Supplementary material for "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_4 dimer
14	TA	Tartaric acid
15	C3D	C_3 dimer
16	MA	Malonic acid

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

Reaction Number	Aqueous phase Reactions	K_{298} (M^nS^{-1})	E/R (K)	References
1	H_2O_2+hv=>2OH	Using the gas phase photolysis rate, increased by a factor of 1.5		Barth et al. (2003)
2	H_2O_2+OH=>HO_2+H_2O	2.7E+07		Lim et al. (2005)
3	H_2O_2+HO_2=>OH+H_2O	3.7E+00		Tan et al. (2009)
4	HO_2+HO_2=>H_2O_2+O_2	9.7E+05	2500	Lim et al. (2005)
5	OH+HO_2=>H_2O + O_2	7.1E+09		Lim et al. (2005)
6	O_3 + hv => H_2O_2	Using the gas phase photolysis rate, increased by a factor of 1.5		Barth et al. (2003)
7	OH + O_3 => HO_2	2.0E+09		Pandis and Seinfeld (1989)
8	HO_2 + O_3 => OH	1.0E+04		Pandis and Seinfeld (1989)
9	O_2^- + O_3 => OH + OH^-	1.5E+09	1500	Pandis and Seinfeld (1989)
10	OH^- + O_3 => $O2^-$ + HO_2	7.0E+01		Pandis and Seinfeld (1989)
11	HO_2^- + O_3 => OH +O_2^-	2.8E+06		Pandis and Seinfeld (1989)
12	NO + NO_2 => 2NO_2^- + 2H^+	2.0E+08	1500	Pandis and Seinfeld (1989)

13	$NO_2 + NO_2 => NO_2^- + NO_3^- + 2H^+$	1.0E+08	1500	Pandis and Seinfeld (1989)
14	$NO + OH => NO_2^- + H^+$	2.0E+10	1500	Pandis and Seinfeld (1989)
15	$NO_2 + OH => NO_3^- + H^+$	1.3E+09	1500	Pandis and Seinfeld (1989)
16	HONO + hv => NO + OH	Using the gas phase photolysis rate, increased by a factor of 1.5		Pandis and Seinfeld (1989)
17	HNO_2^- + hv => NO + OH	Using the gas phase photolysis rate, increased by a factor of 1.5		Barth et al. (2003)
18	HONO+ OH => NO_2	1.0E+09	1500	Pandis and Seinfeld (1989)
19	$NO_2^- + OH => NO_2 + OH^-$	1.0E+10	1500	Pandis and Seinfeld (1989)
20	$NO_2^- + O_3 => NO_3^-$	5.0E+05	6950	Pandis and Seinfeld (1989)
21	$NO_2^- + CO_3^- => NO_2 + CO_3^{2-}$	4.0E+05	0.	Pandis and Seinfeld (1989)
22	$NO_2^- + NO_3 => NO_2 + NO_3^-$	1.2E+09	1500	Pandis and Seinfeld (1989)
23	NO_3^- + hv => NO_2 + OH + OH^-	Using the same as gas-phase HNO3 photolysis, increased a factor of 1.5		Barth et al. (2003)
24	NO_3 + hv => NO	Using the gas phase photolysis rate, increased by a factor of 1.5		Barth et al. (2003)
25	$NO_3 + HO_2 => NO_3^- + H^+$	1.2E+09	1500	Jacob (1989)
26	$NO_3 + O_2^- => NO_3^-$	1.0E+09	1500	Jacob (1989)

27	$NO_3 + H_2O_2 => NO_3^- + HO_2 + H^+$	1.0E+06	2800	Pandis and Seinfeld (1989)
28	$HO_2+O_2^-=>H_2O_2 + OH^-$	1.0E+08	1500	Pandis and Seinfeld (1989)
29	$SO_2+O_3=>H_2SO_4$	2.4E+04		Pandis and Seinfeld (1989)
30	HSO_3-+O_3=>HSO_4-	3.7E+05	5530	Pandis and Seinfeld (1989)
31	$SO_3^{-2} + O_3 => SO_4^{-2}$	1.5E+09	5280	Pandis and Seinfeld (1989)
32	$SO_2+H_2O_2 => H_2SO_4$	1.3E+06	4430	Pandis and Seinfeld (1989)
33	HSO_3- + H_2O_2=> HSO_4^-	5.2E+06	3650	Pandis and Seinfeld (1989)
34	$SO_3^{-2} + H_2O_2 => SO_4^{-2}$	5.2E+06	3650	Pandis and Seinfeld (1989)
35	$SO_3^{-2} + OH => SO_5^- + OH^-$	4.6E+09	1500	Pandis and Seinfeld (1989)
36	$HSO_3^-+OH => SO_5^-$	4.2E+09	1500	Pandis and Seinfeld (1989)
37	$SO_5^- + HSO_3^- => SO_5^- + HSO_5^-$	3.0E+05	3100	Pandis and Seinfeld (1989)
38	$SO_5^- + SO_3^{-2} => SO_4^{-2} + SO_4^-$	1.3E+07	2000	Jacob (1989)
39	$SO_5^- + O_2^- => HSO_5^- + OH^-$	1.0E+08	1500	Jacob (1989)
40	$SO_5^- + HCOOH => HSO_5^- + CO_2 + HO_2$	2.0E+02	5300	Jacob (1989)

41	$SO_5^- + HCOO^- \Rightarrow HSO_5^- + CO_2 + O_2^-$	1.4E+04	4000	Jacob (1989)
42	$SO_5^- + SO_5^- \Rightarrow 2SO_4^-$	2.0E+08	1500	Jacob (1989)
43	$HSO_5^- + OH \Rightarrow SO_5^-$	1.7E+07	1900	Jacob (1989)
44	$HSO_5^- + SO_4^- \Rightarrow SO_5^- + SO_4^{-2} + H^+$	1.0E+05	0.	Jacob (1989)
45	$HSO_5^- + NO_2^- \Rightarrow HSO_4^- + NO_3^-$	3.1E-01	6650	Jacob (1989)
46	$SO_4^- + HSO_3^- \Rightarrow SO_5^- + SO_4^{-2} + H^+$	1.3E+09	1500	Jacob (1989)
47	$SO_4^- + SO_3^{-2} \Rightarrow SO_5^- + SO_4^{-2}$	5.3E+08	1500	Jacob (1989)
48	$SO_4^- + HO_2 \Rightarrow SO_4^{-2} + H^+$	5.0E+09	1500	Jacob (1989)
49	$SO_4^- + O_2^- \Rightarrow SO_4^{-2}$	5.0E+09	1500	Jacob (1989)
50	$SO_4^- + OH^- \Rightarrow SO_4^{-2} + OH$	8.0E+07	1500	Jacob (1989)
51	$SO_4^- + H_2O_2^- \Rightarrow SO_4^{-2} + HO_2 + H^+$	1.2E+07	2000	Pandis and Seinfeld (1989)
52	$SO_4^- + NO_2^- \Rightarrow SO_4^{-2} + NO_2$	8.8E+08	1500	Jacob (1989)
53	$SO_4^- + HCO_3^- \Rightarrow SO_4^{-2} + CO_3^- + H^+$	9.1E+06	2100	Pandis and Seinfeld (1989)
54	$SO_4^- + HCOO^- \Rightarrow SO_4^{-2} + CO_2 + HO_2$	1.7E+08	1500	Jacob (1989)
55	$SO_4^- + HCOOH \Rightarrow SO_4^{-2} + CO_2 + HO_2 + H^+$	1.4E+06	2700	Jacob (1989)
56	$SO_2 + HO_2 \Rightarrow H_2SO_4 + OH$	1.0E+06	0.	Pandis and Seinfeld (1989)
57	$SO_4^- + CH_3OH \Rightarrow SO_4^{-2} + HCHO + HO_2 + H^+$	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^nS^{-1})	E/R (K)	References
1	GLYX+OH=> GLYAC+HO_2	1.1E+09	1564	Lim et al. (2005)
2	GLYAC+OH=>OXLAC+H_2O	3.62E+08	962	Herrmann (2003)
3	GLYAC- + OH => OXLAC- + H_2O	2.8E+09	4330	Herrmann (2003)
4	OXLAC +OH => $2CO_2$ + $2H_2O$	1.4E+06		Lim et al. (2005)
5	OXLAC- + OH => $2CO_2$ + 2 H_2O	4.7E+07		Lim et al. (2005)
6	OXLAC= + OH => $2CO_2$ + $2H_2O$	7.7E+06		Lim et al. (2005)
7	$H_2C(OH)_2$ + OH => HCOOH + HO_2	2.0E+09	1500	Pandis and Seinfeld (1989)
8	$HCOO^-$ + NO_3 => NO_3^- + CO_2 + HO_2	6.0E+07	1500	Jacob (1989)
9	HCOOH + O_3 => CO_2 + HO_2 +OH	5.0E+00	0	Pandis and Seinfeld (1989)
10	$HCOO^-$ + O_3 => CO_2 + OH + O_2^-	1.0E+02	0	Pandis and Seinfeld (1989)
11	$HCOO^-$ + CO_3- => CO_2 + HCO_3^- + HO_2 + OH-	1.1E+05	3400	Pandis and Seinfeld (1989)
12	CH_3O_2 + HO_2 => CH3OOH	4.3E+05	3000	Jacob (1989)
13	CH_3O_2 + O_2^- => CH3OOH+ OH-	5.0E+07	1600	Jacob (1989)
14	CH_3OOH + hv => HCHO + OH + HO_2	5.0E-4*j_{NO2}		Pandis and Seinfeld (1989)
15	CH3OOH + OH => CH3O2	2.7E+07	1700	Jacob (1989)
16	CH3OH + OH => HCHO + HO_2	4.5E+06	1500	Pandis and Seinfeld (1989)
17	CH3OH + $CO3^-$ => HCHO + HO_2 + $HCO3^-$	2.6E+03	4500	Pandis and Seinfeld (1989)
18	CH3OOH + OH => HCHO + OH	1.9E+07	1800	Jacob (1989)

19	CH3OH + NO_3 => NO_3^- + H^+ + HCHO + HO_2	1.0E+06	2800	Pandis and Seinfeld (1989)
20	MGLY + OH => 0.92 PRV +0.08 GLYAC + H_2O + HO_2	1.1E+09	1600	Ervens et al. (2004)
21	PRV + OH => CH3C(O)OH + HO_2 + CO_2	1.2E+08	2766	Lim et al. (2005)
22	PRV- + OH => CH3COO- + HO_2 + CO_2	7.0E+08	2285	Lim et al. (2005)
23	CH3COO- + OH => 0.85GLYAC- + 0.15 HCOO-	1.9E+09	1800	Lim et al. (2005)
24	CH3COOH + OH => 0.85GLYAC + 0.15 HCOOH	1.5E+07	1800	Lim et al. (2005)
25	GLYX + OH => 0.03GLYAC +0.97 OXLAC	3.1E+09		Lumped reactions based on Carlton et al. (2007)
26	GLYC + OH => GLYX + HO_2	1.0E+09	1564	Lim et al. (2005)
27	GLYC +OH => GLYAC + $2HO_2$	5.0E+08	1564	Lim et al. (2005)
28	GLYC + NO_3 => GLYAC +HO_2 + NO_3-	1.1E+07		Herrmann et al. (2005)
29	GLYC + NO_3 => GLYX + NO_3- +H_2O	5.5E+06		Herrmann (2003)
30	GLYX + NO_3 => GLYAC + NO_3- + HO_2	6.3E+07		The same as for MGLY+NO3
31	MGLY + NO_3 => 0.92 PRV +0.08 GLYAC + NO_3- + HO_2	6.3E+07		Herrmann et al. (2005)
32	PRV + NO_3 => CH3COOH + HO2 +CO_2 + NO_3-	4.8E+06		Herrmann et al. (2005)
33	PRV- + NO_3 => CH3COO- + HO_2 + CO_2 + NO_3-	4.8E+06		Herrmann et al. (2005)
34	GLYAC + NO_3 => OXLAC + HO_2 + NO_3-	3.0E+06		The same as glyxolic acid from Herrmann et al. (2005)
35	GLYAC- + NO_3 => OXLAC- + HO_2 + NO_3-	1.1E+08		The same as glyxolic acid from Herrmann et al. (2005)

36	OXLAC + NO_3 => $2CO_2$ + NO_3-	6.8E+07		The same as OLAC- + NO_3
37	OXLAC- + NO_3 => $2CO_2$ + NO_3-	6.8E+07		Herrmann et al. (2000)
38	OXLAC= + NO_3 => $2CO_2$ + NO_3-	2.2E+08		Herrmann et al. (2000)

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

Reaction Number	Aqueous phase Reactions	K_{298} (M^nS^{-1})	E/R (K)	References
1	GLYX + H_2O => GLYX_MH	7		Creighton et al. (1988)
2	GLYX_MH=> GLYX	2.0E-02		Creighton et al. (1988)
3	GLYX_MH + H2O =>GLYX_DH	4.0		Ervens and Volkamer (2010)
4	GLYX_DH=>GLYX_MH	2.0E-02		Ervens and Volkamer (2010)
5	GLYX+GLYX_MH=>GLYOLI	1.0E+02		Ervens and Volkamer (2010)
6	GLYOLI=>GLYX+GLYX_MH	5.556		Ervens and Volkamer (2010)
7	GLYX_MH+GLYX_MH=>GLYOLI	1.0E+02		Ervens and Volkamer (2010)
8	GLYOLI=>GLYX_MH+GLYX_MH	5.556		Ervens and Volkamer (2010)
9	GLYX_DH+GLYX_MH=>GLYOLI	1.0E+02		Ervens and Volkamer (2010)
10	GLYOLI=>GLYX_DH+GLYX_MH	5.556		Ervens and Volkamer (2010)
11	GLYX_DH=>GLYOLI	$0.8\ s^{-1} < k < 7s^{-1}$		k scales with OH concentration with highest value at [OH]=10^7 cm^{-3} (Ervens and Volkamer , (2010))

12	GLYX_MH=>GLYOLI	0.8 s^{-1}<k<7s^{-1}		k scales with OH concentration with highest value at $[OH]=10^7$ cm^{-3} (Ervens and Volkamer , (2010))
13	GLYX =>GLYOLI	0.8 s^{-1}<k<7s^{-1}		k scales with OH concentration with highest value at $[OH]=10^7$ 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_2	1.1E+09	1564	Lim et al. (2005)
28	GLYX_MH + OH=> GLYAC+HO_2	1.1E+09	1564	Lim et al. (2005)
29	GLYX_DH + OH=> GLYAC+HO_2	1.1E+09	1564	Lim et al. (2005)

30	GLYAC+OH=>OXLAC+H_2O	3.62E+08	962	Herrmann (2003)
31	GLYAC- + OH => OXLAC- + H_2O	2.8E+09	4330	Herrmann (2003)
32	OXLAC +OH => $2CO_2$ + $2H_2O$	1.4E+06		Lim et al. (2005)
33	OXLAC- + OH => $2CO_2$ + 2 H_2O	4.7E+07		Lim et al. (2005)
34	OXLAC= + OH => $2CO_2$ + $2H_2O$	7.7E+06		Lim et al. (2005)
35	$H_2C(OH)_2$ + OH => HCOOH + HO_2	2.0E+09	1500	Pandis and Seinfeld (1989)
36	$HCOO^-$ + NO_3 => NO_3^- + CO_2 + HO_2	6.0E+07	1500	Jacob (1989)
37	HCOOH + O_3 => CO_2 + HO_2 +OH	5.0E+00	0	Pandis and Seinfeld (1989)
38	$HCOO^-$ + O_3 => CO_2 + OH + O_2^-	1.0E+02	0	Pandis and Seinfeld (1989)
39	$HCOO^-$ + CO_3- => CO_2 + HCO_3^- + HO_2 + OH-	1.1E+05	3400	Pandis and Seinfeld (1989)
40	CH_3O_2 + HO_2 => CH3OOH	4.3E+05	3000	Jacob (1989)
41	CH_3O_2 + O_2^- => CH3OOH+ OH-	5.0E+07	1600	Jacob (1989)
42	CH_3OOH + hv => HCHO + OH + HO_2	5.0E-4*j_{NO2}		Pandis and Seinfeld (1989)
43	CH3OOH + OH => CH3O2	2.7E+07	1700	Jacob (1989)
44	CH3OH + OH => HCHO + HO_2	4.5E+06	1500	Pandis and Seinfeld (1989)
45	CH3OH + $CO3^-$ => HCHO + HO_2 + $HCO3^-$	2.6E+03	4500	Pandis and Seinfeld (1989)
46	CH3OOH + OH => HCHO + OH	1.9E+07	1800	Jacob (1989)
47	CH3OH + NO_3 => NO_3^- + H^+ + HCHO + HO_2	1.0E+06	2800	Pandis and Seinfeld (1989)
48	MGLY + OH => 0.92 PRV +0.08 GLYAC + H_2O + HO_2	1.1E+09	1600	Ervens et al. (2004)
49	MGLY_MH + OH => 0.92 PRV +0.08 GLYAC + H_2O + HO_2	1.1E+09	1600	Ervens et al. (2004)
50	MGLY_DH + OH => 0.92 PRV +0.08 GLYAC + H_2O + HO_2	1.1E+09	1600	Ervens et al. (2004)

51	PRV + OH => CH3C(O)OH + HO_2 + CO_2	1.2E+08	2766	Lim et al. (2005)
52	PRV- + OH => CH3COO- + HO_2 + CO_2	7.0E+08	2285	Lim et al. (2005)
53	CH3COO- + OH => 0.85GLYAC- + 0.15 HCOO-	1.9E+09	1800	Lim et al. (2005)
54	CH3COOH + OH => 0.85GLYAC + 0.15 HCOOH	1.5E+07	1800	Lim et al. (2005)
55	GLYX + OH => 0.03GLYAC +0.97 OXLAC	3.1E+09		Lumped reactions based on Carlton et al. (2007)
56	GLYC + OH => GLYX + HO_2	1.0E+09	1564	Lim et al. (2005)
57	GLYC +OH => GLYAC + 2HO_2	5.0E+08	1564	Lim et al. (2005)
58	GLYC + NO_3 => GLYAC +HO_2 + NO_3-	1.1E+07		Herrmann et al. (2005)
59	GLYC + NO_3 => GLYX + NO_3- +H_2O	5.5E+06		Herrmann (2003)
60	GLYX + NO_3 => GLYAC + NO_3- + HO_2	6.3E+07		The same as for MGLY+NO3
61	GLYX_MH + NO_3 => GLYAC + NO_3- + HO_2	6.3E+07		The same as for MGLY+NO3
62	GLYX_MH + NO_3 => GLYAC + NO_3- + HO_2	6.3E+07		The same as for MGLY+NO3
63	MGLY + NO_3 => 0.92 PRV +0.08 GLYAC + NO_3- + HO_2	6.3E+07		Herrmann et al. (2005)
64	MGLY_MH + NO_3 => 0.92 PRV +0.08 GLYAC + NO_3- + HO_2	6.3E+07		Herrmann et al. (2005)
65	MGLY_DH + NO_3 => 0.92 PRV +0.08 GLYAC + NO_3- + HO_2	6.3E+07		Herrmann et al. (2005)
66	PRV + NO_3 => CH3COOH + HO2 +CO_2 + NO_3-	4.8E+06		Herrmann et al. (2005)
67	PRV- + NO_3 => CH3COO- + HO_2 + CO_2 + NO_3-	4.8E+06		Herrmann et al. (2005)
68	GLYAC + NO_3 => OXLAC + HO_2 + NO_3-	3.0E+06		The same as glyxolic acid from Herrmann et al. (2005)

69	GLYAC- + NO_3 => OXLAC- + HO_2 + NO_3-	1.1E+08		The same as glyxolic acid from Herrmann et al. (2005)
70	OXLAC + NO_3 => 2CO_2 + NO_3-	6.8E+07		The same as OLAC- + NO_3
71	OXLAC- + NO_3 => 2CO_2 + NO_3-	6.8E+07		Herrmann et al. (2000)
72	OXLAC= + NO_3 => 2CO_2 + NO_3-	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} (M^nS^{-1})	E/R (K)	References
1	GLYX + OH => GLYXr * + H_2O	1.1E+09	1564	Tan et al. (2009)
2	GLYXr +O_2 => GLYXOOr	1.0E+06	0	Guzman et al. (2006)
3	GLYXOOr => GLYAC + HO_2	5.0E+01	0	Carter et al. (1979)
4	GLYXOOr* + GLYXOOr => 2HFALDr + 2CO_2 + O_2 + 2HO_2	3.0E+08	0	Lim et al. (2010)
5	HFALDr + O_2 => ACOL + HO_2	5.0E+06	0	Lim et al. (2010)
6	HFALDr + GLYXr => C3D	1.3E+09	0	Guzman et al. (2006)
7	GLYXr + GLYXr => TA	1.3E+09	0	Guzman et al. (2006)
8	GLYAC + OH => GLYACr +H_2O	3.62E+08	962	Tan et al. (2009)
9	GLYACr + O_2 => GACO2r	1.0E+06	0	Guzman et al. (2006)
10	GACO2r => OXLAC + HO_2	5.0E+01	0	Carter et al. (1979)
11	GACO2r + GACO2r => 2CO_2 + HCOOHr	3.0E+08	0	Lim et al. (2010)

12	HCOOHr + O_2 => CO_2 + HO_2	5.0E+06	0	Guzman et al. (2006)
13	HCOOHr + GLYXr => C3D	1.3E+09	0	Guzman et al. (2006)
14	HFALDr + GLYXr => C3D	1.3E+09	0	Guzman et al. (2006)
15	GLYACr + GLYACr => C4D	1.3E+09	0	Guzman et al. (2006)
16	GLYAC- + OH => GLYACr-	2.8E+09	4330	Tan et al. (2009)
17	GLYACr+ GLYXr => C4D	1.3E+09	0	Guzman et al. (2006)
18	GLYACr- + GLYXr => C4D	1.3E+09	0	Guzman et al. (2006)
19	GLYACr- + GLYACr => C4D	1.3E+09	0	Guzman et al. (2006)
20	GLYACr-+ GLYACr- => C3D	1.3E+09	0	Guzman et al. (2006)
21	GLYACr- + HCOOHr => C3D	1.3E+09	0	Guzman et al. (2006)
22	GLYACr- + HFALDr => C3D	1.3E+09	0	Guzman et al. (2006)
23	GLYACr- + O_2 => GACO2r-	1.0E+06	0	Guzman et al. (2006)
24	GACO2r- => OXLAC-	1.0E+02	0	Lim et al. (2010)
25	GACO2r- + GACO2r- => 2CO_2- + 2HCOOHr	3.0E+08	0	Lim et al. (2010)
26	OXLAC + OH => HCOOHr + CO_2 + 2H_2O	1.4E+06	2766	Tan et al. (2009)
27	OXLAC- + OH => HCOOHr + CO_2- + 2H_2O	1.9E+08	2766	Tan et al. (2009)
28	OXLAC-2 + OH => HCOOHr + CO_2- + 2 H_2O	1.6E+08	4330	Tan et al. (2009)
29	CO_2- + O_2 => O_2- + CO_2	2.4E+09	0	Tan et al. (2009)
30	GLYAC + H_2O_2 => ACOL + CO_2 + H_2O	3.0E-01	0	Tan et al. (2009)

31	ACOL + OH => HCOOHr + H_2O	1.0E+08	0	Tan et al. (2009)
32	HCOO- + OH => CO_2- + H_2O	2.4E+09	0	Tan et al. (2009)
33	O_2- + OH => OH- + O_2	1.0E+10	0	Tan et al. (2009)
34	HCOO- + OH => CO_2- + H_2O	1.0E+07	0	Tan et al. (2009)
35	CO_2- + O_2- => CO_2= + O2	6.5E+08	0	Tan et al. (2009)
36	CO_3- + HCOO- => HCO_3- + CO_2-	1.5E+5	0	Tan et al. (2009)
37	CO_3- +H_2O_2 => HCO_3- + HO_2	8.0E+05	0	Tan et al. (2009)
38	C3D + OH => C3Dr + H2O	3.0E+08	0	Lim et al. (2010)
39	C3Dr + O_2 => C3DOOr	1.0E+06	0	Lim et al. (2010)
40	C3DOOr => HO_2	5.0E+01	0	Carter et al. (1979)
41	C3DOOr => 2HCOOHr + 2GLYAC	3.0E+08	0	Lim et al. (2010)
42	C4D + OH => C4Dr + H_2O	1.1E+08	0	Ervens et al. (2003)
43	C4Dr + O_2 => C4DOOr	1.0E+06	0	Guzman et al. (2006)
44	C4DOOr => HO_2	5.0E+01	0	Carter et al. (1979)
45	C4DOOr + C4DOOr => 2GLYAC	3.0E+08	0	Lim et al. (2010)
46	HFALDr + HFALDr => GLYX	1.3E+09		Guzman et al. (2006)
47	HFALDr + HCOOHr => GLYAC	1.3E+09		Guzman et al. (2006)
48	HCOOHr +HCOOHr => OXLAC	1.3E+09	0	Guzman et al. (2006)
49	CO_2- + HCOOHr => OXLAC-	1.3E+09	0	Guzman et al. (2006)
50	CO_2- + CO_2- => OXLAC=	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_2O	1.6E+08	0	Ervens et al. (2003)

54	TA +OH => C4Dr + H_2O	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^nS^{-1})	E/R (K)	References
1	H_2O_2+ Fe^{2+} => Fe^{3+} + OH + OH^-	52.4	5050	Deguillaume et al. (2010)
2	H_2O_2 + FeO^{2+} => Fe^{3+} + HO_2 + OH^-	9.5E+03	2800	Deguillaume et al. (2010)
3	O_2^- + Fe^{2+} + $2H^+$ => H_2O_2 + Fe^{3+}	1.0E+07		Deguillaume et al. (2010)
4	O_2^- + Fe^{3+} => Fe^{2+} + O_2	1.5E+08		Deguillaume et al. (2010)
5	O_2^- + $[Fe(OH)]^{2+}$ => Fe^{2+} + O_2 + OH^-	1.5E+08		Deguillaume et al. (2010)
6	O_2^- + $[Fe(OH)_2]^+$ => Fe^{2+} + O_2 + $2OH^-$	1.5E+08		Deguillaume et al. (2010)
7	HO_2 + Fe^{2+} + H^+ => Fe^{3+} + H_2O_2	1.2E+06	5050	Deguillaume et al. (2010)
8	HO_2 + FeO^{2+} => Fe^{3+} +O_2 + OH^-	2.0E+06		Deguillaume et al. (2010)
9	OH + Fe^{2+} => $[Fe(OH)]^{2+}$	4.6E+08	1100	Deguillaume et al. (2010)
10	OH + FeO^{2+} + H^+ => Fe^{3+} H_2O_2	1.0E+07		Deguillaume et al. (2010)
11	O_3 +Fe^{2+} => FeO^{2+} + O_2	8.2E+05		Deguillaume et al. (2010)
12	FeO^{2+} + H_2O => Fe^{3+} + OH + OH^-	1.3E-02	4100	Deguillaume et al. (2010)
13	FeO^{2+} + Fe^{2+} + H_2O => $2Fe^{3+}$ + $2OH^-$	7.2E+04	840	Deguillaume et al. (2010)
14	FeO^{2+} + Fe^{2+} + H_2O => $Fe(OH)_2Fe^{4+}$	1.8E+04	5050	Deguillaume et al. (2010)

15	$Fe(OH)_2Fe^{4+}$ => $2Fe^{3+} + 2OH^-$	0.49	8800	Deguillaume et al. (2010)
16	$Fe(OH)_2Fe^{4+} + 2H^+$ => $2Fe^{3+} + 2H_2O$	2.0E+00	5650	Deguillaume et al. (2010)
17	$NO_3 + Fe^{2+}$ => $Fe^{3+} + NO_3^-$	8.0E+06		Deguillaume et al. (2010)
18	$NO_2 + Fe^{2+}$ => $Fe^{3+} + NO_2^-$	3.1E+04		Deguillaume et al. (2010)
19	$HNO_2 + FeO^{2+}$ => $Fe^{3+} + NO_2 + OH^-$	1.1E+04	4150	Deguillaume et al. (2010)
20	$NO_2^- + FeO^{2+} + H^+$ => Fe^{3+} $NO_2 + OH^-$	1.0E+05		Deguillaume et al. (2010)
21	$HSO_3^- + [Fe(OH)]^{2+}$ => $Fe^{2+} + SO_3^- + H_2O$	30		Deguillaume et al. (2010)
22	$SO_5^- + Fe^{2+}$ H_2O => $[Fe(OH)]^{2+} + HSO_5^-$	2.65E+07		Deguillaume et al. (2010)
23	$HSO_5^- + Fe^{2+}$ => $[Fe(OH)]^{2+} + SO_4^-$	3.0E+04		Deguillaume et al. (2010)
24	$SO_4^- + Fe^{2+} + H_2O$ => $[Fe(OH)]^{2+} + SO_4^{2-} + H^+$	4.1E+09	-2165	Deguillaume et al. (2010)
25	$O^{2-} + [Fe(SO_4)]^+$ => $Fe^{2+} + SO_4^{2-} + O_2$	1.5E+08		Deguillaume et al. (2010)
26	$HSO^{3-} + FeO^{2+}$ => $Fe^{3+} + SO^{3-} + OH^-$	2.5E+05		Deguillaume et al. (2010)
27	$HCOOH + FeO^{2+} + O_2 + H^+$ => $Fe^{3+} + CO_2 + HO_2 + H_2O$	160	2680	Deguillaume et al. (2010)
28	$HCOO^- + FeO^{2+} + O_2 + H^+$ => $Fe^{3+} + CO_2 + HO_2$ + OH-	3.0E+05		Deguillaume et al. (2010)
29	$CH_2(OH)_2 + FeO^{2+} + O_2$ => $Fe^{3+} + HCOOH + HO_2 + OH^-$	400	5350	Deguillaume et al. (2010)
30	$CO_3^- + Fe^{2+}$ => $Fe^{3+} + CO_3^{2-}$	2.0E+07		Deguillaume et al. (2010)
31	$CH_3O_2 + Fe^{2+}$ => $CH_3O_2Fe^{2+}$	8.6E+05		Deguillaume et al. (2010)
32	$CH_3O_2Fe^{2+}$ => $CH_3O_2 + Fe^{2+}$	1.3E+03		Deguillaume et al. (2010)
33	$CH_3O_2Fe^{2+} + H_2O$ => $Fe^{3+} + CH_3OOH + OH^-$	100		Deguillaume et al. (2010)
34	$CH_3O_2Fe^{2+} + H^+$ => Fe^{3+} +	3.0E+04		Deguillaume et al. (2010)

	CH_3OOH			
35	$Fe^{3+} + SO_4^{2-}$ => $[Fe(SO_4)]^+$	3.2E+03		Deguillaume et al. (2010)
36	$[Fe(SO_4)]^+$ => $Fe^{3+} + SO_4^{2-}$	27		Deguillaume et al. (2010)
37	$[Fe(C_2O_4)]^+$ => $Fe^{3+} + C_2O_4^{2-}$	3.0E-03		Ervens et al. (2003)
38	$Fe^{3+} + C_2O_4^{2-}$ => $[Fe(C_2O_4)]^+$	7.5E+06		Ervens et al. (2003)
39	$[Fe(C_2O_4)_2]^-$ => $[Fe(C_2O_4)]^+ + C_2O_4^{2-}$	3.0E-03		Ervens et al. (2003)
40	$[Fe(C_2O_4)]^+ + C_2O_4^{2-}$ => $[Fe(C_2O_4)_2]^-$	1.89E+04		Ervens et al. (2003)
41	$[Fe(OH)]^{2+}$ + hv => Fe^{2+} + OH	4.51E-03*		Ervens et al. (2003)
42	$[Fe(OH)_2]^+$ + hv => Fe^{2+} + OH + OH^-	5.77E-03*		Ervens et al. (2003)
43	$[Fe(SO_4)]^+$ + hv => $Fe^{2+} + SO_4^-$	6.43E-03*		Ervens et al. (2003)
44	$[Fe(C_2O_4)_2]^-$ + hv + (O_2) => $Fe^{2+} + C_2O_4^{2-} + 2CO_2 + O_2^-$	2.47E-02*		Ervens et al. (2003)

* Ervens et al. (2003) gave the photolysis rates for H_2O_2 and Fe compounds at latitude of 51° N. Based on these rates, we scale the photolysis rates of Fe compounds to the photolysis rates of H_2O_2 in the model.

Table S7. Effective Henry's law constants

Species	H_{298} (mol L^{-1} atm^{-1})	ΔH/R (K)	Mass accommodation coefficient	References
CO_2	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_2	4.6E3	4800	1.0E-2	Lim et al. (2005)
H_2O_2	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_3	2.1E5		5.0E-2	Pandis and Seinfeld (1989)
O_3	1.03E-2	2300	5.3E-4	Lelieveld, 1991, Sander, 1996
NO_2	1.0E-2	2500	6.3E-4	Pandis and Seinfeld (1989)
NO	1.9E-3	1480	5.0E-3	Pandis and Seinfeld (1989)
CH_3O_2	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_3OOH	2.27E2	5610	5.0E-2	Pandis and Seinfeld (1989)
NO_3	2.1E5	8700	1.0E-3	Pandis and Seinfeld (1989)

HONO	5.1E-4	-1260	5.0E-2	Pandis and Seinfeld (1989)
CH_3OH	2.2E2	4900	5.0E-2	Pandis and Seinfeld (1989)
PAN	2.9E0	5910	5.0E-2	Pandis and Seinfeld (1989)
CH_3CO_3	1.0E2		5.0E-2	Pandis and Seinfeld (1989)
CH_3CHO	1.14E+01	6460	5.0E-2	Herrmann (2000)
CH_3COOH	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)
SO2	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}	ΔH/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	$H_2SO_4 = H^+ + HSO4^-$	1.0E+03		Pandis and Seinfeld (1989)
6	$HSO4^- = H^+ + SO_4^{2-}$	1.02E-02	-2720	Pandis and Seinfeld (1989)
7	$H_2O_2 = H^+ + HO_2^-$	2.2E-12	3730	Pandis and Seinfeld (1989)
8	$HO_2 = H^+ + O2^-$	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	$CH_3C(O)OOH = H^+ + CH3C(O)OO^-$	1.78E-04	0	Assumed equal to HCOOH
15	$CH3COOH = H^+ + CH3COO^-$	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)

References

Barth, M. C., Sillman, S., Hudman, R., Jacobson, M. Z., Kim, C.-H., Monod, A., Liang, J.: Summary of the cloud chemistry modeling intercomparison: Photochemical box model simulation, J. Geophys. Res., 108, 4214, doi:10.1029/2002JD002673, 2003.

Betterton, E. A. and Hoffmann, M. R.: Henry's law constants of some environmentally important aldehydes, Environ. Sci. Tech- nol., 22, 1415–1418, 1988.

Carlton, A. G., Turpin, B. J., Altieri, K. E., Seitzinger, S., Reff, A., Lim, H. J. and Ervens, B.: Atmospheric oxalic acid and SOA production from glyoxal: Results of aqueous photooxidation experiments, Atmospheric Environment, 41(35), 7588–7602, doi:10.1016/j.atmosenv.2007.05.035, 2007.

Carter, W. P. L., Darnall, K. R., Graham, R. A., Winer, A. M., and Pittts, Jr., J.: Reactions of C2 and C4 α–Hydroxy radicals with Oxygen, J. Phys. Chem., 83, 2305-2311, 1979

Creighton, D. J., Migliorini, M., Pourmotabbed, T., and Guha, M. K.: Optimization of efficieny in the glyoxylase pathway, Biochem., 27, 7376–7384, 1988.

Deguillaume, L., Leriche, M. and Desboeufs, K.: Transition metals in atmospheric liquid phases: Sources, reactivity, and sensitive parameters, Chemical Reviews-Columbus, 105, 3388-3431, 2005.

Deguillaume, L., Desboeufs, K. V., Leriche, M., Long, Y., and Chaumerliac, N.: Effect of iron dissolution on cloud chemistry: from laboratory measurements to model results, Atmos. Pollut. Res, *1*(4), 220-228, 2010.

Ervens, B., et al.: CAPRAM 2.4 (MODAC mechanism): An extended and condensed tropospheric aqueous phase mechanism and its application, J. Geophys. Res., 108(D14), 4426–, doi:10.1029/2002JD002202, 2003.

Ervens, B. and Volkamer, R.: Glyoxal processing by aerosol multiphase chemistry: towards a kinetic modeling framework of secondary organic aerosol formation in aqueous particles, Atmos. Chem. Phys., 10(17), 8219–8244, doi:10.5194/acp-10-8219-2010, 2010.

Ervens, B., Turpin, B. J. and Weber, R. J.: Secondary organic aerosol formation in cloud droplets and aqueous particles (aqSOA): a review of laboratory, field and model studies, Atmos. Chem. Phys., 11(21), 11069–11102, doi:10.5194/acp-11-11069-2011, 2011.

Guzman, M. I., Colussi, A. J., and Hoffman, M. R.: Photoinduced oligomerization of aqueous pyruvic acid. J. Phys. Chem. A., 110, 3619-3626, 2006.

Herrmann, H.: Kinetics of aqueous phase reactions relevant for atmospheric chemistry, Chem. Rev., 103, 4691–4716, 2003.

Herrmann, H., Ervens, B., Jacobi, H.-W., Wolke, R., Nowacki, P., and Zellner, R.: CAPRAM2.3: A Chemical Aqueous Phase Radical Mechanism for Tropospheric Chemistry, J. Atmos. Chem., 36, 231–284, 2000.

Herrmann, H., Tilgner, A., Barzaghi, P., Majdik, Z., Gligorovski, S., Poulain, L., and Monod, A.: Towards a more detailed description of tropospheric aqueous phase organic chemistry: CAPRAM 3.0, Atmos. Environ, 39, 4351–4363, 2005.

Jacob, D. J.: Chemistry of OH in remote clouds and its role in the production of formic acid and peroxymonosulfate, J. Geophys. Res., 1986.

Lelieveld, J. and Crutzen, P. J.: The role of clouds in tropospheric photochemistry, J Atmos Chem, 12(3), 229–267, doi:10.1007/BF00048075, 1991.

Ip, H. S. S., Huang, X. H. H., Yu, J. Z.: Effective Henry's law constants of glyoxal, glyoxylic acid, and glycolic acid, Geophys. Res. Lett., 36, L01802, doi:10.1029/2008GL036212, 2009.

Lim, H. J., Carlton, A. G., and Turpin, B. J.: Isoprene forms secondary organic aerosol through cloud processing: Model simulations, Environ. Sci. Technol., 39, 4441–4446, 2005.

Lim, Y. B., Tan, Y., Perri, M. J., Seitzinger, S. P. and Turpin, B. J.: Aqueous chemistry and its role in secondary organic aerosol (SOA) formation, Atmos. Chem. Phys., 10(21), 10521–10539, doi:10.5194/acp-10-10521-2010, 2010.

Liu, X., G. Mauersberger and Moeller D., The effects of cloud processes on the tropospheric photochemistry: an improvement of the EURAD model with a coupled gaseous and aqueous chemical mechanism. Atmospheric Environment. 31, 3119-3135, 1997.

Monod, A., Poulain, L., Grubert, S., Voisin, D., and Wortham, H.: Kinetics of OH-initiated oxidation of oxygenated organic compounds in the aqueous phase: new rate constants, structure-activity relationship and atmospheric implications, Atmos. Environ., 39, 7667-7688, 2005.

Monod, A. and Doussin, J. F.: Structure-activity relationship for the estimation of OH-oxidation rate constants of aliphatic organic compounds in the aqueous phase: alkanes, alcohols, organic acids and bases, Atmos. Environ., 42, 7611-7622, 2008.

Pandis, S. N. and Seinfeld, J. H.: Sensitivity analysis of a chemical mechanism for aqueous-phase atmospheric chemistry, J. Geophys. Res., 94(D1), 1105, doi:10.1029/JD094iD01p01105, 1989.

Sander, R and P.J. Crutzen, Model study indicating halogen activation and ozone destruction in polluted air masses transported to the sea, J. Geophys. Res., 101, 9121-9138, 1996.

Sander, S. P., Friedl R. R., D. M. Golden, M.J. Kurylo, R. E. Huie, V. L. Orkin, G. K. Moortgaat, A. R. Ravishankara, C. E. Kolb,M.J. Molina, and B.J. Finlayson-Pitts. Chemical kinetics and photochemical data for use in stratospheric modeling, Evaluation No. 14. JPL 02-25,Jet Propulsion Laboratory, NASA, 2003, available from http://jpldataeval.jpl.nasa.gov/. (Abbrev: JPL 2003).

Tan, Y., Perri, M. J., Seitzinger, S. P., and Turpin, B. J.: Effects of precursor concentration and acidic surfate in aqueous glyoxal-OH radical oxidation and implications for secondary organic aerosol, Environ. Sci. Technol, 43, 8105-8112, 2009.

Warneck P.: The relative importance of various pathways for the oxidation of sulfur dioxide and nitrogen dioxide in sunlit continental fair weather clouds, Phys. Chem. Chem. Phys., 1, 5471-5483, 1999.