

Supplementary Information for

Kinetics of hypochlorous acid reactions with organic and chloride-containing tropospheric aerosol

Spiro D. Jorga^{1*}, Tengyu Liu², Yutong Wang¹, Sumaiya Hassan¹,

Han Huynh^{1,#} and Jonathan P. D. Abbatt^{1*}

¹Department of Chemistry, University of Toronto, Toronto, M5S 3H6, ON, Canada

²Joint International Research Laboratory of Atmospheric and Earth System Sciences, School of Atmospheric Sciences, Nanjing University, Nanjing, 210023, China

[#]now at: Cooperative Institute for Research in Environmental Sciences, University of Colorado, Boulder, Colorado 80309, USA

*Email: spiro.jorga@utoronto.ca, jonathan.abbatt@utoronto.ca

Table S1: Experimental conditions for the chloride-containing aerosol and HOCl experiments.

Exp #	RH (%)	Temperature (°C)	HOCl (ppb)	Cl ⁻ (M)	Malonic acid (M)	Aerosol pH	Ionic Strength (M)	$k_{\text{HOCl} + \text{H}^+ + \text{Cl}^-}$ (M ⁻² s ⁻¹)
1	70	20	600	2.2	2.9	3.6	8.0	5.3×10^4
2	83	20	600	1.5	1.8	3.1	4.2	1.8×10^4
3	78	25	600	1.8	2.7	3.2	5.3	3.4×10^4
4	83	21	600	1.5	1.8	3.1	4.1	1.1×10^4
5	63	22	600	2.5	3.5	3.8	10.5	1.7×10^5
6	63	22	600	2.4	4.2	3.7	9.6	2.7×10^5
7	63	22	600	2.4	4.2	3.7	9.6	2.2×10^5
8	61	21	600	2.5	4.3	3.7	10.3	1.9×10^5
9	61	21	600	2.5	4.3	3.7	10.3	2.5×10^5
10	61	23	600	2.5	4.4	3.7	10.3	2.4×10^5
11	65	21.5	600	2.4	3.6	3.7	9.5	3.4×10^5
12	65	21.5	600	2.4	3.6	3.7	9.5	2.8×10^5
13	65	21.5	600	2.4	3.6	3.7	9.5	2.6×10^5
14	62	21	600	2.5	3.8	3.8	10.5	1.9×10^5
15	62	21	600	2.5	3.8	3.8	10.5	3.2×10^5
16	80	22	600	1.5	3.1	2.9	4.3	5.9×10^3
17	80	22	1200	1.5	3.1	2.9	4.3	1.9×10^4
18	83	21	600	1.5	2.3	3.0	5.2	7.5×10^4
19	83	21	600	1.5	2.3	3.0	5.2	1.0×10^4
20	81	22	600	1.6	2.1	3.1	6.1	1.2×10^4
21	81	22	600	1.6	2.1	3.1	6.1	1.5×10^4
22	81	22	1200	1.6	2.1	3.1	6.1	2.9×10^4
23	78	21.5	1200	1.8	2.4	3.3	5.7	5.9×10^4
24	78	21.5	1200	1.8	2.4	3.3	5.7	6.2×10^4

Table S2: Experimental conditions for the organic aerosol and HOCl experiments.

Exp #	Aerosol type	RH (%)	Temperature (°C)	HOCl (ppm)	Solution pH
1	Coniferaldehyde	70	23	2.4	5.4
2	Coniferaldehyde	70	23	2.4	5.4
3	Coniferaldehyde	71	22	2.4	5.4
4	Coniferaldehyde	71	22	2.4	5.4
5	Coniferaldehyde	68	23	2.4	5.7
6	Coniferaldehyde	69	22	2.4	5.7
7	Furfural	71	22	2.4	4.1
8	Furfural	71	22	2.4	4.1
9	Furfural	66	23	2.4	4.1
10	Furfural	66	23	2.4	4.1
11	Salicylic acid	70	22.5	2.4	3.4
12	Salicylic acid	70	22	2.4	3.4
13	Salicylic acid	67	23	2.4	3.4
14	Salicylic acid	67	23	2.4	3.4
15	Furfural/buffer	75	21.5	2.4	3.9
16	Furfural/buffer	75	21	2.4	3.9
17	Furfural/buffer	75	21	2.4	3.9
18	Furfural/buffer	65	22	2.4	4
19	Furfural/buffer	68	22.5	2.4	4
20	Furfural/buffer	67	22	2.4	4
21	Furfural/buffer/NH4Cl	69	22.5	2.4	3.8
22	Furfural/buffer/NH4Cl	69	22	2.4	3.8
23	Furfural/buffer/NH4Cl	68	22.5	2.4	3.8
24	Furfural/buffer/NH4Cl	69	22	2.4	3.8
25	Furfural/buffer/NH4Cl	76	22	2.4	3.9
26	Furfural/buffer/NH4Cl	75	21	2.4	3.9
27	Furfural/buffer/NH4Cl	76	22	2.4	3.9
28	Furfural/buffer/NH4Cl	63	22	2.4	3.9
29	Biomass/buffer	62	22	2.4	4
30	Biomass/buffer	62	22	2.4	4
31	Biomass/buffer	63	21	2.4	4
32	Biomass/buffer	64	21.5	2.4	3.9
33	Biomass/buffer	64	22	2.4	3.9
34	Biomass/buffer/NH4Cl	64	21.8	2.4	4
35	Biomass/buffer/NH4Cl	64	22	2.4	4
36	Biomass/buffer/NH4Cl	64	22	2.4	4
37	Biomass/buffer/NH4Cl	64	22	2.4	4

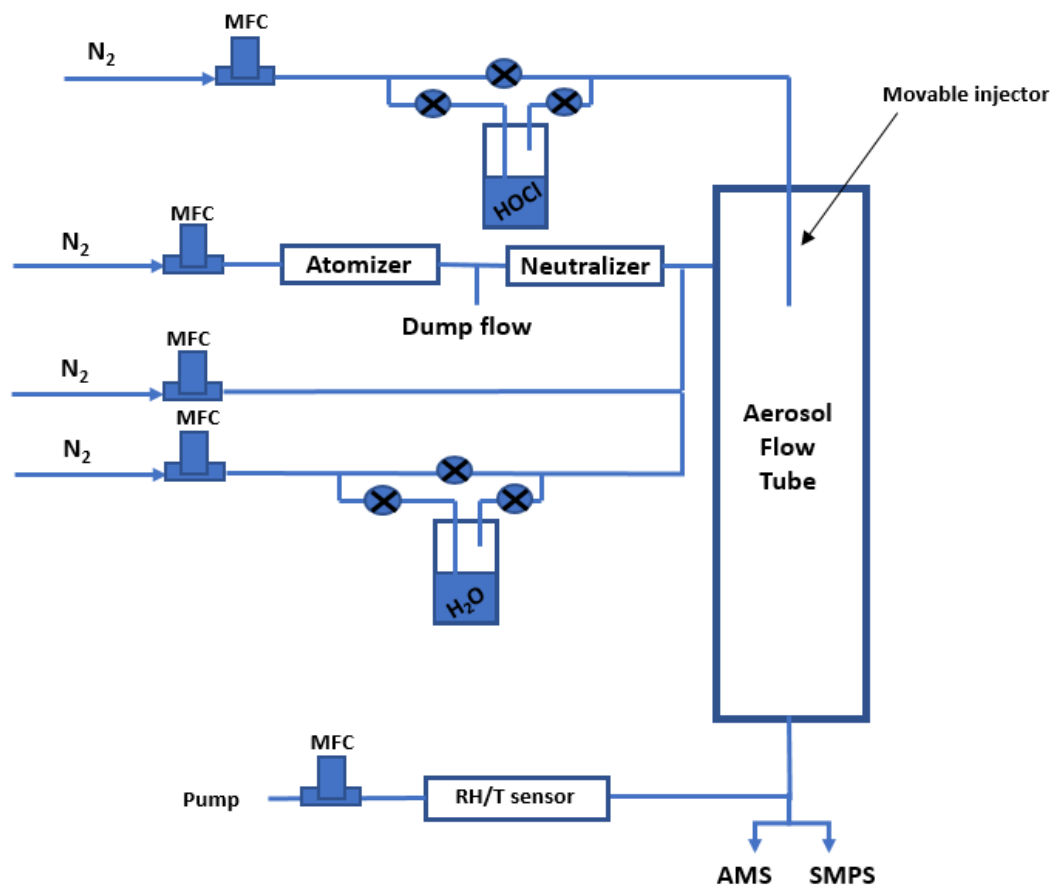


Figure S1: Schematic of the experimental set-up.

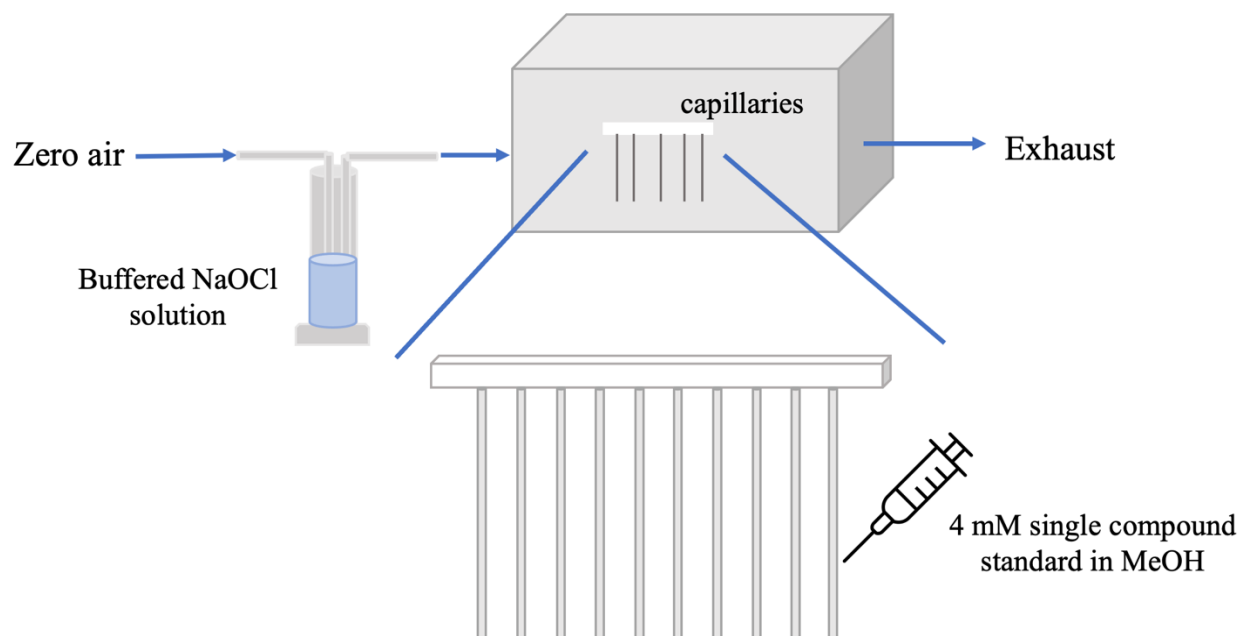


Figure S2: Experimental set-up for coniferaldehyde/salicylic acid HOCl exposure experiment.

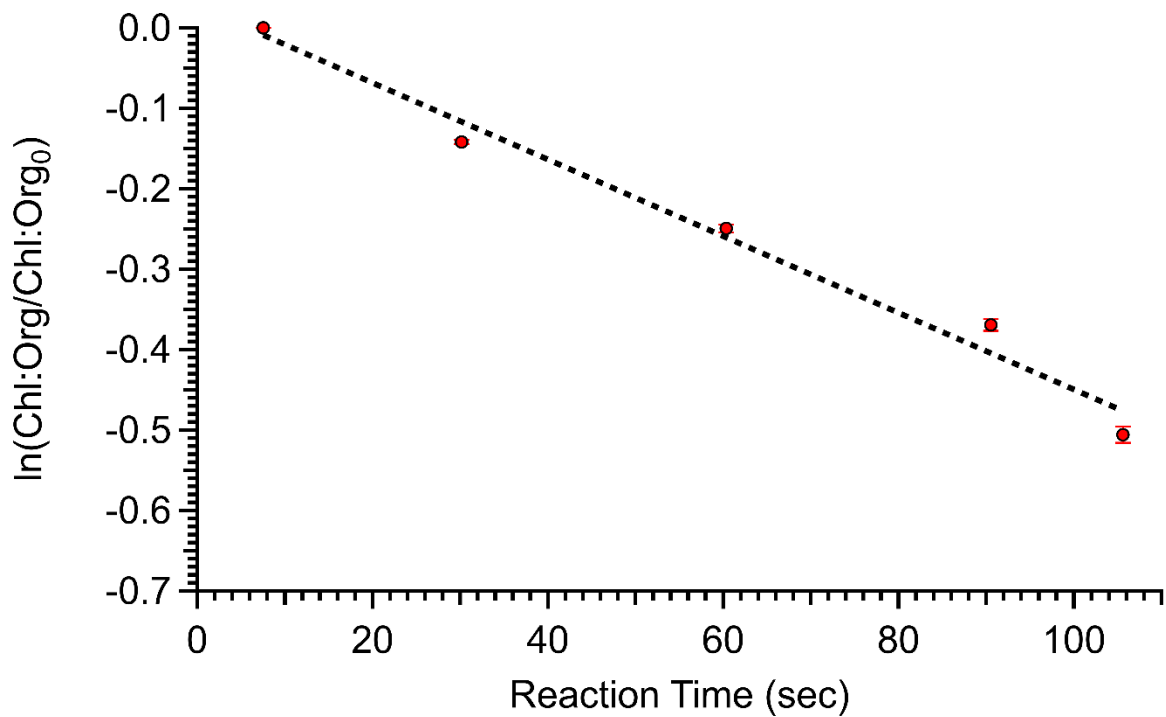


Figure S3: First order decay of $\ln(\text{Chl:Org})$ normalized to the ratio at the start of the experiment versus the reaction time in the flow tube. The results are referring to the HOCl and chloride experiment described in the main text (see Figure 1). The error bars represent one standard deviation and the dotted line the best fit of the slope.

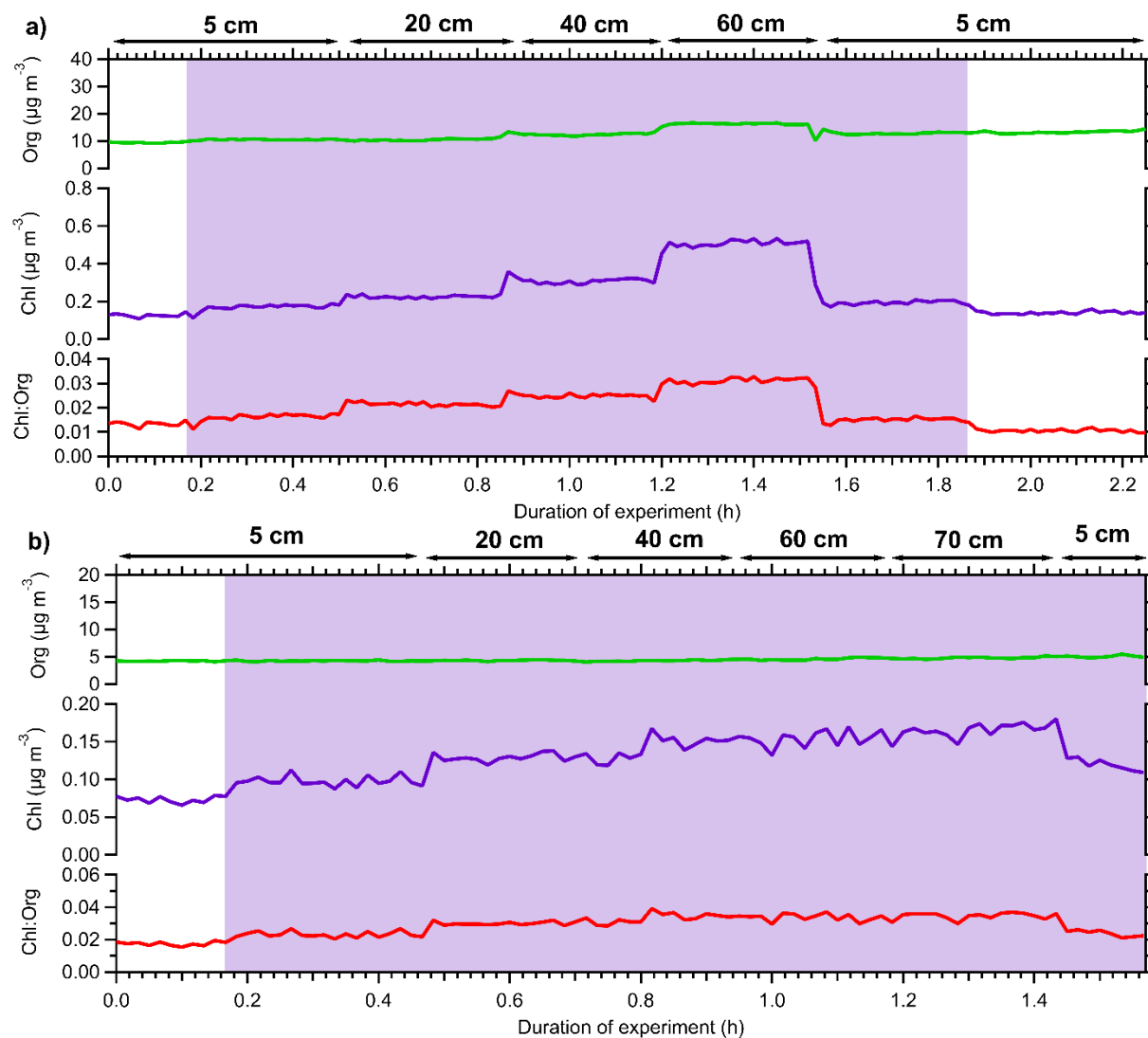


Figure S4: Time series of organic mass loading, chloride mass loading and Chl:Org ratio for a) coniferaldehyde and b) salicylic acid aerosol particles as exposed to HOCl (purple shaded area). Injector position in the flow tube is shown on the upper horizontal axis.

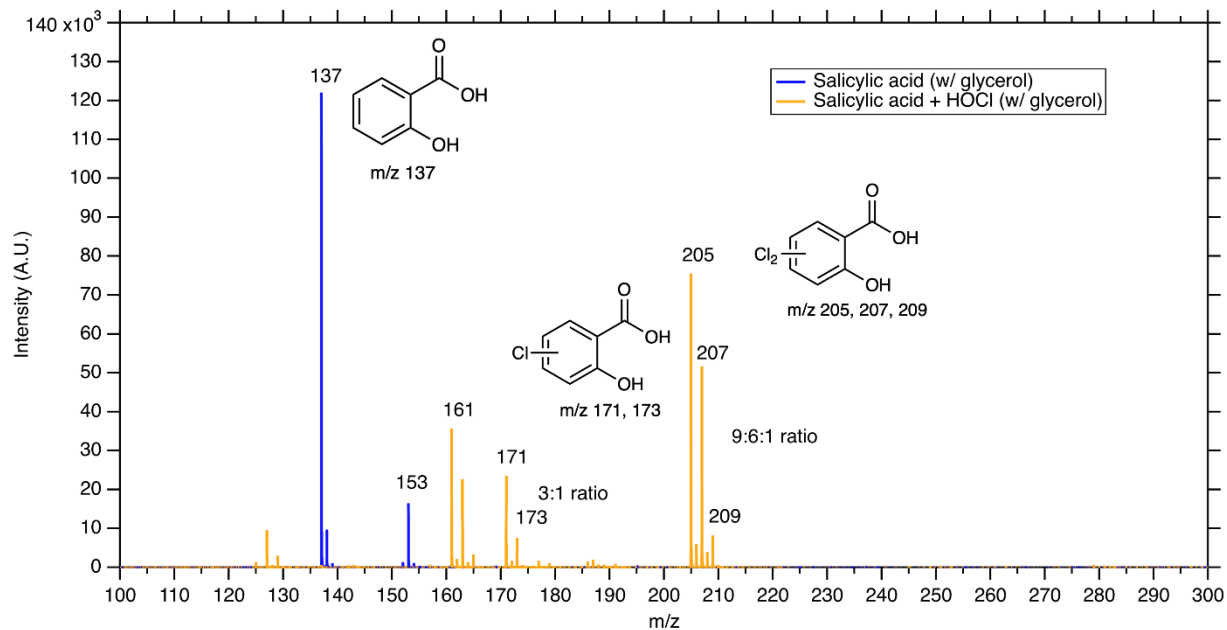


Figure S5: DART mass spectra (negative ion mode) of the glycerol-spiked salicylic acid before (blue) and after (orange) HOCl gaseous exposure. Chemical structures responsible for the corresponding mass peaks are shown along with the m/z of the observed ion and the approximate intensity ratio of clusters of peaks.