Supporting information

Effects of Polysaccharides and Proteins in EPS on DBPs Formation during Iron Release

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Tables:

Table S1 Gas chromatograph (GC) columns and oven temperature programs for the analysis of regulated THMs and HAAs.

	Pretreatment	Analytical Column	Injector Temp.	Detector Temp.	Oven Program	Limits of detection (μg /L)
Regulated THMs	Liquid-liquid extraction with MTBE	HP-5	200°C	290°C	Hold at 35°C for 9 min, ramp to 40°C at 2°C/min, hold for 1 min, ramp to 80°C at 20°C/min, ramp to 160°C at 40°C/min, and hold for 4 min	0.2 ~ 1.2
HAAs	Liquid-liquid extraction with MTBE, derivatization with acidic methanol	HP-5	200°C	290°C	Hold at 35°C for 4 min, ramp to 80°C at 1.5°C/min	1.0 ~ 2.6
HANs	Liquid-liquid extraction with MTBE	HP-5	200°C	290°C	Hold at 35°C for 9 min, ramp to 40°C at 2°C/min, hold for 1 min, ramp to 80°C at 20°C/min, ramp to 160°C at 40°C/min, and hold for 4 min	0.4 ~ 1.9

Table S2 LC50 and genetic potential values of DBPs

DBPs	LC50（M）	value of genetic potential（M）
TCM	9.62×10^{-3}	NA
BDCM	1.15×10^{-2}	NA
DBCM	5.36×10^{-3}	NA
TBM	3.96×10^{-3}	NA
TCAN	1.60×10^{-4}	1.01×10^{-3}
DCAN	5.73×10^{-5}	2.75×10^{-4}
BCAN	8.46×10^{-6}	3.24×10^{-4}
DBAN	5.82×10^{-6}	9.61×10^{-5}
CAA	8.10×10^{-4}	4.11×10^{-4}
BAA	9.60×10^{-6}	1.70×10^{-5}
DCAA	7.30×10^{-3}	NA
TCAA	2.40×10^{-3}	NA
DBAA	5.90×10^{-4}	1.76×10^{-3}

Table S3 Unit cytotoxicity and unit genotoxicity values for DBPs

DBPs	UCI	UGI
TCM	103.95	NA
BDCM	86.96	NA
DBCM	186.57	NA
TBM	252.52	NA
TCAN	6250	990.10
DCAN	17452.01	3636.36
BCAN	118203.30	3086.42
DBAN	350877.20	21231.42
CAA	1234.57	2433.09
BAA	104166.70	58823.53
DCAA	136.99	NA
TCAA	416.67	NA
DBAA	1694.82	568.18

Text

Text S1

Determination of DBPs toxicity

Cytotoxicity and genotoxicity were calculated based on previous studies(Muellner et al., 2007; Wagner and Plewa, 2017). Chronic cytotoxicity was calculated using a 72 h exposure assay in Chinese hamster ovary cells (CHO), and the LC50 value (DBPs concentration at 50% reduction in cell density) was calculated based on the concentration-cell density inhibition curve; for acute genotoxicity, DNA damage was measured by single-cell gel electrophoresis to derive the tail moments of genomic DNA damage, and the genetic potential value was calculated (concentration-tail-moment response curve midpoint value). Unit cytotoxicity (UCI) and unit genotoxicity (UGI) were defined as the reciprocal of cytotoxicity and genetic potential values, respectively, and were used to assess the toxicity of different DBPs. Multiplying the UCI and UGI with the concentration of DBPs in water gives the cytotoxicity value and genotoxicity value. The relevant LC50 and genetic potential values are listed in Table S2 and the UCI and UGI values are shown in Table S3

Figures:

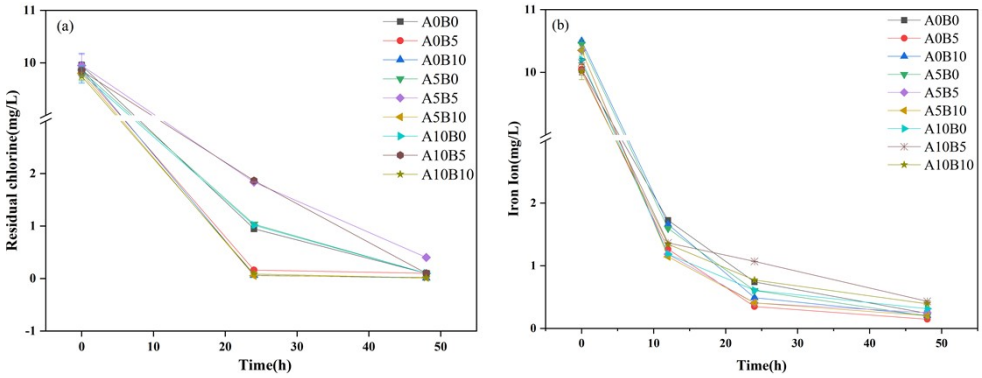

Figure S1 Changes in (a)residual chlorine and (b)iron concentrations during the chlorination process of BSA/SA samples with different concentration gradients. Reaction conditions: [initial chlorine concentration]$_0$ = 10 ± 0.2 mg/L, reaction time = 48 h, T = 25 ± 2 °C.
Variation of residual chlorine, Fe(II) concentration

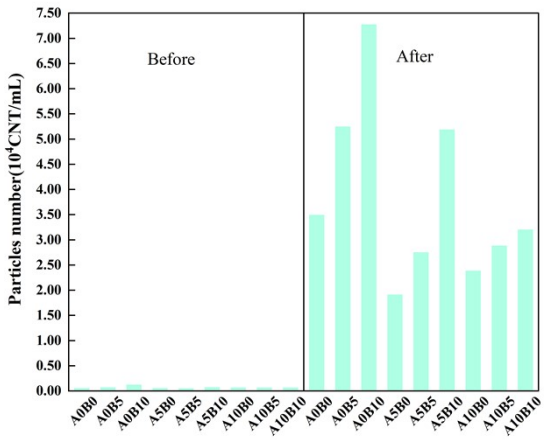

Figure S2 Changes in Particles number during the chlorination process of BSA/SA samples with different concentration gradients. Reaction conditions: $[\text{initial chlorine concentration}]_0 = 10 \pm 0.2$ mg/L, reaction time = 48 h, T = 25 ± 2 °C.

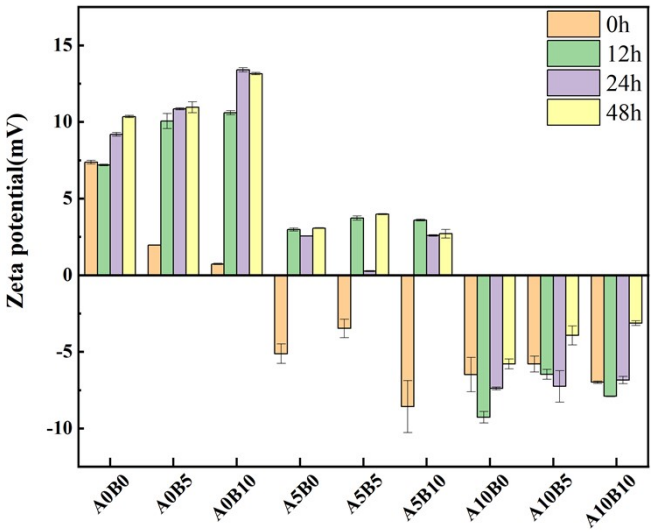

Figure S3 Changes in zeta potential during the chlorination process of BSA/SA samples with different concentration gradients. Reaction conditions: $[\text{initial chlorine concentration}]_0 = 10 \pm 0.2$ mg/L, reaction time = 48 h, T = 25 ± 2 °C.

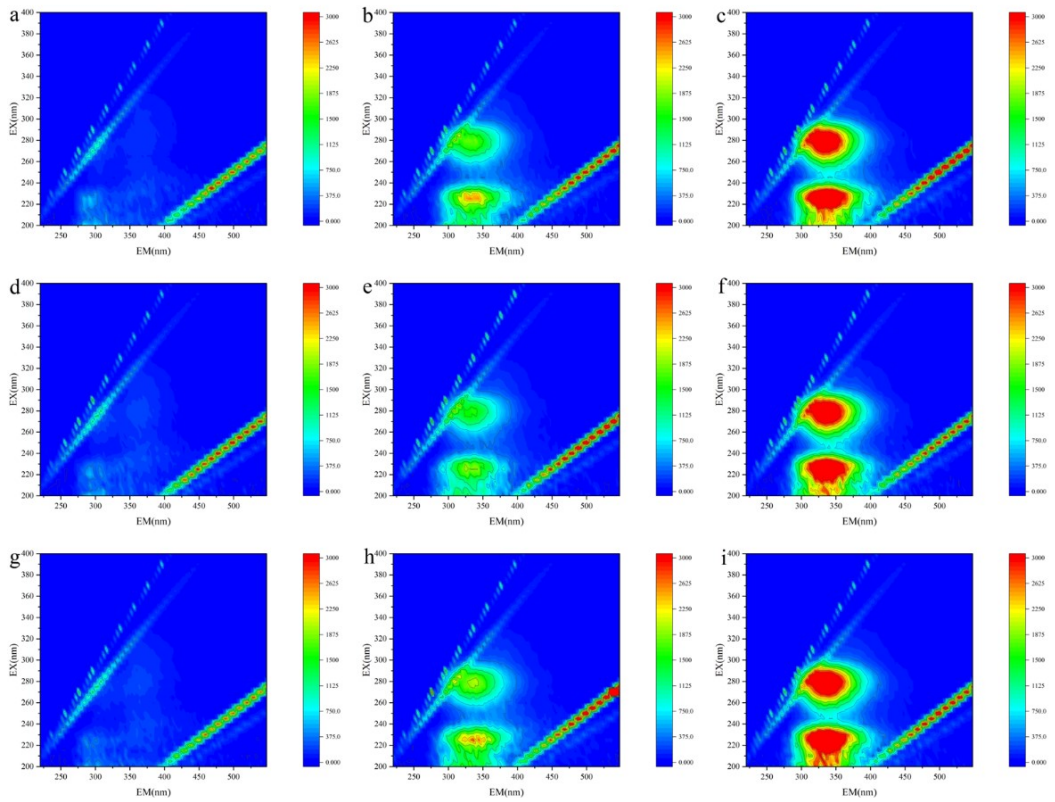

Figure S4 3D-EEM contour plots of BSA/SA samples with different concentration gradients before chlorination reaction. Reaction conditions: $[\text{initial chlorine concentration}]_0 = 10 \pm 0.2$ mg/L, reaction time = 48 h, T = 25 ± 2 °C.

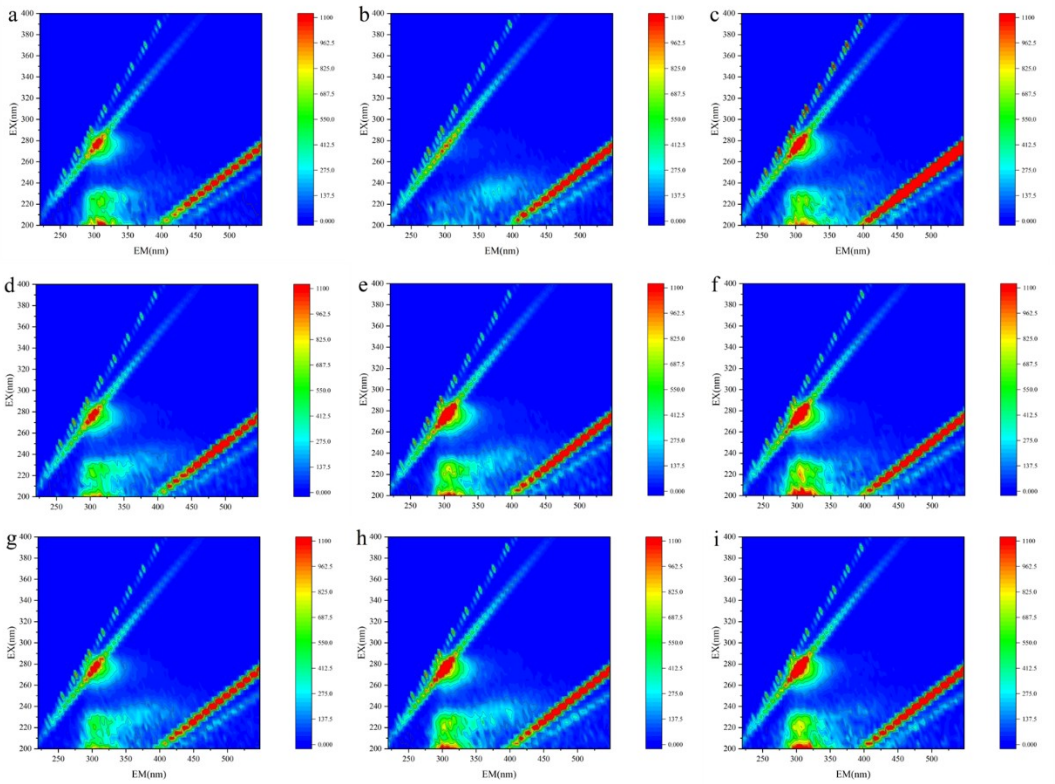

Figure S5 3D-EEM contour plots of BSA/SA samples with different concentration gradients after chlorination reaction. Reaction conditions: $[\text{initial chlorine concentration}]_0 = 10 \pm 0.2$ mg/L, reaction time = 48 h, T = 25 ± 2 °C.

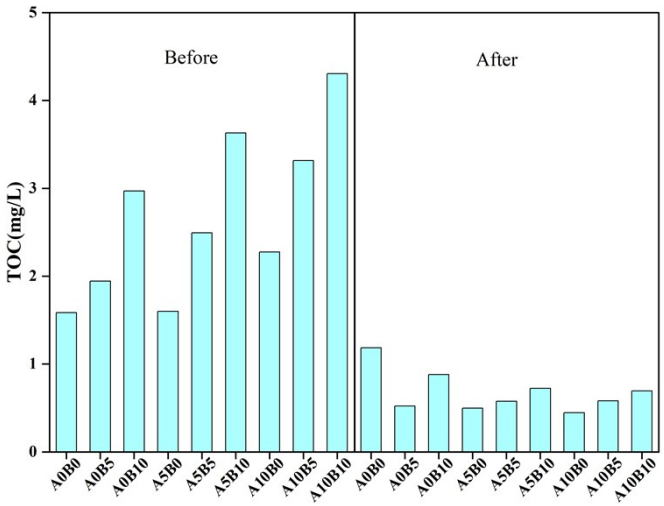

Figure S6 Changes in DOC during the chlorination process of BSA/SA samples with different concentration gradients. Reaction conditions: $[\text{initial chlorine concentration}]_0 = 10 \pm 0.2$ mg/L, reaction time = 48 h, T = 25 ± 2 °C.

References

Muellner, M.G. et al., 2007. Haloacetonitriles vs. Regulated Haloacetic Acids: Are Nitrogen-Containing DBPs More Toxic? Environmental Science & Technology.

Wagner, E.D., Plewa, M.J., 2017. CHO cell cytotoxicity and genotoxicity analyses of disinfection by-products: An updated review. Journal of Environmental Sciences 58,(8), 64-76.