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*Supplement of*

## **Global modeling of SOA: the use of different mechanisms for aqueous-phase formation**

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Table S1. Abbreviations listed in the chemical mechanism tables below.

Species number	Abbreviation	Species name
1	GLYC	Glycolaldehyde
2	GLYX	Glyoxal
3	MGLY	Methylglyoxal
4	GLYAC	Glyoxylic acid
5	OXLAC	Oxalic acid
6	PRV	Pyruvic acid
7	GLYX_MH	Glyoxal monohydrate
8	GLYX_DH	Glyoxal dihydrate
9	MGLY_MH	Methylglyoxal monohydrate
10	MGLY_DH	Methylglyoxal dihydrate
11	GLYOLI	Oligomers from glyoxal
12	MGLOLI	Oligomers from methylglyoxal
13	C4D	C <sub>4</sub> dimer
14	TA	Tartaric acid
15	C3D	C <sub>3</sub> dimer
16	MA	Malonic acid

Table S2. Non-organic chemistry used in the model.

Reaction Number	Aqueous phase Reactions	$K_{298}$ ( $M^n s^{-1}$ )	E/R (K)	References
1	$H_2O_2 + hv \Rightarrow 2OH$	Using the gas phase photolysis rate, increased by a factor of 1.5		Barth et al. (2003)
2	$H_2O_2 + OH \Rightarrow HO_2 + H_2O$	$2.7E+07$		Lim et al. (2005)
3	$H_2O_2 + HO_2 \Rightarrow OH + H_2O$	$3.7E+00$		Tan et al. (2009)
4	$HO_2 + HO_2 \Rightarrow H_2O_2 + O_2$	$9.7E+05$	2500	Lim et al. (2005)
5	$OH + HO_2 \Rightarrow H_2O + O_2$	$7.1E+09$		Lim et al. (2005)
6	$O_3 + hv \Rightarrow H_2O_2$	Using the gas phase photolysis rate, increased by a factor of 1.5		Barth et al. (2003)
7	$OH + O_3 \Rightarrow HO_2$	$2.0E+09$		Pandis and Seinfeld (1989)
8	$HO_2 + O_3 \Rightarrow OH$	$1.0E+04$		Pandis and Seinfeld (1989)
9	$O_2^- + O_3 \Rightarrow OH + OH^-$	$1.5E+09$	1500	Pandis and Seinfeld (1989)
10	$OH^- + O_3 \Rightarrow O_2^- + HO_2$	$7.0E+01$		Pandis and Seinfeld (1989)
11	$HO_2^- + O_3 \Rightarrow OH + O_2^-$	$2.8E+06$		Pandis and Seinfeld (1989)
12	$NO + NO_2 \Rightarrow 2NO_2^- + 2H^+$	$2.0E+08$	1500	Pandis and Seinfeld (1989)

13	$\text{NO}_2 + \text{NO}_2 \Rightarrow \text{NO}_2^- + \text{NO}_3^- + 2\text{H}^+$	1.0E+08	1500	Pandis and Seinfeld (1989)
14	$\text{NO} + \text{OH} \Rightarrow \text{NO}_2^- + \text{H}^+$	2.0E+10	1500	Pandis and Seinfeld (1989)
15	$\text{NO}_2 + \text{OH} \Rightarrow \text{NO}_3^- + \text{H}^+$	1.3E+09	1500	Pandis and Seinfeld (1989)
16	$\text{HONO} + \text{h}\nu \Rightarrow \text{NO} + \text{OH}$	Using the gas phase photolysis rate, increased by a factor of 1.5		Pandis and Seinfeld (1989)
17	$\text{HNO}_2^- + \text{h}\nu \Rightarrow \text{NO} + \text{OH}$	Using the gas phase photolysis rate, increased by a factor of 1.5		Barth et al. (2003)
18	$\text{HONO} + \text{OH} \Rightarrow \text{NO}_2$	1.0E+09	1500	Pandis and Seinfeld (1989)
19	$\text{NO}_2^- + \text{OH} \Rightarrow \text{NO}_2 + \text{OH}^-$	1.0E+10	1500	Pandis and Seinfeld (1989)
20	$\text{NO}_2^- + \text{O}_3 \Rightarrow \text{NO}_3^-$	5.0E+05	6950	Pandis and Seinfeld (1989)
21	$\text{NO}_2^- + \text{CO}_3^{2-} \Rightarrow \text{NO}_2 + \text{CO}_3^{2-}$	4.0E+05	0.	Pandis and Seinfeld (1989)
22	$\text{NO}_2^- + \text{NO}_3 \Rightarrow \text{NO}_2 + \text{NO}_3^-$	1.2E+09	1500	Pandis and Seinfeld (1989)
23	$\text{NO}_3^- + \text{h}\nu \Rightarrow \text{NO}_2 + \text{OH} + \text{OH}^-$	Using the same as gas-phase $\text{HNO}_3$ photolysis, increased a factor of 1.5		Barth et al. (2003)
24	$\text{NO}_3 + \text{h}\nu \Rightarrow \text{NO} + \text{O}_2$	Using the gas phase photolysis rate, increased by a factor of 1.5		Barth et al. (2003)
25	$\text{NO}_3 + \text{HO}_2 \Rightarrow \text{NO}_3^- + \text{H}^+$	1.2E+09	1500	Jacob (1989)
26	$\text{NO}_3 + \text{O}_2^- \Rightarrow \text{NO}_3^-$	1.0E+09	1500	Jacob (1989)

27	$\text{NO}_3^- + \text{H}_2\text{O}_2 \Rightarrow \text{NO}_3^- + \text{HO}_2 + \text{H}^+$	1.0E+06	2800	Pandis and Seinfeld (1989)
28	$\text{HO}_2 + \text{O}_2^- \Rightarrow \text{H}_2\text{O}_2 + \text{OH}^-$	1.0E+08	1500	Pandis and Seinfeld (1989)
29	$\text{SO}_2 + \text{O}_3 \Rightarrow \text{H}_2\text{SO}_4$	2.4E+04		Pandis and Seinfeld (1989)
30	$\text{HSO}_3^- + \text{O}_3 \Rightarrow \text{HSO}_4^-$	3.7E+05	5530	Pandis and Seinfeld (1989)
31	$\text{SO}_3^{-2} + \text{O}_3 \Rightarrow \text{SO}_4^{-2}$	1.5E+09	5280	Pandis and Seinfeld (1989)
32	$\text{SO}_2 + \text{H}_2\text{O}_2 \Rightarrow \text{H}_2\text{SO}_4$	1.3E+06	4430	Pandis and Seinfeld (1989)
33	$\text{HSO}_3^- + \text{H}_2\text{O}_2 \Rightarrow \text{HSO}_4^-$	5.2E+06	3650	Pandis and Seinfeld (1989)
34	$\text{SO}_3^{-2} + \text{H}_2\text{O}_2 \Rightarrow \text{SO}_4^{-2}$	5.2E+06	3650	Pandis and Seinfeld (1989)
35	$\text{SO}_3^{-2} + \text{OH}^- \Rightarrow \text{SO}_5^- + \text{OH}^-$	4.6E+09	1500	Pandis and Seinfeld (1989)
36	$\text{HSO}_3^- + \text{OH}^- \Rightarrow \text{SO}_5^-$	4.2E+09	1500	Pandis and Seinfeld (1989)
37	$\text{SO}_5^- + \text{HSO}_3^- \Rightarrow \text{SO}_5^- + \text{HSO}_5^-$	3.0E+05	3100	Pandis and Seinfeld (1989)
38	$\text{SO}_5^- + \text{SO}_3^{-2} \Rightarrow \text{SO}_4^{-2} + \text{SO}_4^-$	1.3E+07	2000	Jacob (1989)
39	$\text{SO}_5^- + \text{O}_2^- \Rightarrow \text{HSO}_5^- + \text{OH}^-$	1.0E+08	1500	Jacob (1989)
40	$\text{SO}_5^- + \text{HCOOH} \Rightarrow \text{HSO}_5^- + \text{CO}_2 + \text{HO}_2$	2.0E+02	5300	Jacob (1989)

41	$\text{SO}_5^- + \text{HCOO}^- \Rightarrow \text{HSO}_5^- + \text{CO}_2 + \text{O}_2^-$	1.4E+04	4000	Jacob (1989)
42	$\text{SO}_5^- + \text{SO}_5^- \Rightarrow 2\text{SO}_4^-$	2.0E+08	1500	Jacob (1989)
43	$\text{HSO}_5^- + \text{OH}^- \Rightarrow \text{SO}_5^-$	1.7E+07	1900	Jacob (1989)
44	$\text{HSO}_5^- + \text{SO}_4^{2-} \Rightarrow \text{SO}_5^- + \text{SO}_4^- + \text{H}^+$	1.0E+05	0.	Jacob (1989)
45	$\text{HSO}_5^- + \text{NO}_2^- \Rightarrow \text{HSO}_4^- + \text{NO}_3^-$	3.1E-01	6650	Jacob (1989)
46	$\text{SO}_4^- + \text{HSO}_3^- \Rightarrow \text{SO}_5^- + \text{SO}_4^{2-} + \text{H}^+$	1.3E+09	1500	Jacob (1989)
47	$\text{SO}_4^- + \text{SO}_3^{2-} \Rightarrow \text{SO}_5^- + \text{SO}_4^{2-}$	5.3E+08	1500	Jacob (1989)
48	$\text{SO}_4^- + \text{HO}_2 \Rightarrow \text{SO}_4^{2-} + \text{H}^+$	5.0E+09	1500	Jacob (1989)
49	$\text{SO}_4^- + \text{O}_2^- \Rightarrow \text{SO}_4^{2-}$	5.0E+09	1500	Jacob (1989)
50	$\text{SO}_4^- + \text{OH}^- \Rightarrow \text{SO}_4^{2-} + \text{OH}^-$	8.0E+07	1500	Jacob (1989)
51	$\text{SO}_4^- + \text{H}_2\text{O}_2 \Rightarrow \text{SO}_4^{2-} + \text{HO}_2 + \text{H}^+$	1.2E+07	2000	Pandis and Seinfeld (1989)
52	$\text{SO}_4^- + \text{NO}_2^- \Rightarrow \text{SO}_4^{2-} + \text{NO}_2$	8.8E+08	1500	Jacob (1989)
53	$\text{SO}_4^- + \text{HCO}_3^- \Rightarrow \text{SO}_4^{2-} + \text{CO}_3^{2-} + \text{H}^+$	9.1E+06	2100	Pandis and Seinfeld (1989)
54	$\text{SO}_4^- + \text{HCOO}^- \Rightarrow \text{SO}_4^{2-} + \text{CO}_2 + \text{HO}_2$	1.7E+08	1500	Jacob (1989)
55	$\text{SO}_4^- + \text{HCOOH} \Rightarrow \text{SO}_4^{2-} + \text{CO}_2 + \text{HO}_2 + \text{H}^+$	1.4E+06	2700	Jacob (1989)
56	$\text{SO}_2 + \text{HO}_2 \Rightarrow \text{H}_2\text{SO}_4 + \text{OH}^-$	1.0E+06	0.	Pandis and Seinfeld (1989)
57	$\text{SO}_4^- + \text{CH}_3\text{OH} \Rightarrow \text{SO}_4^{2-} + \text{HCHO} + \text{HO}_2 + \text{H}^+$	2.5E+07	1800	Pandis and Seinfeld (1989)

Table S3. Organic chemistry used in cloud and aerosol water to predict carboxylic acids in Case 1

Reaction Number	Aqueous phase Reactions	$K_{298}$ ( $M^n s^{-1}$ )	E/R (K)	References
1	$GLYX + OH \Rightarrow GLYAC + HO_2$	1.1E+09	1564	Lim et al. (2005)
2	$GLYAC + OH \Rightarrow OXLAC + H_2O$	3.62E+08	962	Herrmann (2003)
3	$GLYAC^- + OH \Rightarrow OXLAC^- + H_2O$	2.8E+09	4330	Herrmann (2003)
4	$OXLAC + OH \Rightarrow 2CO_2 + 2H_2O$	1.4E+06		Lim et al. (2005)
5	$OXLAC^- + OH (+ O_2) \Rightarrow 2CO_2 + H_2O (+ O_2^-)$	4.7E+07		Lim et al. (2005)
6	$OXLAC^{2-} + OH (+ O_2) \Rightarrow 2CO_2 + OH^- (+ O_2^-)$	7.7E+06		Lim et al. (2005)
7	$H_2C(OH)_2 + OH \Rightarrow HCOOH + HO_2$	2.0E+09	1500	Pandis and Seinfeld (1989)
8	$HCOO^- + NO_3 \Rightarrow NO_3^- + CO_2 + HO_2$	6.0E+07	1500	Jacob (1989)
9	$HCOOH + O_3 \Rightarrow CO_2 + HO_2 + OH$	5.0E+00	0	Pandis and Seinfeld (1989)
10	$HCOO^- + O_3 \Rightarrow CO_2 + OH + O_2^-$	1.0E+02	0	Pandis and Seinfeld (1989)
11	$HCOO^- + CO_3^- \Rightarrow CO_2 + HCO_3^- + HO_2 + OH^-$	1.1E+05	3400	Pandis and Seinfeld (1989)
12	$CH_3O_2 + HO_2 \Rightarrow CH_3OOH$	4.3E+05	3000	Jacob (1989)
13	$CH_3O_2 + O_2^- \Rightarrow CH_3OOH + OH^-$	5.0E+07	1600	Jacob (1989)
14	$CH_3OOH + h\nu \Rightarrow HCHO + OH + HO_2$	5.0E-4*j <sub>NO2</sub>		Pandis and Seinfeld (1989)
15	$CH_3OOH + OH \Rightarrow CH_3O_2$	2.7E+07	1700	Jacob (1989)
16	$CH_3OH + OH \Rightarrow HCHO + HO_2$	4.5E+06	1500	Pandis and Seinfeld (1989)
17	$CH_3OH + CO_3^- \Rightarrow HCHO + HO_2 + HCO_3^-$	2.6E+03	4500	Pandis and Seinfeld (1989)
18	$CH_3OOH + OH \Rightarrow HCHO + OH$	1.9E+07	1800	Jacob (1989)

19	$\text{CH}_3\text{OH} + \text{NO}_3 \Rightarrow \text{NO}_3^- + \text{H}^+ + \text{HCHO} + \text{HO}_2$	1.0E+06	2800	Pandis and Seinfeld (1989)
20	$\text{MGLY} + \text{OH} \Rightarrow 0.92 \text{ PRV} + 0.08 \text{ GLYAC} + \text{H}_2\text{O} + \text{HO}_2$	1.1E+09	1600	Ervens et al. (2004)
21	$\text{PRV} + \text{OH} \Rightarrow \text{CH}_3\text{C(O)OH} + \text{HO}_2 + \text{CO}_2$	1.2E+08	2766	Lim et al. (2005)
22	$\text{PRV}^- + \text{OH} \Rightarrow \text{CH}_3\text{COO}^- + \text{HO}_2 + \text{CO}_2$	7.0E+08	2285	Lim et al. (2005)
23	$\text{CH}_3\text{COO}^- + \text{OH} \Rightarrow 0.85\text{GLYAC}^- + 0.15 \text{CH}_2(\text{OH})_2$	1.9E+09	1800	Lim et al. (2005)
24	$\text{CH}_3\text{COOH} + \text{OH} \Rightarrow 0.85\text{GLYAC} + 0.15 \text{CH}_2(\text{OH})_2$	1.5E+07	1800	Lim et al. (2005)
25	$\text{GLYC} + \text{OH} \Rightarrow \text{GLYX} + \text{HO}_2$	1.0E+09	1564	Lim et al. (2005)
26	$\text{GLYC} + \text{OH} \Rightarrow \text{GLYAC} + 2\text{HO}_2$	5.0E+08	1564	Lim et al. (2005)
27	$\text{GLYC} + \text{NO}_3 \Rightarrow \text{GLYAC} + \text{HO}_2 + \text{NO}_3^- + \text{H}^+$	1.1E+07		Herrmann et al. (2005)*
28	$\text{GLYC} + \text{NO}_3 \Rightarrow \text{GLYX} + \text{NO}_3^- + \text{H}_2\text{O} + \text{H}^+$	5.5E+06		Herrmann (2003)
29	$\text{GLYX} + \text{NO}_3 \Rightarrow \text{GLYAC} + \text{NO}_3^- + \text{HO}_2 + \text{H}^+$	6.3E+07		The same as for MGLY+NO3
30	$\text{MGLY} + \text{NO}_3 \Rightarrow 0.92 \text{ PRV} + 0.08 \text{ GLYAC} + \text{NO}_3^- + \text{HO}_2 + \text{H}^+$	6.3E+07		Herrmann et al. (2005)*
31	$\text{PRV} + \text{NO}_3 \Rightarrow \text{CH}_3\text{COOH} + \text{HO}_2 + \text{CO}_2 + \text{NO}_3^- + \text{H}^+$	4.8E+06		Herrmann et al. (2005)*
32	$\text{PRV}^- + \text{NO}_3 \Rightarrow \text{CH}_3\text{COO}^- + \text{HO}_2 + \text{CO}_2 + \text{NO}_3^- + \text{H}^+$	4.8E+06		Herrmann et al. (2005)*
33	$\text{GLYAC} + \text{NO}_3 \Rightarrow \text{OXLAC} + \text{HO}_2 + \text{NO}_3^- + \text{H}^+$	3.0E+06		The same as glycolic acid from Herrmann et al. (2005)
34	$\text{GLYAC}^- + \text{NO}_3 \Rightarrow \text{OXLAC}^- + \text{HO}_2 + \text{NO}_3^- + \text{H}^+$	1.1E+08		The same as glycolic acid from Herrmann et al. (2005)
35	$\text{OXLAC} + \text{NO}_3 \Rightarrow 2\text{CO}_2 + \text{NO}_3^- + \text{H}^+$	6.8E+07		The same as OXLAC + NO3
36	$\text{OXLAC}^- + \text{NO}_3 (+ \text{O}_2) \Rightarrow 2\text{CO}_2 + \text{NO}_3^- + \text{H}^+ (+\text{O}_2^-)$	6.8E+07		Herrmann et al. (2000)*



37	$\text{OXLAC}^{2-} + \text{NO}_3 (+ \text{O}_2) \Rightarrow 2\text{CO}_2 + \text{NO}_3^- (+ \text{O}_2^-)$	2.2E+08		Herrmann et al. (2000)*
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\* assuming the same products as the reaction with OH

Table S4. Organic chemistry in aerosol water adopted from Ervens and Volkamer (2010)

Reaction Number	Aqueous phase Reactions	$K_{298} (\text{M}^n \text{s}^{-1})$	E/R (K)	References
1	$\text{GLYX} (+ \text{H}_2\text{O}) \Rightarrow \text{GLYX\_MH}$	7		Creighton et al. (1988)
2	$\text{GLYX\_MH} \Rightarrow \text{GLYX}$	2.0E-02		Creighton et al. (1988)
3	$\text{GLYX\_MH} (+ \text{H}_2\text{O}) \Rightarrow \text{GLYX\_DH}$	4.0		Ervens and Volkamer (2010)
4	$\text{GLYX\_DH} \Rightarrow \text{GLYX\_MH}$	2.0E-02		Ervens and Volkamer (2010)
5	$\text{GLYX} + \text{GLYX\_MH} \Rightarrow \text{GLYOLI}$	1.0E+02		Ervens and Volkamer (2010)
6	$\text{GLYOLI} \Rightarrow \text{GLYX} + \text{GLYX\_MH}$	5.556		Ervens and Volkamer (2010)
7	$\text{GLYX\_MH} + \text{GLYX\_MH} \Rightarrow \text{GLYOLI}$	1.0E+02		Ervens and Volkamer (2010)
8	$\text{GLYOLI} \Rightarrow \text{GLYX\_MH} + \text{GLYX\_MH}$	5.556		Ervens and Volkamer (2010)
9	$\text{GLYX\_DH} + \text{GLYX\_MH} \Rightarrow \text{GLYOLI}$	1.0E+02		Ervens and Volkamer (2010)
10	$\text{GLYOLI} \Rightarrow \text{GLYX\_DH} + \text{GLYX\_MH}$	5.556		Ervens and Volkamer (2010)
11	$\text{GLYX\_DH} \Rightarrow \text{GLYOLI}$	$0.8 \text{ s}^{-1} < k < 7 \text{ s}^{-1}$		k scales with OH concentration with highest value at $[\text{OH}] = 10^7 \text{ cm}^{-3}$ (Ervens and Volkamer, (2010))

12	GLYX_MH=>GLYOLI	$0.8 \text{ s}^{-1} < k < 7 \text{ s}^{-1}$		k scales with OH concentration with highest value at $[\text{OH}] = 10^7 \text{ cm}^{-3}$ (Ervens and Volkamer, (2010))
13	GLYX =>GLYOLI	$0.8 \text{ s}^{-1} < k < 7 \text{ s}^{-1}$		k scales with OH concentration with highest value at $[\text{OH}] = 10^7 \text{ cm}^{-3}$ (Ervens and Volkamer, (2010))
14	MGLY+ H2O => MGLY_MH	1.1E+01		Creighton et al. (1988)
15	MGLY_MH => MGLY	2.0E-02		Creighton et al. (1988)
16	MGLY_MH => MGLY_DH	9.6E-02		
17	MGLY_DH => MGLY_MH	2.0E-02		Assumed the same as monohydrate
18	MGLY +MGLY_MH => MGLOLI	1.0E+02		Assumed the same as glyoxal
19	MGLOLI => MGLY_MH + MGLY	5.556E0		Assumed the same as glyoxal
20	MGLY_MH + MGLY_MH => MGLOLI	1.0E+02		Assumed the same as glyoxal
21	MGLOLI => MGLY_MH + MGLY_MH	5.556E0		Assumed the same as glyoxal
22	MGLY_DH + MGLY_MH => MGLOLI	1.0E+02		Assumed the same as glyoxal
23	MGLOLI => MGLY_MH + MGLY_DH	5.556E0		Assumed the same as glyoxal
24	MGLY_DH => MGLOLI	4.0		Ervens et al. (2011)
25	MGLY_MH => MGLOLI	4.0		Ervens et al. (2011)
26	MGLY => MGLOLI	4.0		Ervens et al. (2011)
27	GLYX + OH=> GLYAC+HO <sub>2</sub>	1.1E+09	1564	Lim et al. (2005)
28	GLYX_MH + OH=> GLYAC+HO <sub>2</sub>	1.1E+09	1564	Lim et al. (2005)
29	GLYX_DH + OH=> GLYAC+HO <sub>2</sub>	1.1E+09	1564	Lim et al. (2005)

30	$\text{GLYAC} + \text{OH} \Rightarrow \text{OXLAC} + \text{H}_2\text{O}$	3.62E+08	962	Herrmann (2003)
31	$\text{GLYAC}^- + \text{OH} \Rightarrow \text{OXLAC}^- + \text{H}_2\text{O}$	2.8E+09	4330	Herrmann (2003)
32	$\text{OXLAC} + \text{OH} \Rightarrow 2\text{CO}_2 + 2\text{H}_2\text{O}$	1.4E+06		Lim et al. (2005)
33	$\text{OXLAC}^- + \text{OH} (+ \text{O}_2) \Rightarrow 2\text{CO}_2 + \text{H}_2\text{O} (+ \text{O}_2^-)$	4.7E+07		Lim et al. (2005)
34	$\text{OXLAC}^{2-} + \text{OH} (+ \text{O}_2) \Rightarrow 2\text{CO}_2 + \text{OH}^- (+ \text{O}_2^-)$	7.7E+06		Lim et al. (2005)
35	$\text{H}_2\text{C}(\text{OH})_2 + \text{OH} \Rightarrow \text{HCOOH} + \text{HO}_2$	2.0E+09	1500	Pandis and Seinfeld (1989)
36	$\text{HCOO}^- + \text{NO}_3 \Rightarrow \text{NO}_3^- + \text{CO}_2 + \text{HO}_2$	6.0E+07	1500	Jacob (1989)
37	$\text{HCOOH} + \text{O}_3 \Rightarrow \text{CO}_2 + \text{HO}_2 + \text{OH}$	5.0E+00	0	Pandis and Seinfeld (1989)
38	$\text{HCOO}^- + \text{O}_3 \Rightarrow \text{CO}_2 + \text{OH} + \text{O}_2^-$	1.0E+02	0	Pandis and Seinfeld (1989)
39	$\text{HCOO}^- + \text{CO}_3^- \Rightarrow \text{CO}_2 + \text{HCO}_3^- + \text{HO}_2 + \text{OH}^-$	1.1E+05	3400	Pandis and Seinfeld (1989)
40	$\text{CH}_3\text{O}_2 + \text{HO}_2 \Rightarrow \text{CH}_3\text{OOH}$	4.3E+05	3000	Jacob (1989)
41	$\text{CH}_3\text{O}_2 + \text{O}_2^- \Rightarrow \text{CH}_3\text{OOH} + \text{OH}^-$	5.0E+07	1600	Jacob (1989)
42	$\text{CH}_3\text{OOH} + h\nu \Rightarrow \text{HCHO} + \text{OH} + \text{HO}_2$	5.0E-4*j <sub>NO2</sub>		Pandis and Seinfeld (1989)
43	$\text{CH}_3\text{OOH} + \text{OH} \Rightarrow \text{CH}_3\text{O}_2$	2.7E+07	1700	Jacob (1989)
44	$\text{CH}_3\text{OH} + \text{OH} \Rightarrow \text{HCHO} + \text{HO}_2$	4.5E+06	1500	Pandis and Seinfeld (1989)
45	$\text{CH}_3\text{OH} + \text{CO}_3^- \Rightarrow \text{HCHO} + \text{HO}_2 + \text{HCO}_3^-$	2.6E+03	4500	Pandis and Seinfeld (1989)
46	$\text{CH}_3\text{OOH} + \text{OH} \Rightarrow \text{HCHO} + \text{OH}$	1.9E+07	1800	Jacob (1989)
47	$\text{CH}_3\text{OH} + \text{NO}_3 \Rightarrow \text{NO}_3^- + \text{H}^+ + \text{HCHO} + \text{HO}_2$	1.0E+06	2800	Pandis and Seinfeld (1989)
48	$\text{MGLY} + \text{OH} \Rightarrow 0.92 \text{ PRV} + 0.08 \text{ GLYAC} + \text{H}_2\text{O} + \text{HO}_2$	1.1E+09	1600	Ervens et al. (2004)
49	$\text{MGLY\_MH} + \text{OH} \Rightarrow 0.92 \text{ PRV} + 0.08 \text{ GLYAC} + \text{H}_2\text{O} + \text{HO}_2$	1.1E+09	1600	Ervens et al. (2004)

50	$\text{MGLY\_DH} + \text{OH} \Rightarrow 0.92 \text{ PRV} + 0.08 \text{ GLYAC} + \text{H}_2\text{O} + \text{HO}_2$	1.1E+09	1600	Ervens et al. (2004)
51	$\text{PRV} + \text{OH} \Rightarrow \text{CH}_3\text{C(O)OH} + \text{HO}_2 + \text{CO}_2$	1.2E+08	2766	Lim et al. (2005)
52	$\text{PRV}^- + \text{OH} \Rightarrow \text{CH}_3\text{COO}^- + \text{HO}_2 + \text{CO}_2$	7.0E+08	2285	Lim et al. (2005)
53	$\text{CH}_3\text{COO}^- + \text{OH} \Rightarrow 0.85 \text{ GLYAC}^- + 0.15 \text{ CH}_2(\text{OH})_2$	1.9E+09	1800	Lim et al. (2005)
54	$\text{CH}_3\text{COOH} + \text{OH} \Rightarrow 0.85 \text{ GLYAC} + 0.15 \text{ CH}_2(\text{OH})_2$	1.5E+07	1800	Lim et al. (2005)
55	$\text{GLYC} + \text{OH} \Rightarrow \text{GLYX} + \text{HO}_2$	1.0E+09	1564	Lim et al. (2005)
56	$\text{GLYC} + \text{OH} \Rightarrow \text{GLYAC} + 2\text{HO}_2$	5.0E+08	1564	Lim et al. (2005)
57	$\text{GLYC} + \text{NO}_3 \Rightarrow \text{GLYAC} + \text{HO}_2 + \text{NO}_3^- + \text{H}^+$	1.1E+07		Herrmann et al. (2005)
58	$\text{GLYC} + \text{NO}_3 \Rightarrow \text{GLYX} + \text{NO}_3^- + \text{H}_2\text{O} + \text{H}^+$	5.5E+06		Herrmann (2003)
59	$\text{GLYX} + \text{NO}_3 \Rightarrow \text{GLYAC} + \text{NO}_3^- + \text{HO}_2 + \text{H}^+$	6.3E+07		The same as for MGLY+NO3
60	$\text{GLYX\_MH} + \text{NO}_3 \Rightarrow \text{GLYAC} + \text{NO}_3^- + \text{HO}_2 + \text{H}^+$	6.3E+07		The same as for MGLY+NO3
61	$\text{GLYX\_MH} + \text{NO}_3 \Rightarrow \text{GLYAC} + \text{NO}_3^- + \text{HO}_2 + \text{H}^+$	6.3E+07		The same as for MGLY+NO3
62	$\text{MGLY} + \text{NO}_3 \Rightarrow 0.92 \text{ PRV} + 0.08 \text{ GLYAC} + \text{NO}_3^- + \text{HO}_2 + \text{H}^+$	6.3E+07		Herrmann et al. (2005)
63	$\text{MGLY\_MH} + \text{NO}_3 \Rightarrow 0.92 \text{ PRV} + 0.08 \text{ GLYAC} + \text{NO}_3^- + \text{HO}_2 + \text{H}^+$	6.3E+07		Herrmann et al. (2005)
64	$\text{MGLY\_DH} + \text{NO}_3 \Rightarrow 0.92 \text{ PRV} + 0.08 \text{ GLYAC} + \text{NO}_3^- + \text{HO}_2 + \text{H}^+$	6.3E+07		Herrmann et al. (2005)
65	$\text{PRV} + \text{NO}_3 \Rightarrow \text{CH}_3\text{COOH} + \text{HO}_2 + \text{CO}_2 + \text{NO}_3^- + \text{H}^+$	4.8E+06		Herrmann et al. (2005)
66	$\text{PRV}^- + \text{NO}_3 \Rightarrow \text{CH}_3\text{COO}^- + \text{HO}_2 + \text{CO}_2 + \text{NO}_3^- + \text{H}^+$	4.8E+06		Herrmann et al. (2005)
67	$\text{GLYAC} + \text{NO}_3 \Rightarrow \text{OXLAC} + \text{HO}_2 + \text{NO}_3^- + \text{H}^+$	3.0E+06		The same as glyxolic acid from Herrmann et al. (2005)

68	$\text{GLYAC}^- + \text{NO}_3 \Rightarrow \text{OXLAC}^- + \text{HO}_2 + \text{NO}_3^- + \text{H}^+$	1.1E+08		The same as glyxolic acid from Herrmann et al. (2005)
69	$\text{OXLAC} + \text{NO}_3 \Rightarrow 2\text{CO}_2 + \text{NO}_3^- + \text{H}^+$	6.8E+07		The same as OXLAC <sup>-</sup> + NO <sub>3</sub>
70	$\text{OXLAC}^- + \text{NO}_3 (+ \text{O}_2) \Rightarrow 2\text{CO}_2 + \text{NO}_3^- + \text{H}^+ (+ \text{O}_2^-)$	6.8E+07		Herrmann et al. (2000)
71	$\text{OXLAC}^{2-} + \text{NO}_3 (+ \text{O}_2) \Rightarrow 2\text{CO}_2 + \text{NO}_3^- (+ \text{O}_2^-)$	2.2E+08		Herrmann et al. (2000)

Table S5. Organic chemistry in cloud water and aerosol water adopted from Lim et al. (2010) which is used in Case 3

Reaction Number	Aqueous phase Reactions	$K_{298} (\text{M}^n \text{s}^{-1})$	E/R (K)	References
1	$\text{GLYX} + \text{OH} \Rightarrow \text{GLYXr}^* + \text{H}_2\text{O}$	1.1E+09	1564	Tan et al. (2009)
2	$\text{GLYXr} + \text{O}_2 \Rightarrow \text{GLYXOOr}$	1.0E+06	0	Guzman et al. (2006)
3	$\text{GLYXOOr} \Rightarrow \text{GLYAC} + \text{HO}_2$	5.0E+01	0	Carter et al. (1979)
4	$\text{GLYXOOr}^* + \text{GLYXOOr} \Rightarrow 2\text{CHOHOH} + 2\text{CO}_2 + \text{O}_2 + 2\text{HO}_2$	3.0E+08	0	Lim et al. (2010)
5	$\text{CHOHOH} + \text{O}_2 \Rightarrow \text{HCOOH} + \text{HO}_2$	5.0E+06	0	Lim et al. (2010)
6	$\text{CHOHOH} + \text{GLYXr} \Rightarrow \text{C3D}$	1.3E+09	0	Guzman et al. (2006)
7	$\text{GLYXr} + \text{GLYXr} \Rightarrow \text{TA}$	1.3E+09	0	Guzman et al. (2006)
8	$\text{GLYAC} + \text{OH} \Rightarrow \text{GLYACr} + \text{H}_2\text{O}$	3.62E+08	962	Tan et al. (2009)
9	$\text{GLYACr} + \text{O}_2 \Rightarrow \text{GLYACO2r}$	1.0E+06	0	Guzman et al. (2006)
10	$\text{GLYACO2r} \Rightarrow \text{OXLAC} + \text{HO}_2$	5.0E+01	0	Carter et al. (1979)

11	$\text{GLYACO2r} + \text{GLYACO2r} \Rightarrow 2\text{CO}_2 + 2\text{HCOOHr}$	3.0E+08	0	Lim et al. (2010)
12	$\text{HCOOHr} + \text{O}_2 \Rightarrow \text{CO}_2 + \text{HO}_2$	5.0E+06	0	Guzman et al. (2006)
13	$\text{HCOOHr} + \text{GLYXr} \Rightarrow \text{C3D}$	1.3E+09	0	Guzman et al. (2006)
14	$\text{CHOHOH} + \text{GLYXr} \Rightarrow \text{C3D}$	1.3E+09	0	Guzman et al. (2006)
15	$\text{GLYACr} + \text{GLYACr} \Rightarrow \text{C4D}$	1.3E+09	0	Guzman et al. (2006)
16	$\text{GLYAC}^- + \text{OH} \Rightarrow \text{GLYACr}^-$	2.8E+09	4330	Tan et al. (2009)
17	$\text{GLYACr} + \text{GLYXr} \Rightarrow \text{C4D}$	1.3E+09	0	Guzman et al. (2006)
18	$\text{GLYACr}^- + \text{GLYXr} \Rightarrow \text{C4D}$	1.3E+09	0	Guzman et al. (2006)
19	$\text{GLYACr}^- + \text{GLYACr} \Rightarrow \text{C4D}$	1.3E+09	0	Guzman et al. (2006)
20	$\text{GLYACr}^+ + \text{GLYACr}^- \Rightarrow \text{C3D}$	1.3E+09	0	Guzman et al. (2006)
21	$\text{GLYACr}^- + \text{HCOOHr} \Rightarrow \text{C3D}$	1.3E+09	0	Guzman et al. (2006)
22	$\text{GLYACr}^- + \text{CHOHOH} \Rightarrow \text{C3D}$	1.3E+09	0	Guzman et al. (2006)
23	$\text{GLYACr}^- + \text{O}_2 \Rightarrow \text{GLYACO2r}^-$	1.0E+06	0	Guzman et al. (2006)
24	$\text{GLYACO2r}^- \Rightarrow \text{OXLAC}^-$	1.0E+02	0	Lim et al. (2010)
25	$\text{GLYACO2r}^- + \text{GLYACO2r}^- \Rightarrow 2\text{CO}_2 + 2\text{COO}^-$	3.0E+08	0	Lim et al. (2010)
26	$\text{OXLAC} + \text{OH} \Rightarrow \text{HCOOHr} + \text{CO}_2 + 2\text{H}_2\text{O}$	1.4E+06	2766	Tan et al. (2009)
27	$\text{OXLAC}^- + \text{OH} \Rightarrow \text{HCOOHr} + \text{CO}_2^- + 2\text{H}_2\text{O}$	1.9E+08	2766	Tan et al. (2009)
28	$\text{OXLAC}^{2-} + \text{OH} \Rightarrow \text{HCOOHr} + \text{CO}_2^- + 2\text{H}_2\text{O}$	1.6E+08	4330	Tan et al. (2009)
29	$\text{CO}_2^- + \text{O}_2 \Rightarrow \text{O}_2^- + \text{CO}_2$	2.4E+09	0	Tan et al. (2009)

30	$\text{GLYAC} + \text{H}_2\text{O}_2 \Rightarrow \text{HCOOH} + \text{CO}_2 + \text{H}_2\text{O}$	3.0E-01	0	Tan et al. (2009)
31	$\text{HCOOH} + \text{OH} \Rightarrow \text{HCOOHr} + \text{H}_2\text{O}$	1.0E+08	0	Tan et al. (2009)
32	$\text{HCOO}^- + \text{OH} \Rightarrow \text{CO}_2^- + \text{H}_2\text{O}$	2.4E+09	0	Tan et al. (2009)
33	$\text{O}_2^- + \text{OH} \Rightarrow \text{OH}^- + \text{O}_2$	1.0E+10	0	Tan et al. (2009)
34	$\text{HCO}_3^- + \text{OH} \Rightarrow \text{CO}_3^- + \text{H}_2\text{O}$	1.0E+07	0	Tan et al. (2009)
35	$\text{CO}_3^- + \text{O}_2^- \Rightarrow \text{CO}_3^{2-} + \text{O}_2$	6.5E+08	0	Tan et al. (2009)
36	$\text{CO}_3^- + \text{HCOO}^- \Rightarrow \text{HCO}_3^- + \text{CO}_2^-$	1.5E+5	0	Tan et al. (2009)
37	$\text{CO}_3^- + \text{H}_2\text{O}_2 \Rightarrow \text{HCO}_3^- + \text{HO}_2$	8.0E+05	0	Tan et al. (2009)
38	$\text{C3D} + \text{OH} \Rightarrow \text{C3Dr} + \text{H}_2\text{O}$	3.0E+08	0	Lim et al. (2010)
39	$\text{C3Dr} + \text{O}_2 \Rightarrow \text{C3DOOr}$	1.0E+06	0	Lim et al. (2010)
40	$\text{C3DOOr} \Rightarrow \text{HO}_2$	5.0E+01	0	Carter et al. (1979)
41	$2\text{C3DOOr} \Rightarrow 2\text{COOH} + 2\text{GLYAC}$	3.0E+08	0	Lim et al. (2010)
42	$\text{C4D} + \text{OH} \Rightarrow \text{C4Dr} + \text{H}_2\text{O}$	1.1E+08	0	Ervens et al. (2003)
43	$\text{C4Dr} + \text{O}_2 \Rightarrow \text{C4DOOr}$	1.0E+06	0	Guzman et al. (2006)
44	$\text{C4DOOr} \Rightarrow \text{HO}_2$	5.0E+01	0	Carter et al. (1979)
45	$\text{C4DOOr} + \text{C4DOOr} \Rightarrow 2\text{GLYAC} + 2\text{GLYACr}$	3.0E+08	0	Lim et al. (2010)
46	$\text{CHOHOH} + \text{CHOHOH} \Rightarrow \text{GLYX}$	1.3E+09		Guzman et al. (2006)
47	$\text{CHOHOH} + \text{HCOOHr} \Rightarrow \text{GLYAC}$	1.3E+09		Guzman et al. (2006)
48	$\text{HCOOHr} + \text{HCOOHr} \Rightarrow \text{OXLAC}$	1.3E+09	0	Guzman et al. (2006)
49	$\text{CO}_2^- + \text{HCOOHr} \Rightarrow \text{OXLAC}^-$	1.3E+09	0	Guzman et al. (2006)
50	$\text{CO}_2^- + \text{CO}_2^- \Rightarrow \text{OXLAC}^{2-}$	1.3E+09	0	Guzman et al. (2006)

51	C3D => MA	1.0E-03	0	Tan et al. (2009)
52	MA => C3D	5.556E-07	0	Tan et al. (2009)
53	MA + OH => C3Dr + H <sub>2</sub> O	1.6E+08	0	Ervens et al. (2003)
54	TA +OH => C4Dr + H <sub>2</sub> O	3.1E+08	0	Monod et al. (2005, 2008)
55	MGLY + OH => 0.2 OXLAC + 0.8 MGLOLI	1.1E+09	1600	

\* r= radical. For example, GLYXr = glyoxal radical; OOr = peroxy radical.

Table S6. Fe chemistry in cloud used in Case 5

Reaction Number	Aqueous phase Reactions	$K_{298}$ (M <sup>n</sup> s <sup>-1</sup> )	E/R (K)	References
1	H <sub>2</sub> O <sub>2</sub> + Fe <sup>2+</sup> => Fe <sup>3+</sup> + OH + OH <sup>-</sup>	52.4	5050	Deguillaume et al. (2010)
2	H <sub>2</sub> O <sub>2</sub> + FeO <sup>2+</sup> => Fe <sup>3+</sup> + HO <sub>2</sub> + OH <sup>-</sup>	9.5E+03	2800	Deguillaume et al. (2010)
3	O <sub>2</sub> <sup>-</sup> + Fe <sup>2+</sup> + 2H <sup>+</sup> => H <sub>2</sub> O <sub>2</sub> + Fe <sup>3+</sup>	1.0E+07		Deguillaume et al. (2010)
4	O <sub>2</sub> <sup>-</sup> + Fe <sup>3+</sup> => Fe <sup>2+</sup> + O <sub>2</sub>	1.5E+08		Deguillaume et al. (2010)
5	O <sub>2</sub> <sup>-</sup> + [Fe(OH)] <sup>2+</sup> => Fe <sup>2+</sup> + O <sub>2</sub> + OH <sup>-</sup>	1.5E+08		Deguillaume et al. (2010)
6	O <sub>2</sub> <sup>-</sup> + [Fe(OH) <sub>2</sub> ] <sup>+</sup> => Fe <sup>2+</sup> + O <sub>2</sub> + 2OH <sup>-</sup>	1.5E+08		Deguillaume et al. (2010)
7	HO <sub>2</sub> + Fe <sup>2+</sup> + H <sup>+</sup> => Fe <sup>3+</sup> + H <sub>2</sub> O <sub>2</sub>	1.2E+06	5050	Deguillaume et al. (2010)
8	HO <sub>2</sub> + FeO <sup>2+</sup> => Fe <sup>3+</sup> + O <sub>2</sub> + OH <sup>-</sup>	2.0E+06		Deguillaume et al. (2010)
9	OH + Fe <sup>2+</sup> => [Fe(OH)] <sup>2+</sup>	4.6E+08	1100	Deguillaume et al. (2010)
10	OH + FeO <sup>2+</sup> + H <sup>+</sup> => Fe <sup>3+</sup> + H <sub>2</sub> O <sub>2</sub>	1.0E+07		Deguillaume et al. (2010)
11	O <sub>3</sub> + Fe <sup>2+</sup> => FeO <sup>2+</sup> + O <sub>2</sub>	8.2E+05		Deguillaume et al. (2010)



12	$\text{FeO}^{2+} + \text{H}_2\text{O} \Rightarrow \text{Fe}^{3+} + \text{OH} + \text{OH}^-$	1.3E-02	4100	Deguillaume et al. (2010)
13	$\text{FeO}^{2+} + \text{Fe}^{2+} + \text{H}_2\text{O} \Rightarrow 2\text{Fe}^{3+} + 2\text{OH}^-$	7.2E+04	840	Deguillaume et al. (2010)
14	$\text{FeO}^{2+} + \text{Fe}^{2+} + \text{H}_2\text{O} \Rightarrow \text{Fe}(\text{OH})_2\text{Fe}^{4+}$	1.8E+04	5050	Deguillaume et al. (2010)
15	$\text{Fe}(\text{OH})_2\text{Fe}^{4+} \Rightarrow 2\text{Fe}^{3+} + 2\text{OH}^-$	0.49	8800	Deguillaume et al. (2010)
16	$\text{Fe}(\text{OH})_2\text{Fe}^{4+} + 2\text{H}^+ \Rightarrow 2\text{Fe}^{3+} + 2\text{H}_2\text{O}$	2.0E+00	5650	Deguillaume et al. (2010)
17	$\text{NO}_3 + \text{Fe}^{2+} \Rightarrow \text{Fe}^{3+} + \text{NO}_3^-$	8.0E+06		Deguillaume et al. (2010)
18	$\text{NO}_2 + \text{Fe}^{2+} \Rightarrow \text{Fe}^{3+} + \text{NO}_2^-$	3.1E+04		Deguillaume et al. (2010)
19	$\text{HNO}_2 + \text{FeO}^{2+} \Rightarrow \text{Fe}^{3+} + \text{NO}_2 + \text{OH}^-$	1.1E+04	4150	Deguillaume et al. (2010)
20	$\text{NO}_2^- + \text{FeO}^{2+} + \text{H}^+ \Rightarrow \text{Fe}^{3+} + \text{NO}_2 + \text{OH}^-$	1.0E+05		Deguillaume et al. (2010)
21	$\text{HSO}_3^- + [\text{Fe}(\text{OH})]^{2+} \Rightarrow \text{Fe}^{2+} + \text{SO}_3^- + \text{H}_2\text{O}$	30		Deguillaume et al. (2010)
22	$\text{SO}_5^- + \text{Fe}^{2+} + \text{H}_2\text{O} \Rightarrow [\text{Fe}(\text{OH})]^{2+} + \text{HSO}_5^-$	2.65E+07		Deguillaume et al. (2010)
23	$\text{HSO}_5^- + \text{Fe}^{2+} \Rightarrow [\text{Fe}(\text{OH})]^{2+} + \text{SO}_4^-$	3.0E+04		Deguillaume et al. (2010)
24	$\text{SO}_4^- + \text{Fe}^{2+} + \text{H}_2\text{O} \Rightarrow [\text{Fe}(\text{OH})]^{2+} + \text{SO}_4^{2-} + \text{H}^+$	4.1E+09	-2165	Deguillaume et al. (2010)
25	$\text{O}^{2-} + [\text{Fe}(\text{SO}_4)]^+ \Rightarrow \text{Fe}^{2+} + \text{SO}_4^{2-} + \text{O}_2$	1.5E+08		Deguillaume et al. (2010)
26	$\text{HSO}_3^- + \text{FeO}^{2+} \Rightarrow \text{Fe}^{3+} + \text{SO}_3^- + \text{OH}^-$	2.5E+05		Deguillaume et al. (2010)
27	$\text{HCOOH} + \text{FeO}^{2+} + \text{O}_2 + \text{H}^+ \Rightarrow \text{Fe}^{3+} + \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	160	2680	Deguillaume et al. (2010)
28	$\text{HCOO}^- + \text{FeO}^{2+} + \text{O}_2 + \text{H}^+ \Rightarrow \text{Fe}^{3+} + \text{CO}_2 + \text{HO}_2 + \text{OH}^-$	3.0E+05		Deguillaume et al. (2010)
29	$\text{CH}_2(\text{OH})_2 + \text{FeO}^{2+} + \text{O}_2 \Rightarrow \text{Fe}^{3+} + \text{HCOOH} + \text{HO}_2 + \text{OH}^-$	400	5350	Deguillaume et al. (2010)
30	$\text{CO}_3^- + \text{Fe}^{2+} \Rightarrow \text{Fe}^{3+} + \text{CO}_3^{2-}$	2.0E+07		Deguillaume et al. (2010)

31	$\text{CH}_3\text{O}_2 + \text{Fe}^{2+} \Rightarrow \text{CH}_3\text{O}_2\text{Fe}^{2+}$	8.6E+05		Deguillaume et al. (2010)
32	$\text{CH}_3\text{O}_2\text{Fe}^{2+} \Rightarrow \text{CH}_3\text{O}_2 + \text{Fe}^{2+}$	1.3E+03		Deguillaume et al. (2010)
33	$\text{CH}_3\text{O}_2\text{Fe}^{2+} + \text{H}_2\text{O} \Rightarrow \text{Fe}^{3+} + \text{CH}_3\text{OOH} + \text{OH}^-$	100		Deguillaume et al. (2010)
34	$\text{CH}_3\text{O}_2\text{Fe}^{2+} + \text{H}^+ \Rightarrow \text{Fe}^{3+} + \text{CH}_3\text{OOH}$	3.0E+04		Deguillaume et al. (2010)
35	$\text{Fe}^{3+} + \text{SO}_4^{2-} \Rightarrow [\text{Fe}(\text{SO}_4)]^+$	3.2E+03		Deguillaume et al. (2010)
36	$[\text{Fe}(\text{SO}_4)]^+ \Rightarrow \text{Fe}^{3+} + \text{SO}_4^{2-}$	27		Deguillaume et al. (2010)
37	$[\text{Fe}(\text{C}_2\text{O}_4)]^+ \Rightarrow \text{Fe}^{3+} + \text{C}_2\text{O}_4^{2-}$	3.0E-03		Ervens et al. (2003)
38	$\text{Fe}^{3+} + \text{C}_2\text{O}_4^{2-} \Rightarrow [\text{Fe}(\text{C}_2\text{O}_4)]^+$	7.5E+06		Ervens et al. (2003)
39	$[\text{Fe}(\text{C}_2\text{O}_4)_2]^- \Rightarrow [\text{Fe}(\text{C}_2\text{O}_4)]^+ + \text{C}_2\text{O}_4^{2-}$	3.0E-03		Ervens et al. (2003)
40	$[\text{Fe}(\text{C}_2\text{O}_4)]^+ + \text{C}_2\text{O}_4^{2-} \Rightarrow [\text{Fe}(\text{C}_2\text{O}_4)_2]^-$	1.89E+04		Ervens et al. (2003)
41	$[\text{Fe}(\text{OH})]^{2+} + \text{h}\nu \Rightarrow \text{Fe}^{2+} + \text{OH}$	4.51E-03*		Ervens et al. (2003)
42	$[\text{Fe}(\text{OH})_2]^+ + \text{h}\nu \Rightarrow \text{Fe}^{2+} + \text{OH} + \text{OH}^-$	5.77E-03*		Ervens et al. (2003)
43	$[\text{Fe}(\text{SO}_4)]^+ + \text{h}\nu \Rightarrow \text{Fe}^{2+} + \text{SO}_4^-$	6.43E-03*		Ervens et al. (2003)
44	$[\text{Fe}(\text{C}_2\text{O}_4)_2]^- + \text{h}\nu + (\text{O}_2) \Rightarrow \text{Fe}^{2+} + \text{C}_2\text{O}_4^{2-} + 2\text{CO}_2 + \text{O}_2^-$	2.47E-02*		Ervens et al. (2003)

\* Ervens et al. (2003) gave the photolysis rates for  $\text{H}_2\text{O}_2$  and Fe compounds at latitude of  $51^\circ$  N. Based on these rates, we scale the photolysis rates of Fe compounds to the photolysis rates of  $\text{H}_2\text{O}_2$  in the model.

Table S7. Effective Henry's law constants

Species	$H_{298}$ (mol L <sup>-1</sup> atm <sup>-1</sup> )	$\Delta H/R$ (K)	Mass accommodation coefficient	References
CO <sub>2</sub>	3.4E-02	-2420	5.0E-2	Pandis and Seinfeld (1989)
GLYX	4.19E+05*	7481	2.3E-2	Ip et al. (2009)
MGLY	3.7E+03*	7481	2.3E-2	Lim et al. (2005)
OH	3.0E+1	4500	5.0E-2	Lim et al. (2005)
HO <sub>2</sub>	4.6E3	4800	1.0E-2	Lim et al. (2005)
H <sub>2</sub> O <sub>2</sub>	8.6E4	6500	1.1E-1	Lim et al. (2005)
GLYAC	1.09E4	4811	1.9E-2	Ip et al. (2009)
OXLAC	3.26E6		1.9E-2	Lim et al., 2009
HNO <sub>3</sub>	2.1E5		5.0E-2	Pandis and Seinfeld (1989)
O <sub>3</sub>	1.03E-2	2300	5.3E-4	Lelieveld, 1991, Sander, 1996
NO <sub>2</sub>	1.0E-2	2500	6.3E-4	Pandis and Seinfeld (1989)
NO	1.9E-3	1480	5.0E-3	Pandis and Seinfeld (1989)
CH <sub>3</sub> O <sub>2</sub>	6.0E0	5600	5.0E-2	Pandis and Seinfeld (1989)
HCHO	6.3E3	6460	5.0E-2	Pandis and Seinfeld (1989)
HCOOH	3.5E3	5740	5.0E-2	Pandis and Seinfeld (1989)
CH <sub>3</sub> OOH	2.27E2	5610	5.0E-2	Pandis and Seinfeld (1989)
NO <sub>3</sub>	2.1E5	8700	1.0E-3	Pandis and Seinfeld (1989)

HONO	5.1E-4	-1260	5.0E-2	Pandis and Seinfeld (1989)
CH <sub>3</sub> OH	2.2E2	4900	5.0E-2	Pandis and Seinfeld (1989)
PAN	2.9E0	5910	5.0E-2	Pandis and Seinfeld (1989)
CH <sub>3</sub> CO <sub>3</sub>	1.0E2		5.0E-2	Pandis and Seinfeld (1989)
CH <sub>3</sub> CHO	1.14E+01	6460	5.0E-2	Herrmann (2000)
CH <sub>3</sub> COOH	3.5E3	5740	5.0E-2	Pandis and Seinfeld (1989)
PRV	3.09E5		1.9E-2	Lim et al. (2005)
GLYC	4.10E4	4600	2.3E-2	Lim et al. (2005)
SO <sub>2</sub>	1.23E0	3120	5.0E-2	Pandis and Seinfeld (1989)

\* When using the organic chemistry in aerosol water adopted from Ervens and Volkamer (2010), the Henry's law constant for glyoxal and methylglyoxal is 5.8 (Ervens and Volkamer (2010)) and 1.4 (Betterton and Hoffmann, 1988), which do not consider the effect of hydration on the solubility of species.

Table S8. Aqueous equilibrium coefficients

Reaction number	Reactions	$K_{aq298}$	$\Delta H/R$	Reference
1	$CO_2 = H^+ + HCO_3^-$	4.46E-07	1000	Pandis and Seinfeld (1989)
2	$HCO_3^- = H^+ + CO_3^{2-}$	4.68E-11	1760	Pandis and Seinfeld (1989)
3	$SO_2 = H^+ + HSO_3^-$	1.23E-02	1960	Pandis and Seinfeld (1989)
4	$HSO_3^- = H^+ + SO_3^{2-}$	6.61E-08	-1500	Sander (1996)
5	$H_2SO_4 = H^+ + HSO_4^-$	1.0E+03		Pandis and Seinfeld (1989)
6	$HSO_4^- = H^+ + SO_4^{2-}$	1.02E-02	-2720	Pandis and Seinfeld (1989)
7	$H_2O_2 = H^+ + HO_2^-$	2.2E-12	3730	Pandis and Seinfeld (1989)
8	$HO_2 = H^+ + O_2^-$	3.5E-05		
9	$HNO_3 = H^+ + NO_3^-$	1.54E+01	-8700	Pandis and Seinfeld (1989)
10	$HONO = H^+ + NO_2^-$	5.1E-04	1260	Pandis and Seinfeld (1989)
11	$NH_3 = OH^- + NH_4^+$	1.7E-05	-4325	Pandis and Seinfeld (1989)
12	$HCHO + H_2O = H_2C(OH)_2$	1.82E+03	-4020	Pandis and Seinfeld (1989); Sander (2004)
13	$HCOOH = H^+ + HCOO^-$	1.78E-04	20	Pandis and Seinfeld (1989)
14	$CH_3C(O)OOH = H^+ + CH_3C(O)OO^-$	1.78E-04	0	Assumed equal to HCOOH
15	$CH_3COOH = H^+ + CH_3COO^-$	1.75E-05	0	Herrmann et al. (2000)
16	$GLYAC = GLYAC^- + H^+$	3.47E-04	267	Lim et al. (2005)
17	$OXLAC = OXLAC^- + H^+$	5.60E-02	453	Lim et al. (2005)
18	$OXLAC^- = OXLAC^{2-} + H^+$	5.42E-02	805	Lim et al. (2005)
19	$PRV = PRV^- + H^+$	3.20E-03	0	Lim et al. (2005)
20	$Fe^{3+} = Fe(OH)^{2+} + H^+$	1.10E-04	0	Ervens et al. (2003)
21	$Fe(OH)^{2+} = Fe(OH)_2^+ + H^+$	1.40E-07	0	Ervens et al. (2003)
22	$Fe^{2+} = Fe(OH)^+ + H^+$	3.22E-10	0	Deguillaume et al. (2005)

Table S9. Comparison of measured dissolved iron concentrations with modeled concentrations.

References	Measured dissolved iron ( $\mu$ mol/L)	Modeled dissolved iron ( $\mu$ mol/L)	Location
Parazols et al. (2006)	0.1-9.1	1.43	puy de Dôme Station, France.
Hutchings et al. (2009)	4.7-30.4	595	Mt. Elden, Arizona, U.S.A.
Arakaki and Faust (1998)	0.08-1.57	0.29	Whiteface Mountain, New York, U.S.A.
Sedlak et al. (1997)	0.06-1.6	0.45	Great Dun Fell, U.K.
Erel et al. (1993)	3-20	100.6	San Pedro Hill, CA, U.S.A

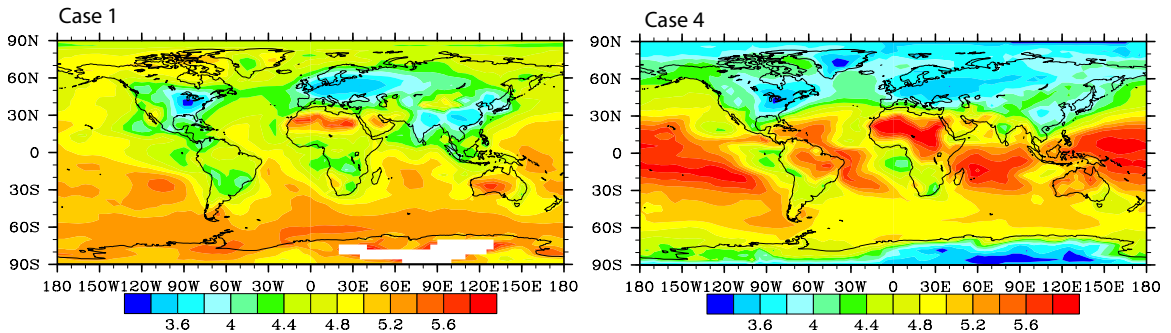


Figure S1. The predicted cloud water pH values in Case 1 and Case 4 near 971 hPa.

Table S10. Comparison of measured pH values in cloud water with modeled pH values

Measured pH values	Location	Time	Reference	Modeled pH (Case 1)	Modeled pH (Case 4)
Average=4.10	Tai Mountain, China	Summer, 2007	Shen et al. (2012)	3.77	3.87

Average=3.77	Tai Mountain, China	Summer, 2008	Shen et al. (2012)	3.77	3.87
Average=3.68	Tai Mountain, China	Spring, 2007	Shen et al. (2012)	4.33	3.92
Average=4.34	Tai Mountain, China	Spring, 2008	Shen et al. (2012)	4.33	3.92
3.5~3.8	Whiteface Mtn, NY, U.S.	July and August	Faust et al. (1993)	3.99	4.20
3.5~4.0	Shenandoah Park, VA	August	Faust et al. (1993)	3.89	4.61
5.6~5.8	Corvallis, OR	Nov. and Jan.	Faust et al. (1993)	4.33	4.12
2.7~3.8	Whiteface Mtn, NY, U.S.	July, 1998	Moore et al. (2004)	3.96	4.29
5.5~7.0	Davis	December 1998–January 1999)	Moore et al. (2004)	4.20	4.12
4.5~5.5	Puy de Dôme, France	February-April, 2001 and February-May, 2002	Marinoni et al. (2004)	3.74	3.70
3.6~5.8	Puy de Dôme, France	February, 2002	Sellegri et al. (2003)	3.61	3.37
4.6~6.6	Sydney, Australia	July-August, 1976	Scott (1978)	4.63	4.78

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