Table A1. Parameters for the calculation of the vertical speed of wind pumping and the effective diffusivity (Thomas et al., 2011).

Parameter	Value	Units	Description
μ	1.6×10^{-5}	$N\,m^{-2}\,s$	air dynamic viscosity
λ_{surf}	3.0×10^{-2}	m	relief wavelength
h	1.5×10^{-2}	m	relief amplitude
α	1	-	horizontal aspect ratio of relief
k	8.0×10^{-10}	m^2	permeability

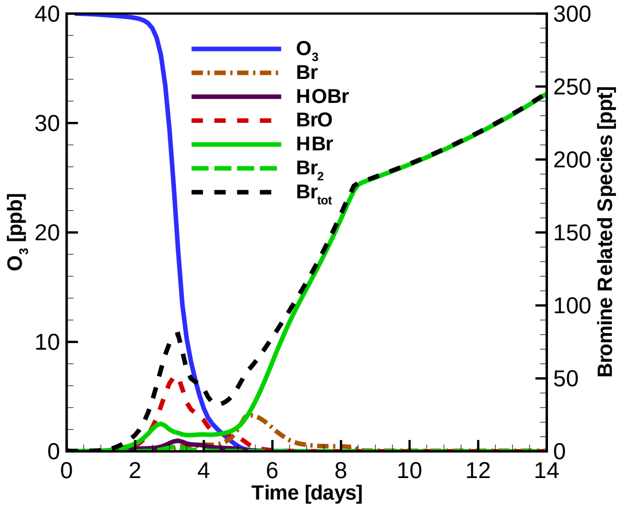
Table A2. The chemical reaction mechanism applied in KINAL-SNOW, with the presence of a 35 cm snowpack which is divided into 7 uniform layers. A constant temperature $T = 258K$ is assumed in the model, and the rate of third-body reactions is estimated as $k = k_\infty \times \frac{k_0/k_\infty}{(1+k_0/k_\infty)} \times F_c^{\frac{1}{1+(\log_{10}(k_0/k_\infty))^2}}$ (Atkinson et al., 2006).

Reaction	k $[(\text{molec. cm}^{-3})^{1-n}\text{s}^{-1}]$	Order n	Reference	Reaction No.
$O_3 + h\nu \rightarrow O(^1D) + O_2$	4.70×10^{-7}	1	Lehrer et al. (2004)	(R1) (×8)
$O(^1D) + O_2 \rightarrow O_3$	$3.20\times10^{-11}\exp(67/T)$	2	Atkinson et al. (2006)	(R2) (×8)
$O(^1D) + N_2 \rightarrow O_3 + N_2$	$1.80\times10^{-11}\exp(107/T)$	2	Atkinson et al. (2006)	(R3) (×8)
$O(^1D) + H_2O \rightarrow 2OH$	2.20×10^{-10}	2	Atkinson et al. (2006)	(R4) (×8)
$Br + O_3 \rightarrow BrO + O_2$	$1.70\times10^{-11}\exp(-800/T)$	2	Atkinson et al. (2006)	(R5) (×8)
$Br_2 + h\nu \rightarrow 2Br$	0.021	1	Lehrer et al. (2004)	(R6) (×8)
$BrO + h\nu \xrightarrow{O_2} Br + O_3$	0.014	1	Lehrer et al. (2004)	(R7) (×8)
$BrO + BrO \rightarrow 2Br + O_2$	2.70×10^{-12}	2	Atkinson et al. (2006)	(R8) (×8)
$BrO + BrO \rightarrow Br_2 + O_2$	$2.90\times10^{-14}\exp(840/T)$	2	Atkinson et al. (2006)	(R9) (×8)
$BrO + HO_2 \rightarrow HOBr + O_2$	$4.5\times10^{-12}\exp(500/T)$	2	Atkinson et al. (2006)	(R10) (×8)
$HOBr + h\nu \rightarrow Br + OH$	3.00×10^{-4}	1	Lehrer et al. (2004)	(R11) (×8)
$CO + OH(+M) \xrightarrow{O_2} HO_2 + CO_2(+M)$	$1.44\times10^{-13}(1+\frac{[N_2]}{4\times10^{19}})$	2	Atkinson et al. (2006)	(R12) (×8)
$Br + HO_2 \rightarrow HBr + O_2$	$7.70\times10^{-12}\exp(-450/T)$	2	Atkinson et al. (2006)	(R13) (×8)
$HOBr + HBr \xrightarrow{aerosol} Br_2 + H_2O$	See Sect. 2.2 of the manuscript			(R14) (×8)
$Br + HCHO \xrightarrow{O_2} HBr + CO + HO_2$	$7.70\times10^{-12}\exp(-580/T)$	2	Atkinson et al. (2006)	(R15) (×8)
$Br + CH_3CHO \xrightarrow{O_2} HBr + CH_3CO_3$	$1.80\times10^{-11}\exp(-460/T)$	2	Atkinson et al. (2006)	(R16) (×8)
$Br_2 + OH \rightarrow HOBr + Br$	$2.0\times10^{-11}\exp(240/T)$	2	Atkinson et al. (2006)	(R17) (×8)
$HBr + OH \rightarrow H_2O + Br$	$5.50\times10^{-12}\exp(205/T)$	2	Atkinson et al. (2006)	(R18) (×8)
$Br + C_2H_2 \xrightarrow{3O_2} 2CO + 2HO_2 + Br$	4.20×10^{-14}	2	Borken (1996)	(R19) (×8)
$Br + C_2H_2 \xrightarrow{2O_2} 2CO + HO_2 + HBr$	8.92×10^{-14}	2	Borken (1996)	(R20) (×8)
$Br + C_2H_4 \xrightarrow{3.5O_2} 2CO + 2HO_2 + Br + H_2O$	2.52×10^{-13}	2	Barnes et al. (1993)	(R21) (×8)
$Br + C_2H_4 \xrightarrow{2.5O_2} 2CO + HO_2 + HBr + H_2O$	5.34×10^{-13}	2	Barnes et al. (1993)	(R22) (×8)
$CH_4 + OH \xrightarrow{O_2} CH_3O_2 + H_2O$	$1.85\times10^{-12}\exp(-1690/T)$	2	Atkinson et al. (2006)	(R23) (×8)
$BrO + CH_3O_2 \rightarrow Br + HCHO + HO_2$	1.60×10^{-12}	2	Aranda et al. (1997)	(R24) (×8)
$BrO + CH_3O_2 \rightarrow HOBr + HCHO + 0.5O_2$	4.10×10^{-12}	2	Aranda et al. (1997)	(R25) (×8)

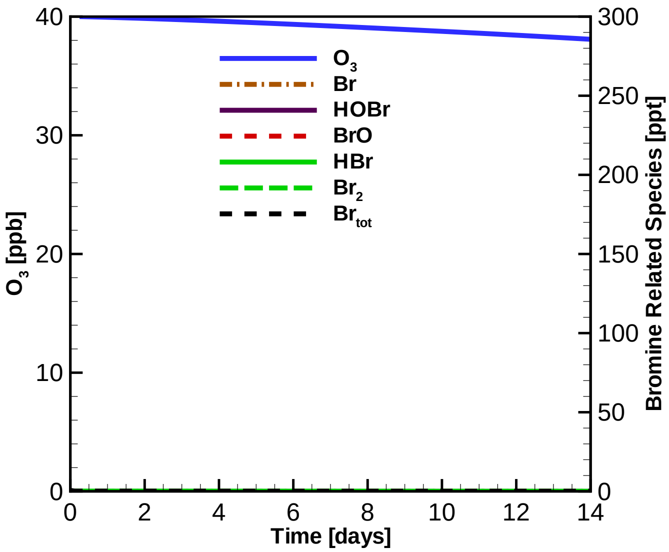
Reaction	k $[(\text{molec. cm}^{-3})^{1-n}\text{s}^{-1}]$	Order n	Reference	Reaction No.
$OH+O_3 \rightarrow HO_2+O_2$	$1.70\times10^{-12}\exp(-940/T)$	2	Atkinson et al. (2006)	(R26) (×8)
$OH+HO_2 \rightarrow H_2O+O_2$	$4.80\times10^{-11}\exp(250/T)$	2	Atkinson et al. (2006)	(R27) (×8)
$OH+H_2O_2 \rightarrow HO_2+H_2O$	$2.90\times10^{-12}\exp(-160/T)$	2	Atkinson et al. (2006)	(R28) (×8)
$OH+OH \xrightarrow{O_2} H_2O+O_3$	$6.20\times10^{-14}(T/298)^{2.6}\exp(945/T)$	2	Atkinson et al. (2006)	(R29) (×8)
$HO_2+O_3 \rightarrow OH+2O_2$	$2.03\times10^{-16}(T/300)^{4.57}\exp(693/T)$	2	Atkinson et al. (2006)	(R30) (×8)
$HO_2+HO_2 \rightarrow O_2+H_2O_2$	$2.20\times10^{-13}\exp(600/T)$	2	Atkinson et al. (2006)	(R31) (×8)
$C_2H_6+OH \rightarrow C_2H_5+H_2O$	$6.90\times10^{-12}\exp(-1000/T)$	2	Atkinson et al. (2006)	(R32) (×8)
$C_2H_5+O_2 \rightarrow C_2H_4+HO_2$	3.80×10^{-15}	2	Atkinson et al. (2006)	(R33) (×8)
$C_2H_5+O_2(+M) \rightarrow C_2H_5O_2(+M)$	$k_0=5.90\times10^{-29}(T/300)^{-3.8}[N_2]$ $k_\infty=7.80\times10^{-12}$ $F_c=0.58\exp(-T/1250)$ $+0.42\exp(-T/183)$	2	Atkinson et al. (2006)	(R34) (×8)
$C_2H_4+OH(+M) \xrightarrow{1.5O_2} CH_3O_2+CO+H_2O(+M)$	$k_0=8.60\times10^{-29}(T/300)^{-3.1}[N_2]$ $k_\infty=9.00\times10^{-12}(T/300)^{-0.85}$ $F_c=0.48$	2	Atkinson et al. (2006)	(R35) (×8)
$C_2H_4+O_3 \rightarrow HCHO+CO+H_2O$	4.33×10^{-19}	2	Sander et al. (1997)	(R36) (×8)
$C_2H_2+OH(+M) \xrightarrow{1.5O_2} HCHO+CO+HO_2(+M)$	$k_0=5.00\times10^{-30}(T/300)^{-1.5}[N_2]$ $k_\infty=1.00\times10^{-12}$ $F_c=0.37$	2	Atkinson et al. (2006)	(R37) (×8)
$C_3H_8+OH \xrightarrow{2O_2} C_2H_5O_2+CO+2H_2O$	$7.60\times10^{-12}\exp(-585/T)$	2	Atkinson et al. (2006)	(R38) (×8)
$HCHO+OH \xrightarrow{O_2} CO+H_2O+HO_2$	$5.40\times10^{-12}\exp(135/T)$	2	Atkinson et al. (2006)	(R39) (×8)
$CH_3CHO+OH \xrightarrow{O_2} CH_3CO_3+H_2O$	$4.40\times10^{-12}\exp(365/T)$	2	Atkinson et al. (2006)	(R40) (×8)
$CH_3O_2+HO_2 \rightarrow CH_3O_2H+O_2$	$3.42\times10^{-13}\exp(780/T)$	2	Atkinson et al. (2006)	(R41) (×8)
$CH_3O_2+HO_2 \rightarrow HCHO+H_2O+O_2$	$3.79\times10^{-14}\exp(780/T)$	2	Atkinson et al. (2006)	(R42) (×8)
$CH_3OOH+OH \rightarrow CH_3O_2+H_2O$	$1.00\times10^{-12}\exp(190/T)$	2	Atkinson et al. (2006)	(R43) (×8)
$CH_3OOH+OH \rightarrow HCHO+OH+H_2O$	$1.90\times10^{-12}\exp(190/T)$	2	Atkinson et al. (2006)	(R44) (×8)
$CH_3OOH+Br \rightarrow CH_3O_2+HBr$	$2.66\times10^{-12}\exp(-1610/T)$	2	Mallard et al. (1993)	(R45) (×8)
$CH_3O_2+CH_3O_2 \rightarrow CH_3OH+HCHO+O_2$	$6.29\times10^{-14}\exp(365/T)$	2	Atkinson et al. (2006)	(R46) (×8)
$CH_3O_2+CH_3O_2 \xrightarrow{O_2} 2HCHO+2HO_2$	$3.71\times10^{-14}\exp(365/T)$	2	Atkinson et al. (2006)	(R47) (×8)
$CH_3OH+OH \xrightarrow{O_2} HCHO+HO_2+H_2O$	$2.42\times10^{-12}\exp(-345/T)$	2	Atkinson et al. (2006)	(R48) (×8)
$C_2H_5O_2+C_2H_5O_2 \rightarrow C_2H_5O+C_2H_5O+O_2$	6.40×10^{-14}	2	Atkinson et al. (2006)	(R49) (×8)
$C_2H_5O+O_2 \rightarrow CH_3CHO+HO_2$	7.44×10^{-15}	2	Sander et al. (1997)	(R50) (×8)
$C_2H_5O+O_2 \rightarrow CH_3O_2+HCHO$	7.51×10^{-17}	2	Sander et al. (1997)	(R51) (×8)
$C_2H_5O_2+HO_2 \rightarrow C_2H_5OOH+O_2$	$3.80\times10^{-13}\exp(900/T)$	2	Atkinson et al. (2006)	(R52) (×8)
$C_2H_5OOH+OH \rightarrow C_2H_5O_2+H_2O$	8.21×10^{-12}	2	Sander et al. (1997)	(R53) (×8)
$C_2H_5OOH+Br \rightarrow C_2H_5O_2+HBr$	5.19×10^{-15}	2	Sander et al. (1997)	(R54) (×8)
$OH+OH(+M) \longrightarrow H_2O_2(+M)$	$k_0=6.90\times10^{-31}(T/300)^{-0.8}[N_2]$ $k_\infty=2.60\times10^{-11}$ $F_c=0.50$	2	Atkinson et al. (2006)	(R55) (×8)
$H_2O_2+h\nu \rightarrow 2OH$	2.00×10^{-6}	1	Lehrer et al. (2004)	(R56) (×8)
$HCHO+h\nu \xrightarrow{2O_2} 2HO_2+CO$	5.50×10^{-6}	1	Lehrer et al. (2004)	(R57) (×8)
$HCHO+h\nu \rightarrow H_2+CO$	9.60×10^{-6}	1	Lehrer et al. (2004)	(R58) (×8)
$C_2H_4O+h\nu \rightarrow CH_3O_2+CO++HO_2$	6.90×10^{-7}	1	Lehrer et al. (2004)	(R59) (×8)
$CH_3O_2H+h\nu \rightarrow OH+HCHO+HO_2$	1.20×10^{-6}	1	Lehrer et al. (2004)	(R60) (×8)
$C_2H_5O_2H+h\nu \rightarrow C_2H_5O+OH$	1.20×10^{-6}	1	Lehrer et al. (2004)	(R61) (×8)

Reaction	k $[(\text{molec. cm}^{-3})^{1-n}\text{s}^{-1}]$	Order n	Reference	Reaction No.
$NO + O_3 \rightarrow NO_2 + O_2$	$1.40\times10^{-12}\exp(-1310/T)$	2	Atkinson et al. (2006)	(R62) (×8)
$NO + HO_2 \rightarrow NO_2 + OH$	$3.60\times10^{-12}\exp(270/T)$	2	Atkinson et al. (2006)	(R63) (×8)
$NO_2 + O_3 \rightarrow NO_3 + O_2$	$1.40\times10^{-13}\exp(-2470/T)$	2	Atkinson et al. (2006)	(R64) (×8)
$NO_2 + OH(+M) \rightarrow HNO_3(+M)$	$k_0 = 3.30\times10^{-30}(T/300)^{-3.0}[N_2]$ $k_\infty = 4.10\times10^{-11}$ $F_c = 0.40$	2	Atkinson et al. (2006)	(R65) (×8)
$NO + NO_3 \rightarrow 2NO_2$	$1.80\times10^{-11}\exp(110/T)$	2	Atkinson et al. (2006)	(R66) (×8)
$HONO + OH \rightarrow NO_2 + H_2O$	$2.50\times10^{-12}\exp(260/T)$	2	Atkinson et al. (2006)	(R67) (×8)
$HO_2 + NO_2(+M) \rightarrow HNO_4(+M)$	$k_0 = 1.80\times10^{-31}(T/300)^{-3.2}[N_2]$ $k_\infty = 4.70\times10^{-12}$ $F_c = 0.60$	2	Atkinson et al. (2006)	(R68) (×8)
$HNO_4(+M) \rightarrow NO_2 + HO_2(+M)$	$k_0 = 4.10\times10^{-5}\exp(-10650/T)[N_2]$ $k_\infty = 4.80\times10^{15}\exp(-11170/T)$ $F_c = 0.60$	1	Atkinson et al. (2006)	(R69) (×8)
$HNO_4 + OH \rightarrow NO_2 + H_2O + O_2$	$3.20\times10^{-13}\exp(690/T)$	2	Atkinson et al. (2006)	(R70) (×8)
$NO + OH(+M) \rightarrow HONO(+M)$	$k_0 = 7.40\times10^{-31}(T/300)^{-2.4}[N_2]$ $k_\infty = 3.30\times10^{-11}(T/300)^{-0.3}$ $F_c = 0.81$	2	Atkinson et al. (2006)	(R71) (×8)
$OH + NO_3 \rightarrow NO_2 + HO_2$	2.00×10^{-11}	2	Atkinson et al. (2006)	(R72) (×8)
$HNO_3 + h\nu \rightarrow NO_2 + OH$	4.40×10^{-8}	1	Lehrer et al. (2004)	(R73) (×8)
$NO_2 + h\nu \xrightarrow{O_2} NO + O_3$	3.50×10^{-3}	1	Lehrer et al. (2004)	(R74) (×8)
$NO_3 + h\nu \xrightarrow{O_2} NO_2 + O_3$	1.40×10^{-1}	1	Lehrer et al. (2004)	(R75) (×8)
$NO_3 + h\nu \rightarrow NO + O_2$	1.70×10^{-2}	1	Lehrer et al. (2004)	(R76) (×8)
$NO + CH_3O_2 \xrightarrow{O_2} HCHO + HO_2 + NO_2$	$2.30\times10^{-12}\exp(360/T)$	2	Atkinson et al. (2006)	(R77) (×8)
$NO_3 + CH_3OH \xrightarrow{O_2} HCHO + HO_2 + HNO_3$	$9.40\times10^{-13}\exp(-2650/T)$	2	Atkinson et al. (2006)	(R78) (×8)
$NO_3 + HCHO \xrightarrow{O_2} CO + HO_2 + HNO_3$	5.60×10^{-16}	2	Atkinson et al. (2006)	(R79) (×8)
$NO + C_2H_5O_2 \xrightarrow{O_2} CH_3CHO + NO_2 + HO_2$	$2.60\times10^{-12}\exp(380/T)$	2	Atkinson et al. (2006)	(R80) (×8)
$NO + CH_3CO_3 \xrightarrow{O_2} CH_3O_2 + NO_2 + CO_2$	$7.50\times10^{-12}\exp(290/T)$	2	Atkinson et al. (2006)	(R81) (×8)
$NO_2 + CH_3CO_3(+M) \rightarrow PAN(+M)$	$k_0 = 2.70\times10^{-28}(T/300)^{-7.1}[N_2]$ $k_\infty = 1.20\times10^{-11}(T/300)^{-0.9}$ $F_c = 0.30$	2	Atkinson et al. (2006)	(R82) (×8)
$Br + NO_2(+M) \rightarrow BrNO_2(+M)$	$k_0 = 4.20\times10^{-31}(T/300)^{-2.4}[N_2]$ $k_\infty = 2.70\times10^{-11}$ $F_c = 0.55$	2	Atkinson et al. (2006)	(R83) (×8)
$Br + NO_3 \rightarrow BrO + NO_2$	1.60×10^{-11}	2	Atkinson et al. (2006)	(R84) (×8)
$BrO + NO_2(+M) \rightarrow BrONO_2(+M)$	$k_0 = 4.70\times10^{-31}(T/300)^{-3.1}[N_2]$ $k_\infty = 1.80\times10^{-11}$ $F_c = 0.40$	2	Atkinson et al. (2006)	(R85) (×8)
$BrO + NO \rightarrow Br + NO_2$	$8.70\times10^{-12}\exp(260/T)$	2	Atkinson et al. (2006)	(R86) (×8)
$BrONO_2 + h\nu \rightarrow NO_2 + BrO$	3.40×10^{-4}	1	Lehrer et al. (2004)	(R87) (×8)
$BrNO_2 + h\nu \rightarrow NO_2 + Br$	9.30×10^{-5}	1	Lehrer et al. (2004)	(R88) (×8)
$BrONO_2 + H_2O \xrightarrow{\text{aerosol}} HOBr + HNO_3$	See Sect. 2.2 of the manuscript			(R89) (×8)
$PAN + h\nu \rightarrow NO_2 + CH_3CO_3$	6.79×10^{-7}	1	Fishman and Carney (1984)	(R90) (×8)

Reaction	k $[(\text{molec. cm}^{-3})^{1-n}\text{s}^{-1}]$	Order n	Reference	Reaction No.
$HOBr_{(BL)} \rightarrow HOBr_{(SIA,i)}$	See Sect. 2.1.1 of the manuscript			(R721) (×7)
$BrONO_{2(BL)} \rightarrow BrONO_{2(SIA,i)}$	See Sect. 2.1.1 of the manuscript			(R728) (×7)
$HOBr_{(SIA,i)} \rightarrow HOBr_{(liquid,i)}$	See Sect. 2.1.2 of the manuscript			(R735) (×7)
$HOBr_{(liquid,i)} \rightarrow HOBr_{(SIA,i)}$	See Sect. 2.1.2 of the manuscript			(R742) (×7)
$BrONO_{2(SIA,i)} + H_2O \rightarrow HOBr_{(liquid,i)} + H^+_{(liquid,i)} + NO^-_{3(liquid,i)}$	See Sect. 2.1.2 of the manuscript			(R749) (×7)
$HOBr_{(liquid,i)} + H^+_{(liquid,i)} + Br^-_{(liquid,i)} \rightarrow Br_{2(liquid,i)} + H_2O_{(liquid,i)}$	See Sect. 2.1.3 of the manuscript	3	Beckwith et al. (1996)	(R756) (×7)
$Br_{2(liquid,i)} + H_2O_{(liquid,i)} \rightarrow HOBr_{(liquid,i)} + H^+_{(liquid,i)} + Br^-_{(liquid,i)}$	See Sect. 2.1.3 of the manuscript	1	Beckwith et al. (1996)	(R763) (×7)
$HOBr_{(liquid,i)} + H^+_{(liquid,i)} + Cl^-_{(liquid,i)} \rightarrow BrCl_{(liquid,i)} + H_2O_{(liquid,i)}$	See Sect. 2.1.3 of the manuscript	3	Wang et al. (1994)	(R770) (×7)
$BrCl_{(liquid,i)} + H_2O_{(liquid,i)} \rightarrow HOBr_{(liquid,i)} + H^+_{(liquid,i)} + Cl^-_{(liquid,i)}$	See Sect. 2.1.3 of the manuscript	1	Wang et al. (1994)	(R777) (×7)
$BrCl_{(liquid,i)} + Br^-_{(liquid,i)} \rightarrow Br_2Cl_{(liquid,i)}$	See Sect. 2.1.3 of the manuscript	2	Michalowski et al. (2000)	(R784) (×7)
$Br_2Cl_{(liquid,i)} \rightarrow BrCl_{(liquid,i)} + Br^-_{(liquid,i)}$	See Sect. 2.1.3 of the manuscript	1	Wang et al. (1994)	(R791) (×7)
$Br_2Cl_{(liquid,i)} \rightarrow Br_{2(liquid,i)} + Cl^-_{(liquid,i)}$	See Sect. 2.1.3 of the manuscript	1	Wang et al. (1994)	(R798) (×7)
$Br_{2(liquid,i)} + Cl^-_{(liquid,i)} \rightarrow Br_2Cl_{(liquid,i)}$	See Sect. 2.1.3 of the manuscript	2	Michalowski et al. (2000)	(R805) (×7)
$Br_{2(SIA,i)} \rightarrow Br_{2(liquid,i)}$	See Sect. 2.1.4 of the manuscript			(R812) (×7)
$Br_{2(liquid,i)} \rightarrow Br_{2(SIA,i)}$	See Sect. 2.1.4 of the manuscript			(R819) (×7)
$Br_{2(SIA,i)} \rightarrow Br_{2(BL)}$	See Sect. 2.1.5 of the manuscript			(R826) (×7)
$NO_{(SIA,i)} \rightarrow NO_{(BL)}$	See Sect. 2.4 of the manuscript			(R833) (×7)
$NO_{2(SIA,i)} \rightarrow NO_{2(BL)}$	See Sect. 2.4 of the manuscript			(R840) (×7)
$HONO_{(SIA,i)} \rightarrow HONO_{(BL)}$	See Sect. 2.4 of the manuscript			(R847) (×7)
$H_2O_{2(SIA,i)} \rightarrow H_2O_{2(BL)}$	See Sect. 2.4 of the manuscript			(R854) (×7)
$HCHO_{(SIA,i)} \rightarrow HCHO_{(BL)}$	See Sect. 2.4 of the manuscript			(R861) (×7)
$NO_{(BL)} \rightarrow NO_{(SIA,i)}$	See Sect. 2.4 of the manuscript			(R868) (×7)
$NO_{2(BL)} \rightarrow NO_{2(SIA,i)}$	See Sect. 2.4 of the manuscript			(R875) (×7)
$HONO_{(BL)} \rightarrow HONO_{(SIA,i)}$	See Sect. 2.4 of the manuscript			(R882) (×7)
$H_2O_{2(BL)} \rightarrow H_2O_{2(SIA,i)}$	See Sect. 2.4 of the manuscript			(R889) (×7)
$HCHO_{(BL)} \rightarrow HCHO_{(SIA,i)}$	See Sect. 2.4 of the manuscript			(R896) (×7)



(a)



(b)

Fig. A1. Temporal evolution of the mixing ratios of ozone and bromine species in the ambient air of the 200 m boundary layer when the initial PH value of the snowpack is (a) 7 and (b) 10.

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