Supplement of Atmos. Chem. Phys., 16, 14853–14873, 2016
http://www.atmos-chem-phys.net/16/14853/2016/
doi:10.5194/acp-16-14853-2016-supplement

Atmospheric Chemistry and Physics
Open Access

Supplement of

Derivation of the reduced reaction mechanisms of ozone depletion events in the Arctic spring by using concentration sensitivity analysis and principal component analysis

Le Cao et al.

Correspondence to: Le Cao (le.cao@nuist.edu.cn)

Table S1. The original chemical reaction mechanism with an assumption of a 200 m boundary layer. A constant temperature $T = 258$ K 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). For Reactions (SR14) and (SR90), the parameter r in the column of k denotes the average radius of the suspended aerosols. D_g is the molecular diffusivity. v_therm represents the mean molecular speed of HOBr and $BrONO_2$ for Reactions (SR14) and (SR90), respectively. γ denotes the uptake coefficient of the gas-phase HOBr or $BrONO_2$ by the suspended aerosols. $\alpha_\mathrm{eff,aerosol}$ is the effective aerosol surface area density. With respect to Reactions (SR15) and (SR92), r_a, r_b and r_c in the column of k represent the aerodynamic resistance, quasi-laminar resistance due to molecular diffusion, and surface resistance, respectively. $\alpha_\mathrm{eff,ice}$ is the surface area density of the ice-/snow-covered surfaces under the condition of a 200 m boundary layer.

Reaction Number	Reaction	k $[(\mathrm{molec.\ cm^{-3}})^{1-n}\mathrm{s^{-1}}]$	Order n	Reference
(SR1)	$O_3 + h\nu \rightarrow O(^1D) + O_2$	4.70×10^{-7}	1	Lehrer et al. (2004)
(SR2)	$O(^1D) + O_2 \rightarrow O_3$	$3.20\times10^{-11}\exp(67/T)$	2	Atkinson et al. (2006)
(SR3)	$O(^1D) + N_2 \rightarrow O_3 + N_2$	$1.80\times10^{-11}\exp(107/T)$	2	Atkinson et al. (2006)
(SR4)	$O(^1D) + H_2O \rightarrow 2OH$	2.20×10^{-10}	2	Atkinson et al. (2006)
(SR5)	$Br + O_3 \rightarrow BrO + O_2$	$1.70\times10^{-11}\exp(-800/T)$	2	Atkinson et al. (2006)
(SR6)	$Br_2 + h\nu \rightarrow 2Br$	0.021	1	Lehrer et al. (2004)
(SR7)	$BrO + h\nu \xrightarrow{O_2} Br + O_3$	0.014	1	Lehrer et al. (2004)
(SR8)	$BrO + BrO \rightarrow 2Br + O_2$	2.70×10^{-12}	2	Atkinson et al. (2006)
(SR9)	$BrO + BrO \rightarrow Br_2 + O_2$	$2.90\times10^{-14}\exp(840/T)$	2	Atkinson et al. (2006)
(SR10)	$BrO + HO_2 \rightarrow HOBr + O_2$	$4.5\times10^{-12}\exp(500/T)$	2	Atkinson et al. (2006)
(SR11)	$HOBr + h\nu \rightarrow Br + OH$	3.00×10^{-4}	1	Lehrer et al. (2004)
(SR12)	$CO + OH(+M) \xrightarrow{O_2} HO_2 + CO_2(+M)$	$1.44\times10^{-13}(1+\frac{[N_2]}{4\times10^{19}})$	2	Atkinson et al. (2006)
(SR13)	$Br + HO_2 \rightarrow HBr + O_2$	$7.70\times10^{-12}\exp(-450/T)$	2	Atkinson et al. (2006)
(SR14)	$HOBr + HBr \xrightarrow{aerosol} Br_2 + H_2O$	$(\frac{r}{D_\mathrm{g}} + \frac{4}{v_\mathrm{therm}\gamma})^{-1}\alpha_\mathrm{eff,aerosol}$		Cao et al. (2014)
(SR15)	$HOBr + H^+ + Br^- \xrightarrow{ice} Br_2 + H_2O$	$(r_a + r_b + r_c)^{-1}\alpha_\mathrm{eff,ice}$		Cao et al. (2014)
(SR16)	$Br + HCHO \xrightarrow{O_2} HBr + CO + HO_2$	$1.70\times10^{-11}\exp(-800/T)$	2	Sander et al. (2003)
(SR17)	$Br + CH_3CHO \xrightarrow{O_2} HBr + CH_3CO_3$	$1.80\times10^{-11}\exp(-460/T)$	2	Atkinson et al. (2006)
(SR18)	$Br_2 + OH \rightarrow HOBr + Br$	$2.0\times10^{-11}\exp(240/T)$	2	Atkinson et al. (2006)
(SR19)	$HBr + OH \rightarrow H_2O + Br$	$5.50\times10^{-12}\exp(205/T)$	2	Atkinson et al. (2006)
(SR20)	$Br + C_2H_2 \xrightarrow{3O_2} 2CO + 2HO_2 + Br$	4.20×10^{-14}	2	Borken (1996)
(SR21)	$Br + C_2H_2 \xrightarrow{2O_2} 2CO + HO_2 + HBr$	8.92×10^{-14}	2	Borken (1996)
(SR22)	$Br + C_2H_4 \xrightarrow{3.5O_2} 2CO + 2HO_2 + Br + H_2O$	2.52×10^{-13}	2	Barnes et al. (1993)
(SR23)	$Br + C_2H_4 \xrightarrow{2.5O_2} 2CO + HO_2 + HBr + H_2O$	5.34×10^{-13}	2	Barnes et al. (1993)
(SR24)	$CH_4 + OH \xrightarrow{O_2} CH_3O_2 + H_2O$	$1.85\times10^{-12}\exp(-1690/T)$	2	Atkinson et al. (2006)
(SR25)	$BrO + CH_3O_2 \rightarrow Br + HCHO + HO_2$	1.60×10^{-12}	2	Aranda et al. (1997)
(SR26)	$BrO + CH_3O_2 \rightarrow HOBr + HCHO + 0.5O_2$	4.10×10^{-12}	2	Aranda et al. (1997)
(SR27)	$OH + O_3 \rightarrow HO_2 + O_2$	$1.70\times10^{-12}\exp(-940/T)$	2	Atkinson et al. (2006)
(SR28)	$OH + HO_2 \rightarrow H_2O + O_2$	$4.80\times10^{-11}\exp(250/T)$	2	Atkinson et al. (2006)
(SR29)	$OH + H_2O_2 \rightarrow HO_2 + H_2O$	$2.90\times10^{-12}\exp(-160/T)$	2	Atkinson et al. (2006)
(SR30)	$OH + OH \xrightarrow{O_2} H_2O + O_3$	$6.20\times10^{-14}(T/298)^{2.6}\exp(945/T)$	2	Atkinson et al. (2006)
(SR31)	$HO_2 + O_3 \rightarrow OH + 2O_2$	$2.03\times10^{-16}(T/300)^{4.57}\exp(693/T)$	2	Atkinson et al. (2006)
(SR32)	$HO_2 + HO_2 \rightarrow O_2 + H_2O_2$	$2.20\times10^{-13}\exp(600/T)$	2	Atkinson et al. (2006)
(SR33)	$C_2H_6 + OH \rightarrow C_2H_5 + H_2O$	$6.90\times10^{-12}\exp(-1000/T)$	2	Atkinson et al. (2006)
(SR34)	$C_2H_5 + O_2 \rightarrow C_2H_4 + HO_2$	3.80×10^{-15}	2	Atkinson et al. (2006)
(SR35)	$C_2H_5 + O_2(+M) \rightarrow C_2H_5O_2(+M)$	$k_0 = 5.90\times10^{-29}(T/300)^{-3.8}[N_2]$ $k_\infty = 7.80\times10^{-12}$ $F_c = 0.58\exp(-T/1250)$ $+0.42\exp(-T/183)$	2	Atkinson et al. (2006)

Reaction Number	Reaction	k $[(\text{molec. cm}^{-3})^{1-n}\text{s}^{-1}]$	Order n	Reference
(SR36)	$C_2H_4 + OH(+M) \xrightarrow{1.5O_2} CH_3O_2 + CO + H_2O(+M)$	$k_0 = 8.60\times10^{-29}(T/300)^{-3.1}[N_2]$ $k_\infty = 9.00\times10^{-12}(T/300)^{-0.85}$ $F_c = 0.48$	2	Atkinson et al. (2006)
(SR37)	$C_2H_4 + O_3 \rightarrow HCHO + CO + H_2O$	4.33×10^{-19}	2	Sander et al. (1997)
(SR38)	$C_2H_2 + OH(+M) \xrightarrow{1.5O_2} HCHO + CO + HO_2(+M)$	$k_0 = 5.00\times10^{-30}(T/300)^{-1.5}[N_2]$ $k_\infty = 1.00\times10^{-12}$ $F_c = 0.37$	2	Atkinson et al. (2006)
(SR39)	$C_3H_8 + OH \xrightarrow{2O_2} C_2H_5O_2 + CO + 2H_2O$	$7.60\times10^{-12}\exp(-585/T)$	2	Atkinson et al. (2006)
(SR40)	$HCHO + OH \xrightarrow{O_2} CO + H_2O + HO_2$	$5.40\times10^{-12}\exp(135/T)$	2	Atkinson et al. (2006)
(SR41)	$CH_3CHO + OH \xrightarrow{O_2} CH_3CO_3 + H_2O$	$4.40\times10^{-12}\exp(365/T)$	2	Atkinson et al. (2006)
(SR42)	$CH_3O_2 + HO_2 \rightarrow CH_3O_2H + O_2$	$3.42\times10^{-13}\exp(780/T)$	2	Atkinson et al. (2006)
(SR43)	$CH_3O_2 + HO_2 \rightarrow HCHO + H_2O + O_2$	$3.79\times10^{-14}\exp(780/T)$	2	Atkinson et al. (2006)
(SR44)	$CH_3OOH + OH \rightarrow CH_3O_2 + H_2O$	$1.90\times10^{-12}\exp(190/T)$	2	Atkinson et al. (2006)
(SR45)	$CH_3OOH + OH \rightarrow HCHO + OH + H_2O$	$1.00\times10^{-12}\exp(190/T)$	2	Atkinson et al. (2006)
(SR46)	$CH_3OOH + Br \rightarrow CH_3O_2 + HBr$	$2.66\times10^{-12}\exp(-1610/T)$	2	Mallard et al. (1993)
(SR47)	$CH_3O_2 + CH_3O_2 \rightarrow CH_3OH + HCHO + O_2$	$6.71\times10^{-14}\exp(365/T)$	2	Atkinson et al. (2006)
(SR48)	$CH_3O_2 + CH_3O_2 \xrightarrow{O_2} 2HCHO + 2HO_2$	$3.29\times10^{-14}\exp(365/T)$	2	Atkinson et al. (2006)
(SR49)	$CH_3OH + OH \xrightarrow{O_2} HCHO + HO_2 + H_2O$	$2.42\times10^{-12}\exp(-345/T)$	2	Atkinson et al. (2006)
(SR50)	$C_2H_5O_2 + C_2H_5O_2 \rightarrow C_2H_5O + C_2H_5O + O_2$	6.40×10^{-14}	2	Atkinson et al. (2006)
(SR51)	$C_2H_5O + O_2 \rightarrow CH_3CHO + HO_2$	7.44×10^{-15}	2	Sander et al. (1997)
(SR52)	$C_2H_5O + O_2 \rightarrow CH_3O_2 + HCHO$	7.51×10^{-17}	2	Sander et al. (1997)
(SR53)	$C_2H_5O_2 + HO_2 \rightarrow C_2H_5OOH + O_2$	$3.80\times10^{-13}\exp(900/T)$	2	Atkinson et al. (2006)
(SR54)	$C_2H_5OOH + OH \rightarrow C_2H_5O_2 + H_2O$	8.21×10^{-12}	2	Sander et al. (1997)
(SR55)	$C_2H_5OOH + Br \rightarrow C_2H_5O_2 + HBr$	5.19×10^{-15}	2	Sander et al. (1997)
(SR56)	$OH + OH(+M) \longrightarrow H_2O_2(+M)$	$k_0 = 6.90\times10^{-31}(T/300)^{-0.8}[N_2]$ $k_\infty = 2.60\times10^{-11}$ $F_c = 0.50$	2	Atkinson et al. (2006)
(SR57)	$H_2O_2 + h\nu \rightarrow 2OH$	2.00×10^{-6}	1	Lehrer et al. (2004)
(SR58)	$HCHO + h\nu \xrightarrow{2O_2} 2HO_2 + CO$	5.50×10^{-6}	1	Lehrer et al. (2004)
(SR59)	$HCHO + h\nu \rightarrow H_2 + CO$	9.60×10^{-6}	1	Lehrer et al. (2004)
(SR60)	$C_2H_4O + h\nu \rightarrow CH_3O_2 + CO + + HO_2$	6.90×10^{-7}	1	Lehrer et al. (2004)
(SR61)	$CH_3O_2H + h\nu \rightarrow OH + HCHO + HO_2$	1.20×10^{-6}	1	Lehrer et al. (2004)
(SR62)	$C_2H_5O_2H + h\nu \rightarrow C_2H_5O + OH$	1.20×10^{-6}	1	Lehrer et al. (2004)
(SR63)	$NO + O_3 \rightarrow NO_2 + O_2$	$1.40\times10^{-12}\exp(-1310/T)$	2	Atkinson et al. (2006)
(SR64)	$NO + HO_2 \rightarrow NO_2 + OH$	$3.60\times10^{-12}\exp(270/T)$	2	Atkinson et al. (2006)
(SR65)	$NO_2 + O_3 \rightarrow NO_3 + O_2$	$1.40\times10^{-13}\exp(-2470/T)$	2	Atkinson et al. (2006)
(SR66)	$NO_2 + OH(+M) \rightarrow HNO_3(+M)$	$k_0 = 3.30\times10^{-30}(T/300)^{-3.0}[N_2]$ $k_\infty = 4.10\times10^{-11}$ $F_c = 0.40$	2	Atkinson et al. (2006)
(SR67)	$NO + NO_3 \rightarrow 2NO_2$	$1.80\times10^{-11}\exp(110/T)$	2	Atkinson et al. (2006)
(SR68)	$HONO + OH \rightarrow NO_2 + H_2O$	$2.50\times10^{-12}\exp(260/T)$	2	Atkinson et al. (2006)
(SR69)	$HO_2 + NO_2(+M) \rightarrow HNO_4(+M)$	$k_0 = 1.80\times10^{-31}(T/300)^{-3.2}[N_2]$ $k_\infty = 4.70\times10^{-12}$ $F_c = 0.60$	2	Atkinson et al. (2006)
(SR70)	$HNO_4(+M) \rightarrow NO_2 + HO_2(+M)$	$k_0 = 4.10\times10^{-5}\exp(-10650/T)[N_2]$ $k_\infty = 4.80\times10^{15}\exp(-11170/T)$ $F_c = 0.60$	1	Atkinson et al. (2006)

Reaction Number	Reaction	k $[(\text{molec. cm}^{-3})^{1-n}\text{s}^{-1}]$	Order n	Reference
(SR71)	$HNO_4 + OH \rightarrow NO_2 + H_2O + O_2$	$3.20\times10^{-13}\exp(690/T)$	2	Atkinson et al. (2006)
(SR72)	$NO + OH(+M) \rightarrow HONO(+M)$	$k_0 = 7.40\times10^{-31}(T/300)^{-2.4}[N_2]$ $k_\infty = 3.30\times10^{-11}(T/300)^{-0.3}$ $F_c = 0.81$	2	Atkinson et al. (2006)
(SR73)	$OH + NO_3 \rightarrow NO_2 + HO_2$	2.00×10^{-11}	2	Atkinson et al. (2006)
(SR74)	$HNO_3 + h\nu \rightarrow NO_2 + OH$	4.40×10^{-8}	1	Lehrer et al. (2004)
(SR75)	$NO_2 + h\nu \xrightarrow{O_2} NO + O_3$	3.50×10^{-3}	1	Lehrer et al. (2004)
(SR76)	$NO_3 + h\nu \xrightarrow{O_2} NO_2 + O_3$	1.40×10^{-1}	1	Lehrer et al. (2004)
(SR77)	$NO_3 + h\nu \rightarrow NO + O_2$	1.70×10^{-2}	1	Lehrer et al. (2004)
(SR78)	$NO + CH_3O_2 \xrightarrow{O_2} HCHO + HO_2 + NO_2$	$2.30\times10^{-12}\exp(360/T)$	2	Atkinson et al. (2006)
(SR79)	$NO_3 + CH_3OH \xrightarrow{O_2} HCHO + HO_2 + HNO_3$	$9.40\times10^{-13}\exp(-2650/T)$	2	Atkinson et al. (2006)
(SR80)	$NO_3 + HCHO \xrightarrow{O_2} CO + HO_2 + HNO_3$	5.60×10^{-16}	2	Atkinson et al. (2006)
(SR81)	$NO + C_2H_5O_2 \xrightarrow{O_2} CH_3CHO + NO_2 + HO_2$	$2.60\times10^{-12}\exp(380/T)$	2	Atkinson et al. (2006)
(SR82)	$NO + CH_3CO_3 \xrightarrow{O_2} CH_3O_2 + NO_2 + CO_2$	$7.50\times10^{-12}\exp(290/T)$	2	Atkinson et al. (2006)
(SR83)	$NO_2 + CH_3CO_3(+M) \rightarrow PAN(+M)$	$k_0 = 2.70\times10^{-28}(T/300)^{-7.1}[N_2]$ $k_\infty = 1.20\times10^{-11}(T/300)^{-0.9}$ $F_c = 0.30$	2	Atkinson et al. (2006)
(SR84)	$Br + NO_2(+M) \rightarrow BrNO_2(+M)$	$k_0 = 4.20\times10^{-31}(T/300)^{-2.4}[N_2]$ $k_\infty = 2.70\times10^{-11}$ $F_c = 0.55$	2	Atkinson et al. (2006)
(SR85)	$Br + NO_3 \rightarrow BrO + NO_2$	1.60×10^{-11}	2	Atkinson et al. (2006)
(SR86)	$BrO + NO_2(+M) \rightarrow BrONO_2(+M)$	$k_0 = 4.70\times10^{-31}(T/300)^{-3.1}[N_2]$ $k_\infty = 1.80\times10^{-11}$ $F_c = 0.40$	2	Atkinson et al. (2006)
(SR87)	$BrO + NO \rightarrow Br + NO_2$	$8.70\times10^{-12}\exp(260/T)$	2	Atkinson et al. (2006)
(SR88)	$BrONO_2 + h\nu \rightarrow NO_2 + BrO$	3.40×10^{-4}	1	Lehrer et al. (2004)
(SR89)	$BrNO_2 + h\nu \rightarrow NO_2 + Br$	9.30×10^{-5}	1	Lehrer et al. (2004)
(SR90)	$BrONO_2 + H_2O \xrightarrow{\text{aerosol}} HOBr + HNO_3$	$(\frac{r}{D_g} + \frac{4}{v_{\text{therm}}\gamma})^{-1}\alpha_{\text{eff,aerosol}}$		Cao et al. (2014)
(SR91)	$PAN + h\nu \rightarrow NO_2 + CH_3CO_3$	6.79×10^{-7}	1	Fishman and Carney (1984)
(SR92)	$BrONO_2 + H_2O \xrightarrow{\text{ice}} HOBr + HNO_3$	$(r_a + r_b + r_c)^{-1}\alpha_{\text{eff,ice}}$		Cao et al. (2014)

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