Supplementary Material

Chemical Insights, Explicit Chemistry and Yields of Secondary Organic Aerosol from Methylglyoxal and Glyoxal

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The supporting information contains 10 pages with following information: the chemical model (Table S1); the simulated concentration of dissolved oxygen during an experiment (Fig. S1); atmospheric CSTR simulated SOA yields (Fig. S2).

Table S1. Reactions and rate/equilibrium constants used in the full kinetic model of unified glyoxal/methylglyoxal + OH

	Reactions	**Rate constants (M^{1-n} s^{-1})**	**Ref**
1	$H_2O_2 \rightarrow 2OH$	1.1e-4×Trans[a]	T, e
2	$OH + H_2O_2 \rightarrow HO_2 + H_2O$	2.7e7	T
3	$HO_2 + H_2O_2 \rightarrow OH + H_2O + O_2$	3.7	T
4	$2\ HO_2 \rightarrow H_2O_2 + O_2$	8.3e5	T
5	$OH + HO_2 \rightarrow H_2O + O_2$	7.1e9	T
6	$HO_2 + O_2^- + H^+ \rightarrow H_2O_2 + O_2$	1e8	T
7	$2OH \rightarrow H_2O_2$	5.5e9	T
8	$OH + O_2^- \rightarrow OH^- + O_2$	1e10	T
9	$O_{2g} \leftrightarrow O_2$	K_{eq} = 1.3e-3 k_r = 5.3e2	T, W
10	$CO_{2g} \leftrightarrow CO_2$	K_{eq} = 3.4e-2 k_r = 5.3e2	T, W
11	$CO_2 \leftrightarrow H^+ + HCO_3^-$	K_{eq} = 4.3e-7 k_r = 5.6e4	T
12	$HCO_3^- \rightarrow H^+ + CO_3^{-2}$	K_{eq} = 4.69e-11 k_r = 5.0e10	T
13	$CO_2^- + O_2 \rightarrow O_2^- + CO_2$	2.4e9	T
14	$HCO_3^- + OH \rightarrow CO_3^- + H_2O$	1e7	T
15	$CO_3^- + O_2^- \rightarrow CO_3^{-2} + O_2$	6.5e8	T
16	$CO_3^- + HCO_2^- \rightarrow HCO_3^- + CO_2^-$	1.5e5	T
17	$CO_3^- + H_2O_2 \rightarrow HCO_3^- + HO_2$	8e5	T
18	GCOLAC + OH → GCOLAC* + H2O	6.0e8	T
19	GCOLAC* + O_2 → GCOLACOO*	1e6	G, L’
20	GCOLACOO* → GLYAC + HO_2	5e1	C
21	2GCOLACOO* → 2GCOLACO* + O_2	3e8*0.95	L’, e
22	2GCOLACOO* → GLYAC + OXLAC + O_2	3e8*0.05	L’, e
23	GCOLACO* → HCO_2H + CO_2	I	Gi, e
24	GCOLACO* → GLYAC*	1e7	Gi, e
25	GCOLAC ↔ H^+ + $GCOLAC^-$	K_{eq} = 1.48e-4 k_r = 2.0e10	T
26	$GCOLAC^-$ + OH → $GCOLAC^{*-}$ + H_2O	6.0e8	T
27	$GCOLAC^{*-}$ + O_2 → $GCOLACOO^{*-}$	1e6	G, L’
28	$GCOLACOO^{*-}$ → $GLYAC^-$ + HO_2	5e1	C
29	$2GCOLACROO^{*-}$ → $2GCOLACO^{*-}$ + O_2	3e8×0.95	L’, e
30	2 $GCOLACROO^{*-}$ → $GLYAC^-$ + $OXLAC^-$+ O_2	3e8×0.05	L’, e
31	$GCOLACO^{*-}$ → HCO_2H + CO_2^-	I	Gi, e
32	$GCOLACO^{*-}$→ $GLYAC^{*-}$	1e7	Gi, e
33	GLY + OH → GLY* + H_2O	1.1e9	T
34	GLY* + O_2 → GLYOO*	1e6	G, L’
35	GLYOO* → GLYAC + HO_2	5e1	C
36	2GLYOO* → 2*CHOHOH + 2CO_2 + O_2 + 2H_2O	3e8	L’
37	*CHOHOH + O_2 → HCO_2H + HO_2	5e6	G, L’
38	GLYAC + OH → GLYAC* + H_2O	3.62e8	T
39	GLYAC* + O_2 → GLYACOO*	1e6	G, L’
40	GLYACOO* → OXLAC + HO_2	5e1	C

41	2GLYACOO* $\rightarrow$ 2CO_2 + 2COOH	3e8	L'
42	*COOH + O_2 $\rightarrow$ CO_2 + HO_2	5e6	G, L'
43	GLYAC $\leftrightarrow$ H^+ + $GLYAC^-$	K_{eq} = 3.47e-4 K_r = 2.0e10	T
44	$GLYAC^-$ + OH $\rightarrow$ $GLYAC^{*-}$ + H_2O	1.28e7	T
45	$GLYAC^-$ + OH $\rightarrow$ GLYAC* + OH^-	2.9e9	T
46	$GLYAC^{*-}$ + O_2 $\rightarrow$ $GLYACOO^{*-}$	1e6	G, L'
47	$GLYACOO^{*-}$ $\rightarrow$ $OXLAC^-$ + HO_2	1e2	C, L'
48	2$GLYACOO^{*-}$ $\rightarrow$ 2CO_2^- + 2*COOH	3e8	L'
49	MGLY + OH $\rightarrow$ MGLY* + H_2O	7.0e8×0.92	T
50	MGLY + OH $\rightarrow$ *MGLY + H_2O	7.0e8×0.08	T
51	MGLY* + O_2 $\rightarrow$ MGLYOO*	1e6	G, L'
52	MGLYOO* $\rightarrow$ PYRAC + HO_2	5e1	C
53	2MGLYOO* $\rightarrow$ 2CO_2 + 2CH_3CO_2H + O_2	3e8	L'
54	*MGLY + O_2 $\rightarrow$ *OOMGLY	1e6	G, L'
55	2*OOMGLY $\rightarrow$ 2*OMGLY + O_2	3e8×0.95	L', e
56	2*OOMGLY $\rightarrow$ HOMGLY + OMGLY + O_2	3e8×0.05	L', e
57	*OMGLY $\rightarrow$ HCHO + GLY*	I	Gi, e
58	*OMGLY $\rightarrow$ *HOMGLY	1e7	Gi, e
59	HOMGLY + OH $\rightarrow$ *HOMGLY + H_2O	4.10e7	M
60	*HOMGLY + O_2 $\rightarrow$ *OOHOMGLY	1e6	G, L'
61	*OOHOMGLY $\rightarrow$ OMGLY + HO_2	5e1	C
62	OMGLY + OH $\rightarrow$ *OMGLY + H_2O	6.17e9	M
63	*OMGLY + O_2 $\rightarrow$ *OOOMGLY	5e1	C
64	GLY* + *CHOHOH $\rightarrow$ C3D	1.3e9	G, L'
65	2GLY* $\rightarrow$ C4D	1.3e9	G, L'
66	GLY* + *COOH $\rightarrow$ C3D	1.3e9	G, L'
67	GLYAC* + *COOH $\rightarrow$ C3D	1.3e9	G, L'
68	GLYAC* + *CHOHOH $\rightarrow$ C3D	1.3e9	G, L'
69	2GLYAC* $\rightarrow$ C4D	1.3e9	G, L'
70	GLYAC* + GLY* $\rightarrow$ C4D	1.3e9	G, L'
71	$GLYAC^{*-}$ + GLY* $\rightarrow$ C4D	1.3e9	G, L'
72	$GLYAC^{*-}$ + GLYAC* $\rightarrow$ C4D	1.3e9	G, L'
73	2$GLYAC^{*-}$ $\rightarrow$ C4D	1.3e9	G, L'
74	$GLYAC^{*-}$ + *COOH $\rightarrow$ C3D	1.3e9	G, L'
75	$GLYAC^{*-}$ + *CHOHOH $\rightarrow$ C3D	1.3e9	G, L'
76	$GLYCOL^{*1}$ + *CHOHOH $\rightarrow$ C3D	1.3e9	G, L'
77	$GLYCOL^{*1}$ + GLY* $\rightarrow$ C4D	1.3e9	G, L'
78	$GLYCOL^{*1}$ + *COOH $\rightarrow$ C3D	1.3e9	G, L'
79	$GLYCOL^{*1}$ + GLYAC* $\rightarrow$ C4D	1.3e9	G, L'
80	$GLYCOL^{*1}$ + $GLYAC^{*-}$ $\rightarrow$ C4D	1.3e9	G, L'
81	$GLYCOL^{*2}$ + *CHOHOH $\rightarrow$ C3D	1.3e9	G, L'
82	$GLYCOL^{*2}$ + GLY* $\rightarrow$ C4D	1.3e9	G, L'
83	$GLYCOL^{*2}$ + *COOH $\rightarrow$ C3D	1.3e9	G, L'
84	$GLYCOL^{*2}$ + GLYAC* $\rightarrow$ C4D	1.3e9	G, L'
85	GCOLAC* + *CHOHOH $\rightarrow$ C3D	1.3e9	G, L'
86	GCOLAC* + GLY* $\rightarrow$ C4D	1.3e9	G, L'
87	GCOLAC* + *COOH $\rightarrow$ C3D	1.3e9	G, L'
88	GCOLAC* + GLYAC* $\rightarrow$ C4D	1.3e9	G, L'
89	GCOLAC* + $GLYAC^{*-}$ $\rightarrow$ C4D	1.3e9	G, L'

90	GCOLAC* + GLYCOL*^{1} → C4D	1.3e9	G, L’
91	GCOLAC* + GLYCOL*^{2} → C4D	1.3e9	G, L’
92	GCOLAC* + GCOLAC* → C4D	1.3e9	G, L’
93	GCOLAC*$^-$ + *CHOHOH → C3D	1.3e9	G, L’
94	GCOLAC*$^-$ + GLY* → C4D	1.3e9	G, L’
95	GCOLAC*$^-$ + *COOH → C3D	1.3e9	G, L’
96	GCOLAC*$^-$ + GLYAC* → C4D	1.3e9	G, L’
97	GCOLAC*$^-$ + GLYAC*$^-$ → C4D	1.3e9	G, L’
98	GCOLAC*$^-$ + GLYAC*$^-$ → C4D	1.3e9	G, L’
99	GCOLAC*$^-$ + GLYCOL*^{1} → C4D	1.3e9	G, L’
100	GCOLAC*$^-$ + GLYCOL*^{2} → C4D	1.3e9	G, L’
101	GCOLAC*$^-$ + GCOLAC* → C4D	1.3e9	G, L’
102	2 GCOLAC*$^-$ → C4D	1.3e9	G, L’
103	2MGLY* → C6D	1.3e9	G, L’
104	MGLY* + *CHOHOH → C4D	1.3e9	G, L’
105	MGLY* + GLY* → C5D	1.3e9	G, L’
106	MGLY* + *COOH → C4D	1.3e9	G, L’
107	MGLY* + GLYAC* → C5D	1.3e9	G, L’
108	MGLY* + GLYAC*$^-$ → C5D	1.3e9	G, L’
109	MGLY* + GLYCOL*^{1} → C5D	1.3e9	G, L’
110	MGLY* + GLYCOL*^{2} → C5D	1.3e9	G, L’
111	MGLY* + GCOLAC* → C5D	1.3e9	G, L’
112	MGLY* + GCOLAC*$^-$ → C5D	1.3e9	G, L’
113	MGLY* + CH_3CO* → C5D	1.3e9	G, L’
114	MGLY* + *HOPYRAC → C6D	1.3e9	G, L’
115	2*HOPYRAC → C6D	1.3e9	G, L’
116	MGLY* + *HOPYRAC$^-$ → C6D	1.3e9	G, L’
117	*HOPYRAC$^-$ + *HOPYRAC$^-$ → C6D	1.3e9	G, L’
118	*HOPYRAC + *HOPYRAC$^-$ → C6D	1.3e9	G, L’
119	CH_3CO* + *HOPYRAC → C6D	1.3e9	G, L’
120	CH_3CO* + *HOPYRAC$^-$ → C6D	1.3e9	G, L’
121	2LA* → C6D	1.3e9	G, L’
122	LA* + MGLY* → C6D	1.3e9	G, L’
123	LA* + *CHOHOH → C4D	1.3e9	G, L’
124	LA* + GLY* → C5D	1.3e9	G, L’
125	LA* + *COOH → C4D	1.3e9	G, L’
126	LA* + GLYAC* → C5D	1.3e9	G, L’
127	LA* + GLYAC*$^-$ → C5D	1.3e9	G, L’
128	LA* + GLYCOL*^{1} → C5D	1.3e9	G, L’
129	LA* + GLYCOL*^{2} → C5D	1.3e9	G, L’
130	LA* + GCOLAC* → C5D	1.3e9	G, L’
131	LA* + GCOLAC*$^-$ → C5D	1.3e9	G, L’
132	LA* + CH_3CO* → C5D	1.3e9	G, L’
133	2CH_3CO* → C4D	1.3e9	G, L’
134	LA* + *HOPYRAC → C6D	1.3e9	G, L’
135	LA* + *HOPYRAC$^-$ → C6D	1.3e9	G, L’
136	OXLAC + OH → COOH + CO_2 + H_2O	1.4e6	T
137	OXLAC ↔ H^+ + OXLAC$^-$	K_{eq} = 5.67e-2 k_r = 5.0e10	T
138	OXLAC$^-$ + OH → COOH + CO_2^- + H_2O	2.0e7	T, L’

139	$OXLAC^- \leftrightarrow H^+ + OXLAC^{-2}$	K_{eq} = 5.42e-5 k_r = 5e10	T
140	$OXLAC^{-2} + OH \rightarrow *COOH + CO_2^- + OH^-$	4.0e7	T, L’
141	$LA + OH \rightarrow LA* + H_2O$	4.3e8	H
142	$LA* + O_2 \rightarrow LAOO*$	1e6	G, L’
143	$LAROO* \rightarrow PYRAC + HO_2$	5e1	C
144	$LA \leftrightarrow LA^- + H^+$	K_{eq} = 1.38e-4 k_r = 5.0e10	E&C
145	$LA^- + OH \rightarrow LA*^- + H_2O$	3e8	B
146	$LA*^- + O_2 \rightarrow LAOO*^-$	1e6	G, L’
147	$LAOO*^- \rightarrow PYRAC^- + HO_2$	5e1	C
148	$PYRAC + OH \rightarrow PYRAC* + H_2O$	6.0e7×0.85	T
149	$PYRAC + OH \rightarrow CH_3CO* + CO_2 + H_2O$	6.0e7×0.15	T
150	$CH_3CO* + O_2 \rightarrow CH_3C(O)OO*$	1e6	G, L’
151	$CH3C(O)OO* \rightarrow CH_3CO_2H + HO_2$	5e1	C
152	$2CH3C(O)OO* \rightarrow 2CH_3C(O)O* + O_2$	3e8	L’
153	$CH_3C(O)O* \rightarrow CO_2 + HCHO$	1e7	Gi
154	$PYRAC* + O_2 \rightarrow PYRACOO*$	1e6	G, L’
144	$2PYRACOO* \rightarrow 2PYRACO* + O_2$	3e8×0.95	L’, e
145	$2PYRACOO* \rightarrow HOPYRAC + OPYRAC + O_2$	3e8×0.15	L’, e
146	$PYRACO* \rightarrow HCHO + GLYAC*$	I	Gi, e
147	$PYRACO* \rightarrow *HOPYRAC$	1e7	Gi, e
148	$HOPYRAC + OH \rightarrow *HOPYRAC + H_2O$	3.6e8	H
149	$*HOPYRAC + O_2 \rightarrow *OOHOPYRAC$	1e6	G, L’
150	$*OOHOPYRAC \rightarrow OPYRAC + HO_2$	5e1	C
151	$OPYRAC + OH \rightarrow *OPYRAC + H_2O$	5e7	e
152	$*OPYRAC + O_2 \rightarrow *OO(O)PYRAC$	1e6	G, L’
153	$*OO(O)PYRAC \rightarrow MOXLAC + HO_2$	5e1	C
154	$PYRAC \leftrightarrow PYRAC^- + H^+$	K_{eq} = 3.2e-3 k_r = 2e10	T
155	$PYRAC^- + OH \rightarrow PYRAC*^- + H_2O$	6.0e7×0.95	T
156	$PYRAC^- + OH \rightarrow CH3CO* + CO_2 + OH^-$	6.0e7×0.05	T
157	$PYRAC*^- + O_2 \rightarrow PYRACOO*^-$	5e1	C
158	$2PYRACOO*^- \rightarrow 2PYRACO*^- + O_2$	3e8×0.95	L’, e
159	$2PYRACOO*^- \rightarrow HOPYRAC^- + OPYRAC^- + O_2$	3e8×0.05	L’, e
160	$PYRACO*^- \rightarrow HCHO + GLYAC*^- + O_2$	I	Gi, e
161	$PYRACO*^- \rightarrow *HOPYRAC^-$	1e7	Gi, e
162	$HOPYRAC \leftrightarrow HOPYRAC^- + H^+$	K_{eq} = 3.2e-3 k_r = 2e10	e
163	$OPYRAC \leftrightarrow OPYRAC^- + H^+$	K_{eq} = 3.2e-3 k_r = 2e10	e
164	$HOPYRAC^- + OH \rightarrow *HOPYRAC^- + H_2O$	2.6e9	H
165	$*HOPYRAC^- + O_2 \rightarrow *OOHOPYRAC^-$	1e6	G, L’
166	$*OOHOPYRAC^- \rightarrow OPYRAC^- + HO_2$	5e1	C
167	$OPYRAC^- + OH \rightarrow *OPYRAC^- + H_2O$	5e7	M
168	$*OPYRAC^- + O2 \rightarrow *OO(O)PYRAC^-$	1e6	G, L’
169	$*OO(O)PYRAC^- \rightarrow MOXLAC^- + HO_2$	5e1	C
170	$MOXLAC + OH \rightarrow GLYAC* + CO_2 + H_2O$	5.7e7	Gl
171	$MOXLAC^- + OH \rightarrow GLYAC*^- + CO_2 + H_2O$	7.85e7	e
172	$MOXLAC^{-2} + OH \rightarrow GLYAC*^- + CO_2 + OH^-$	1.0e8	H

173	$MOXLAC \leftrightarrow MOXLAC^- + H^+$	K_{eq} = 3.16e-3 k_r = 5e10	H
174	$MOXLAC^- \leftrightarrow MOXLAC^{-2} + H^+$	K_{eq} = 1.5e-2 k_r = 5e10	V
175	$CH_3CO_2H + OH \rightarrow *CH_2CO_2H + H_2O$	1.36e7	T
176	$CH_3CO_2H + OH \rightarrow CO_2 + HCHO + HO_2 + H_2O$	2.40e6	T
177	$*CH_2CO_2H + O_2 \rightarrow *OOCH_2CO_2H$	1e6	G, L’
178	$2*OOCH_2CO_2H \rightarrow 2*OCH_2CO_2H + O_2$	3e8*0.95	L’, e
179	$2*OOCH_2CO_2H \rightarrow GLYAC + GCOLAC + O_2$	3e8*0.05	L’, e
180	$*OCH_2CO_2H \rightarrow 2CO_2 + 2HCHO$	I	Gi, e
181	$*OCH_2CO_2H \rightarrow GCOLAC*$	1e7	Gi, e
182	$CH_3CO_2H \leftrightarrow CH_3CO_2^- + H^+$	K_{eq} = 1.75e-5 k_r = 5.0e10	T
183	$CH_3CO_2^- + OH \rightarrow *CH_2CO_2^- + H_2O$	7.23e7	T
184	$CH_2CO_2^- + OH \rightarrow CO_2 + HCHO + HO_2 + OH^-$	1.28e7	T
185	$*CH_2CO_2^- + O_2 \rightarrow *OOCH_2CO_2^-$	1e6	G, L’
186	$2*OOCH_2CO_2n1 \rightarrow 2*OCH_2CO_2 + O_2$	3e8×0.95	L’, e
187	$2*OOCH_2CO_2^- \rightarrow GLYAC^- + GCOLAC^- + O2$	3e8×0.05	L’, e
188	$*OCH_2CO_2^- \rightarrow 2CO_2^- + 2HCHO$	I	Gi, e
189	$*OCH_2CO_2^- \rightarrow GCOLAC*^-$	1e7	Gi, e
190	$H_2O \leftrightarrow H^+ + OH^-$	K_{eq} = 1.0e-14 k_r = 1.4e11	T
191	$HO_2 \leftrightarrow H^+ + O_2^-$	K_{eq} = 1.6e-5 k_r = 5.0e10	T
192	$HCO_2H + OH \rightarrow *COOH + H_2O$	1e8	T
193	$HCO_2^- + OH \rightarrow CO_2^- + H_2O$	2.4e9	T
194	$HCO_2H \leftrightarrow H^+ + HCO_2^-$	K_{eq} = 1.77e-4 k_r = 5.0e10	T
195	$GLYAC + H_2O_2 \rightarrow HCO_2H + CO_2 + H_2O$	0.3	T
196	$PYRAC + H_2O_2 \rightarrow CH_2CO_2H + H_2O + CO_2$	0.11	T
197	$PYRAC^- + H_2O_2 \rightarrow CH_2CO_2^- + H_2O + CO_2$	0.11	T
198	$MOXLAC + H_2O_2 \rightarrow OXLAC + CO_2 + H_2O$	0.5	T
199	$MOXLAC^- + H_2O_2 \rightarrow OXLAC^- + CO_2 + H_2O$	0.5	T
200	$HCO_2H + OH \rightarrow COOH + H_2O$	1e8	T
201	$HCO_2^- + OH \rightarrow CO_2^- + H_2O$	2.4e9	T
202	$HCO_2H \leftrightarrow H^+ + HCO_2^-$	K_{eq} = 1.77e-4 k_r = 5.0e10	T
203	$2*CHOHOH \rightarrow GLY$	1.3e9	G, L’
204	$*CHOHOH + *COOH \rightarrow GLYAC$	1.3e9	G, L’
205	$2*COOH \rightarrow OXLAC$	1.3e9	G, L’
206	$C3D \leftrightarrow MA + H2O$	K_{eq} = 1e5 k_r = 1e-8	L’
207	$MA + OH \rightarrow C3D* + H_2O$	1.6e7	E
208	$TA + OH \rightarrow C4D* + H_2O$	3.1e8	M
209	$2*COOH \rightarrow OXLAC$	1.3e9	G, L’
210	$CO_2^- + *COOH \rightarrow OXLAC^-$	1.3e9	G, L’
211	$2CO_2^- \rightarrow OXLAC^{-2}$	1.3e9	G, L’
212	$PYRAC^- \rightarrow 0.45CH_3CO_2^{-}$ [b]	1e-4 [b]	C, e

[a]Trans = Transmittance = $10^{-18.4 \times 0.80 \times [H_2O_2]}$; * = radical (e.g., glyoxal* = glyoxal radical); *[n] = radical type n (e.g., GLYCOLAC*[1] = glycolic acid radical type 1); O* (or *O) = alkoxy radical ; OO* (or *OO) = peroxy radical; CnD = C_n dimer (e.g., C2D = C_2 dimer); X_g = X in the gas phase (e.g., O_{2g} = O_2 in the gas

phase); MGLY = methylglyoxal, PYRAC = pyruvic acid, GLYAC = glyoxylic acid, GLYCOL = glycolaldehyde, GLYCOLAC = glycolic acid, LA = lactic acid, MOXLAC = mesoxalic acid, OXLAC = oxalic acid; n = n^{th} order; K_{eq} = the equilibrium constant (M), k_r = the reverse rate constant for corresponding K_{eq}., Thus, the forward rate constant can be calculated by $K_{eq} \times k_r$; (g) = in the gas phase; I (= the decomposition rate constant from alkoxy radicals) = 5e6 s^{-1} for ~10μM acetic acid/methylglyoxal, 8e6 s^{-1} for ~10^2 μM acetic acid/methylglyoxal, and 2e7 s^{-1} for ~10^3μM acetic acid/ 3.2e7 s^{-1} for ~10^3μM methylglyoxal; [b] PYRAC is assumed to photolyze to produce only 45% acetic acid with 5 times slower than the literature value (Carlton et al., 2006).

Reference
T = Tan et al., 2009, 2010 and 2012
G = Guzman et al., JPCA, 2006
C = Carter et al., JPC, 1979
H = Herrmann et al., AE, 2005
E = Ervens et al., PCCP, 2003
M = Monod et al., AE, 2005, 2008
L = Lim et al.,EST, 2005
L' = Lim et al., ACP, 2010
W = Warneck, PCCP, 1999
E&C = Eyal and Canari, Ind. Eng. Chem. Res., 1995
B = Buxton et al., JPCRD, 1988
Gi = Gilbert et al., 1976 and 1981
V = Volgger et al., J. Chrom. A, 1997
e = Estimation by fitting

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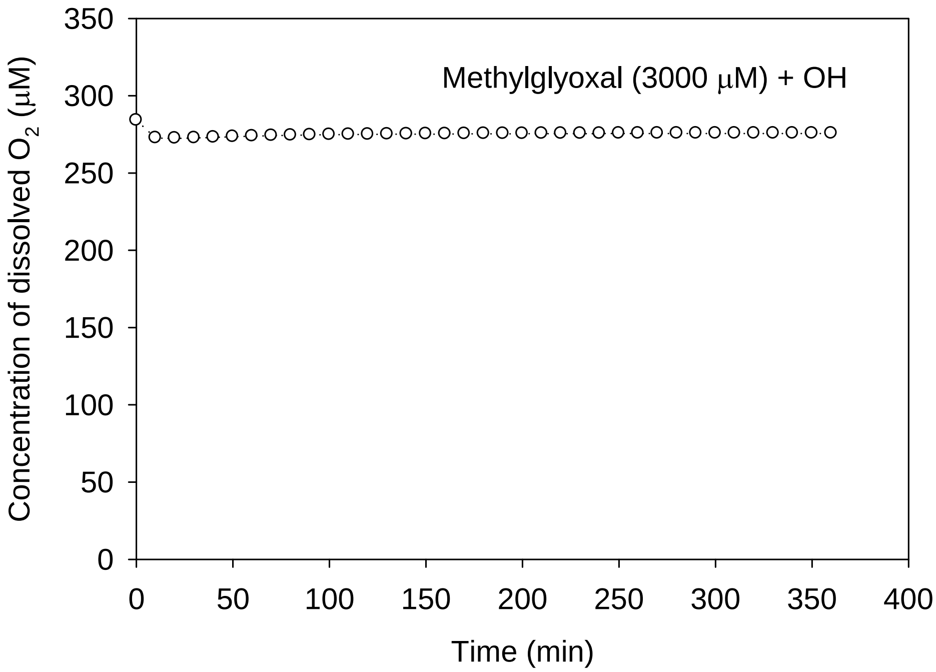

Figure S1. The simulated concentration of dissolved O_2 during the reaction of methylglyoxal (3000 μM) + OH

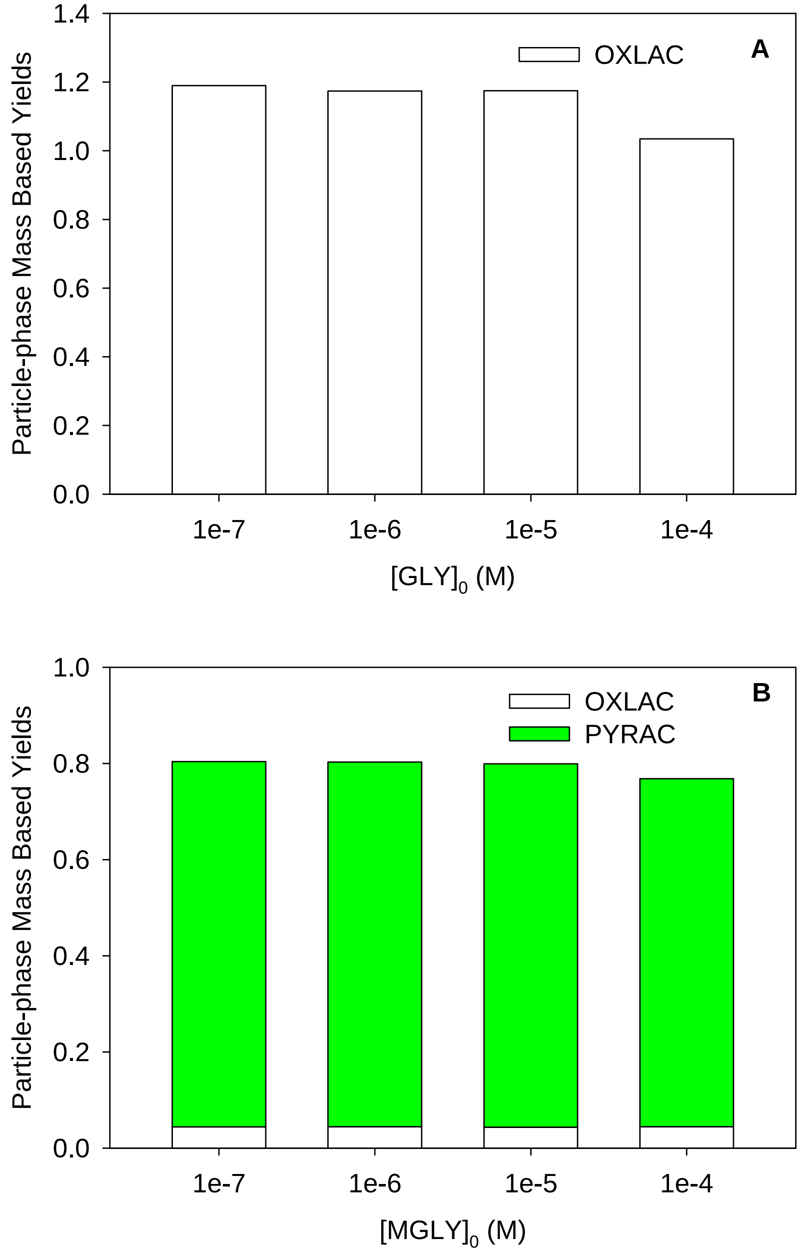

Figure S2. Atmospheric CSTR simulations **(A)** for particle-phase mass yields of oxalate (Y_{OXLAC}) with increasing initial concentrations of glyoxal ($[GLY]_0$) for aqueous-phase OH radical reactions ($Y_{OXLAC} = 1.19/(1+1450[GLY]_0)$; $Y_{SOA}(GLY) = Y_{OXLAC}$), and **(B)** for particle-phase mass yields of oxalate (Y_{OXLAC}) and pyruvate (Y_{PYRAC}) with increasing initial concentrations of methylglyoxal ($[MGLY]_0$) for aqueous-phase OH radical reactions($Y_{PYRAC} = 0.759/(1+495[MGLY]_0)$; $Y_{OXLAC} = 0.0439/(1-127[MGLY]_0)$; $Y_{SOA}(MGLY) = Y_{PYRAC} + Y_{OXLAC}$).