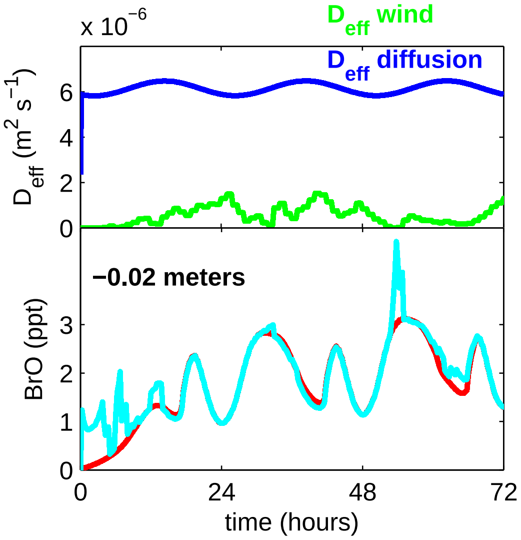

Figure 4: Contribution of the effective diffusion constant (m^2 s^{-1}) from wind pumping and molecular diffusion at a depth of 2 cm in the firn using the measured hourly averaged surface wind speed to calculate the wind pumping speed (upper panel) and the the modeled BrO mixing ratio at a depth of 2 cm for the base case run (red) using a constant 3 m/s 10 meter wind speed and a sensitivity run (cyan) using the hourly averaged measured 10 meter wind speed. See the following figures for the difference in the atmosphere and at a depth of 10 cm.

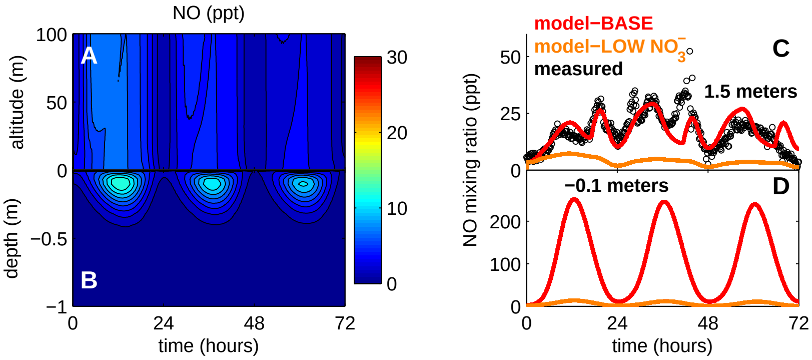

Figure 5: HNO_3 Sensitivity Run 1: Modeled NO mixing ratios with the initial NO_3^- and H^+ concentrations in the liquid layer equal to 2.3×10^{-4} M (LOW NO_3^-) in the atmosphere (A) and interstitial (B) air. Modeled mixing ratios for this and the base case run in the atmosphere at an altitude of 1.5 m above the snowpack are compared with measurements in panel C. Predicted interstitial air mixing ratios 10 cm below the snow surface are shown in panel D. The predicted NO mixing ratios using this initialization indicate it is not consistent with the measured NO mixing ratios.

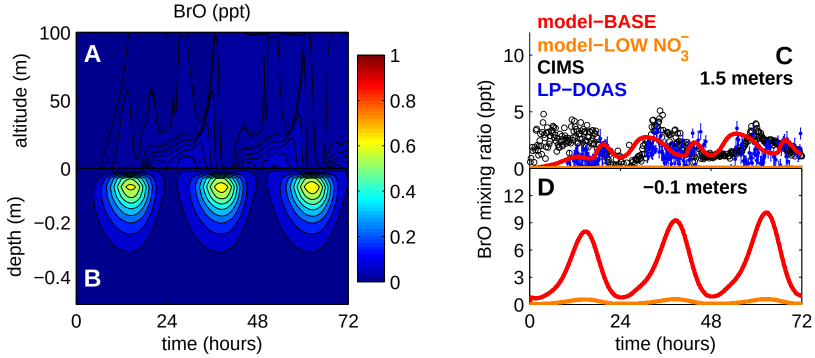

Figure 6: HNO_3 Sensitivity Run 1: Modeled BrO mixing ratios with the initial NO_3^- and H^+ concentrations in the liquid layer equal to 2.3×10^{-4} M (LOW NO_3^-) in the atmosphere (A) and interstitial (B) air. Modeled mixing ratios for this and the base case run in the atmosphere at an altitude of 1.5 m above the snowpack are compared with measurements in panel C. Predicted interstitial air mixing ratios 10 cm below the snow surface are shown in panel D. The predicted BrO mixing ratios using this initialization indicate it is not consistent with the measured BrO mixing ratios.

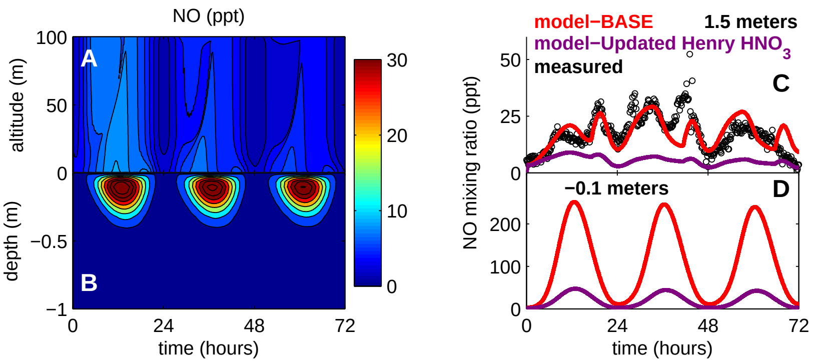

Figure 7: HNO_3 Sensitivity Run 2: Modeled NO mixing ratios with the initial NO_3^- and H^+ concentrations in the liquid layer equal to 1.17×10^{-3} M and with a higher Henry's law constant for HNO_3 according to Chameides (1984). The predicted NO mixing ratios for this run indicate that it is not consistent with the measured NO mixing ratios in ambient air.

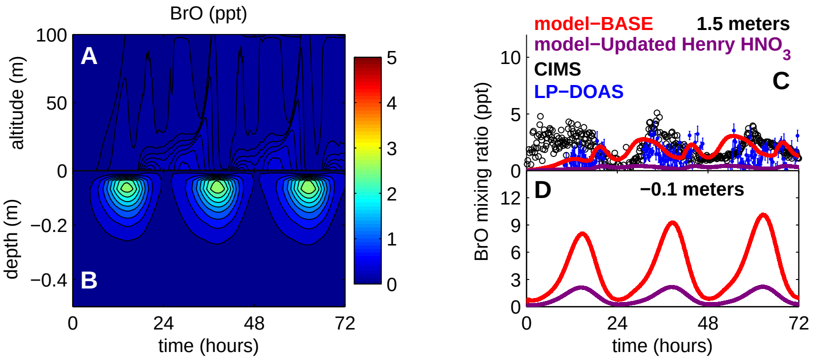

Figure 8: HNO_3 Sensitivity Run 2: Modeled BrO mixing ratios with the initial NO_3^- and H^+ concentrations in the liquid layer equal to 1.17×10^{-3} M and with a higher Henry's law constant for HNO_3 according to (Chameides 1984). The predicted BrO mixing ratios for this run indicate that it is not consistent with the measured BrO mixing ratios in ambient air.

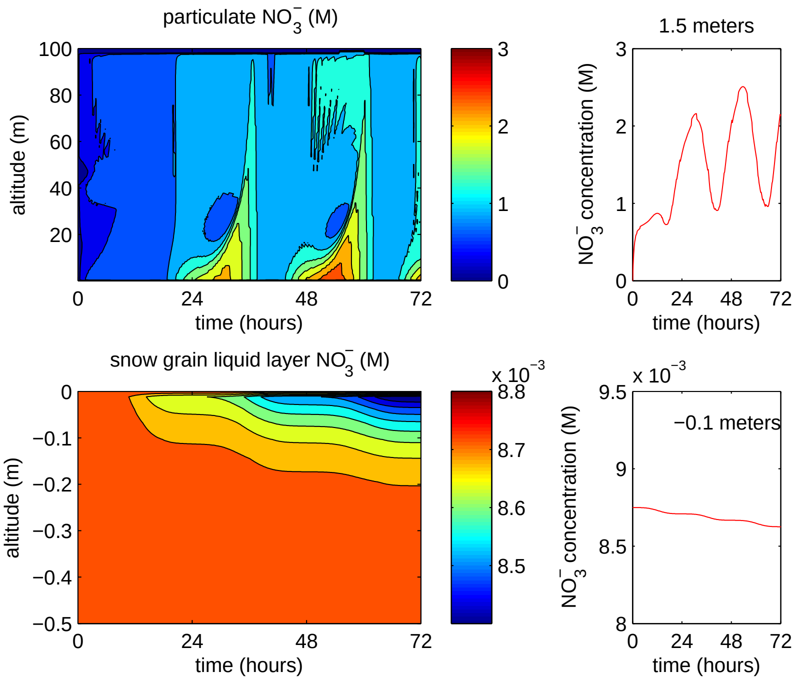

Figure 9: Modeled NO$_3^-$ in the snow liquid layer and in the atmosphere throughout the three day model run.

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