Supplementary Materials

Probing into the mechanisms of disinfection byproduct formation from natural organic matter and model compounds after UV/chlorine treatment

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Lists of Captions

Table S1. Rate constants of NOM and model compounds with free chlorine and radicals at pH 7.0.

□	$k_{chlorine}$ (M^{-1} s^{-1})	$k_{HO\bullet}$ (M^{-1} s^{-1})	$k_{Cl\bullet}$ (M^{-1} s^{-1})	$k_{Cl_2\bullet^-}$ (M^{-1} s^{-1})	$k_{ClO\bullet}$ (M^{-1} s^{-1})
NOM	2.4 [1]	3×10^8 [2]	1.6×10^8 [2]	1.7×10^7 [2]	5.4×10^8 [3]
Phenol	18 [4]	6.6×10^9 [5]	1.1×10^{10} [5]	3.2×10^8 [5]	3.4×10^6 [b]
Resorcinol	4×10^3 [4]	1.2×10^{10} [6]	1.4×10^{10} [a]	8.6×10^9 [a]	2.2×10^6 [b]
Benzoic acid	Negligible [4]	5.9×10^9 [7]	1.8×10^{10} [7]	2×10^6 [7]	$< 1 \times 10^6$ [7]
Methylamine	3.2×10^4 [4]	N.D.	N.D.	N.D.	N.D.
Dimethylamine	8.9×10^3 [4]	N.D.	N.D.	N.D.	N.D.
Tyrosine	~1×10^4 [4]	1.3×10^{10} [6]	1.2×10^{10} [a]	4.6×10^8 [a]	N.D.
Asparagine	~1×10^4 [4]	4.9×10^7 [6]	7.2×10^8 [a]	Negligible [a]	N.D.

N.D. = Not determined.

[a] Determined in this study.

[b] Assumed in this study.

Table S2. Alteration of UV absorbance at 254 nm (UV_{254}), DOC concentration and specific UV absorbance (SUVA) of NOM after chlorination, UV/chlorine and UV treatments.

□	UV_{254} (cm^{-1})	DOC (mg/L)	SUVA (L/mg/m)
Untreated NOM	0.1112	3	3.7
Chlorination	0.0892	2.7	3.3
UV/chlorine	0.0456	2.4	1.9
UV	0.1063	2.9	3.7

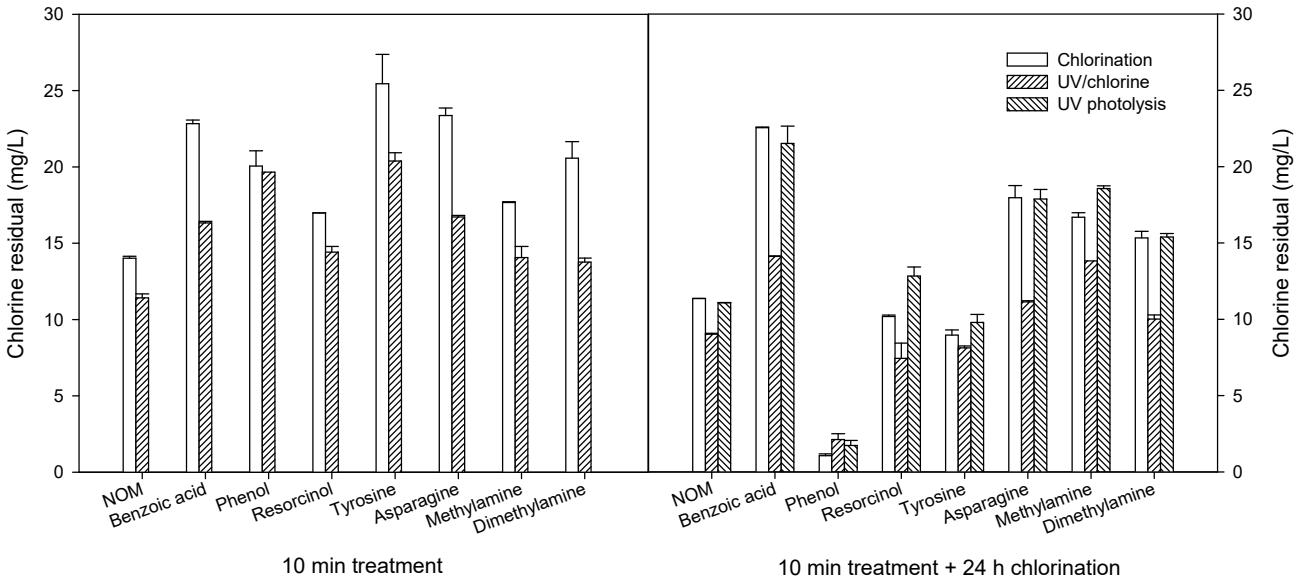

Figure S1. Chlorine residuals after 10 min UV, chlorination and UV/chlorine treatment, and 24 h post chlorination. Conditions: [NOM] = 3 mg/L, [model compounds] = 50 μM, [chlorine] = 15 mg/L for NOM, 300 μM for benzoate, methylamine, and dimethylamine, 500 μM for phenol, resorcinol, and asparagine, and 750 μM for tyrosine, pH = 7.0.

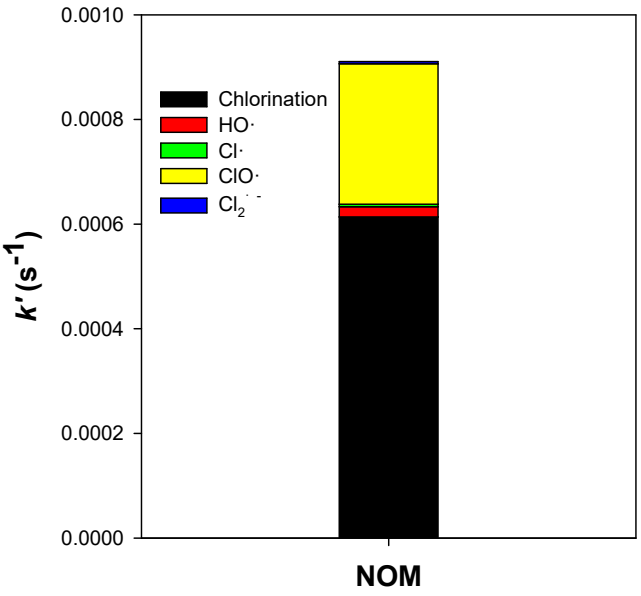

Figure S2. The contributions of reactive species to NOM transformation in the UV/chlorine process. Conditions: [NOM] = 3 mg/L, [chlorine] = 15 mg/L, pH = 7.0.

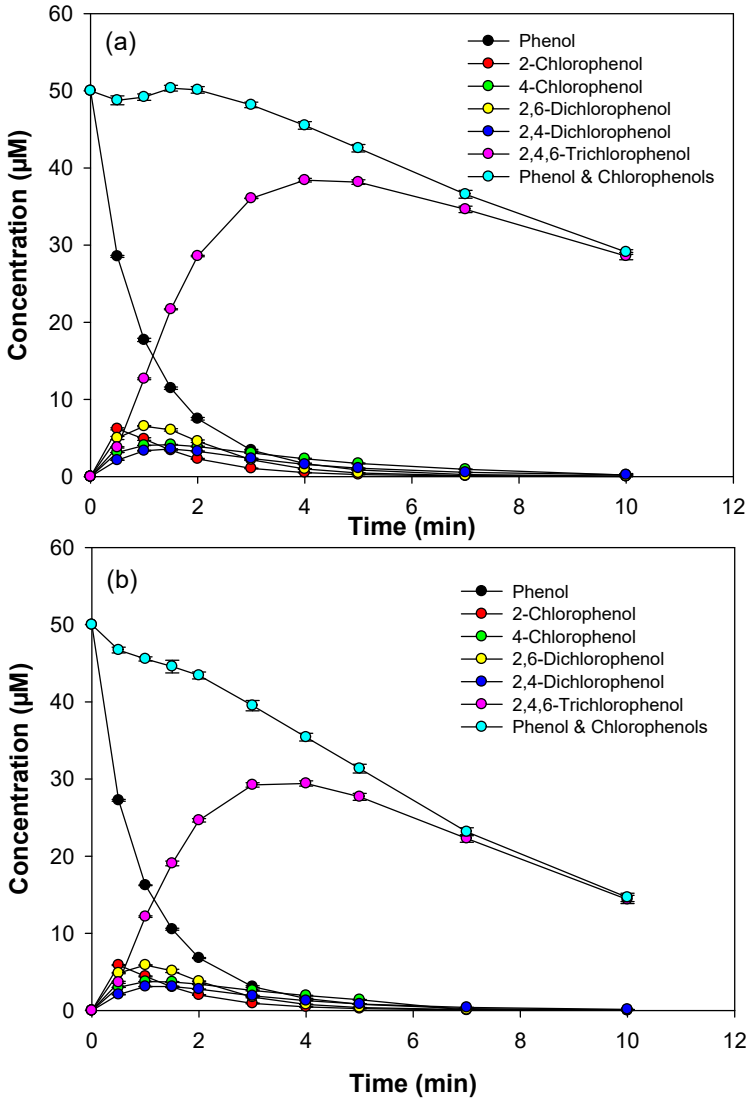

Figure S3. The degradation of phenol and the formation of chlorophenols in chlorination (a) and UV/chlorine process (b). Conditions: [phenol] = 50 μM, [chlorine] = 500 μM, pH = 7.0.

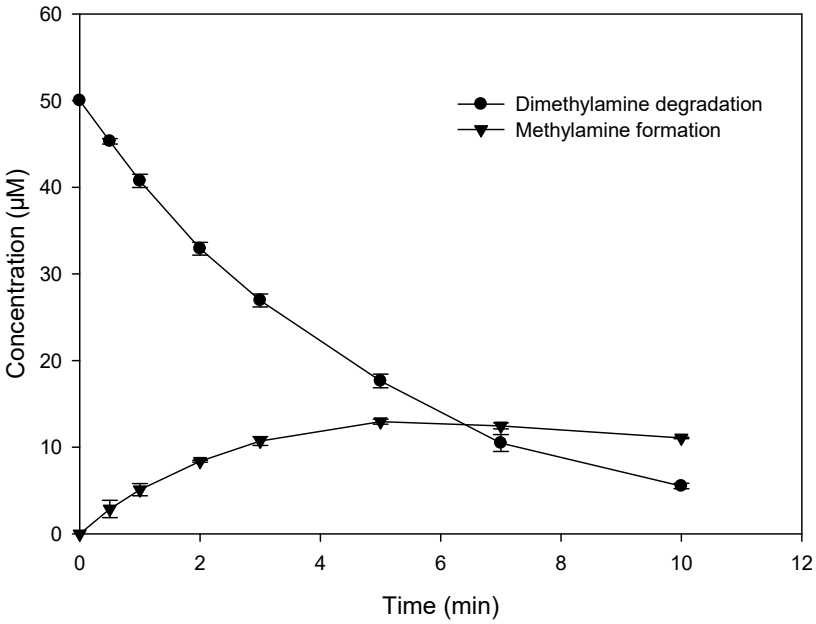

Figure S4. The formation of methylamine from dimethylamine during UV/chlorine treatment. Conditions: $[\text{dimethylamine}]_0$ = 50 μM, [chlorine] = 300 μM, pH = 7.0.

References

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