Electronic Supplementary Material (ESI) for Environmental Science: Water Research & Technology.

Supporting Information for:

Formation and Sorption of Trihalomethanes from Cross-Linked Polyethylene Pipes Following Chlorinated Water Exposure

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(a) (b) (c)

Figure S1. Pictures of pipe coils of (a) PEX-a pipe, (b) PEX-b pipe, and (c) PEX-c pipe.

(a) (b)

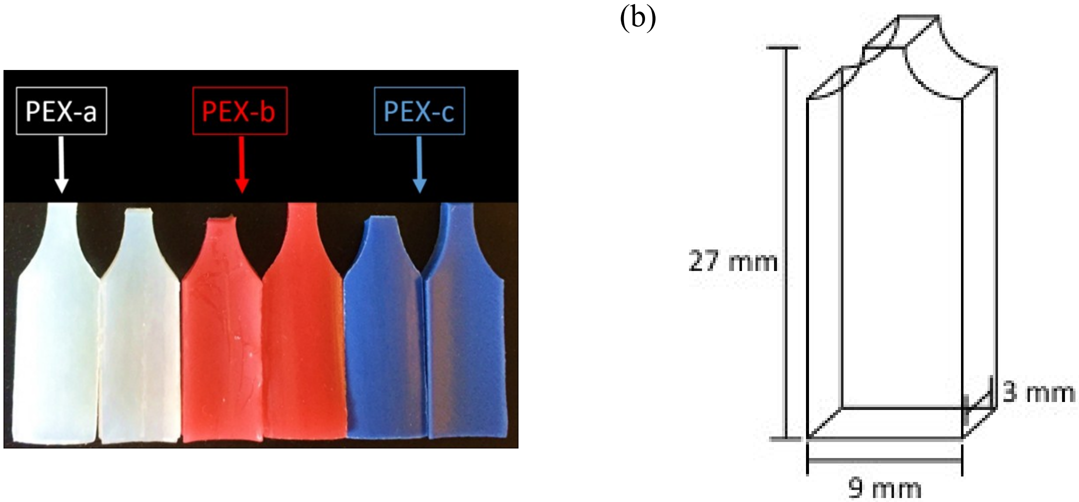

Figure S2. The (a) shape and (b) dimensions (length, width, and thickness) of the half-dog-bone shape pipe pieces.

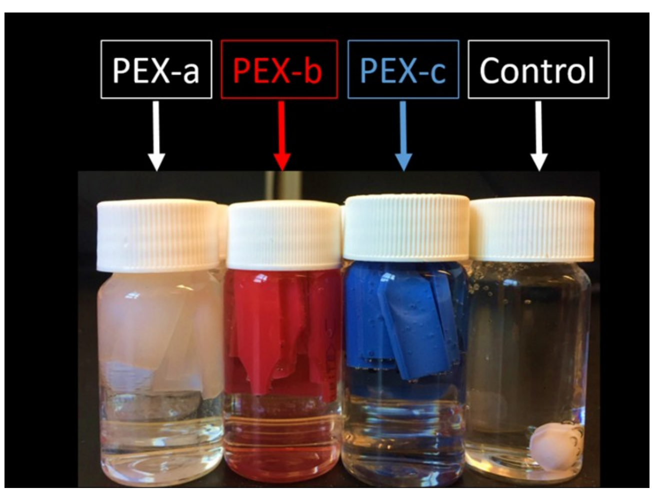

Figure S3. Pictures of the reactors used for the sorption experiments.

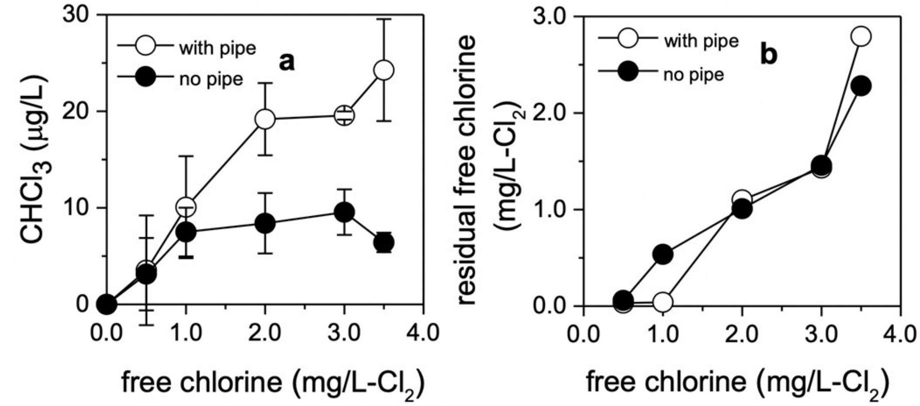

Figure S4. Effect of the initial free chlorine dose on (a) $CHCl_3$ formation and (b) the residual free chlorine concentration, after 120 h of free chlorine exposure from the PEX-a pipe (pH 7.3±0.2, $[TOC]_0$ = 3.2 mg/L-C, FP 1, 22 °C).

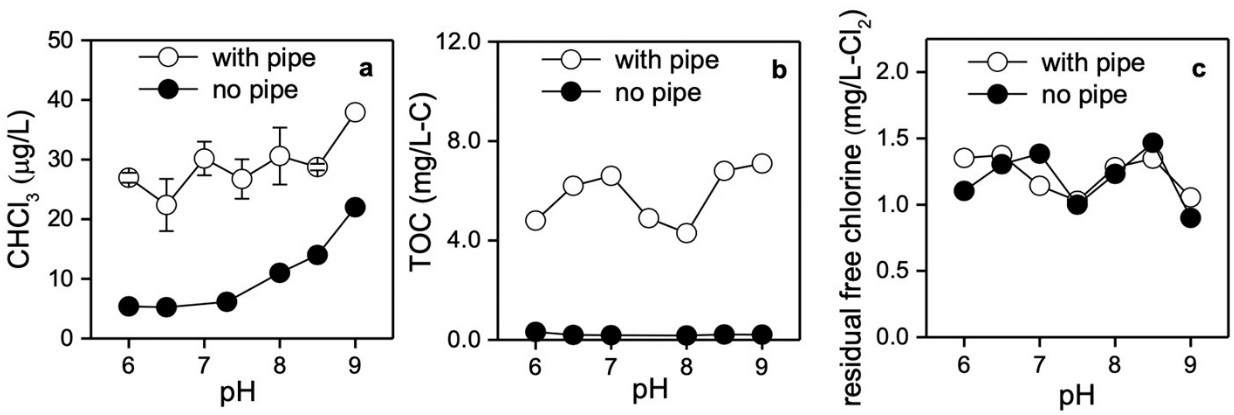

Figure S5. Effect of varying pH on (a) $CHCl_3$ formation, (b) TOC leaching and (c) the residual free chlorine after 120 h of chlorination (pH 6.0 to 9.0, 22 °C, $[\text{free chlorine}]_0$ = 2 mg/L-Cl_2, $[Br^-]_0$ = 0 µg/L) from the PEX-a pipe after FP 1 and bottle-only controls.

Table S1. A summary of the conditions used to assess THM formation from the kinetic and dosage experiments.

Type	**Varied Parameter**	**Pipe Type**	**Flushing Period**	**Temperature (°C)**	**pH**	**$[Br^-]$ (µg/L)**	**Free Chlorine Dosage (mg/L – Cl_2)**	**Quenching Times**
Kinetic	Pipe Type	PEX-a PEX-b PEX-c	FP1, FP2, FP3	22	7.0	0	2.0	Periodically over 120 h
Kinetic	Temperature	PEX-a	FP1	22 and 55	7.0	0	2.0	Periodically over 120 h
Kinetic	Temperature with Bromide	PEX-a	FP1	22 and 55	7.0	78	2.0	Periodically over 120 h
Dosage-based	Temperature	PEX-a	FP1	4, 22, and 55	7.0	0	2.0	After 120 h
Dosage-based	pH	PEX-a	FP1	22	6.0 – 9.0	0	2.0	After 120 h
Dosage-based	Bromide	PEX-a	FP1	22	7.0	0 – 195	2.0	After 120 h
Dosage-based	Disinfectant Dose	PEX-a	FP1	22	7.0	0	0 – 3.5	After 120 h

Table S2. Values obtained when evaluating sorption of each THM to each PEX pipe type at 22 and 55 °C. These values include: (i) k' values obtained when fitting the sorption kinetic model to the experimental data to assess THM sorption to PEX at 22 and 55 °C, and (ii) the slope and R^2 values for the linear regressions obtained when plotting the log K_d values with the log K_{ow} values.

		$CHCl_3$	$CHBrCl_2$	$CHBr_2Cl$	$CHBr_3$	Linear Regression for K_d ($K_d = slope \cdot K_{ow} + b$)	
PEX Type	temperature (°C)	k' (1/h)	k' (1/h)	k' (1/h)	k' (1/h)	Slope	R^2
a	22	4.3E-02	7.2E-02	8.3E-02	9.1E-02	0.72	0.99
b	22	2.4E-02	3.8E-02	5.2E-02	6.3E-02	0.47	0.96
c	22	3.1E-02	3.9E-02	5.0E-02	5.6E-02	0.62	0.78
a	55	1.9E-01	3.6E-01	4.3E-01	4.5E-01	0.70	0.98
b	55	2.4E-01	4.0E-01	4.3E-01	4.3E-01	0.75	0.99
c	55	1.5E-01	2.4E-01	3.0E-01	2.8E-01	0.77	0.98

Text S1. Surface area calculations for the dog-bone pieces.

The total surface area of each dog-bone piece was calculated by first measuring its dimensions including the various heights (H: H1, H2, H3), lengths (L: L1, L2), and the width (W) of the dog-bone piece, as described by the figure below. All of these dimensions were measured with a ruler, except for the curved H2 value, which was measured by aligning a string to the curved side, marking on the string and then measuring the length of the marked string. After obtaining all of these dimensions, the total surface area was calculated by summing up the surface areas of different parts of the dog-bone piece. Most of the parts were rectangles and the area were calculated by multiplying the corresponding length by the width. An approximation was made when calculating the shaded part of the dog-bone piece (see Fig. 1 below), where the area was calculated assuming rectangle and trapezoid shapes.

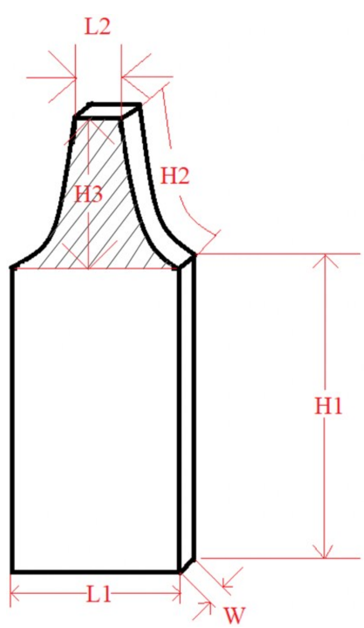

Figure 1. Dimensions of the dog-bone piece used to calculate the surface area.

Text S2. Description of the derivation of the analytical solution of the kinetic surface adsorption model.

An analytical solution was derived for the differential equation provided in eq. 6 from the main text, which represented how surface adsorption occurred over time through a kinetic adsorption model. This model was also adjusted to include a distribution coefficient (K_d) instead of K_{eq}, since the sorption data in Fig. 3 did not reach equilibrium conditions. This equation was integrated using the integration factor method.[1] Two boundary conditions were used when integrating this equation and included: (1) at time = 0, $C_{liquid} = C_{liquid,0}$ = ~ 50 μg/L and (2) at time = t, $C_{liquid} = C_{liquid}$. After integration, the solution for this equation is provided below (eq. S1):

$$C_{liquid} = C_{liquid,0} \cdot e^{-\alpha \cdot t} + \frac{\beta}{\alpha} \cdot \left(1 - e^{-\alpha \cdot t} \right) \qquad where\ \alpha = \frac{k' \cdot V_{liquid}}{M_{PEX} \cdot K_d} + k' \tag{S1}$$

$$where\ \beta = \frac{k' \cdot M_{Total}}{M_{PEX} \cdot K_d}$$

References

1 J. L. Schnoor, *Environmental Modeling: Fate and Transport of Pollutants in Water, Air, and Soil*, Wiley-Interscience, New York, NY, 1996.