



Supplement of

Multiphase processes in the EC-Earth model and their relevance to the atmospheric oxalate, sulfate, and iron cycles

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Supplementary Tables

Table S1: Averaged factors for the years 2000-2014 used to represent the Fe-containing aerosols in the emitted fine and coarse aerosols of the model, as applied to a) the calculated dust mineral emissions as derived from the updated mineralogy maps originally created by Claquin et al. (1999), b) the CMIP6 anthropogenic emission sectors (Hoesly et al., 2018) as retrieved based on estimates from Ito et al. (2018) for the emitted submicron carbonaceous particulate matter (i.e., sum of OC and BC) and inorganic matter, and c) the CMIP6 biomass burning emissions (van Marle et al., 2017) also based on Ito et al. (2018) estimates. In parentheses, the standard deviation (where available) is also provided.

Fe types	Fine aerosols	Coarse aerosols
a) Dust minerals Illite Smectite Kaolinite Feldspars	0.048 0.164 0.007 0.025	
Iron oxides	0.660	
b) Anthropogenic sectors Energy Industrial Residential & Commercial Shipping Waste treatment	$1.861 \cdot 10^{-2} (\pm 6.281 \cdot 10^{-4})$ $1.459 \cdot 10^{-2} (\pm 1.414 \cdot 10^{-3})$ $4.336 \cdot 10^{-6} (\pm 3.485 \cdot 10^{-7})$ $3.751 \cdot 10^{-2} (\pm 9.043 \cdot 10^{-9})$ $1.389 \cdot 10^{-3} (\pm 9.622 \cdot 10^{-11})$	$\begin{array}{l} 3.528 \bullet 10^{-1} (\pm 1.190 \bullet 10^{-2}) \\ 2.764 \bullet 10^{-1} (\pm 2.681 \bullet 10^{-2}) \\ 1.350 \bullet 10^{-5} (\pm 1.085 \bullet 10^{-6}) \\ 1.398 \bullet 10^{-2} (\pm 4.454 \bullet 10^{-9}) \\ 3.595 \bullet 10^{-3} (\pm 8.487 \bullet 10^{-10}) \end{array}$
c) Biomass Burning	6.292 • 10 ⁻³	2.296 • 10 ⁻²

Table S2. Aqueous phase chemical mechanism and reaction rate constants. The photolysis frequencies (J) are expressed in s⁻¹, and the aqueous reactions (K) are expressed in L mol⁻¹ s⁻¹.

Plotopia Plotopia $ -$ 100 <tdt< th=""><th></th><th>Aqueous-phase Reactions</th><th></th><th></th><th>J_{max}/K₂₉₈</th><th>E_a/R</th><th>Reference</th></tdt<>		Aqueous-phase Reactions			J _{max} /K ₂₉₈	E _a /R	Reference
101 0) - $h^{-}(+16)$ -1 100 + 0, -0, -0, -0 103 NO + h^{-} - NO + 0, -0, -0 - 103 NO + h^{-} - NO + 0, -0, -0 - 103 NO + h^{-} NO + 0, -0, -0 - 105 NO + $h^{+}(H^{+})$ - NO + 0H - 106 NO + $h^{+}(H^{+})$ - NO + 0H - 108 Ca ⁺ + $h^{+}(H^{+})$ - NO + 0H - - 108 Ca ⁺ + $h^{+}(H^{+})$ - NO + 0H + HO - - - 109 Fe(OH) ⁺ + h^{-} - Fe ⁺ + OH + HO - - Deguillaume et al. (2001) 110 Ferdon (+ D_0) - Fe ⁺ + OH + HO 7.52 10 ⁻³ Deguillaume et al. (2010) 110 Ferdon (+ D_0) - Fe ⁺ + OH + HO 1.10 ⁴ Deguillaume et al. (2010) 110 Ferdon (+ D_0) - OH + 20, - 1.10 ⁴ Deguillaume et al. (2010) 110 Otho (- O, - - OH + 20, - 1.10 ⁴ Deguillaume et al. (2010) 1100		Photolysis					
102 $Hot + hv$ - 2.0H - 103 Not + hv - Not + 0v - 104 Not + hv (+H) - Not + 0v - 105 Not + hv (+H) - Not + 0H - 106 Not + hv (+H) - Not + 0H - 107 CH(0AH + hv (+O) - F(2/OH)H + HV - Hegee 108 Fe ³ + hv (+Hz0) - Fe ³ + 0H + HT 6.410 ^{4 + h} Deguillame et al (2004) 108 Fe ³ + hv (+Hz0) - Fe ³ + 0H + HT 6.410 ^{4 + h} Deguillame et al (2004) 111 FerdStall + hv (+O) - Fe ³ + OL + Or + 0P 2.4710 ^{2 + h} Deguillame et al (2004) 112 FerdStall + hv (+O) - Fe ³ + OL + 0P + 0	J01	$O_3 + hv (+ H_2O)$	\rightarrow	$H_2O_2 + O_2$	a		
103 NO, + hr NO + 0, * 105 NO, + hr (+ H) NO + 0H * 105 NO, + hr (+ H) NO + 0H * 107 CH:0,H + hr (+ HO) Te ² + 0H + HC 6.41 10 ^{4 + h} Deguilaume et al. (2004) 109 [Fe(10]] ^{2 + hr} Te ^{2 + 0} OH + HC 5.61 10 ^{3 + hr} Deguilaume et al. (2004) 109 [Fe(10]] ^{2 + hr} Te ^{2 + 0} OH + HC 5.61 10 ^{3 + hr} Deguilaume et al. (2004) 111 [Fe(20]] ^{2 + hr} (+ HO) Te ^{2 + 0} OH + HC 4.51 10 ^{4 + hr} Deguilaume et al. (2004) 111 [Fe(20]] ^{2 + hr} (+ HO) Te ^{2 + 0} OH + O ² 2.47 10 ^{2 + hr} Ervers et al. (2003) 111 [Fe(20]] ^{2 + hr} (+ HO) Te ^{2 + 0} OH + O ² 1.10 ⁴ Deguilaume et al. (2010) 112 [Fe(20,H] + hr (+HO) O + 0 ^{2 + 1} O ² 1.10 ¹⁰ Deguilaume et al. (2010) 110 IP O + O ² O + 10 O + 10 O + 10 D + 0.10 ¹⁰ Deguilaume et al. (2010) 1100 10 0 ¹⁰ Expense tal. (2003) Evense tal. (2003) Evense tal. (2003) 1100 0 - 0 + HO 1.10 ¹⁰ Deguilaume et al. (2010)	J02	$H_2O_2 + hv$	\rightarrow	2 OH	a		
104 NO, + hr - NO, + 0, + 105 NO, + hr (+ H) - NO, + 0H + 106 NO, + hr (+ H) - NO, + 0H + 107 CH, 0, H + hr (+ 0,) - FC(-1, 0, H + hr (+ 0,) - 108 Fc ² + hr (+ H, 0,) - Fc ² + 0, H + Hr 6.41 10 ^{6 +} Deguillaume et al. (2004) 110 IFG(OB) ² + hr - Fc ² + 0, H + HO 7.52 10 ³ + Deguillaume et al. (2004) 111 IFG(OS, I) + hr (+ 0,) - Fc ² + 0, V + 2 CO ₂ 2.47 10 ² + Deguillaume et al. (2010) 110 IFG(OS, I) + hr (+ 0,) - Fc ² + 0, V + 2 CO ₂ 2.47 10 ² + Deguillaume et al. (2010) 120 O ₁ + HO - HO ₂ + 0, + 1.0 10 ⁴ Deguillaume et al. (2010) 120 O ₁ + HO - O ₁ + HO 1.0 10 ⁴ Deguillaume et al. (2010) 120 O ₁ + HO - O ₁ + HO 1.0 10 ⁴ Deguillaume et al. (2010) 120 O ₁ + O ₁ HO ₂ + O ₂ 0	J03	$NO_3 + hv$	\rightarrow	$NO + O_2$	a		
105 NO; $z + hr (+ H')$ NO $z + 0H$ * 107 CH: $0H_3 + hr (z + 0)$ - CH: $0H_3 + hr (z + 0)$ - CH: $0H_3 + hr (z + 0)$ 107 CH: $0H_3 + hr (z + 0)$ - CH: $0H_3 + hr (z + 0)$ - CH: $0H_3 + hr (z + 0)$ Deguillaume et al. (2004) 109 [Fe(0Th] ²⁺ hr - Fe ²⁺ + 0H + HO 5.51 0 ³ hr Deguillaume et al. (2004) 111 [Fe(SDi] ³⁺ hr (z + HO) - Fe ²⁺ + 0H + HO 7.52 10 ³ hr Deguillaume et al. (2004) 111 [Fe(SDi] ³⁺ hr (z + HO) - Fe ²⁺ + 0H + HO 7.52 10 ³ hr Deguillaume et al. (2004) 111 [Fe(SDi] ³⁺ hr (z + HO) - Fe ²⁺ + 0A ²⁺ + 0C ² c 2.47 10 ^{2 hr} Ervers et al. (2003) 111 [Fe(SDi] ³⁺ hr (z + HO) - HO + 0, 0 1.10 ⁴ Deguillaume et al. (2010) 1000 0.4 (z + HO) - 0.4 + HO 1.10 ⁴ Deguillaume et al. (2010) 1001 Deguillaume et al. (2010) - 0.4 + HO 1.10 ¹⁰ Ervers et al. (2033) 1000 HO + 0 + HO + 0 + HO + 0 1.10 ¹⁰ Deguillaume et al. (2010)	J04	$NO_3 + hv$	\rightarrow	$NO_2 + O_3$	a		
106 NO: $+ hv (+ R)$ - NO: $+ hv (+ R)$ - NO: $+ hv (+ R)$ - Rest (204) 108 $Fe^{-3} + hv (+ R, O)$ - $Fe^{-3} + OR + R + R + OR + R + R + R + R + R +$	J05	$NO_2^- + hv (+ H^+)$	\rightarrow	NO + OH	a		
107 CH ₂ (OH + hr(+ C ₀) → CH ₂ (OH + HC) + - 109 $[F_{q}(OH)]^{b} + hv$ → $F_{q}^{b} + OH$ 5.61 10 ^b Deguillame et al. (2004) 109 $[F_{q}(OH)]^{b} + hv$ → $F_{q}^{b} + OH$ 5.21 10 ^b Deguillame et al. (2004) 111 $[F_{q}(OL)_{1}^{b} + hv$ (+ HO) → $F_{q}^{b} + SO^{2} + OH$ 4.51 10 ^b Deguillame et al. (2004) 121 $[F_{q}(OL)_{1}^{b} + hv$ (+ HO) → $F_{q}^{b} + SO^{2} + OH$ 4.51 10 ^b Deguillame et al. (2010) 111 $[F_{q}(OL)_{1}^{b} + hv$ (+ HO) → $F_{q}^{b} + SO^{2} + OH$ 1.1 10 ^a Deguillame et al. (2010) 1000 0, + HO, → HO, + OC 1.1 10 ^a Deguillame et al. (2010) 1000 0, + OF → HO, + OC 8.1 0 ^a 2.200 Deguillame et al. (2010) 1000 HO, + CH → HO, + OC 8.1 0 ^a 2.700 Evens et al. (2003) 1080 HO, 2 + OH → HO, - O_{2} 8.1 0 ^a 2.700 Evens et al. (2003) 1080 HO, 2 + OH → HO, 2 + OH HO, 2 + OH	J06	$NO_{3}^{-} + hv (+ H^{+})$	\rightarrow	$NO_2 + OH$	a		
108 $Fe^{-2} + hr (+ HzO)$ \rightarrow $Fe^{-2} + OH + HC$ 6.5 (10 ⁻⁶) Deguilaume et al. (2004) 110 $Fe(-5O_1)^2 + hr$ \rightarrow $Fe^{-2} + OH + HC$ 7.5 (21) ⁻⁵ Deguilaume et al. (2004) 111 $Fe(-5O_1)^2 + hr (+HO)$ \rightarrow $Fe^{-2} + OH + HC$ 7.5 (21) ⁻⁵ Deguilaume et al. (2004) 112 $Fe(-5O_1)^2 + hr (+HO)$ \rightarrow $Fe^{-2} + OX^{1,2} + O_2 + 2 CO_2$ 2.4 (10 ^{-2, 5} Deguilaume et al. (2010) 112 $Fe(-5O_1)^2 + hr (+Fe)^2$ \rightarrow $Fe^{-2} + OX^{1,2} + O_2^{-2} + 2 CO_2$ 2.4 (10 ^{-2, 5} Deguilaume et al. (2010) 112 $Fe(-5O_1)^2 + hr (+Fe)^2$ \rightarrow $Fe^{-2} + OH + HC$ 1.1 (0 ⁴ Deguilaume et al. (2010) 112 $Fe(-5O_1)^2 + hr (-5O_1)^2$ 1.0 10 ⁴⁰ Deguilaume et al. (2010) Ervens et al. (2003) 1100 $O_1 + O_2$ $O_1 + O_2$ PTO_1 PTO_2 Ervens et al. (2003) 1100 $PO_1 + O_1$ $PO_1 + O_2$ PTO_1 PTO_2 Ervens et al. (2010) 1100 $PO_2 + OH$ $PO_1 + D_2$ PTO_2 PTO_2 Ervens et al. (2003) 1100 $PO_2 + HT$ $PO_1 + D_2$	J07	$CH_{3}O_{2}H + hv (+ O_{2})$	\rightarrow	$CH_2(OH)_2 + HO_2 + OH$	a		
109 [Fe(0H)] ¹⁺ hv \rightarrow Fe ³⁺ + OH 5.3 (10 ³⁻⁵) Deguillame et al. (2004) 111 [Fe(0S,0]] ¹⁺ hv(+HO) \rightarrow Fe ³⁺ sOA ²⁺ OH + H° 4.51 (10 ³⁻⁵) Deguillame et al. (2004) 111 [Fe(0S,0]] ¹⁺ hv(+HO) \rightarrow Fe ³⁺ sOA ²⁺ OH + H° 4.51 (10 ³⁻⁵) Deguillame et al. (2004) 111 [Fe(0S,0]] ¹⁺ hv(+HO) \rightarrow Fe ³⁺ sOA ²⁺ OH + H° 4.51 (10 ³⁻⁵) Deguillaume et al. (2010) 111 [Fe(0S,0]] ¹⁺ hv(+HO) \rightarrow He ³⁺ SOA ²⁺ OH + H° 1.0 (10 ³) Deguillaume et al. (2010) 111 \rightarrow OH + O2 \rightarrow OH + 2O ₂ 1.0 (10 ³) Deguillaume et al. (2010) 111 \rightarrow OH + O2 \rightarrow OH + O2 1.0 (10 ³) Ervens et al. (203) 111 \rightarrow OP + HO 1.0 (10 ³) Ervens et al. (203) Ervens et al. (203) 111 \rightarrow OP + HO 1.0 (10 ³) Ervens et al. (203) Ervens et al. (203) 111 \rightarrow OP + HO 1.0 (10 ³) Ervens et al. (203) Ervens et al. (203) 111 \rightarrow OP + HO \rightarrow HO ₂ + O ₂ \rightarrow 10 ³ 1060 Ervens et al. (203) 111 \rightarrow OP + H ¹ \rightarrow HO ₂ + DO \rightarrow NO ₂ + H \rightarrow NO<	J08	$Fe^{+3} + hv (+ H_2O)$	\rightarrow	$Fe^{+2} + OH + H^+$	6.41 10 ^{-6 b}		Deguillaume et al. (2004)
10 [Fe(OH ₃) ⁺ + hv] → Fe^{2+} + OH + HO 7.5 (210 ⁺⁵⁾ Deguilaume et al. (2004) 11 [Fe(OXL)] ⁺ + hv (+O) → Fe^{2+} SOA ⁺ + Of + H ⁺ 4.5 110 ⁺⁵ Deguilaume et al. (2004) 110 [Fe(OXL)] ⁺ + hv (+O ₂) → Fe^{2+} SOA ⁺ + Of + 2 CO ₂ 2.47 10 ²⁻⁵ Deguilaume et al. (2010) 100 0, + OH → HO ₂ + O ₂ 1.0 10 ⁴ Deguilaume et al. (2010) 1000 0, + HO → OH + 2,O ₂ 1.0 10 ⁴⁰ Deguilaume et al. (2010) 1000 0, + O ₂ OH + 0,O ₂ + HO 1.0 10 ⁴⁰ Ervens et al. (2003) 1000 HO ₂ + O ₁ → O ₂ + HO 1.0 10 ⁴⁰ Ervens et al. (2003) 1000 HO ₂ + O ₁ → O ₂ + HO 1.0 10 ⁴⁰ Ervens et al. (2003) 1000 HO ₂ + O ₁ → O ₂ + HO 3.0 10 ⁴ 1680 Ervens et al. (2003) 1000 HO ₂ + OH → HO ₂ + HO 3.0 10 ⁴ 1680 Ervens et al. (2010) 1010 NO + OH → NO ₂ + HT 3.0 10 ⁴ Ervens et al. (2010) 10110 <t< td=""><td>J09</td><td>$[Fe(OH)]^{2+} + hv$</td><td>\rightarrow</td><td>$Fe^{2+} + OH$</td><td>5.63 10^{-3 b}</td><td></td><td>Deguillaume et al. (2004)</td></t<>	J09	$[Fe(OH)]^{2+} + hv$	\rightarrow	$Fe^{2+} + OH$	5.63 10 ^{-3 b}		Deguillaume et al. (2004)
J11 [Fe(SO ₀)] ⁺ hw(+H ₂ O) \rightarrow Fe ²⁺ + O ₂ ⁺ + O ₂ ⁺ + O ₂ ⁺ + O ₂ ⁺ $2.47 \ 10^{-5}$ Deguillaume et al. (2004) H ₀ , chemistry \rightarrow HO ₂ + O ₂ $2.47 \ 10^{-5}$ Ervers et al. (2003) K001 O ₁ + OH \rightarrow HO ₂ + O ₂ $1.1 \ 10^{6}$ Deguillaume et al. (2010) K002 O ₁ + O ₁ \rightarrow OH + 2 O ₂ $1.0 \ 10^{6}$ Deguillaume et al. (2010) K003 O ₁ + O ₁ (+ H ₂) \rightarrow OH + 0 ₂ + HO $1.0 \ 10^{60}$ Ervers et al. (2003) K004 HO ₂ + O ₁ \rightarrow O ₂ + HO $1.0 \ 10^{60}$ Ervers et al. (2003) K005 O ₂ + O ₁ \rightarrow O ₂ + HO $1.0 \ 10^{60}$ Ervers et al. (2003) K006 HO ₂ + O ₁ \rightarrow HO ₂ + O ₂ $9.1 \ 10^{60}$ Ervers et al. (2003) K007 HO ₂ + O ₁ \rightarrow HO ₂ + HO $3.0 \ 10^{6}$ Ervers et al. (2003) K008 OH + O ₁ \rightarrow HO ₂ + HO $3.0 \ 10^{6}$ Ervers et al. (2003) K018 NO ₂ + O ₁ \rightarrow NO ₂ + HT $3.0 \ 10^{6}$ Ervers et al. (2003)	J10	$[Fe(OH)_2]^+ + hv$	\rightarrow	$Fe^{2+} + OH + HO^{-}$	7.52 10 ^{-3 b}		Deguillaume et al. (2004)
112 [Fe ² + 0XL ² + 02 + 2 CO ₂ 2.47 10 ^{2 b} Erems et al. (2003) K001 O ₁ + 0H → HO ₂ + 0C ₂ 1.10 ⁶ Deguillaume et al. (2010) K002 O ₁ + HO ₂ → OH + 2O ₂ 1.10 ¹⁰ Deguillaume et al. (2010) K003 O ₁ + HO ₂ → OH + 0 ₂ + HO 1.510 ⁹ 2200 Deguillaume et al. (2010) K004 HO ₂ + OH → O ₂ + HO 1.110 ¹⁰ Ervens et al. (2003) K005 O ₁ + OH → O ₂ + HO 8.10 ¹⁰ 2120 Ervens et al. (2003) K006 HO ₂ + HO → H ₂ O ₂ + O ₂ 8.10 ¹⁰ 2120 Ervens et al. (2003) K007 HO ₂ + O ₁ C → H ₂ O ₂ + O ₂ 8.10 ¹⁰ 2120 Ervens et al. (2003) K008 HO ₂ + HI → HO ₂ + H ₂ O 3.010 ¹⁰ If N = NO N = NO K010 NO + H → HO ₂ + H ₂ O 3.010 ¹⁰ Ervens et al. (2003) K010 NO + HO → NO ₂ + H ¹ 3.010 ¹⁰ Ervens et al. (2003) K011 NO ₁ + O ₁ + H ¹	J11	$[Fe(SO_4)]^+ + hv (+ H_2O)$	\rightarrow	$Fe^{2+}+SO_4^{2-}+OH+H^+$	4.51 10 ⁻⁵ b		Deguillaume et al. (2004)
H.O. chemistry H.O. + OH \rightarrow HO, + D_2 1.1 10 ⁴ Deguillaume et al. (2010) K002 O, + HO, \rightarrow OH + 2, 0 1.5 10 ⁶ 220 Deguillaume et al. (2010) K003 O, + O; (+ HO) \rightarrow OH + 0, + HO 1.5 10 ⁶ 220 Deguillaume et al. (2010) K004 HO, + O; (+ HO) \rightarrow O, + HO 1.1 10 ¹⁰ Ervens et al. (2003) K005 O, + O; (+ HO) \rightarrow H-0 1.1 10 ¹⁰ Ervens et al. (2003) K006 HO, + HO; \rightarrow H-0 8.3 10 ⁵ 2720 Ervens et al. (2003) K007 HO, + O; (+ H ⁺) \rightarrow H-0 3.0 10 ⁷ 1660 Ervens et al. (2003) K008 OH + O1; (+ H_2) \rightarrow NO; + H 2.1 0 ¹⁰ Deguillaume et al. (2010) K010 NO + NO (+ H_2) \rightarrow NO; + H ⁺ 3.0 10 ⁷ Deguillaume et al. (2010) K011 NO + NO (+ H_2) \rightarrow NO; + O; H A 10 ¹⁰ -2900 Ervens et al. (2003) K011 NO + NO (+ H_2) \rightarrow NO; + O; 3.0 10 ⁷ Ervens et al. (2003) K011 NO +	J12	$[Fe(OXL)_2] + hv(+O_2)$	\rightarrow	$Fe^{+2} + OXL^{2} + O_2^{-2} + 2 CO_2$	2.47 10 ^{-2 b}		Ervens et al. (2003)
K001 $0_1 + 0_1$ \rightarrow HO ₂ + 0 1.10^{6} Deguilaume et al. (2010) K002 $0_1 + HO_2$ 0 $0H + 2_2 O_2$ 0 $0H = 20$ K003 $0_1 + 0_2$ 0 $0H + 2_2 O_2$ 0 $0H = 01$ K004 $HO_2 + HO$ $1.0^{10^{10}}$ $Erves et al. (2003)$ K005 $0_2 + HO$ $1.10^{10^{10}}$ 2120 $Erves et al. (2003)$ K006 $HO_2 + HO_2$ 9.710^{10} 106 $Erves et al. (2003)$ K007 $HO_1 + C_1$ $HO_2 + HO_2$ 9.710^{10} 106 $Erves et al. (2003)$ K008 $HO_1 + HI$ $HO_2 + HO$ 3010^{10} 106 $Erves et al. (2010)$ K008 $HO_1 + HI$ $HO_2 + HT$ 3010^{10} $Deguillaume et al. (2010)$ K011 $NO_1 + HI_2O$ $2.0^{10^{10} + 1HO$ 3010^{10} $Erves et al. (2003)$ K011 $NO_1 + 0_2$ $NO_1 + 0_2$ $10^{10} + 10^{10}$ $Deguillaume et al. (2010)$ K011 $NO_1 + 0_2$ $NO_1 + 0_2$ $10^{10} 0^{10}$ </td <td></td> <td>H_xO_y chemistry</td> <td></td> <td></td> <td></td> <td></td> <td></td>		H _x O _y chemistry					
K002 O ₁ + HO ₂ \rightarrow OH + 2 O ₂ 1.0 10 ⁴ Deguillaume et al. (2010) K003 O ₁ + O ₂ (+ H ₂ O) \rightarrow O ₂ + H ₂ O 1.0 10 ¹⁰ Ervens et al. (2003) K006 HO ₂ + HO \rightarrow O ₂ + HO 1.0 10 ¹⁰ Ervens et al. (2003) K006 HO ₂ + HO ₂ \rightarrow H ₂ O ₂ + O ₂ 8.3 10 ⁵ 27.20 Ervens et al. (2003) K007 HO ₂ + O ₂ \rightarrow H ₂ O ₂ + O ₂ \rightarrow $3.0 10^{5}$ Ervens et al. (2003) K008 OH + OH \rightarrow HO ₂ + H ₂ O $3.0 10^{6}$ Deguillaume et al. (2010) K008 N + OH \rightarrow HO ₂ + H ₂ O $3.0 10^{6}$ Deguillaume et al. (2010) K010 NO + OH \rightarrow NO ₂ + H ² $3.0 10^{6}$ Ervens et al. (2003) K011 NO ₁ + H ₂ O \rightarrow NO ₂ + H ² $3.0 10^{6}$ Ervens et al. (2003) K011 NO ₁ + H ₂ O \rightarrow NO ₁ + O ₂ A NO ₁ + O ₁ A K011 NO ₁ + H ₁ O A <	K001	$O_3 + OH$	\rightarrow	$HO_2 + O_2$	1.1 108		Deguillaume et al. (2010)
K003 $0_1 + 0_7 + (H_2O)$ \rightarrow $0_1 + 0_1 + 0_1O^2$ $15 \ 10^9$ 2200 Deguillaume et al. (2010) K004 $0_1 + 0_1O^2$ $-0_7 + H_2O$ $1.1 \ 10^{10}$ 2120 $Ervens et al. (2003)$ K005 $0_7 + 0H$ \rightarrow $0_2 + HO$ $1.1 \ 10^{10}$ 2120 $Ervens et al. (2003)$ K006 $HO_2 + HO_2$ $H \ 10_2 + O_2$ $9.7 \ 10^7$ 1060 $Ervens et al. (2003)$ K008 $HO_1 + O_1^* (H^*)$ $H \ 10_2 + I_0$ $3.0 \ 10^7$ 1500 Deguillaume et al. (2010) K010 $NO + OH$ \rightarrow $HO_2 + H_2$ $3.0 \ 10^7$ 1500 Deguillaume et al. (2010) K011 $NO_1 + OH$ \rightarrow $NO_7 + H^*$ $2.1 \ 10^{10}$ Ervens et al. (2003) K011 $NO_1 + NO_2 + H^*$ $3.0 \ 10^9$ Ervens et al. (2003) $1.0 \ 10^{10}$ Ervens et al. (2003) K014 $NO_1 + H_2$ \rightarrow $NO_7 + O_2$ $3.0 \ 10^9$ Ervens et al. (2003) K014 $NO_1 + O_2$ \rightarrow $NO_7 + O_7$ $3.0 \ 10^9$ Ervens et al. (2003) K014 $NO_1 + O_2$ $NO_7 + O_7$ <td< td=""><td>K002</td><td>$O_3 + HO_2$</td><td>\rightarrow</td><td>$OH + 2 O_2$</td><td>1.0 104</td><td></td><td>Deguillaume et al. (2010)</td></td<>	K002	$O_3 + HO_2$	\rightarrow	$OH + 2 O_2$	1.0 104		Deguillaume et al. (2010)
K004 HO ₂ +OH \rightarrow O ₂ +HO 1.0 10 ¹⁰ Ervens et al. (2003) K005 O ₂ +HO ₂ H ₂ O ₂ +O ₂ 8.3 10 ⁵ 2720 Ervens et al. (2003) K006 HO ₂ +HO ₂ 9.7 10 ⁷ 1060 Ervens et al. (2003) K007 HO ₂ +O ₂ (+H ⁻) H ₂ O ₂ +O ₂ 9.7 10 ⁷ 1060 Ervens et al. (2003) K008 OH+OH +HO ₂ +H ₂ O 3.0 10 ⁷ 1680 Ervens et al. (2010) K009 HO ₂ +HO +HO ₂ +H ₂ O 3.0 10 ⁷ 1680 Ervens et al. (2010) K011 NO ₂ +H ⁺ 2.1 0 ¹⁰ Deguillaume et al. (2010) Ervens et al. (2003) K012 NO ₂ +H ₂ O HON + NO ₂ +H ⁺ 2.1 0 ¹⁰ Ervens et al. (2003) K011 NO ₂ +H ₂ O HON + NO ₂ +H ⁺ 2.1 0 ¹⁰ Ervens et al. (2003) K014 NO ₂ +H ₂ O HON + NO ₂ +H ⁺ 3.0 10 ⁹ Ervens et al. (2003) K014 NO ₂ +H ₂ O NO ₁ +O ₂ +H ⁺ 3.0 10 ⁹ Ervens et al. (2003) K014 NO ₁ +O ₂ NO ₁ +O ₂ +H ⁺ 3.0 10 ⁹ Ervens et al. (2003) K015 NO ₁ +O ₂ NO ₁ +O ₂ +	K003	$O_3 + O_2^- (+ H_2O)$	\rightarrow	$OH + O_2 + HO^2$	1.5 109	2200	Deguillaume et al. (2010)
K005 $0_7 + 0H$ $\rightarrow 0_2 + HO$ 1.1 10 ¹⁰ 2120 Ervens et al. (2003) K006 HO ₂ + HO ₂ $H_{20} + O_2$ $9.7 10^7$ 1060 Ervens et al. (2003) K008 HO ₂ + O ₂ ' + H ⁻) \rightarrow HO ₂ + HO ₂ $3.6 10^9$ 930 Deguillaume et al. (2010) K008 HO ₂ + OH \rightarrow HO ₂ + HO $3.6 10^9$ 930 Deguillaume et al. (2010) Nitrogen chemistry Nitrogen chemistry $8.1 10^9$ 1680 Ervens et al. (2003) K010 NO + OH \rightarrow NO ₇ + H ⁺ $2.2 10^{10}$ 1500 Deguillaume et al. (2010) K011 NO ₇ + OH \rightarrow NO ₇ + H ⁺ $2.2 10^{10}$ Ervens et al. (2003) Ervens et al. (2003) K012 NO ₇ + OH \rightarrow NO ₇ + H ⁺ $2.1 0^{10}$ Ervens et al. (2003) Ervens et al. (2003) K014 NO ₇ + OH \rightarrow NO ₇ + H ⁺ $3.0 10^9$ Ervens et al. (2003) Ervens et al. (2003) K014 NO ₇ + HO ₂ $NO_7 + O_2$ $3.0 10^9$ Ervens et al. (2003) Ervens et al. (2003) K014 NO ₇ + O ₂ $NO_7 + O_2$ $3.0 10^9$ Ervens et al. (2003) Ervens e	K004	$HO_2 + OH$	\rightarrow	$O_2 + H_2O$	$1.0\ 10^{10}$		Ervens et al. (2003)
K006 HO ₂ + HO ₂ \rightarrow H ₂ O ₂ + O ₂ 8.3 10 ⁶ 2720 Evens et al. (2003) K007 HO ₂ + O ₁ (+ H ⁺) \rightarrow H ₂ O ₂ + O ₂ 9.7 10 ⁷ 1060 Evens et al. (2003) K008 OH + OH \rightarrow H ₂ O ₂ + O ₂ 9.7 10 ⁷ 1060 Evens et al. (2003) K009 HO ₂ + HOH \rightarrow HO ₂ + H ₂ O 3.0 10 ⁷ 1800 Deguillaume et al. (2010) K010 NO + OH \rightarrow NO ₂ + H ² 2.10 ¹⁰⁰ 1500 Deguillaume et al. (2010) K011 NO ₂ + H ₂ O \rightarrow 100 ⁷ + H ² 3.0 10 ⁸ Deguillaume et al. (2010) K012 NO ₂ + NO ₁ (+ H ₂ O) \rightarrow 100 ⁷ + H ² 3.0 10 ⁹ Ervens et al. (2003) K013 NO ₂ + OH \rightarrow NO ₂ + H ² 3.0 10 ⁹ Ervens et al. (2003) K014 NO ₂ + O ₂ \rightarrow NO ₁ + O ₂ 3.0 10 ⁹ Ervens et al. (2003) K014 NO ₂ + O ₂ \rightarrow NO ₂ + HO ₂ 3.0 10 ⁹ Ervens et al. (2003) K014 NO ₂ + O ₂ \rightarrow NO ₁ + HO ₂ \rightarrow 10 ¹⁰ Ervens et al. (2003) K014 NO ₂ + O ₁ \rightarrow NO ₁ + HO ₂ $=$ 10 ¹⁰ Ervens et a	K005	$O_2 + OH$	\rightarrow	$O_2 + HO^2$	$1.1\ 10^{10}$	2120	Ervens et al. (2003)
K007 H0, + 0; + (H + T) \rightarrow H ₂ 0; + 0; 9, 10 ⁷ 1060 Ervens et al. (2003) K008 OH + OH \rightarrow H ₂ 0; 3, 6 10 ⁹ 930 Deguillaume et al. (2010) Nurogen chemistry \rightarrow H0; + H ₂ O 3, 0 10 ⁸ Ervens et al. (2003) K010 NO + OH \rightarrow NO; + H ² 2, 2 10 ¹⁰ 1500 Deguillaume et al. (2010) K011 NO; + OH \rightarrow 2, NO; + H ² 3, 0 10 ⁸ Deguillaume et al. (2010) K012 NO; + NO; (+ H ₂ O) \rightarrow 2, NO; + H ² 8, 4 10 ⁷ -2900 Ervens et al. (2003) K013 NO; + O(+ H ₂ O) \rightarrow NO; + H ² 3, 0 10 ⁹ Ervens et al. (2003) K014 NO; + HO; \rightarrow NO; + 10 ² \rightarrow NO; + 0; Ervens et al. (2003) K016 NO; + HO; \rightarrow NO; + 0; 3, 0 10 ⁹ Ervens et al. (2003) K016 NO; + HO; \rightarrow NO; + 0; 3, 0 10 ⁹ Ervens et al. (2003) K016 NO; + HO; \rightarrow NO; + 0; 1, 0 10 ⁹ Deguillaume et al. (2010) K017 NO; + 0;	K006	$HO_2 + HO_2$	\rightarrow	$H_2O_2 + O_2$	8.3 105	2720	Ervens et al. (2003)
K009 $H + OH$ \rightarrow $H_{O_2} + H_{CO}$ $3.6 10^9$ 930 Deguillaume et al. (2010) K009 $H_{O_2} + OH$ \rightarrow $HO_2 + H_{EO}$ $3.0 10^7$ 1680 Ervens et al. (2003) K010 NO + OH \rightarrow $NO_2 + H^*$ $2.1 0^{10}$ 1500 Deguillaume et al. (2010) K011 NO_2 + NO (+H_2O) \rightarrow HON $0 + NO_1 + H^*$ $3.0 10^7$ Deguillaume et al. (2010) K012 NO_2 + NO (+H_2O) \rightarrow HON $0 + NO_2 + H^*$ $3.0 10^7$ Ervens et al. (2003) K013 NO_2 + OH \rightarrow NO_3 + O_2 + H^* $3.0 10^7$ Ervens et al. (2003) K014 NO_3 + HO_2 \rightarrow NO_3 + O_2 + H^* $3.0 10^7$ Ervens et al. (2003) K015 NO_3 + O_2 \rightarrow NO_3 + O_2 $3.0 10^7$ Ervens et al. (2003) K016 NO_3 + HO_2 \rightarrow NO_3 + O_2 $3.0 10^7$ Ervens et al. (2003) K018 NO_2 + OH \rightarrow NO_3 + O_2 $3.0 10^7$ Ervens et al. (2003) K019 HON + OH \rightarrow NO_2 + O_2 $5.0 10^6$ Ervens et al. (2003)	K007	$HO_2 + O_2^- (+ H^+)$	\rightarrow	$H_2O_2 + O_2$	9.7 10 ⁷	1060	Ervens et al. (2003)
K009 H $_{2}$ D ₂ + 0H \rightarrow HD ₂ + H ₂ O $3.0 10^7$ 1680 Errors et al. (2003) K010 NO + 0H \rightarrow NO ₂ + H ⁺ $2.2 10^{10}$ 1500 Deguillaume et al. (2010) K011 NO ₂ + NO ₁ (+ H ₂ O) \rightarrow 2 NO ⁺ + 2 H ⁺ $3.0 10^6$ Deguillaume et al. (2010) K012 NO ₂ + NO ₂ (+ H ₂ O) \rightarrow HONO + NO ₃ + H ⁺ $3.0 10^6$ Ervens et al. (2003) K013 NO ₂ + OH \rightarrow NO ₃ + H ⁺ $3.0 10^6$ Ervens et al. (2003) K014 NO ₃ + HO ₂ \rightarrow NO ₃ + O ₂ $3.0 10^6$ Ervens et al. (2003) K016 NO ₃ + HO ₂ \rightarrow NO ₃ + O ₂ $3.0 10^6$ Ervens et al. (2003) K015 NO ₃ + O ₂ \rightarrow NO ₃ + O ₂ $3.0 10^6$ Ervens et al. (2003) K016 NO ₃ + HO ₂ \rightarrow NO ₃ + O ₂ $3.0 10^6$ Ervens et al. (2003) K017 NO ₄ + HO ₂ \rightarrow NO ₅ + O ₂ $3.0 10^6$ Ervens et al. (2003) K018 NO ₂ + O ₃ \rightarrow NO ₂ + H ₂ O $1.0 10^6$ Evens et al. (2003) K020 NO ₂ + O ₃ $NO_2 + O_3^2^+$ $6.6 10^5$ 850 Ervens et al. (2003)	K008	OH + OH	\rightarrow	H ₂ O ₂	3.6 109	930	Deguillaume et al. (2010)
Nitrogen chemistry Nitrogen chemistry No2 + H ² 2 10 ¹⁰ 1500 Deguillaume et al. (2010) K011 NO2 + NO (+ H ₂ O) \rightarrow HONO + NO3 + H ² 3.0 10 ⁶ Deguillaume et al. (2010) K012 NO2 + NO2 (+ H ₂ O) \rightarrow HONO + NO3 + H ² 8.4 10 ⁷ -2900 Ervens et al. (2003) K013 NO2 + OH \rightarrow NO3 + O2 + H ² 3.0 10 ⁹ Ervens et al. (2003) K014 NO3 + HO2 \rightarrow NO3 + O2 + H ² 3.0 10 ⁹ Ervens et al. (2003) K015 NO4 + O2 \rightarrow NO3 + O2 + H ² 3.0 10 ⁹ Ervens et al. (2003) K016 NO3 + HO2 \rightarrow NO3 + O2 + H ² 4.9 10 ⁶ 2000 Deguillaume et al. (2004) K017 NO3 + HO2 \rightarrow NO3 + O2 \rightarrow NO3 + O2 \rightarrow NO3 + O2 K018 NO2 + O3 \rightarrow NO3 + O2 \rightarrow NO2 + HO2 \rightarrow 1.0 10 ⁰ Ervens et al. (2003) K021 NO2 + O3 \rightarrow NO2 + CO3 a a NO3 <t< td=""><td>K009</td><td>$H_2O_2 + OH$</td><td>\rightarrow</td><td>$HO_2 + H_2O$</td><td>3.0 107</td><td>1680</td><td>Ervens et al. (2003)</td></t<>	K009	$H_2O_2 + OH$	\rightarrow	$HO_2 + H_2O$	3.0 107	1680	Ervens et al. (2003)
K010 NO + OH \rightarrow NO ₂ + H ² 2.2 10 ¹⁰ 1500 Deguillaume et al. (2010) K011 NO ₂ + NO ₁ (+H ₂ O) \rightarrow 2 NO + 2 H ² 3.0 10 ⁸ Deguillaume et al. (2010) K012 NO ₂ + NO ₂ (+H ₂ O) \rightarrow 2 NO + 2 H ² 3.0 10 ⁸ Deguillaume et al. (2003) K013 NO ₂ + OH \rightarrow NO ₃ + H ² 1.0 10 ¹⁰ Ervens et al. (2003) K014 NO ₃ + O ₂ : \rightarrow NO ₃ + H ² 3.0 10 ⁹ Ervens et al. (2003) K014 NO ₃ + O ₂ : \rightarrow NO ₃ + H ² 3.0 10 ⁹ Ervens et al. (2003) K015 NO ₃ + O ₂ : \rightarrow NO ₃ + H ² 3.0 10 ⁹ Ervens et al. (2003) K016 NO ₃ + H ₂ O \rightarrow NO ₃ + HO ₂ + H ⁴ 4.9 10 ⁶ 2000 Deguillaume et al. (2004) K017 NO ₄ + HO ₂ \rightarrow NO ₃ + HO ₂ + H ⁴ 5.0 10 ⁵ 7000 Ervens et al. (2003) K018 NO ₂ + O ₃ \rightarrow NO ₂ + HO ₂ 1.0 10 ¹⁰ Deguillaume et al. (2010) K020 NO ₂ + O ₃ \rightarrow NO ₂ + CO ₃ ² 5.0 10 ⁵ 7000		Nitrogen chemistry					× ,
K011 NO2 + NO (+ H2O) \rightarrow 2 NO + 2 H ² 3.0 10 ⁸ Deguillaume et al. (2010) K012 NO2 + NO; (+ H2O) \rightarrow HONO + NO3 + H ² 8.4 10 ⁷ -2900 Ervens et al. (2003) K013 NO2 + 0H \rightarrow NO3 + H2 1.2 10 ¹⁰ Ervens et al. (2003) K014 NO3 + H02 \rightarrow NO3 + 02 + H ² 3.0 10 ⁹ Ervens et al. (2003) K015 NO3 + O2 \rightarrow NO3 + 02 + H ² 3.0 10 ⁹ Ervens et al. (2003) K016 NO3 + H02 \rightarrow NO3 + 02 + H ² 3.0 10 ⁹ Ervens et al. (2003) K016 NO3 + H02 \rightarrow NO3 + 02 + H ² 3.0 10 ⁹ Ervens et al. (2003) K017 NO3 + H07 \rightarrow NO3 + 02 + H ² 5.0 10 ⁵ 7000 Ervens et al. (2003) K018 NO2 + 03 \rightarrow NO3 + 02 + C03 5.0 10 ⁵ 7000 Ervens et al. (2010) K019 HON + 0H $NO_2 + HO2$ 1.0 10 ¹⁰ Ervens et al. (2003) M01 K021 NO2 + C03 \rightarrow $NO_2 + 02$ 3.7 10 ⁵ 5530 Seinfeld and Pandis (2006) M02	K010	NO + OH	\rightarrow	$NO_{2}^{-} + H^{+}$	2.2 1010	1500	Deguillaume et al. (2010)
K012 N02 + N02 (+ H2O) \rightarrow HONO + N03 + H ⁺ 8.4 107 -2900 Ervens et al. (2003) K013 N02 + OH \rightarrow N03 + H ⁺ 1.2 10 ¹⁰ Ervens et al. (2003) K014 N03 + O2 \rightarrow N03 + O2 + H ⁺ 3.0 10° Ervens et al. (2003) K015 N03 + O2 \rightarrow N03 + O2 + H ⁺ 4.9 106 2000 Deguillaume et al. (2004) K016 N03 + H02 + H ⁺ 4.9 106 2000 Deguillaume et al. (2004) 5.0 105 7000 Ervens et al. (2003) K018 N05 + O3 \rightarrow N05 + HO 9.4 107 2700 Ervens et al. (2003) K018 N05 + O3 \rightarrow N05 + O2 5.0 105 7000 Ervens et al. (2003) K018 N05 + O3 \rightarrow N05 + HO 1.0 10 ¹⁰ Deguillaume et al. (2010) K019 HONO + OH \rightarrow N02 + HO ² 6.6 105 850 Ervens et al. (2003) K021 N05 + O3 \rightarrow HSO4 + O2 3.7 105 5530 Seinfeld and Pandis (2006) K023 HSO3 + O3 \rightarrow HSO4 + O2 1.5 10 ⁰	K011	$NO_2 + NO (+ H_2O)$	\rightarrow	$2 \text{ NO}^{-} + 2 \text{ H}^{+}$	3.0 108		Deguillaume et al. (2010)
K013 NQ ₂ + OH \rightarrow NQ ₅ + H ⁺ 1.2 10 ¹⁰ Ervens et al. (2003) K014 NQ ₅ + HQ ₂ \rightarrow NQ ₅ + Q ₂ + H ⁺ 3.0 10 ⁹ Ervens et al. (2003) K016 NQ ₅ + Q ₂ \rightarrow NQ ₅ + Q ₂ + H ⁺ 3.0 10 ⁹ Ervens et al. (2003) K016 NQ ₅ + HQ ₂ \rightarrow NQ ₅ + HQ ₂ + H ⁺ 4.9 10 ⁶ 2000 Deguillaume et al. (2004) K017 NQ ₅ + HO \rightarrow NQ ₅ + O ₂ \rightarrow NQ ₅ + O ₂ 5.0 10 ⁶ 7000 Ervens et al. (2003) K018 NQ ₂ + O ₃ \rightarrow NQ ₅ + H ₂ O 1.0 10 ¹⁰ Deguillaume et al. (2010) K019 HONO + OH \rightarrow NQ ₂ + H ₂ O 1.0 10 ¹⁰ Deguillaume et al. (2003) K021 NQ ₂ + CO ₃ \rightarrow NQ ₂ + CO ₃ ² 6.6 10 ⁶ 850 Ervens et al. (2003) K022 SQ ₂ + O ₃ (+ H ₂ O) \rightarrow HSQ ₄ + O ₂ + H ⁺ 2.4 10 ⁴ Seinfeld and Pandis (2006) K023 HSQ ₁ + H ₂ O \rightarrow HSQ ₄ + O ₂ + H ⁺ 2.4 10 ⁴ Seinfeld and Pandis (2006) K024 SQ ₃ ² + O ₃ \rightarrow SQ ₄ ² + O ₂ 1.5 10 ⁹ 5280 Seinfeld and Pandis (2006) K025 HSQ ₁ + H ₂ O) <t< td=""><td>K012</td><td>$NO_2 + NO_2 (+ H_2O)$</td><td>\rightarrow</td><td>$HONO + NO_3 + H^+$</td><td>8.4 107</td><td>-2900</td><td>Ervens et al. (2003)</td></t<>	K012	$NO_2 + NO_2 (+ H_2O)$	\rightarrow	$HONO + NO_3 + H^+$	8.4 107	-2900	Ervens et al. (2003)
K014 NO3 ⁺ + HO2 \rightarrow NO3 ⁺ + Q2 + H ⁺ 3.010^9 Ervens et al. (2003) K015 NO3 + Q2 3.010^9 Ervens et al. (2003) K016 NO3 + HO2 \rightarrow NO3 ⁺ + O2 + H ⁺ 4.910^6 2000 Deguillaume et al. (2004) K016 NO3 + HO2 \rightarrow NO3 ⁺ + O2 + H ⁺ 4.910^6 2000 Deguillaume et al. (2003) K018 NO2 + O3 \rightarrow NO3 ⁺ + O2 5.010^5 7000 Ervens et al. (2003) K019 HONO + OH \rightarrow NO2 ⁺ + H2O 1.010^{10} Deguillaume et al. (2003) K021 NO2 ⁺ + O3 \rightarrow NO2 ⁺ + H2O 1.010^{10} Deguillaume et al. (2003) K021 NO2 ⁺ + O3 \rightarrow NO2 ⁺ + H2O 1.010^{10} Ervens et al. (2003) K022 NO2 ⁺ + O3 \rightarrow NO2 ⁺ + H2O 1.010^{10} Ervens et al. (2003) K021 NO2 ⁺ + O3 \rightarrow NO2 ⁺ + C9 ⁺ H ⁺ 2.410^4 Seinfeld and Pandis (2006) K023 HSO3 ⁺ + O3 \rightarrow SO3 ⁺ + O2 3.710^5 5330 Seinfeld and Pandis (2006) K024 <td>K013</td> <td>$NO_2 + OH$</td> <td>\rightarrow</td> <td>$NO_3^- + H^+$</td> <td>$1.2 \ 10^{10}$</td> <td></td> <td>Ervens et al. (2003)</td>	K013	$NO_2 + OH$	\rightarrow	$NO_3^- + H^+$	$1.2 \ 10^{10}$		Ervens et al. (2003)
K015 NO ₃ + O ₂ ⁻ → NO ₅ ⁺ + O ₂ ⁻ 3.0 10 ⁹ Ervens et al. (2003) K016 NO ₃ + H ₂ O ₂ → NO ₅ ⁺ + HO ₂ + H ⁺ 4.9 10 ⁶ 2000 Deguillaume et al. (2004) K017 NO ₃ + HO ² → NO ₅ ⁺ + O ₂ 5.0 10 ⁶ 7000 Ervens et al. (2003) K018 NO ₂ + O ₃ → NO ₅ ⁺ + O ₂ 5.0 10 ⁶ 7000 Ervens et al. (2003) K019 HONO + OH → NO ₂ + HO ² 1.0 10 ¹⁰ Deguillaume et al. (2003) K020 NO ₂ + CO ₃ → NO ₂ + HO ² 1.0 10 ¹⁰ Ervens et al. (2003) K021 NO ₂ + CO ₃ → NO ₂ + CO ₃ ⁻² 6.6 10 ⁵ 850 Ervens et al. (2003) K022 SO ₂ + O ₃ → HSO ₄ + O ₂ + H ⁺ 2.4 10 ⁴ Seinfeld and Pandis (2006) K023 HSO ₃ ⁺ + O ₃ → HSO ₄ + O ₂ + H ⁺ 2.4 10 ⁴ Seinfeld and Pandis (2006) K024 SO ₃ ⁺ + H ₂ O → HSO ₄ + O ₂ 3.7 10 ⁵ 5530 Seinfeld and Pandis (2006) K025 HSO ₃ ⁺ + H ₂ O ₁ + H ⁺ DO → HSO ₄ ⁺ +	K014	$NO_3 + HO_2$	\rightarrow	$NO_{3}^{-} + O_{2} + H^{+}$	3.010^9		Ervens et al. (2003)
K016 $NO_3 + H_2O_2$ \rightarrow $NO_5^+ + HO_2 + H^+$ 4.9 10 ⁶ 2000 Deguillaume et al. (2004) K017 $NO_3 + HO^ \rightarrow$ $NO_5^+ + OH$ 9.4 10 ⁷ 2700 Ervens et al. (2003) K018 $NO_2^+ + O_3$ \rightarrow $NO_5^+ + O_2$ 5.0 10 ⁵ 7000 Ervens et al. (2003) K019 $HONO + OH$ \rightarrow $NO_2 + H_2O$ 1.0 10 ¹⁰ Deguillaume et al. (2010) K020 $NO_2^+ + OH$ $NO_2 + HO^-$ 1.1 10 ¹⁰ Ervens et al. (2003) K021 $NO_2^+ + CO_3^ \rightarrow$ $NO_2^+ + O_2^- + H^+$ 2.4 10 ⁴ Seinfeld and Pandis (2006) K022 $SO_2^+ O_3 + O_2$ 1.5 10 ⁰ S280 Seinfeld and Pandis (2006) K023 $HSO_3^+ + O_2$ $SO_3^+ + O_2$ 1.5 10 ⁰ S280 Seinfeld and Pandis (2006) K024 $SO_3^+ + O_3$ \rightarrow $H_2SO_4 + H_2O$ $NO_4^+ + H^+$ $SO_4^+ + O_2^- + H^+$ Seinfeld and Pandis (2006) K025 $HSO_3 + H_2O_2(+ H^+)$ \rightarrow $H_2SO_4 + H_2O$ S Seinfeld and Pandis (2006) K026 $SO_2 + O_2^+ (+H_2O)$ $H_2SO_4 + H_2$ $NO_2^+ CH_3OH$	K015	$NO_3 + O_2^-$	\rightarrow	$NO_{3}^{-} + O_{2}$	3.0 109		Ervens et al. (2003)
K017 N03 + H0 ⁻ → N05 ⁺ + 0H 9.4 10 ⁷ 2700 Ervens et al. (2003) K018 N05 ⁺ + 05 → N03 ⁺ + 02 5.0 10 ⁵ 7000 Ervens et al. (2003) K019 HON0 + 0H → N02 ⁺ H20 1.0 10 ¹⁰⁰ Deguillaume et al. (2010) K020 N02 ⁺ + C0F N02 ⁺ H0 ⁻ 1.1 10 ¹⁰ Ervens et al. (2003) K021 N02 ⁺ + C03 ⁻ → N02 ⁺ + H ² 6.6 10 ⁵ 850 Ervens et al. (2003) K022 S02 ⁺ + C03 ⁻ → N02 ⁺ + H ² 2.4 10 ⁴ Seinfeld and Pandis (2006) K023 HS03 ⁺ + 03 → HS04 ⁺ + 02 3.7 10 ⁵ 5530 Seinfeld and Pandis (2006) K024 S03 ²⁺ + 03 → S04 ²⁺ + 02 3.7 10 ⁵ 5530 Seinfeld and Pandis (2006) K025 HS03 ⁺ + H02 ⁺ → S04 ²⁺ + 02 1.5 10 ⁹ 5280 Seinfeld and Pandis (2006) K026 S02 ⁺ + H02 ⁺ → S04 ²⁺ + 02 1.0 10 ⁶ Seinfeld and Pandis (2006) K027 S02 ⁺ + O13 → S04 ²⁺ + CH3OH + 2H ⁺⁺ 1.0 10 ⁶ Seinfeld	K016	$NO_3 + H_2O_2$	\rightarrow	$NO_3^- + HO_2 + H^+$	4.9 106	2000	Deguillaume et al. (2004)
K018 $NO_2^+ + O_3^ \rightarrow NO_3^- + O_2^ 5.0 \ 10^5$ 7000 Ervens et al. (2003)K019HON0 + OH $\rightarrow NO_2 + H_2O$ $1.0 \ 10^{10}$ Deguillaume et al. (2010)K020 $NO_2^+ + OH$ $NO_2 + HO^ 1.1 \ 10^{10}$ Ervens et al. (2003)K021 $NO_2^+ + O_3^ \rightarrow NO_2 + CO_3^ 6.6 \ 10^5$ 850 Ervens et al. (2003)Sulfur chemistry $K022$ $SO_2 + O_3(+ H_2O)$ $\rightarrow HSO_4 + O_2 + H^+$ $2.4 \ 10^4$ Seinfeld and Pandis (2006)K023 $HSO_3^+ + O_3$ $\rightarrow HSO_4^+ + O_2$ $3.7 \ 10^5$ 5530 Seinfeld and Pandis (2006)K024 $SO_3^+ + O_3$ $\rightarrow HSO_4 + H_2O$ $5.0 \ 10^6$ Seinfeld and Pandis (2006)K025 $HSO_3^+ + O_3$ $\rightarrow H2SO_4 + H_2O$ $5.0 \ 10^6$ Seinfeld and Pandis (2006)K025 $HSO_3^+ + O_2$ $1.5 \ 10^9$ 5280 Seinfeld and Pandis (2006)K025 $HSO_3^+ + O_2$ $hESO_4 + H_2O$ $5.0 \ 10^6$ Seinfeld and Pandis (2006)K026 $SO_2 + HO_2 (+ H_2O)$ $\rightarrow H2SO_4 + HO^ 1.0 \ 10^6$ Seinfeld and Pandis (2006)K027 $SO_2^- + O_3^- + O_4 + HO^ 1.0 \ 10^6$ Seinfeld and Pandis (2006)K028 $HSO_3^+ + O_4 + H^ -SO_3^- + O_4 + H^+$ $1.7 \ 10^7$ 1900 Ervens et al. (2003)K039 $CO_3^- + OH$ $\rightarrow CO_3^- + HO^ 3.9 \ 10^6$ 2840 Ervens et al. (2003)K031 $HCO_3^- + NO_3$ $\rightarrow CO_3^- + NO_3^ 4.1 \ 10^7$ Ervens et al. (2003)K032 $CO_3^- + NO_3$ $\rightarrow CO_3^- + N$	K017	$NO_3 + HO^2$	\rightarrow	$NO_3^- + OH$	9.4 107	2700	Ervens et al. (2003)
K019HONO + OH \rightarrow NO2 + H2O1.0 10 ⁴⁰ Deguillaume et al. (2010)K020NO2 + OHNO2 + HO1.1 10 ⁴⁰ Ervens et al. (2003)K021NO2 + CO3 \rightarrow NO2 + CO3 ^{2/2} 6.6 10 ⁵ 850Ervens et al. (2003)K021NO2 + CO3 \rightarrow NO2 + CO3 ^{2/2} 6.6 10 ⁵ 850Ervens et al. (2003)K022SO2 + O3 (+ H2O) \rightarrow HSO4 + O2 + H ⁺ 2.4 10 ⁴ Seinfeld and Pandis (2006)K023HSO3 + O3 \rightarrow HSO4 + O23.7 10 ⁵ 5530Seinfeld and Pandis (2006)K024SO3 ²⁺ + O3 \rightarrow H2SO4 + H2O8Seinfeld and Pandis (2006)K025HSO3 + H2O2 (+ H ⁺) \rightarrow H2SO4 + H2O8Seinfeld and Pandis (2006)K026SO2 + HO2 (+ H2O) \rightarrow H2SO4 + H2O8Seinfeld and Pandis (2006)K027SO2 + O2 (+ H2O) \rightarrow H2SO4 + OH1.0 10 ⁶ Seinfeld and Pandis (2006)K028HSO3 + CH3O2H (+ H ⁺) \rightarrow SO3 ²⁺ + O11.0 10 ⁵ Seinfeld and Pandis (2006)K029HCO3 + OH \rightarrow CO3 + HO3.9 10 ⁸ 2840Ervens et al. (2003)K030CO3 ²⁺ + OH \rightarrow CO3 + HO3.9 10 ⁸ 2840Ervens et al. (2003)K032CO3 ²⁺ + NO3 \rightarrow CO3 + NO3 \rightarrow CO3 + NO34.1 10 ⁷ Ervens et al. (2003)K032CO3 ²⁺ + NO3 \rightarrow CO3 + NO3 \rightarrow CO3 + NO34.1 10 ⁷ Ervens et al. (2003)K032CO3 ²⁺ + NO3 \rightarrow CO3 + NO	K018	$NO_{2}^{-} + O_{3}$	\rightarrow	$NO_3^- + O_2$	$5.0 10^5$	7000	Ervens et al. (2003)
K020 $NO_2 + OH$ $NO_2 + HO^2$ $1.1 \ 10^{10}$ Ervens et al. (2003)K021 $NO_2 + CO_3^2$ $O_2 + CO_3^{2^2}$ $6.6 \ 10^5$ 850 Ervens et al. (2003)Sulfur chemistry $Sulfur chemistry$ $Sulfur chemistry$ $Sulfur chemistry$ $Sulfur chemistry$ K022 $SO_2 + O_3 (+ H_2O)$ \rightarrow HSO ₄ + $O_2 + H^+$ $2.4 \ 10^4$ Seinfeld and Pandis (2006)K023HSO_3 + O_3 \rightarrow HSO ₄ + O_2 $3.7 \ 10^5$ 5530 Seinfeld and Pandis (2006)K024 $SO_3^2 + O_3$ \rightarrow SO ₄ ² + O_2 $1.5 \ 10^9$ 5280 Seinfeld and Pandis (2006)K025HSO_3 + H_2O_2 (+ H^+) \rightarrow H_2SO ₄ + H_2O s Seinfeld and Pandis (2006)K026SO_2 + HO_2 (+ H_2O) \rightarrow HSO ₃ + OH + HO' $1.0 \ 10^6$ Seinfeld and Pandis (2006)K028HSO_3 + CH_3O_2H (+ H^+) \rightarrow SO ₄ ² + CH ₃ OH + 2H^+ $1.7 \ 10^7$ 3160 Seinfeld and Pandis (2006)K029HCO_3 + OH \rightarrow CO ₅ + H ₂ O $1.7 \ 10^7$ 1900 Ervens et al. (2003)K030CO ₃ ² + OH \rightarrow CO ₅ + HO ⁷ $3.9 \ 10^8$ 2840 Ervens et al. (2003)K031HCO ₃ + NO ₃ \rightarrow CO ₅ + NO ₅ + H ⁺ $4.1 \ 10^7$ Ervens et al. (2003)K032CO ₃ + NO ₃ \rightarrow CO ₅ + NO ₅ $4.1 \ 10^7$ Ervens et al. (2003)	K019	HONO + OH	\rightarrow	$NO_2 + H_2O$	1.0 1010		Deguillaume et al. (2010)
K021 $NO_2^{-r} + CO_3^{-r}$ $\rightarrow NO_2^{-r} + CO_3^{-2r}$ $6.6 \ 10^5$ 850 Ervens et al. (2003) Sulfur chemistry K K $Sulfur chemistry$ $Sulfur chemistry$ K022 $SO_2 + O_3 (+ H_2O)$ $\rightarrow HSO_4 + O_2 + H^+$ $2.4 \ 10^4$ Seinfeld and Pandis (2006) K023 $HSO_3^{-r} + O_3$ $\rightarrow HSO_4^{-r} + O_2$ $3.7 \ 10^5$ 5530 Seinfeld and Pandis (2006) K024 $SO_3^{2-r} + O_3$ $\rightarrow SO_4^{2-r} + O_2$ $1.5 \ 10^9$ 5280 Seinfeld and Pandis (2006) K025 $HSO_3^{-r} + D_3$ $\rightarrow SO_4^{2-r} + O_2$ $1.5 \ 10^9$ 5280 Seinfeld and Pandis (2006) K025 $HSO_3^{-r} + H_2^{-r} + H_2^{-r}$ $1.5 \ 10^9$ 5280 Seinfeld and Pandis (2006) K026 $SO_2^{-r} + H_2^{-r} + H_2^{-r}$ $1.0 \ 10^6$ Seinfeld and Pandis (2006) K028 $HSO_3^{-r} + CH_3O_2 + (+H^+)$ $\rightarrow SO_4^{-r} + CH_3O + 2H^+$ $1.7 \ 10^7$ 3160 Seinfeld and Pandis (2006) K029 $HCO_3^{-r} + OH$ $\rightarrow CO_3^{-r} + HO^{-r}$ $3.9 \ 10^8$ 2840 Ervens et al. (2003) K031 $HCO_3^{-r} + NO_3$ $\rightarrow CO_3^{-r} + NO_3^{-r} + H^{-r}$ $4.$	K020	$NO_2 + OH$		$NO_2 + HO^2$	$1.1\ 10^{10}$		Ervens et al. (2003)
Sulfur chemistryK022S0 ₂ + 0 ₃ (+ H ₂ O)→HSO ₄ + 0 ₂ + H ⁺ 2.4 10 ⁴ Seinfeld and Pandis (2006)K023HSO ₃ ⁺ + 0 ₃ →HSO ₄ + 0 ₂ 3.7 10 ⁵ 5530Seinfeld and Pandis (2006)K024SO ₃ ⁺ + 0 ₃ →SO ₄ ² + 0 ₂ 1.5 10 ⁹ 5280Seinfeld and Pandis (2006)K025HSO ₃ ⁺ + 0 ₃ →H ₂ SO ₄ + H ₂ O ⁸ Seinfeld and Pandis (2006)K026SO ₂ + HO ₂ (+ H ⁺)→H ₂ SO ₄ + H ₂ O ⁸ Seinfeld and Pandis (2006)K027SO ₂ + O ₂ (+ H ₂ O)→HSO ₃ + OH + HO ⁻ 1.0 10 ⁶ Seinfeld and Pandis (2006)K028HSO ₃ + CH ₃ O ₂ H (+ H ⁺)→SO ₂ ² + CH ₃ OH + 2H ⁺ 1.7 10 ⁷ 3160Seinfeld and Pandis (2006)Carbonate chemistryK039CO ₃ ² + OH→CO ₃ ⁻ + HO ⁻ 3.9 10 ⁸ 2840Ervens et al. (2003)K031HCO ₃ + NO ₃ →CO ₃ ⁻ + NO ₃ +CO ₃ ⁻ + NO ₃ 4.1 10 ⁷ Ervens et al. (2003)K032CO ₃ ⁻² + NO ₃ →CO ₃ ⁻ + NO ₃ 4.1 10 ⁷ Ervens et al. (2003)	K021	$NO_2^- + CO_3^-$	\rightarrow	$NO_2 + CO_3^{2-}$	6.6 10 ⁵	850	Ervens et al. (2003)
K022 SO ₂ + O ₃ (+ H ₂ O) → HSO ₄ + O ₂ + H ⁺ 2.4 10 ⁴ Seinfeld and Pandis (2006) K023 HSO ₃ + O ₃ → HSO ₄ + O ₂ 3.7 10 ⁵ 5530 Seinfeld and Pandis (2006) K024 SO ₃ ² + O ₃ → HSO ₄ + O ₂ 1.5 10 ⁹ 5280 Seinfeld and Pandis (2006) K025 HSO ₃ + H ₂ O ₂ (+ H ⁺) → H ₂ SO ₄ + H ₂ O \$ Seinfeld and Pandis (2006) K026 SO ₂ + HO ₂ (+ H ₂ O) → H ₂ SO ₄ + OH 1.0 10 ⁶ Seinfeld and Pandis (2006) K027 SO ₂ + O ₂ (+ H ₂ O) → HSO ₃ + OH + HO ⁺ 1.0 10 ⁶ Seinfeld and Pandis (2006) K028 HSO ₃ + H ₂ O ₂ H(H ⁺) → HSO ₃ + CH ₃ OH + 2H ⁺ 1.7 10 ⁷ 3160 Seinfeld and Pandis (2006) K028 HCO ₃ + OH → CO ₃ ⁺ + H ₂ O 1.7 10 ⁷ 3160 Seinfeld and Pandis (2006) K039 CO ₃ ⁺ + OH → CO ₃ ⁺ + H ₂ O 1.7 10 ⁷ 1900 Ervens et al. (2003) K039 CO ₃ ⁺ + OH → CO ₃ ⁺ + HO ² 3.9 10 ⁸ 2840 Ervens et al. (2003) K031		Sulfur chemistry					× ,
K023HSO3 + O3 \rightarrow HSO4 + O2 $3.7 10^5$ 5530 Seinfeld and Pandis (2006)K024SO32 + O3 \rightarrow SO42 + O2 $1.5 10^9$ 5280 Seinfeld and Pandis (2006)K025HSO3 + H2O2 (+ H1) \rightarrow H2SO4 + H2O 8 Seinfeld and Pandis (2006)K026SO2 + HO2 (+ H2O) \rightarrow HSO3 + OH + HO $1.0 10^6$ Seinfeld and Pandis (2006)K027SO2 + O2 (+ H2O) \rightarrow HSO3 + OH + HO $1.0 10^6$ Seinfeld and Pandis (2006)K028HSO3 + CH3O2H (+ H1) \rightarrow SO42 + CH3OH + 2H1 $1.7 10^7$ 3160 Seinfeld and Pandis (2006)K029HCO3 + OH \rightarrow CO3 + H2O $1.7 10^7$ 1900 Ervens et al. (2003)K030CO32 + OH \rightarrow CO3 + HO7 $3.9 10^8$ 2840 Ervens et al. (2003)K031HCO3 + NO3 \rightarrow CO3 + NO3 \rightarrow CO3 + H07 $4.1 10^7$ Ervens et al. (2003)K032CO3 + NO3 \rightarrow CO3 + NO3 \rightarrow CO3 + NO3 $4.1 10^7$ Ervens et al. (2003)	K022	$SO_2 + O_3 (+ H_2O)$	\rightarrow	$HSO_{4} + O_{2} + H^{+}$	$2.4 10^4$		Seinfeld and Pandis (2006)
K024 $SO_3^{2^2} + O_3$ \rightarrow $SO_4^{2^2} + O_2$ $1.5 \ 10^9$ 5280 Seinfeld and Pandis (2006)K025 $HSO_3 + H_2O_2(+H^+)$ \rightarrow $H_2SO_4 + H_2O$ s Seinfeld and Pandis (2006)K026 $SO_2 + HO_2(+H_2O)$ \rightarrow $H_2SO_4 + OH$ $1.0 \ 10^6$ Seinfeld and Pandis (2006)K027 $SO_2 + O_2(+H_2O)$ \rightarrow $HSO_3 + OH + HO^ 1.0 \ 10^6$ Seinfeld and Pandis (2006)K028 $HSO_3^- + CH_3O_2H(+H^+)$ \rightarrow $SO_4^{2^2} + CH_3OH + 2H^+$ $1.7 \ 10^7$ 3160 Seinfeld and Pandis (2006)K029 $HCO_3^- + OH$ \rightarrow $CO_3^- + HO^ 3.9 \ 10^8$ 2840 Ervens et al. (2003)K039 $CO_3^{2^2} + OH$ \rightarrow $CO_3^- + HO^ 3.9 \ 10^8$ 2840 Ervens et al. (2003)K031 $HCO_3^- + NO_3$ \rightarrow $CO_3^- + NO_3^ 4.1 \ 10^7$ Ervens et al. (2003)K032 $CO_3^{-2^2} + NO_3$ \rightarrow $CO_3^- + NO_3^ 4.1 \ 10^7$ Ervens et al. (2003)	K023	$HSO_3 + O_3$	\rightarrow	$HSO_4 + O_2$	3.7 105	5530	Seinfeld and Pandis (2006)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	K024	$SO_3^{2-} + O_3$	\rightarrow	$SO_4^2 + O_2$	1.5 109	5280	Seinfeld and Pandis (2006)
K026 $SO_2 + HO_2(+H_2O)$ \rightarrow $H_2SO_4 + OH$ $1.0\ 10^6$ Seinfeld and Pandis (2006) K027 $SO_2 + O_2(+H_2O)$ \rightarrow $HSO_3 + OH + HO^\circ$ $1.0\ 10^5$ Seinfeld and Pandis (2006) K028 $HSO_3 + CH_3O_2H (+H^+)$ \rightarrow $SO_4^2 + CH_3OH + 2H^+$ $1.7\ 10^7$ 3160 Seinfeld and Pandis (2006) K029 $HCO_3 + CH_3O_2H (-H^+)$ \rightarrow $CO_3^2 + H_2O$ $1.7\ 10^7$ 1900 Ervens et al. (2003) K039 $CO_3^2 + OH$ \rightarrow $CO_3^2 + HO^\circ$ $3.9\ 10^8$ 2840 Ervens et al. (2003) K031 $HCO_3^2 + NO_3$ \rightarrow $CO_3^2 + H^+$ $4.1\ 10^7$ Ervens et al. (2003) K032 $CO_3^2 + NO_3$ \rightarrow $CO_3^2 + NO_3$ \rightarrow $CO_3^2 + NO_3$ K032 $CO_3^2 + NO_3$ \rightarrow $CO_3^2 + NO_3$ \rightarrow $CO_3^2 + NO_3$ K032 $CO_3^2 + NO_3$ \rightarrow $CO_3^2 + O_3^2$ $4.1\ 10^7$ Ervens et al. (2003)	K025	$HSO_{3}^{-} + H_{2}O_{2}(+H^{+})$	\rightarrow	$H_2SO_4 + H_2O_1$	s		Seinfeld and Pandis (2006)
K027 SO ₂ + O ₂ '(+ H ₂ O)' \rightarrow HSO ₃ + OH + HO' 1.0 10 ⁵ Seinfeld and Pandis (2006) K028 HSO ₃ + CH ₃ O ₂ H (+ H ⁺) \rightarrow SO ₄ ²⁺ + CH ₃ OH + 2H ⁺ 1.7 10 ⁷ 3160 Seinfeld and Pandis (2006) Carbonate chemistry \rightarrow CO ₃ + H ₂ O 1.7 10 ⁷ 3160 Seinfeld and Pandis (2006) K029 HCO ₃ + OH \rightarrow CO ₃ + H ₂ O 1.7 10 ⁷ 1900 Ervens et al. (2003) K030 CO ₃ ²⁻ + OH \rightarrow CO ₃ + HO' 3.9 10 ⁸ 2840 Ervens et al. (2003) K031 HCO ₃ + NO ₃ \rightarrow CO ₃ + HO' 4.1 10 ⁷ Ervens et al. (2003) K032 CO ₂ + NO ₃ \rightarrow CO ₃ + NO ₃ \rightarrow CO ₃ + NO ₃ (C) + O ₂ (C) + O ₂	K026	$SO_2 + HO_2 (+ H_2O)$	\rightarrow	$H_2SO_4 + OH$	$1.0\ 10^{6}$		Seinfeld and Pandis (2006)
K028 HSO ₃ + CH ₃ O ₂ H (+ H ⁺) \rightarrow SO ₄ ²⁻ + CH ₃ OH + 2H ⁺ 1.7 10 ⁷ 3160 Seinfeld and Pandis (2006) Carbonate chemistry \sim CO ₅ ⁺ + H ₂ O 1.7 10 ⁷ 1900 Ervens et al. (2003) K039 CO ₃ ²⁻ + OH \rightarrow CO ₅ ⁺ + HO ⁻ 3.9 10 ⁸ 2840 Ervens et al. (2003) K031 HCO ₃ ⁻ + NO ₃ \rightarrow CO ₅ ⁻ + NO ₅ + H ⁺ 4.1 10 ⁷ Ervens et al. (2003) K032 CO ₂ ⁻² + NO ₃ \rightarrow CO ₃ ⁻ + NO ₅ 4.1 10 ⁷ Ervens et al. (2003)	K027	$SO_2 + O_2 + H_2O$	\rightarrow	$HSO_3 + OH + HO$	$1.0\ 10^{5}$		Seinfeld and Pandis (2006)
Carbonate chemistryK029HCO3 + OH \rightarrow CO3 + H2O1.7 1071900Ervens et al. (2003)K039CO32 + OH \rightarrow CO3 + HO3.9 1082840Ervens et al. (2003)K031HCO3 + NO3 \rightarrow CO3 + NO3 + H ⁺ 4.1 107Ervens et al. (2003)K032CO32 + NO3 \rightarrow CO3 + NO34.1 107Ervens et al. (2003)K032CO32 + NO3 \rightarrow CO3 + NO34.1 107Ervens et al. (2003)	K028	$HSO_3^- + CH_3O_2H (+ H^+)$	\rightarrow	$SO_4^{2^+} + CH_3OH + 2H^+$	$1.7 10^7$	3160	Seinfeld and Pandis (2006)
K029 HCO ₃ + OH \rightarrow CO ₃ + H ₂ O 1.7 10 ⁷ 1900 Ervens et al. (2003) K039 CO ₃ ² + OH \rightarrow CO ₃ + HO ⁷ 3.9 10 ⁸ 2840 Ervens et al. (2003) K031 HCO ₃ + NO ₃ \rightarrow CO ₃ + NO ₃ + H ⁺ 4.1 10 ⁷ Ervens et al. (2003) K032 CO ₃ ² + NO ₃ \rightarrow CO ₃ + NO ₅ [*] 4.1 10 ⁷ Ervens et al. (2003) K032 CO ₃ + O ₃ \rightarrow CO ₃ + NO ₅ [*] 4.1 10 ⁷ Ervens et al. (2003)		Carbonate chemistry					
K039 $CO_3^{2^2} + OH$ \rightarrow $CO_3^2 + HO^2$ $3.9 10^8$ 2840 Ervens et al. (2003) K031 HCO_3^2 + NO_3 \rightarrow $CO_3^2 + HO^2$ $4.1 10^7$ Ervens et al. (2003) K032 $CO_3^2 + NO_3$ \rightarrow $CO_3^2 + NO_3^2$ $4.1 10^7$ Ervens et al. (2003) K032 $CO_3^2 + NO_3$ \rightarrow $CO_3^2 + NO_3^2$ $4.1 10^7$ Ervens et al. (2003)	K029	$HCO_3 + OH$	\rightarrow	CO_3 + H ₂ O	$1.7 \ 10^{7}$	1900	Ervens et al. (2003)
K031HCO ₃ + NO ₃ \rightarrow CO ₃ + NO ₃ + H ⁺ 4.1 10 ⁷ Ervens et al. (2003)K032CO ₂ + NO ₃ \rightarrow CO ₃ + NO ₃ 4.1 10 ⁷ Ervens et al. (2003)K032CO ₂ + O ₃ \rightarrow CO ₃ + NO ₃ 4.1 10 ⁷ Ervens et al. (2003)	K039	$CO_3^{2-} + OH$	\rightarrow	$CO_3 + HO^2$	3.910^8	2840	Ervens et al. (2003)
$\begin{array}{cccc} \text{K032} & \text{CO}_3^{-2} + \text{NO}_3 & \rightarrow & \text{CO}_3^{-1} + \text{NO}_3^{-1} & & \text{H} 110^7 & \text{Ervens et al. (2003)} \\ \text{K032} & \text{CO}_3^{-2} + \text{NO}_3 & \rightarrow & \text{CO}_3^{-1} + \text{NO}_3^{-1} & & \text{H} 110^7 & \text{Ervens et al. (2003)} \\ \text{K032} & \text{CO}_3^{-1} + \text{O}_3 & & \text{H} 10^7 & \text{Ervens et al. (2003)} \\ \text{K032} & \text{CO}_3^{-1} + \text{O}_3 & & \text{H} 10^7 & \text{Ervens et al. (2003)} \\ \text{K032} & \text{CO}_3^{-1} + \text{O}_3^{-1} & & \text{H} 10^7 & \text{Ervens et al. (2003)} \\ \text{K032} & \text{CO}_3^{-1} + \text{O}_3^{-1} & & \text{H} 10^7 & \text{Ervens et al. (2003)} \\ \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} \\ \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} \\ \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} \\ \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} \\ \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} \\ \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} \\ \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} \\ \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} \\ \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} \\ \text{K032} & \text{K032} & \text{K032} & \text{K032} \\ \text{K032} & \text{K032} & \text{K032} & \text{K032} \\ \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} \\ \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} \\ \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} \\ \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} \\ \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} & \text{K032} \\ \text{K032} & $	K031	$HCO_3 + NO_3$	\rightarrow	$CO_3^- + NO_3^- + H^+$	4.110^{7}		Ervens et al. (2003)
$V_{022} = C_0 + $	K032	$CO_3^{2-} + NO_3$	\rightarrow	$CO_3 + NO_3$	4.1 107		Ervens et al. (2003)
$\kappa_{000} \rightarrow C_{00} + $	K033	$CO_3 + O_3$	\rightarrow	$CO_2 + O_2 + O_2$	1.0 105		Ervens et al. (2003)

K034	$CO_3^- + HO_2$	\rightarrow	$HCO_3 + O_2$	6.5 10 ⁸		Ervens et al. (2003)
K035	$CO_{3}^{-} + O_{2}^{-}$	\rightarrow	$CO_3^{2^2} + O_2^{2^2}$	6.5 10 ⁸		Ervens et al. (2003)
K036	CO_3 ⁻ + H ₂ O ₂	\rightarrow	$HCO_3^- + HO_2$	4.3 105		Ervens et al. (2003)
K037	$CO_3^- + NO_2$	\rightarrow	$CO_2 + NO_3$	1.0 109		Ervens et al. (2003)
K038	$CO_3 + CO_3 (+ O_2)$	\rightarrow	$2 O_2^{-} + 2 CO_2$	2.2 10		Ervens et al. (2003)
K030	CH ₂ O ₂ H + OH	_	$0.8(CH_{2}O_{2} + H_{2}O) + 0.2(HCOOH + HO_{2})$	3 0 107	1680	Ervens et al. (2003)
K040	$CH_3O_2H + CO_3^-$	\rightarrow	$CH_{2}O_{2} + HCO_{2}$	4310^{5}	1080	Ervens et al. (2003)
K041	$CH_3O_2 + HO_2$	\rightarrow	$CH_3O_2H + O_2$	4.2 105	3000	Deguillaume et al. (2010)
K042	$CH_3O_2 + O_2 + H_2O$	\rightarrow	$CH_3O_2H + O_2 + HO^2$	4.8 107	1600	Deguillaume et al. (2010)
K043	$CH_{3}O_{2} + CH_{3}O_{2}(+H_{2}O)$	\rightarrow	$CH_3OH + CH_2(OH)_2 + O_2$	$1.7 \ 10^8$	2200	Ervens et al. (2003)
K044	$CH_{3}O_{2} + CH_{3}O_{2} (+ 2 O_{2} + 2 O_{2})$	\rightarrow	$2 CH_2(OH)_2 + 2 HO_2 + O_2$	$3.6 10^{7}$	2200	Ervens et al. (2003)
No 45	H ₂ O)			1.0.109	1020	
K045	$CH_2(OH)_2 + OH (+ O_2)$ $CH_2(OH)_2 + NO_2 (+ O_2)$	\rightarrow	$HCOOH + HO_2 + H_2O$ $HCOOH + HO_2 + NO_2 + H^+$	1.0 10'	1020	Ervens et al. (2003)
K040 K047	$CH_2(OH)_2 + NO_3(+O_2)$ $CH_2OH + OH(+O_2)$	\rightarrow	$CH_2(OH)_2 + HO_2 + H_2O$	1.010^9	580	Ervens et al. (2003)
K048	$CH_3OH + NO_3 (+ O_2)$	\rightarrow	$CH_2(OH)_2 + HO_2 + HO_3^-$	5.4 10 ⁵	4300	Ervens et al. (2003)
K049	$CH_{3}OH + CO_{3}(+O_{2})$	\rightarrow	$CH_2(OH)_2 + HO_2 + HCO_3$	2.6 10 ³		Ervens et al. (2003)
K050	$HCOOH + OH (+ O_2)$	\rightarrow	$CO_2 + HO_2 + H_2O$	1.3 108	1000	Ervens et al. (2003)
K051	$HCOO^{-} + OH (+ O_2)$	\rightarrow	$CO_2 + HO_2 + HO_3$	3.2 109	1000	Ervens et al. (2003)
K052	$HCOOH + NO_3 (+ O_2)$	\rightarrow	$CO_2 + HO_2 + NO_3^- + H^+$	3.8 103	3400	Ervens et al. (2003)
K053 K054	$HCOO + NO_3 (+ O_2)$ $HCOO + CO_2 (+ O_2)$	\rightarrow	$CO_2 + HO_2 + NO_3$ 2 $CO_2 + O_2 + HO_3$	5.1 10 ⁷ 1 4 10 ⁵	2200	Ervens et al. (2003) Ervens et al. (2003)
K054 K055	$CH_{2}CH(OH)_{2} + OH(+O_{2})$	\rightarrow	$CH_{3}COOH + HO_{2} + H_{2}O$	1.410 1.210^{9}	5500	Ervens et al. (2003)
K056	$CH_3CH(OH)_2 + NO_3 (+ O_2)$	\rightarrow	$CH_3COOH + HO_2 + NO_3^- + H^+$	1.9 106		Ervens et al. (2003)
K057	$CH_3CH(OH)_2 + CO_3 + (+O_2)$	\rightarrow	$CH_3COOH + HO_2 + CO_2$	$1.0\ 10^4$		Ervens et al. (2003)
K058	$GLYAL + OH (+ O_2)$	\rightarrow	$GLY + HO_2$	$1.0\ 10^9$		Lim et al. (2005)
K059	$GLYAL + OH (+ O_2)$	\rightarrow	$GLX + 2 HO_2$	5.0 10 ⁸		Lim et al. (2005)
K060	$GLYAL + NO_3 (+ O_2)$	\rightarrow	$GLY + HO_2 + NO_3^- + H^-$	1.1 10'		Herrmann et al. (2005)
K061 K062	$GLYAL + NO_3 (+ O_2)$ $GLY + OH (+ O_2)$	\rightarrow	$GLX + 2 HO_2 + NO_3 + H + H_2O$ $GLX + HO_1 + H_2O$	$5.5 10^{\circ}$ 1 1 10 ⁹	1516	Fryens et al. (2003)
K063	GLY + OH	\rightarrow	GLXOLIG ^c	3 0 10 ¹⁰	1510	Carlton et al. (2007)
K064	GLYOLIG ° + OH	\rightarrow	OXL	3.0 10 ¹⁰		Carlton et al. (2007)
K065	GLYOLIG ° + OH	\rightarrow	GLX	$1.0\ 10^9$		Carlton et al. (2007)
K066	$GLY + NO_3 (+ O_2)$	\rightarrow	$GLX + HO_2 + NO_3^- + H^+$	$1.1\ 10^{6}$	3368	Ervens et al. (2003)
K067	$CH_3CH_2OH + OH (+ O_2)$	\rightarrow	$CH_3CH(OH)_2 + HO_2$	1.9 10 ⁹		Ervens et al. (2003)
K068	$CH_3CH_2OH + NO_3 (+ O_2)$	\rightarrow	$CH_3CH(OH)_2 + HO_2 + NO_3 + H^+$	2.2 106		Ervens et al. (2003)
K069	$CH_3CH_2OH + CO_3^- (+ O_2)$	\rightarrow	$CH_3CH(OH)_2 + HO_2 + CO_2$	1.5 10*	1220	Ervens et al. (2003)
K070 K071	$CH_3COOH + OH (+ O_2)$ $CH_3COOT + OH (+ O_2)$	\rightarrow	$0.85 \text{ GLX} + 0.15 \text{ CH}_2(\text{OH})_2 + 0.15 \text{ CO}_2 + \text{HO}_2$ $0.85 \text{ GLX}^2 + 0.15 \text{ CH}_2(\text{OH})_2 + 0.15 \text{ CO}_2 + \text{HO}_2$	1.5 10	1330	Ervens et al. (2003) Ervens et al. (2003)
K072	$CH_2COOH + NO_2(+ O_2)$	\rightarrow	$0.85 \text{ GLX} + 0.15 \text{ CH}_2(\text{OH})_2 + 0.15 \text{ CO}_2 + \text{HO}_2$ 0.85 GLX + 0.15 CH ₂ (OH) ₂ + 0.15 CO ₂ + NO ₂ ⁻ + H ⁺	$1.0\ 10^{4}$	3800	Ervens et al. (2003)
K073	$CH_3COO^2 + NO_3 (+ O_2)$	\rightarrow	$0.85 \text{ GLX}^{-} + 0.15 \text{ CH}_2(\text{OH})_2 + 0.15 \text{ CO}_2 + \text{NO}_3^{-} + \text{H}^+$	$2.9 10^6$	3800	Ervens et al. (2003)
K074	$CH_3COO^- + CO_3^- (+ O_2)$	\rightarrow	$0.85 \text{ GLX} + 0.15 \text{ CH}_2(\text{OH})_2 + 1.15 \text{ CO}_2$	5.8 10 ²		Ervens et al. (2003)
K075	HYAC + OH	\rightarrow	$MGLY + HO_2$	$1.2\ 10^9$		Herrmann et al. (2005)
K076	$HYAC + NO_3$	\rightarrow	$MGLY + NO_3 + H^+$	1.7 106		Herrmann et al. (2005)
K077	$MGLY + OH (+ O_2)$	\rightarrow	$0.92 \text{ PRV} + 0.08 \text{ GLX} + 0.08 \text{ CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	1.1 109	1600	Ervens et al. (2004)
K078	MGLY + OH	\rightarrow	$0.8 \text{ MGLYOLIG}^\circ + 0.2 \text{ OXL}$	1.1 10 ⁹	1600	Lin et al. (2014) (Tan et al., 2012)
K079 K080	$MGLY + NO_3 (+ O_2)$ $PPV + OH (+ O_2)$	\rightarrow	$0.92 \text{ PKV} + 0.08 \text{ GLX} + 0.08 \text{ CO}_2 + \text{HO}_2 + \text{NO}_3 + \text{H}^2$	$0.3 10^{\circ}$ 1 2 10 ⁸	2800	Herrmann et al. (2005)
K080	$PRV^{-} + OH$	\rightarrow	$CH_2COO^2 + HO_2 + CO_2$	$7.0 \ 10^8$	2285	Herrmann et al. (2005)
K082	$PRV + NO_3 (+ O_2 + H_2O)$	\rightarrow	$CH_3COOH + CO_2 + HO_2 + NO_3^- + H^+$	4.8 106		Herrmann et al. (2005)
K083	$PRV + NO_3 (+ O_2 + H_2O)$	\rightarrow	$CH_{3}COO^{-} + CO_{2} + HO_{2} + NO_{3}^{-} + H^{+}$	1.9 10 ⁸		Herrmann et al. (2005)
K084	$GLX + OH (+ O_2)$	\rightarrow	$OXL + HO_2 + H_2O$	3.6 108	1000	Deguillaume et al. (2009)
K085	$GLX^{-} + OH (+ O_2)$	\rightarrow	$OXL^2 + HO_2 + H_2O$	2.6 109	4330	Deguillaume et al. (2009)
K086	$GLX + NO_3 (+ O_2)$	\rightarrow	$OXL + HO_2 + NO_3^- + H^+$	3.0 10°		as for glycolic acid from Herrmann et al. (2005)
K08/	$GLX^2 + NO_3(+O_2)$	\rightarrow	$OXL^{2} + HO_{2} + NO_{3}^{2} + H^{2}$	1.1 10°		as for glycolic acid from Herrmann et al. (2005)
K088	$OXL + OH(+O_2)$ $OXL + OH(+O_2)$	\rightarrow	$2CO_2 + HO_2 + H_2O$	$3.2 10^7$		Ervens et al. (2004) Ervens et al. (2003)
K090	$OXL^{2-} + OH(+O_2)$	\rightarrow	$2CO_2 + O_2 + H_2O_2$	5.3 106		Ervens et al. (2003)
K091	$OXL + NO_3 (+ O_2)$	\rightarrow	$2CO_2 + NO_3 + H^+ + HO_2$	6.8 10 ⁷		
K092	$OXL^2 + NO_3 (+ O_2)$	\rightarrow	$2CO_2 + NO_3 + H^+ + O_2$	6.8 10 ⁷		Ervens et al. (2003)
K093	$OXL^{2-} + NO_3 (+ O_2)$	\rightarrow	$2CO_2 + NO_3 + O_2$	$2.2 \ 10^8$		Ervens et al. (2003)
	Iron chemistry		P ² +	4 5 4 08		E
K094 K095	$Fe^{(0+1)} + O_2$	\rightarrow	$Fe^{2+} + O_2$ $Fe^{2+} + O_2 + H_2O_2$	1.5 10° 1.3 10 ⁵		Ervens et al. (2003) Ervens et al. (2003)
K095	$[Fe(OH)]^{2+} + O_2^{-}$	\rightarrow	$Fe^{2+} + O_2 + HO^{-}$	1.510^{8}		Ervens et al. (2003)
K097	$Fe^{3+} + SO_4^{2-}$	\rightarrow	$[Fe(SO_4)]^+$	3.2 10 ³		Deguillaume et al. (2004)
K098	$[Fe(SO_4)]^+$	\rightarrow	$Fe^{3+} + SO_4^{2-}$	$2.7 \ 10^{1}$		Deguillaume et al. (2004)
K099	$[Fe(SO_4)]^+ + HO_2$	\rightarrow	$Fe^{2+} + SO_4^{2-} + O_2 + H^+$	1.0 105		Deguillaume et al. (2004)
K100	$[Fe(SO_4)]^+ + O_2^-$	\rightarrow	$Fe^{2+} + SO_4^{2-} + O_2$	1.5 108		Deguillaume et al. (2004)
K101	$Fe^{2+} + OH$	\rightarrow	$[Fe(OH)]^{2^{+}}$	4.3 10°	1100	Ervens et al. (2003)
K102 K103	$Fe^{2+} + HO_2(+H)$ $Fe^{2+} + O_2^{-}(+2H^+)$	\rightarrow	$Fe^{-4} + H_2O_2$ $Fe^{3+} + H_2O_2$	$1.2 \ 10^{-7}$	3030	Ervens et al. (2003) Ervens et al. (2003)
K105	$Fe^{2+} + H_2O_2$	\rightarrow	$Fe^{3+} + OH + HO^{-}$	5 0 10 ¹		Ervens et al. (2003)
K105	$Fe^{2+} + O_3$	\rightarrow	$FeO^{2+} + O_2$	8.2 105		Ervens et al. (2003)
K106	$Fe^{2+} + NO_2$	\rightarrow	$Fe^{3+} + NO_2^{-}$	3.1 104		Deguillaume et al. (2004)
K107	$Fe^{2+} + NO_3$	\rightarrow	$Fe^{3+} + NO_3^{-}$	8.0 106		Deguillaume et al. (2004)
K108	$Fe^{2^+} + CO_3^-$	\rightarrow	$Fe^{3+} + CO_3^{2-}$	2.7 10'		Ervens et al. (2003)
K109	$Fe^{2^{+}} + CH_3O_2$ $Fe^{-O^{2^{+}}} + OH(+H^{+})$	\rightarrow	Fe^{3+} + CH_3O_2H + HO^2	8.6 10 ⁹		Ervens et al. (2003)
K110 K111	$FeO^{2+} + HO_{2}$	\rightarrow	$Fe^{3+} + \Pi_2 O_2$ $Fe^{3+} + O_2 + HO^2$	2.0.106		Ervens et al. (2003) Ervens et al. (2003)
K112	$FeO^{2+} + H_2O_2$		$Fe^{3+} + HO_2 + HO^2$	$9.5 10^3$	2766	Ervens et al. (2003)
K113	$FeO^{2+} + H_2O$	\rightarrow	$Fe^{3+} + OH + HO$	2.34 10-4	4089	Ervens et al. (2003)
K114	$FeO^{2+} + Fe^{2+} (+ H_2O)$	\rightarrow	$2 \text{ Fe}^{3+} + 2 \text{ HO}^{-}$	$1.8 \ 10^4$	5052	Ervens et al. (2003)
K115	FeO ²⁺ + HONO	\rightarrow	$Fe^{3+} + NO_2 + HO^{-}$	1.1 104	4150	Ervens et al. (2003)
K116	$FeO^{2+} + NO_2 (+ H^+)$	\rightarrow	$Fe^{3+} + NO_2 + HO^{-}$	1.0 105	5252	Ervens et al. (2003)
K117 V119	$FeO^{2+} + CH_2(OH)_2 (+ O_2)$ $FeO^{2+} + HCOOH (+ O_2 + H^{+})$	\rightarrow	Fe^{3+} + HCOOH + HO ₂ + HO ⁻ Fe^{3+} + HO ₂ + CO ₂ + H O	4.0 10 ²	5352	Ervens et al. (2003)
K118 K110	$FeO^{2+} + HCOO^{-} (+O_2 + H^{-})$ $FeO^{2+} + HCOO^{-} (+O_2)$	\rightarrow	$Fe^{-7} + HO_2 + CO_2 + H_2O$ $Fe^{3+} + O_2^{-7} + CO_2 + HO^{-7}$	1.0 10 ⁵	2080	Ervens et al. (2003) Ervens et al. (2003)
K120	$Fe^{3+} + OXL^{2-}$	\rightarrow	$[Fe(OXL)]^+$	7.5 10		Ervens et al. (2003)
K121	[Fe(OXL)] ⁺	\rightarrow	$Fe^{3+} + OXL^{2-}$	3.0 10-3		Ervens et al. (2003)
K122	$[Fe(OXL)]^+ + OXL^2$	\rightarrow	[Fe(OXL) ₂] ⁻	$1.89 \ 10^4$		Ervens et al. (2003)
K123	[Fe(OXL) ₂]	\rightarrow	$[Fe(OXL)]^{+} + OXL^{2-}$	3.0 10-3		Ervens et al. (2003)
K124	$[Fe(OXL)]^+ + HO_2$	\rightarrow	$Fe(OXL) + O_2 + H^+$	1.2 105		Sedlak and Hoigné (1993)
K125	$[Fe(OXL)]^{+} + O_2^{-}$	\rightarrow	$Fe(OXL) + O_2$	1.0 10°		Sedlak and Hoigné (1993)

K126	$Fe(OXL) + H_2O_2$	\rightarrow	$[Fe(OXL)]^+ + OH + HO^-$	$3.1 10^4$	Sedlak and Hoigné (1993)
K127	$Fe^{2+} + OXL^{2-}$	\rightarrow	Fe(OXL)	3.67 10 ⁵	Sedlak and Hoigné (1993)
K128	Fe(OXL)	\rightarrow	$Fe^{2+} + OXL^{2-}$	3.0 10-3	as for K121 and K123

a) using the calculated gas-phase photolysis frequencies.

b) aqueous-phase photolysis rates at noontime scaled on model's H2O2 gas-phase photolysis frequencies.

c) representing large multifunctional compounds (see Carlton et al., 2007).

Table S3: Henry's law solubility constants (Η), mass accommodation coefficients (α) and gas phase diffusion coefficients (Dg) used in aqueous-phase chemistry scheme.

Trace gas	H (mol m ⁻³ Pa ⁻¹)	-ΔH R ⁻¹ (K)	Reference	α	Reference	$D_{g}(m^{2} s^{-1})$	Reference
O ₃	1.0 10 ⁻⁴	2800	1	0.05	2	1.48 10-5	2
H ₂ O ₂	9.1 10 ²	6600	1	0.11	2	1.46 10-5	2
HO ₂	6.8		1	0.01	2	1.04 10-5	2
OH	3.8 10-1		1	0.05	2	1.53 10-5	2
NO	1.9 10-5	1600	1	as for NO ₂	2	as for NO ₂	
NO ₂	9.9 10 ⁻⁵		1	0.0015	2	1.92 10-5	2
NO ₃	3.8 10-4		1	0.004	2	1.00 10-5	2
HONO	4.8 10 ⁻¹	4800	1	0.5	2	1.30 10-5	2
HNO ₃	8.8 10 ²		1	0.054	2	1.32 10-5	2
SO ₂	1.3 10-2	2900	1	0.035	2	1.28 10-5	2
CO ₂	3.3 10-4	2400	1	0.0002	2	1.55 10-5	2
CH ₃ O ₂	1.5 10-1	3700	1	as for CH ₃ O ₂ H	2	as for CH ₃ O ₂ H	2
CH ₃ O ₂ H	2.9	5200	1	0.0038	2	1.31 10-5	2
НСНО	3.2 10-1	6800	1	0.02	2	1.64 10-5	2
CH ₃ OH	2.0	5600	1	0.015	2	1.16 10-5	2
НСООН	8.8 10 ¹	6100	1	0.012	2	1.53 10-5	2
GLYAL	4.1 10 ²	4600	1	as for GLY		as for GLY	
GLY	$4.1\ 10^3$	7500	1	0.023	3	1.15 10-5	3
MGLY	3.4 10 ¹	7500	1	as for GLY		as for GLY	
HYAC	$7.7 \ 10^{1}$		1	0.0176	4	9.50 10-7	4
CH ₃ CHO	1.3 10-1	5900	1	0.03	2	1.22 10-5	2
CH ₃ CH ₂ OH	1.9	6400	1	0.0082	2	9.50 10-6	2
CH ₃ COOH	4.0 10 ¹	6200	1	0.019	3	1.24 10-5	2
PRV	3.1 10 ³	5100	1	as for CH ₃ COOH as for CH ₃ COOH			
GLX	$1.1 \ 10^2$	4800	1	as for CH ₃ COOH		as for CH ₃ COOH	
H ₂ OXL	3.1 104	7300	1	as for CH ₃ COOH		as for CH ₃ COOH	

1) Sander (2015) and references therein.

2) Herrmann et al. (2000) and references therein.

3) Lim et al. (2005) and references therein. 4) Ervens et al. (2003) and references therein

Table S4. Dissolution scheme for iron-containing combustion and mineral dust aerosols.

	Iron pool	Scheme ^g	K298 ^a	m ^b	Keq ^c	n ^d	Reference
D01	Combustion Fe ^e	H^+	5.24 10-8	0.36			Ito (2015)
D02		OXL	3.85 10-6	1			Ito (2015)
D03		hv^{f}	4.10 10-6	1			Ito (2015)
D04	Ferrihydrite	H^+	7.13 10-5	1.1	1550	3	Ito and Shi (2016)
D05		OXL	4.61 10-8	0.069	1550	3	Ito and Shi (2016)
D06		hv^{f}	4.61 10 ⁻⁸	0.069			Ito and Shi (2016)
D07	Nano-Fe oxides	H^+	1.43 10-4	1.6	42	2.75	Ito and Shi (2016)
D08		OXL	1.28 10 ⁻⁸	0.069	1550	3	Ito and Shi (2016)
D09		hv^{f}	1.28 10 ⁻⁸	0.069			Ito and Shi (2016)
D10	Aluminosilicates	H^{+}	5.85 10-8	0.76	3.3	2.85	Ito and Shi (2016)
D11		OXL	1.68 10 ⁻⁹	0.056	1500	3	Ito and Shi (2016)
D12		hv^{f}	1.68 10 ⁻⁹	0.056			Ito and Shi (2016)

The dissolution rate constants (K) for combustion and mineral dust aerosols are expressed in mol Fe g⁻¹ s⁻¹ and defined as:

 $K = K_{228} \cdot exp \left[E_{pH} \cdot (1/298 - 1/T) \right]$

b)

where, $E_{pH} = -1.56 \ 10^3 \ pH + 1.08 \ 10^4$ (Bibi et al., 2014; Ito and Shi, 2016) m is the reaction order (Ito, 2015; Ito and Shi, 2016) K_{eq} is the equilibrium constant (mol² kg⁻²) (Bonneville et al., 2004; Ito and Shi, 2016) c) d)

n is the stoichiometric ratio (Bonneville et al., 2004; Ito and Shi, 2016). e)

The unit for combustion aerosol is converted from moles m⁻² s⁻¹ to mol Fe g⁻¹ s⁻¹ (Ito, 2015) f)

Photoinduced dissolution rate constants are scaled on the model's H₂O₂ gas-phase photolysis frequencies. g)

For the proton-promoted dissolution, suppressions are taken into account when the solution becomes supersaturated with respect to Fe(III), but any suppression due to OXL is neglected (i.e., $0 \le f_i \le 1$ and $g_i = 1$). For oxalate-promoted dissolution, the formation of amorphous Fe(OH)₃(s) (Shi et al., 2009, 2015) is assumed to inhibit the adsorption of OXL and, thus, the Fe release from the minerals' surface (i.e., $0 \le f_i \le 1$ and $0 \le g_i \le 1$). For combustion aerosols, both the OXL-promoted and photo-induced dissolution rates are also considered to be suppressed by the formation of amorphous Fe(OH)₃(s) (Ito, 2015).

Table S5: Aqueous phase equilibrium constants (E_k) used in aqueous-phase chemistry scheme.

Equilibrium Reaction			Ek298 (mol L ⁻¹)	-ΔH R ⁻¹ (K)	Reference
H ₂ O	\leftrightarrow	$HO^{-} + H^{+}$	1.0 10 ⁻¹⁴	-6710	1
H ₂ O ₂	\leftrightarrow	$HO_{2}^{-} + H^{+}$	2.2 10-12	-3730	1
HO ₂	\leftrightarrow	$O_2^- + H^+$	3.5 10-5		1
$CO_2 (+ H_2O)$	\leftrightarrow	H ₂ CO ₄	7.7 10-7	-750	2
H ₂ CO ₄	\leftrightarrow	$HCO_3^- + H^+$	2.0 10-4		2
HCO3 ⁻	\leftrightarrow	$CO_3^{2-} + H^+$	4.69 10-11	-1820	2
NH4OH	\leftrightarrow	$NH_4^+ + HO^-$	1.7 10-5	-450	1
SO ₂ ·H ₂ O	\leftrightarrow	$HSO_3^- + H^+$	1.3 10-2	1960	1
HSO3 ⁻	\leftrightarrow	$SO_4^{2-} + H^+$	6.6 10-8	1500	1
HONO	\leftrightarrow	$NO_{2}^{-} + H^{+}$	5.1 10-4	-1260	1
HNO ₃	\leftrightarrow	$NO_{3}^{-} + H^{+}$	15.4	8700	1
НСООН	\leftrightarrow	$HCOO^{-} + H^{+}$	1.77 10-4	-12	3
CH3COOH	\leftrightarrow	$CH_3COO^- + H^+$	1.75 10-5	-46	3
PRV	\leftrightarrow	$PRV^{-} + H^{+}$	3.2 10-3		4
GLX	\leftrightarrow	$GLX^- + H^+$	3.47 10-4	-267	4
H ₂ OXL	\leftrightarrow	$HOXL^{-} + H^{+}$	5.6 10-2	-453	4
HOXL-	\leftrightarrow	$OXL^{=} + H^{+}$	5.42 10-5	-805	4
Fe^{3+} (+ H ₂ O)	\leftrightarrow	$[Fe(OH)]^{2+} + H^{+}$	1.1 10 ⁻⁴		3
$[Fe(OH)]^{2+}$ (+ H ₂ O)	\leftrightarrow	$[Fe(OH)_2]^+ + H^+$	1.4 10-7		3
1) Seinfeld and Pandis ((2006) and refe	rences therein			

Seinfeld and Pandis (2006) and references therein. Herrmann et al. (2000) and references therein.

2) 3)

Ervens et al. (2003) and references therein. 4)

Lim et al. (2005) and references therein.

Supplementary Equations

Mathematical formulas for correlation coefficient (R; Eq. S1), normalized mean bias (nMB; Eq. S2), and the normalized root mean square error (nRMSE; Eq. S3), used for the statistical analysis of model comparison against observations; O_i and P_i stand for observations and predictions, respectively. N is the number of pairs (observations, predictions) that are compared.

$$R = \left[\frac{\frac{1}{N}\sum_{i=1}^{N} (O_i - \overline{O})(P_i - \overline{P})}{\sigma_o \sigma_P}\right]$$
(Eq. S1)

$$NMB = \frac{\sum_{i=1}^{N} (M_i - O_i)}{\sum_{i=1}^{N} O_i} \times 100$$
(Eq. S2)

$$nRMSE = \frac{\sqrt{\frac{1}{N}\sum_{i=1}^{N} (P_i - O_i)^2}}{\sum_{i=1}^{N} O_i}$$
(Eq. S3)

Supplementary Figures



Figure S1: Annual mean zonal mean concentrations of a) OH radicals $(10^6 \text{ molec. cm}^{-3})$, c) glyoxal (ppt), e) glycolaldehyde (ppt), g) methylglyoxal (ppt), and i) acetic acid (ppt), as simulated for the EC-Earth simulation, averaged for the period 2000-2014, and the absolute differences to the ERA-Interim simulation (b,d,f,h,j).



Figure S2: Annual mean of a) zonal mean concentrations of cloud water (g m⁻³), c) surface concentrations of aerosol water associated with accumulation aerosols (μ g m⁻³), and e) surface concentrations of aerosol water associated with coarse aerosols (μ g m⁻³), as simulated for the EC-Earth simulation, averaged for the period 2000-2014, and the respective absolute differences to the ERA-Interim simulation (b,d,f).



Figure S3: Annual mean a) vertical-column-integrated (VCI) liquid-water-weighted cloud water pH, c) accumulation aerosol pH at the surface, e) and coarse aerosol pH at the surface, as calculated for the EC-Earth simulation, averaged for the period 2000-2014, and the respective absolute differences to the ERA-Interim simulation (b,d,f).



Figure S4: Annual mean emission fluxes (mg m⁻² yr⁻¹) of a) DMS, c) sea salt, e) mineral dust, and g) calcite (in mg Ca m⁻² yr⁻¹), as calculated for the EC-Earth simulation, averaged for the period 2000-2014, and the respective absolute differences to the ERA-Interim simulation (b,d,f,h).



Figure S5: Scatterplot comparisons of cruise observations (see text) for accumulation aerosols (top), coarse aerosols (middle), and total suspended matter (bottom) of dissolved iron (DFe; a,d,g), total iron (TFe; b,e,h) aerosols (ng m⁻³) and the derived aerosol solubility (SFe=%DFe/TFe; c,f,i) of EC-Earth (orange circles) and ERA-Interim (light blue triangles) simulations; the solid line represents the 1 : 1 correspondence and the dashed lines show the 10 : 1 and 1 : 10 relationships, respectively. The color-coded error bars represent the model's standard error of the multi-annual mean for the individual observational period. Summary statistics (color-coded) for all points are also included.



Figure S6: Observed total iron (TFe) concentrations (ng m⁻³) of a) accumulation aerosols, b) coarse aerosols, and c) total suspended particles (tsp), the respective absolute differences to the ERA-Interim simulation (d,e,f), and the comparison to observations (black x-line) in latitudinal order (g,e,f) with the EC-Earth (orange circle-line) and ERA-Interim (light blue triangle-line) simulations; the grey shaded areas correspond to the standard deviation of the observations and the color-coded error bars/shaded areas correspond to the model's standard error of the multi-annual mean for the individual observational period.

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