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

Supplementary Information for
Environmental Life Cycle Comparison of Conventional and Biological Filtration Alternatives for Drinking Water Treatment

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S1. Water Quality Regulations

Table S1. Total organic carbon (TOC) percent removal requirements, as a function of source water TOC and alkalinity, as defined by the enhanced coagulation requirement in the Stage 1 DBP Rule.[1,2]

Source Water TOC (mg/L C)	Source Water Alkalinity (mg/L $CaCO_3$)		
	<60	**60 to 120**	**>120**
>2 to 4	35%	25%	15%
>4 to 8	45%	35%	25%
>8	50%	40%	30%

S2. Life Cycle Inventory and Impact Assessment Categories

Table S2. Life cycle unit process data and descriptions. Data were from the ecoinvent v3 database[3] except for unit process data on anthracite coal, which was from US-EI 2.2 database.[4] The relative amount of US electricity produced by each electrical grid is stated under application (percent contribution);[5] n/a is not available.

Description	Calc. Section #	Unit Process Name	Application
Alum	A3.1	Aluminium sulfate, powder {RoW}| production | Alloc Def, U	Coagulation
Anthracite	A4.1	Anthracite coal, at mine NREL/RNA U	Filter media
Caustic Soda	A5	Sodium hydroxide, without water, in 50% solution state {RoW}| chlor-alkali electrolysis, membrane cell | Alloc Def, U	pH adjustment
Chlorine	[6]	Sodium hypochlorite, without water, in 15% solution state {RoW}| sodium hypochlorite production, product in 15% solution state | Alloc Def, U	Disinfection (free chlorine from NaOCl and was adjusted as such)
Concrete	[6]	Concrete, 20MPa {RoW}| concrete production 20MPa, RNA only | Alloc Def, U	Chlorine contact basin
Electricity	A4.2, [6]	Electricity, medium voltage {ASCC}| market for | Alloc Def, U	ASCC grid (n/a)
		Electricity, medium voltage {FRCC}| market for | Alloc Def, U	FRCC grid (6% US electricity)
		Electricity, medium voltage {NPCC, US only}| market for | Alloc Def, U	NPCC grid (7% US electricity)
		Electricity, medium voltage {MRO, US only}| market for | Alloc Def, U	MRO grid (17% US electricity)
		Electricity, medium voltage {RFC}| market for | Alloc Def, U	RFC grid (20% US electricity)
		Electricity, medium voltage {SERC}| market for | Alloc Def, U	SERC grid (17% US electricity)
		Electricity, medium voltage {SPP}| market for | Alloc Def, U	SPP grid (6% US electricity)
		Electricity, medium voltage {TRE}| market for | Alloc Def, U	TRE grid (9% US electricity)
		Electricity, medium voltage {WECC, US only}| market for | Alloc Def, U	WECC grid (18% US electricity)
		Electricity, medium voltage {HICC}| market for | Alloc Def, U	HICC grid (n/a)
Ferric Chloride	A3.1	Iron (III) chloride, without water, in 40% solution state {RoW}| iron (III) chloride production, product in 40% solution state | Alloc Def, U	Coagulation
Hauling	A4.3	Trasport freight, lorry 3.5-7.5 metric ton, EURO6 {RoW}| transport, freight, lorry 3.5-7.5 metric ton, EURO6 | Alloc Def, U	Solids and chemical hauling
Lime	A5	Lime, hydrated, loose weight {RoW}| production | Alloc Def, U	pH adjustment
Reinforcing Steel	[6]	Reinforcing steel {RoW}| market for | Alloc Def, U	Chlorine contact basin
Sand	A4.1	Sand {GLO}| market for | Alloc Def, U	Sand (filter media)
Soft Plastic	[6]	Polyethylene, high density, granulate {RoW}| production | Alloc Def, U	Plastic cylindrical tank (contact basin)
Stainless Steel	A4.1, [6]	Steel, chromium steel 18/8, hot rolled {RoW}| production | Alloc Def, U	Filter housing, steel baffles, ozone generator
Tap Water	[6]	Tap water {RoW}| tap water production, conventional treatment | Alloc Def, U	Dilution water (chlorine solution)

Table S3. Material, energy, and chemical quantities for the 3 filtration alternatives. Values are for the entire functional unit (i.e., treatment of 2,700 m^3/day over 40 years) normalized to 1 m^3 of treated water. These results are for the treatment of the typical source water under the enhanced coagulation treatment scenario, assuming typical values for each uncertainty parameter (Table S12) Unit process details are in Table S10. Chlorine mass is kg free chlorine from NaOCl.

Inventory Unit Process (Units/m^3 water treated)	Filtration Alternatives		
	Conventional Filtration	Nonozonated Biofiltration	Ozonated Biofiltration
Alum (kg)	1.30E-02	1.20E-02	1.00E-02
Anthracite (kg)	1.37E-04	1.37E-04	1.37E-04
Backwash Energy (kWh)	9.46E-04	9.46E-04	9.46E-04
Baffle Steel (kg)	3.61E-04	3.61E-04	3.61E-04
Caustic (kg)	1.28E-02	1.22E-02	1.08E-02
Chemicals Hauling (tkm)	5.75E-04	5.43E-04	5.43E-04
Chlorine (kg)	1.40E-03	1.40E-03	1.40E-03
Chlorine Dose (mg free Cl_2/L)	1.4	1.4	1.4
Chlorine Pump Energy (kWh)	6.26E-06	6.26E-06	6.26E-06
Polyethylene Chlorine Storage Tank (kg)	9.38E-07	9.38E-07	9.38E-07
Concrete (m^3)	1.72E-06	1.72E-06	1.72E-06
Contactor Pump Energy (kWh)	9.71E-09	9.71E-09	9.71E-09
Stainless Steel Filter Housing (kg)	7.45E-04	7.45E-04	7.45E-04
Filter Operational Energy (kWh)	1.37E-02	1.39E-02	1.39E-02
Rebar (kg)	7.78E-06	7.78E-06	7.78E-06
Sand (kg)	1.71E-04	1.71E-04	1.71E-04
Solids Hauling (tkm)	2.61E-04	2.41E-04	2.41E-04
Ozone Energy (kWh)	N/A	N/A	3.22E-02
Stainless Steel Ozone Generator (kg)	N/A	N/A	3.79E-05

S3. TOC Removal Design Calculations

S3.1 Coagulation

Alum and Ferric Chloride coagulation is affected most by pH and specific ultraviolet absorbance (SUVA), both of which are affected by alkalinity and TOC. Also, alum and Ferric Chloride lower the water's pH and alkalinity. Due to these complex interactions, the following approach was used to determine the alum dose needed for a specific percent TOC removal target. An alum dose and TOC removal table (Table S4) was generated for every source water scenario to determine the proper alum dose for coagulation using 6 main steps. First, the source water quality was defined in terms of TOC, alkalinity, pH, SUVA, and temperature. Second, a comprehensive range of possible alum doses was generated (from 0 to 122 mg/L, in 1 mg/L increments). Third, the pH of the coagulated water was calculated by iteratively solving Eq. S1 from the U.S. EPA's Water Treatment Plant Model v2.[7] Fourth, the coagulated water TOC was calculated using Eq. S2 with values for the coagulated water pH and alkalinity input as well as variables from the Edwards Model.[8] Fifth, the SUVA of coagulated water was determined (Eq. S3). Sixth, the percent TOC removal was calculated based on the source water TOC and final TOC. Table S4 shows example alum doses and the corresponding percent TOC removals for an example source water. The same strategy was used for Ferric Chloride. Overall, the required alum dose for a specified source water quality and TOC removal target was found from these tables. For the enhanced coagulation TOC removal scenario, the selected alum dose was the smallest dose associated with any of the follow situations, as long as that value was above the minimum allowable value (10 mg/L alum, uncertainty parameter, Table S11): (i) percent TOC removal target, (ii) 2 mg/L coagulated water TOC, or (iii) 2 L/mg/m coagulated water SUVA. Table S5 shows the alum doses needed for all of these conditions for an example source water. Note that coagulant ecoinvent data is for dry weights of coagulant chemicals without water as verified through correspondence with ecoinvent.

Table S4. Example alum dose and TOC removal table. Values were calculated for the national average source water scenario (77 mg/L $CaCO_3$, 3.2 mg/L TOC, 15 °C) and enhanced coagulation TOC removal.

Alum Dose (mg/L)	Coagulated Water pH	Coagulated Water TOC (mg/L)	Coagulated Water SUVA	TOC Removal (%)
0	7.50	3.20	3.13	0%
1	7.43	3.16	2.53	1.2%
2	7.37	3.12	2.40	2.4%
…	…	…	…	…
13	6.94	2.64	2.01	17%

Table S5. The four alum dose options for the national average source water scenario (77 mg/L $CaCO_3$, 3.2 mg/L TOC, 15 °C) and enhanced coagulation TOC removal. The smallest, above the minimum allowable alum dose, was chosen as the modeled alum dose (green shade).

Purpose	Alum Dose (mg/L)	Coagulated Water TOC (mg/L)	Coagulated Water SUVA	TOC Removal (%)
Turbidity removal (minimum allowable dose)	10	2.78	2.06	13%
SUVA (≤ 2 L/mg/m)	14	2.60	2.00	19%
TOC (≤ 2 mg/L)	30	1.99	1.81	38%
%TOC removal	19	2.38	1.94	25%

$$(\boldsymbol{\alpha_1} + (2 * \boldsymbol{\alpha_2})) * [\mathbf{Ct_{CO3}}] + \left[\frac{\mathbf{k_w}}{[\mathbf{H^+}]}\right] - [\mathbf{H^+}] = [\boldsymbol{\alpha_1} * \mathbf{C_{TCO3}}] + 2 * [\boldsymbol{\alpha_2} * \mathbf{C_{TCO3}}] + \left[\frac{\mathbf{k_w}}{[\mathbf{H^+}]}\right] - [\mathbf{H^+}] - 6 * [\mathbf{Alum}] \qquad \textbf{Eq. S1a}$$

$$\boldsymbol{\alpha_1} = \frac{\mathbf{k_{1CO3}} * [\mathbf{H^+}]}{[\mathbf{H^+}]^2 + \mathbf{k_{1CO3}} * [\mathbf{H^+}] + \mathbf{k_{1CO3}} * \mathbf{k_{2CO3}}} \qquad \textbf{Eq. S1b}$$

$$\boldsymbol{\alpha_2} = \frac{\mathbf{k_{1CO3}} * \mathbf{k_{2CO3}}}{[\mathbf{H^+}]^2 + \mathbf{k_{1CO3}} * [\mathbf{H^+}] + \mathbf{k_{1CO3}} * \mathbf{k_{2CO3}}} \qquad \textbf{Eq. S1c}$$

$$\mathbf{C_{TCO3}} = \frac{[\mathbf{Alk}] + [\mathbf{H}] - [\mathbf{OH}]}{\boldsymbol{\alpha_1} + (2 * \boldsymbol{\alpha_2})} \qquad \textbf{Eq. S1d}$$

$$\mathbf{k_{1CO3}} = \mathbf{exp}\left\{\left[\left(\frac{\mathbf{7700}\frac{\mathbf{J}}{\mathbf{mole}}}{\mathbf{8.314}\frac{\mathbf{J}}{\mathbf{K * mole}}}\right)\left(\frac{\mathbf{1}}{\mathbf{298.15\ K}} - \frac{\mathbf{1}}{\mathbf{T}}\right)\right] - \mathbf{14.5}\right\} \qquad \textbf{Eq. S1e}$$

$$\mathbf{k_{2CO3}} = \mathbf{exp}\left\{\left[\left(\frac{\mathbf{14900}\frac{\mathbf{J}}{\mathbf{mole}}}{\mathbf{8.314}\frac{\mathbf{J}}{\mathbf{K * mole}}}\right)\left(\frac{\mathbf{1}}{\mathbf{298.15\ K}} - \frac{\mathbf{1}}{\mathbf{T}}\right)\right] - \mathbf{14.5}\right\} \qquad \textbf{Eq. S1f}$$

Where:

$[OH^-]$ = Concentration of hydroxide (M)
$[H^+]$ = Concentration of hydrogen (M)
$[CO_3^{2-}]$ = Concentration of carbonate (M)
$[HCO_3^-]$ = Concentration of bicarbonate (M)
[Alum] = Concentration of dry alum added (M)
α_1 = Water chemistry equilibrium value for the second hydrogen state (Eq. S1b)
α_2 = Water chemistry equilibrium value for the third hydrogen state (Eq. S1c)
C_{TCO3} = Total concentration of all carbonate species (M)
k_{1CO3} = Carbonate equilibrium constant for second hydrogen[9]
k_{2CO3} = Carbonate equilibrium constant for second hydrogen[9]
k_w = Water equilibrium constant (4.52E-15)
[Alk] = Concentration of influent alkalinity eq/L
T = Influent water temperature (K)

$$\mathbf{DOC_i = (1 - (SUVA * K_1) - K_2) * TOC} \qquad \textbf{Eq. S2a}$$

$$\mathbf{Al^{3+} = \frac{Dry\ Alum * \left(\frac{2\ mmol\ Al^{3+}}{1\ mmol\ Alum}\right)}{\left(\frac{342.15\ mg\ dry\ Alum}{1\ mmol\ Alum}\right)}} \qquad \textbf{Eq. S2b}$$

$$\mathbf{a = (x_1 * pH^3 + x_2 * pH^2 + x_3 * pH)} \qquad \textbf{Eq. S2c}$$

$$\mathbf{\frac{DOC_i - [C]_{eq}}{Al^{3+}} = \frac{a * b * [C]_{eq}}{1 + b * [C]_{eq}}} \qquad \textbf{Eq. S2d}$$

$$\mathbf{[C]_{eq} = \frac{\sqrt{\left(b^2 * (DOC_i - a * Al^{3+})^2 + (2b * (DOC_i + a * Al^{3+}) + 1)\right)} + \left(\boldsymbol{b} * \left(DOC_i - a * Al^{3+}\right)\right) - 1}{2b}} \qquad \textbf{Eq. S2e}$$

$$\mathbf{TOC_{coagulated} = [C]_{eq} + (TOC - DOC_i)} \qquad \textbf{Eq. S2f}$$

$$\mathbf{TOC\ Removal = \frac{TOC - TOC_{coagulated}}{TOC}} \qquad \textbf{Eq. S2g}$$

Where:

DOC$_i$ = Sorbable DOC of coagulation influent water (mg/L)
SUVA = Specific ultraviolet absorbance of influent water (L/mg/m)
K$_1$ = Constant: (-0.075)[8]
K$_2$ = Constant: (0.56)[8]
TOC = Influent TOC (mg/L)
Alum = Alum dose added (mg/L)
Al^{3+} = Aluminum ions present (mM)
a = Maximum TOC sorption per mM of Al^{3+} added
x$_1$ = Constant: (284)[8]
x$_2$ = Constant: (-74.2)[8]
x$_3$ = Constant: (4.91)[8]
[C]$_{eq}$ = Amount of sorbable TOC remaining after coagulation (mg/L)
b = Constant: (0.147)[8]
TOC = Influent TOC (mg/L)
TOC$_{coagulated}$ = Coagulated water TOC concentration (mg/L)
TOC Removal = Amount of TOC removed from source water (%)

$$\mathbf{SUVA_{coagulated} = \frac{(5.716*(UVA)^{1.0894}*(3*Al^{3+})^{0.306}*(pH)^{-0.9513})}{TOC_{coagulated}} * \frac{100cm}{m}} \qquad \textbf{Eq. S3}$$

Where:

SUVA$_{coagulated}$ = Specific ultraviolet absorbance of coagulated water (L/mg/m)
UVA = ultraviolet absorbance at 254 nm of influent water (1/cm)

S3.2 Coagulated and Biological TOC Removal

Table S6 and Table S7 shows experimental data from the literature on biodegradable TOC removal using Table S6 for coagulation and Table S7 for nonozonated biofiltration and ozonated biofiltration, for systems that match the treatment process configuration in this LCA).

Table S6. Experimental data from the published literature that shows coagulated biodegradable TOC removal efficacy at different SUVAs. (Volk and LeChavellier, 2002; Volk et al., 2000)[10,11]

SUVA	Coagulation percent TOC removal		
	25th percentile	75th percentile	Average
< 3 (L/mg/m)	2%	5%	4%
≥ 3 (L/mg/m)	7.5%	13.5%	9%

Table S7. Experimental data from the published literature that shows nonozonated biofiltration and ozonated biofiltration TOC removal efficacy at different temperatures. Table data was adapted from Terry and Summers, 2018.[12]

Temperature	Nonozonated Biofilter percent TOC removal			Ozonated Biofilter percent TOC removal		
	Min	Max	Median	Min	Max	Median
≤10 °C	2%	14%	7%	3%	24%	11%
10 - 20 °C	5%	22%	10%	3%	47%	13%
≥20 °C	10%	22%	15%	6%	45%	20%

S3.3 City of Boulder Betasso Drinking Water Pilot Plant

S3.3.1 Methods

Pilot filters were set up at the City of Boulder's (CO) Betasso Water Treatment Plant (Betasso WTP) and source water, a combination of Barker Reservoir and Lakewood Reservoir was sent to the raw water tank, from which water was pumped to the treatment train. The Betasso WTP pilot was composed of a pilot treatment train operated at a flow rate of 2 gal/min. The train consists of rapid mix, three stage tapered flocculation, sedimentation, and filtration. The pilot plant schematic is represented by Figure S1 and a detailed schematic of the biofilters can be seen in Figure S2. The water passed through the static mixer, into three flocculation basins with tapered paddles, into a sedimentation basin with plate settlers, then split into one of two filters. For coagulation, aluminum sulfate was added at the front of the pilot plant. Chlorine was added at the front of the second filter to allow comparison of a biofilter (BF) and a conventional filter (RMF).

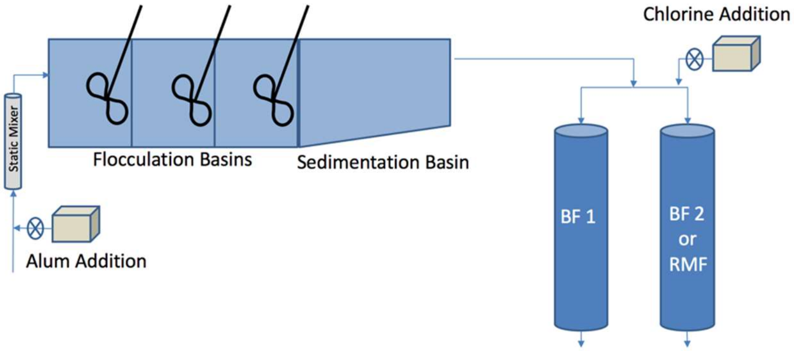

Figure S1. Pilot Plant Schematic.

Biologically active anthracite media from a full-scale filter, which was in operation for over seven years at the City of Longmont (CO) Nelson Flanders Drinking Water Treatment Plant, was used to pack the biofilter column. Inert anthracite was used to pack the conventional filter. The anthracite media had an effective size of 1.0 mm and an approximate uniformity coefficient of 1.3. The pilot system was modified and two columns were fabricated with depth taps to achieve filter depth samples, as seen in Table S8. The placement of the sampling ports allowed for measurement of only removal associated with the biological media and not the feed system. The filters were backwashed once per week with chlorinated water. Flow rates were monitored online via a flow analyzer. The analyzer installed was a Blue White F-400N Inline Rotameter with a range of 0.025 – 0.25 gpm. The flow was changed by adjusting the ball valve at the end of each filter. The flow rate was measured after each filter using in-line flow meters and averaged at 0.04 gpm, and the hydraulic loading rate averaged 2 m/hr.

Table S8. Pilot Filter Design Parameters

Filters	*Media Type*	*Experiment*	*Target EBCTs (min)*	*Media Height (cm)*	*Inner Diameter (mm)*	*Support Media Height (cm)*	*Flow Rate (gpm)*
Fresh (conventional) and Acclimated (biofilter)	Anthracite	Pilot with taps	5 15 30	17 50 100	76	8	0.04

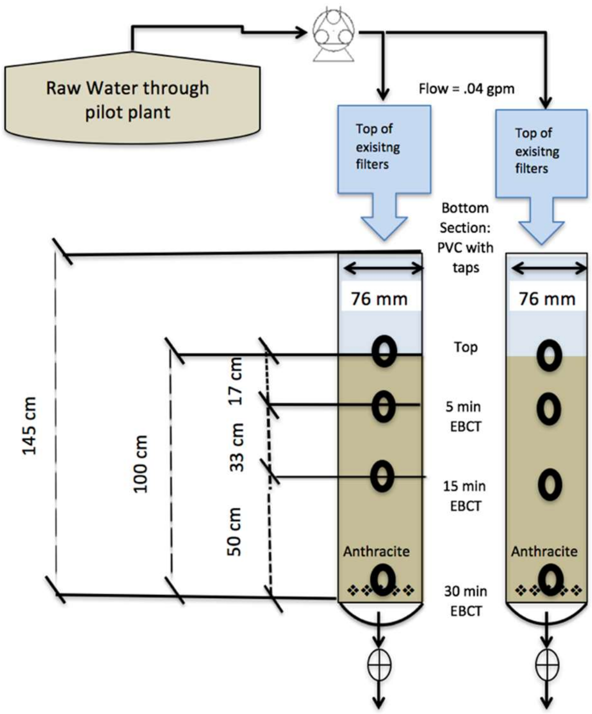

Figure S2. Biofilters Pilot Schematic

Influent feed water samples were collected at the tap directly between the sedimentation basin and the filters. Subsequent EBCT samples were taken at the corresponding EBCT tap. Liquid samples were collected in amber glassware that had been previously cleaned with deionized water and muffled at 550 ˚C for 3 hours. Samples were then transported to the University of Colorado, Boulder to be analyzed.

DOC concentrations were measured at the University of Colorado, Boulder on a Sievers M5310 C Laboratory Organic Carbon Analyzer using the ultraviolet irradiation/persulfate oxidation method (SM 5310C). The samples were collected and immediately filtered through a 0.45 mm membrane filter (Pall Life Sciences). Filters were first rinsed with 250 mL of reverse osmosis water to ensure that carbon leaching from the filters did not occur. After filtration, the samples were stored at 4°C until DOC analysis. All DOC analysis was performed within the hold time of 2 weeks of sample collection. Samples were taken in duplicate and analyzed in groups of four with a blank in between as a quality control measure to ensure stable operations and no organic carbon carryover from previous samples. The instrument was calibrated in accordance with the Operations and Maintenance manual. Quality assurance and quality control tests were performed monthly to ensure instrument accuracy.

S3.3.2 Results

Drinking water treatment utilities are required to remove a certain percentage of influent TOC (15 – 50%) based on source water TOC and alkalinity per the Stage 1 DBP Rule (termed the enhanced coagulation requirement). Utilities have multiple ways of meeting this regulation. The pilot plant was used to determine the trade-offs between DOC removal from coagulant addition and biofiltration. Figure S3 demonstrates the best optimization of biofiltration and coagulant addition to meet the Stage 1 DBP Rule requirements. If the utility is required to remove 30% of the influent TOC, the utility can either dose at 20 mg/L alum to achieve 33% DOC removal or dose at 15mg/L alum and run a biofilter with an EBCT of 30 minutes to achieve 32%. If the source water changes and the utility needs to remove 20% of the influent TOC, the utility can dose 15 mg/L alum to achieve 25% DOC removal or dose 10 mg/L alum and run a biofilter with an EBCT of 30 minutes to achieve 23% DOC removal.

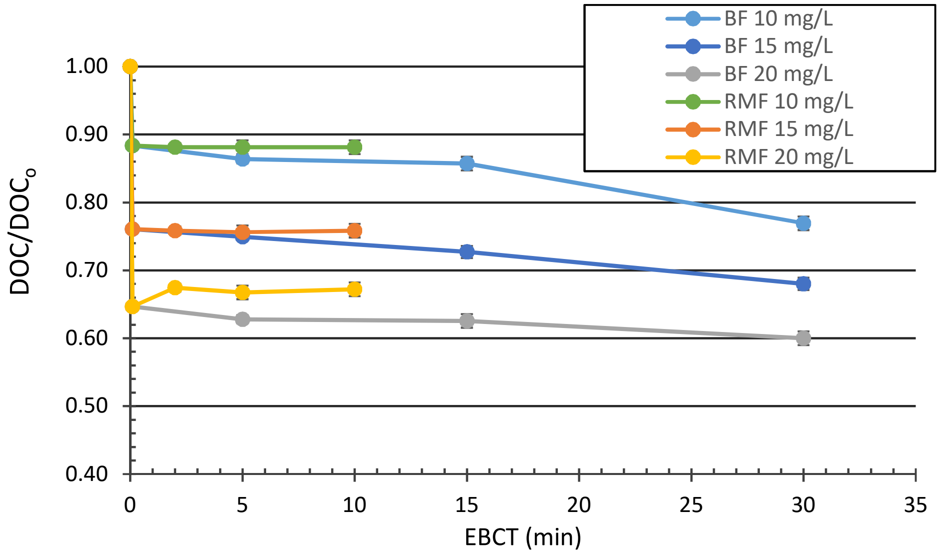

Figure S3. DOC removal throughout the coagulation and filtration process as a function of EBCT for a biological filter (BF) and a conventional rapid media filter (RMF) at 3 different aluminum sulfate doses: 10, 15 and 20 mg/L.

S4. Filter Design Calculations

Major materials and energy requirements to operate each filter were accounted for over the functional unit timeframe (40 years). A dual media filter of anthracite over sand was chosen for the rapid media filter design due to its prevalence in practice.

S4.1 Filter Materials

For each filter, the filter area was calculated using Eq. S4. The mass of media was calculated using Eq. S5. These equations assumed values for hydraulic loading rate and media depth, respectively, which were uncertainty parameters based on typical values for each type of filter (Table S11).[13] The total filter depth included the (packed) media depth and freeboard (0.3 m).[13] Filter volume was calculated using this total depth and Eq. S6. Then, the mass of steel needed for the filter housing was calculated using Eq. S7; this equation assumed a square cross section and typical steel thickness,[14] which was an uncertainty parameter (S6. Uncertainty and Sensitivity Analysis).

$$\mathbf{A_T = \frac{Q}{HLR}} \qquad \textbf{Eq. S4}$$

Where:

A_T = Total filter area requirement (m^2)
Q = Plant capacity flow rate (m3/hr)
HLR = Filter design hydraulic loading rate (m/hr)

$$\mathbf{M_{media} = A_T * D_{media} * \rho_{media}} \qquad \textbf{Eq. S5}$$

Where:

M_{media} = Mass of filter media (kg)
D_{media} = Media Depth (m) (Table S11)
ρ_{media} = Media density (kg/m^3): (1,500 kg/m^3 sand, and 800 kg/m^3 anthracite)[15]

$$\mathbf{V_{Filter} = A_T * \left(D_{media} + H_{fb} + D_{expansion}\right)} \qquad \textbf{Eq. S6}$$

Where:

V_{Filter} = Required filter volume (m^3)
H_{fb} = freeboard (m)
$D_{expansion}$ = Backwash filter expansion depth (m): Assumed 50% bed expansion[16]

$$\mathbf{M_{steel} = \Bigg\{\Bigg(\Bigg(\bigg(\sqrt{\frac{V_{filter}}{D_{total}}}\bigg) * t_b\Bigg) + \Bigg(4{t_w}^2 + 4\bigg(\sqrt{\frac{V_{filter}}{D_{total}}}\bigg) * t_w\Bigg) * (D_{total} + t_B)\Bigg\} * \rho_{steel}} \qquad \textbf{Eq. S7}$$

Where:

D_{total} = Sum of media depth and filter head requirement (m)
t_b = Thickness of filter base (m)
t_w = Thickness of filter walls (m)
ρ_{steel} = Density of steel (kg/m^3): (7,500 kg/m^3)[17]

S4.2 Filter Energy Requirements

Pumping energy (for operation and backwash) was determined using Eq. S8. Filter operational head loss uncertainty was accounted for because media depth and water height above media were uncertainty parameters (Table S11).[13] Typical values were used to estimate the backwash flowrate and pressure[18] and ultimately to determine head loss during backwashing; both were uncertainty parameters (Table S11). Other than the 10 minutes of backwash every day, constant filtration was assumed.

$$\mathbf{P} = \frac{(\mathbf{Q} * \boldsymbol{\rho} * \mathbf{g} * \mathbf{H})}{\left(\mathbf{1000}\frac{\mathbf{W}}{\mathbf{kW}} * \boldsymbol{\eta}\right)} \qquad \textbf{Eq. S8}$$

Where:

P = Power (kW)
Q = Flow rate (m^3/s): water treatment plant flow rate or backwash flow rate
ρ = Density of liquid solution (kg/m^3): 1000 kg/m^3 for water
g = Gravity (9.81 m/s^2)
H = Head loss (m): filter operational head loss or backwash pressure
η = Efficiency (60%)

S4.3 Solids and Chemical Hauling Requirements

The hauling requirements, in tonne kilometers, were determined for solid coagulation waste and all chemicals (Eq. S9). The masses of alum, caustic soda, and chlorine were based on their treatment doses. The hauling distance was assumed to be the same for all chemicals and was an uncertainty parameter (Table S11). The solid waste generated from coagulation and sedimentation was conservatively estimated as the alum mass plus the mass of TOC removed. This waste was hauled to a landfill; the distance was an uncertainty parameter (Table S11).

$$\mathbf{tkm} = \mathbf{M_T} * \mathbf{L_T} \qquad \textbf{Eq. S9}$$

Where:

tkm = tonne kilometers (tkm)
M_T = Mass of chemicals or solids (tonne)
L_T = Transport Distance (km)

S5. pH Adjustment

The final water's pH was raised to 8.2 at the end of the plant with caustic soda (sodium hydroxide). Other cases were considered where there was no pH adjustment as well as pH adjustment to the source water pH. Similar to the alum dose calculations, the caustic soda and lime doses were determined by generating a caustic soda (Table S10) or lime dose and final pH table for every source water scenario using three main steps. First, the pH after chlorination was calculated using Eq. S10. Second, a comprehensive range of possible caustic and lime doses was generated (from 0 to 2,000 mg/L in 0.1 mg/L increments until 15 mg/L, then 1.0 mg/L increments until 50 mg/L, then 5.0 mg/L increments until 300 mg/L, and then 100 mg/L increments until 2,000 mg/L). Third, the pH of the final adjusted water was calculated by iteratively solving Eq. S11, based on the U.S. EPA's Water Treatment Plant Model v2.[7] Overall, the required caustic or lime dose for the pH adjustment needed was found from the table. Figure S4 shows an example of how pH changed throughout the treatment train and displays the input and output pH at the point of each chemical addition. Table S10 shows example caustic doses and the corresponding final water pH (when the starting pH was 7.5).

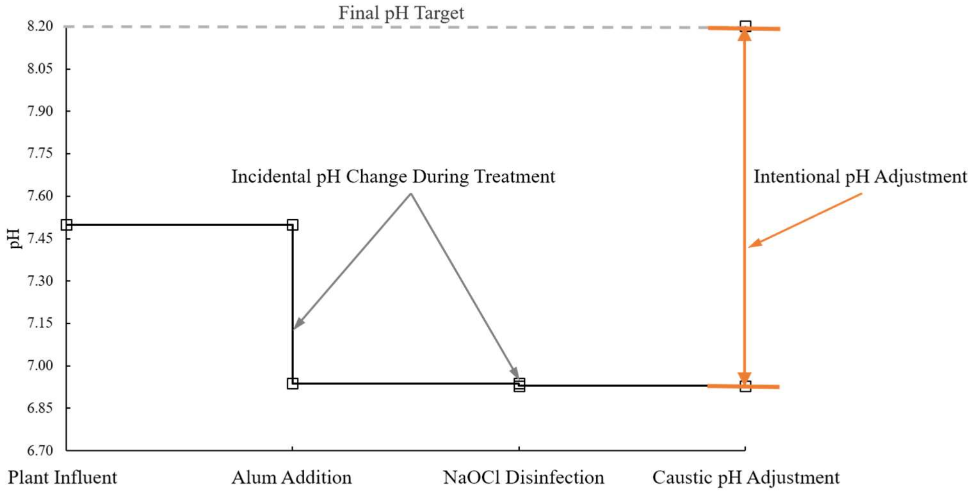

Figure S4. Example pH changes throughout the treatment process. Values were calculated for an example source water (77 mg/L $CaCO_3$, 3.2 mg/L TOC, 7.6 pH, 3.1 SUVA, 15 °C) and enhanced coagulation TOC removal.

Table S9. Example chlorine dose and free chlorine before the distribution system. Values were calculated for an example source water representing national averages (77 mg/L $CaCO_3$, 3.2 mg/L TOC, 7.6 pH, 3.1 SUVA, 15 °C) for enhanced coagulation TOC removal.

Initial Chlorine Added (mg/L as free Cl_2)	Final Chlorine Before Distribution (mg/L as free Cl_2)
1	0.66
1.1	0.75
…	…
1.4	1.01

Table S10. Example caustic dose and final pH table. Values were calculated for an example source water representing national averages (77 mg/L $CaCO_3$, 3.2 mg/L TOC, 7.6 pH, 3.1 SUVA, 15 °C) for enhanced coagulation TOC removal.

Caustic Added (mg/L)	Final pH
0	6.93
0.2	6.94
0.5	6.95
0.8	6.96
…	…
12.8	8.21

$$\left((\alpha_1 + 2) * \alpha_2 * \left[CO_3{}^{2-}\right]\right) + [OH^-] - [H^+] = [HCO_3{}^-] + 2 * \left[CO_3{}^{2-}\right] + [OH^-] - [H^+] - \left(\frac{[Ct_{OCl-}]}{1 + \frac{[H^+]}{k_{ocl-}}}\right)$$ **Eq. S10a**

$$[Ct_{OCl^-}] = [Ct_{NaOCl}] = \frac{Cl_2\ Dose}{1000\frac{mg}{g} * \left(\frac{(2 * 35)g\ Cl_2}{1\ mol\ Cl_2}\right) * \left(\frac{1\ mol\ Cl_2}{2\ mol\ NaOCl}\right)}$$ **Eq. S10b**

$$k_{OCl^-} = \exp\left\{\left[\left(\frac{13800\frac{J}{mol}}{8.314\frac{J}{K * mol}}\right)\left(\frac{1}{298.15\ K} - \frac{1}{T}\right)\right] - 17.5\right\}$$ **Eq. S10c**

$$\left((\alpha_1 + 2) * \alpha_2 * \left[CO_3{}^{2-}\right]\right) + [OH^-] - [H^+] = [HCO_3{}^-] + 2 * \left[CO_3{}^{2-}\right] + [OH^-] - [H^+] + [Caustic]$$ **Eq. S11**

Where:

$[OH^-]$ = Concentration of hydroxide (M)
$[H^+]$ = Concentration of hydrogen (M): Known target
$[CO_3{}^{2-}]$ = Concentration of carbonate (M)
$[HCO_3{}^-]$ = Concentration of bicarbonate (M)
$[Ct_{NaOCl}]$ = Concentration of sodium hypochlorite added (M) (Eq. S10ab)
$[Ct_{OCl}$-] = Concentration of hypochlorite chlorine (M) (Eq. S10ab)
k_{ocl}- = Hypochlorite equilibrium constant[9]
α_1 = Water chemistry equilibrium value for the second hydrogen state (Eq. S1b)
α_2 = Water chemistry equilibrium value for the third hydrogen state (Eq. S1c)
[Caustic] = Amount of caustic added (M)
T = Influent water temperature (K)
[Cl_2 Dose] = Required residual chlorine dose (mg Cl_2/L): Using Jones et. al.[6]

S6. Uncertainty and Sensitivity Analysis

Table S11. The low (L) and high (H) values of each uncertainty parameter. The typical (T) value represents the most likely value expected based on the range. Uncertainty parameters 1 to 8 used a triangular distribution with the known L, H, and T values; the rest had uniform distributions based on the known L and H values.

#	Uncertainty Parameter	Low Value	High Value	Typical Value	Basis and Citations
1	Minimum allowable alum dose (mg alum/L)	6.0	17	10	L=25th percentile value[19], H=75th percentile value[19], T=median[19]
2	Source water BDOC/TOC ratio	14%	27%	20%	L=min[12], H=max[12], T=median[12]
3	Ozonated water BDOC/TOC ratio	20%	38%	30%	L=min[12], H=max[12], T=median[48]
4	Biodegradable fraction of TOC removed by coagulation, when source water SUVA<3 L/mg/m	2.0%	5.0%	4.0%	L=25th percentile[10,11], H=75th percentile[10,11], T=average[10,11]
5	Biodegradable fraction of TOC removed by coagulation, when source water SUVA>3 L/mg/m	7.5%	14%	9.0%	L=25th percentile[10,11], H=75th percentile[10,11], T=average[10,11]
6	Nonozonated biofilter percent TOC removal (of the available biodegradable fraction of TOC) for 10°C to 20°C	5.0%	22%	10%	L=min[12], H=max[12], T=median[12]
7	Ozonated biofilter TOC removal (of the available biodegradable fraction of TOC) for 10°C to 20°C	3.0%	47%	13%	L=min[12], H=max[12], T=median[12]
8	Pre-ozonation dose (g O_3/g TOC)	0.25	1.6	0.50	L=min[12], H=max[12], T=median[12]
9	Air-fed ozone specific energy use (kWh/g O_3 generated)	0.018	0.022	0.020	L[20], H[21,22], T=average of L&H
10	Steel Tank Thickness (m)	0.14	0.55	0.27	L/H[14], T=Average
11	Steel Life Expectancy (yr)	30	60	45	L/H[23], T[24]
12	Backwash Flowrate ($m^3/h/m^2$)	30	60	50	L/H[18], T=expert judgment
13	Backwash Pressure (m)	8	10	9	L/H[18], T=average
14	Water Height Above Media (m)	1.5	2.5	2	L/H[13], T=average
15	Media Lifetime (yr)	15	25	20	Expert judgment
16	Hydraulic Loading Rate (m/h)	10	25	15	L/H[13], T=expert judgment
17	Anthracite Depth (m)	0.405	0.5	0.45	B= 0.45[13], L/H = ±10% of T
18	Sand Depth (m)	0.27	0.33	0.3	B= 0.3[13], L/H = ±10% of T
19	Chlorine Storage Tank Lifetime (yr)	30	35	30	L/H[23], T[24]
20	Chlorine Delivery Rate (trips/week)	0.5	2	1	L=every other week, H=twice a week, T=weekly
21	Chlorine Pump Head (m)	1.22	70.3	70.3	L/H[25], T=conservative
22	Concrete Basin Base Thickness (m)	0.30	0.61	0.46	L/H[26], T=average
23	Concrete Basin Wall Thickness (m)	0.23	0.46	0.46	L/H[26], T=same as base thickness
24	Baffling Factor for Tank with 2 Baffles	0.3	0.5	0.4	L/H[14], T=average
25	Baffle Thickness (cm)	3.8	4.5	4.5	L[27], H=[28](Fig. 1), T=conservative
26	Steel Baffle Life Expectancy (yr)	30	60	45	L/H[23], T[24]
27	Concrete Life Expectancy (yr)	30	60	30	L/H[23], T[24]
28	Chlorine Storage Tank Thickness (cm)	1.3	5.1	3.2	L/H[14], T=average
29	Landfill Hauling Distance (km)	20	100	20	L[29], H=expert judgement, T=most reliable estimate[29]
30	Chemical Hauling Distance (km)	20	100	20	L[29], H=expert judgement, T=most reliable estimate[29]
31	Ozone generator mass (kg/(g/hr))	0.8	18.7	9.8	L[30], H[31], T=average

S7. Typical Source Water Analysis

S7.1 UV Disinfection Compared to Chlorine Disinfection

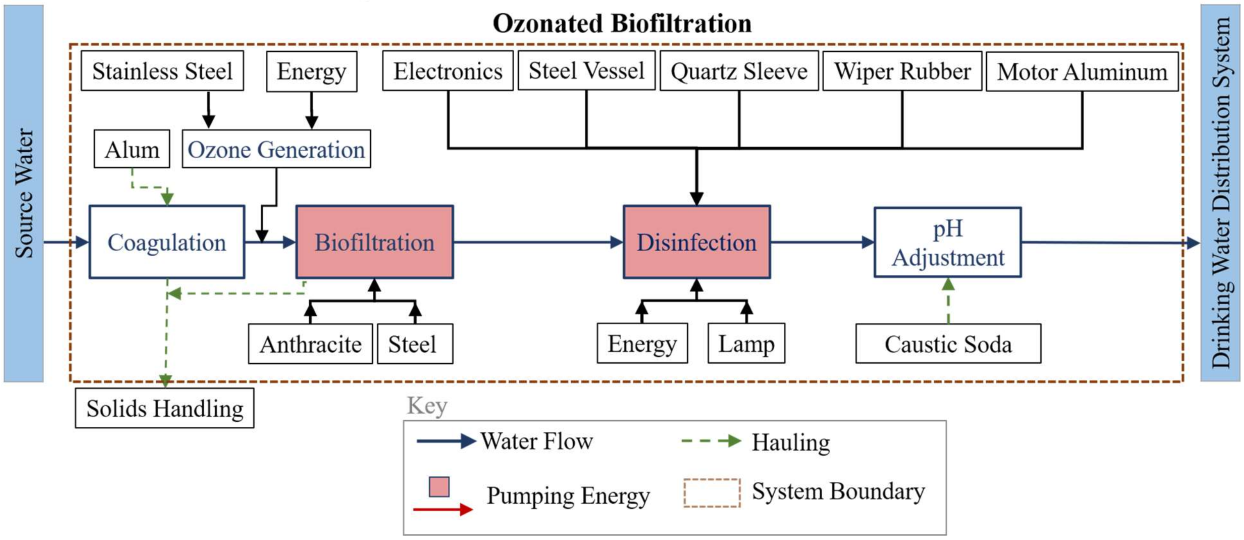

Figure S5. The LCA system boundary of the UV disinfection alternative treatment train, which included treatment processes (blue text and lines) as well as LCI unit processes for the materials and chemicals (black text and lines), for hauling (dashed green lines), and for energy (red lines or red fill color). Refer to the web version for proper interpretation of references to color in this figure.

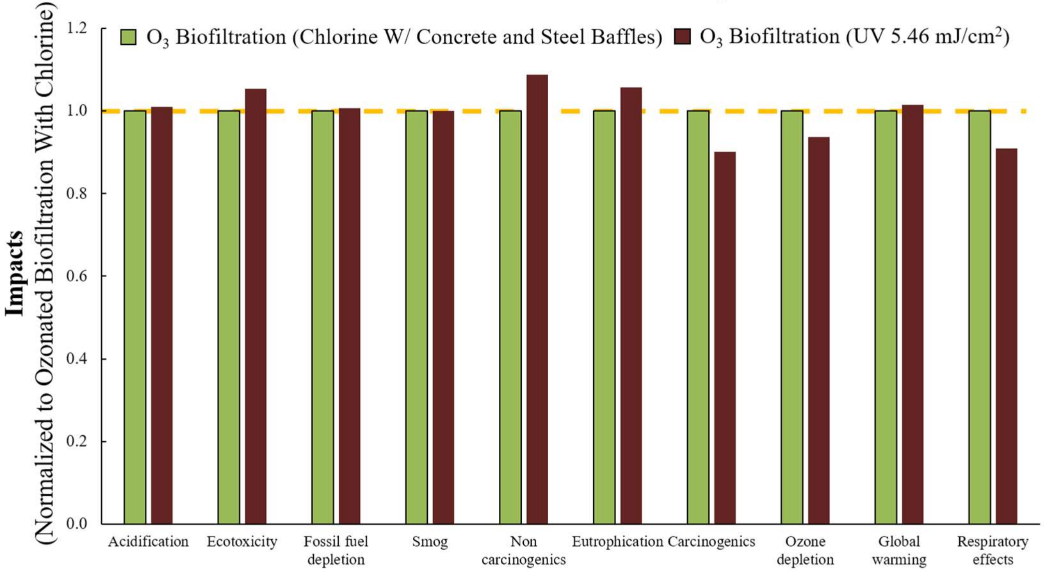

Figure S6. Ozonated biofiltration impacts using chlorine and ultraviolet (UV) disinfection using the model developed by Jones et. al. 2018, where the results are consistent for a comparison of chlorine with a concrete contact zone and steel baffles vs. UV (5.46 mJ/cm^2 dose) without chlorination.[6] Infrastructure and operations were scaled to the flow rate used in this manuscript (2730 m^3/day), and virus removal was expected to be achieved by ozonation and biofiltration. Ultimately, disinfection plays a minor role to total impacts compared to alum and caustic chemical dosing, and results were not significantly different across all impact categories. For detailed analysis of these trends see Jones et. al. 2018.[6]

S7.2 Typical Source Water Scenario Process Contribution

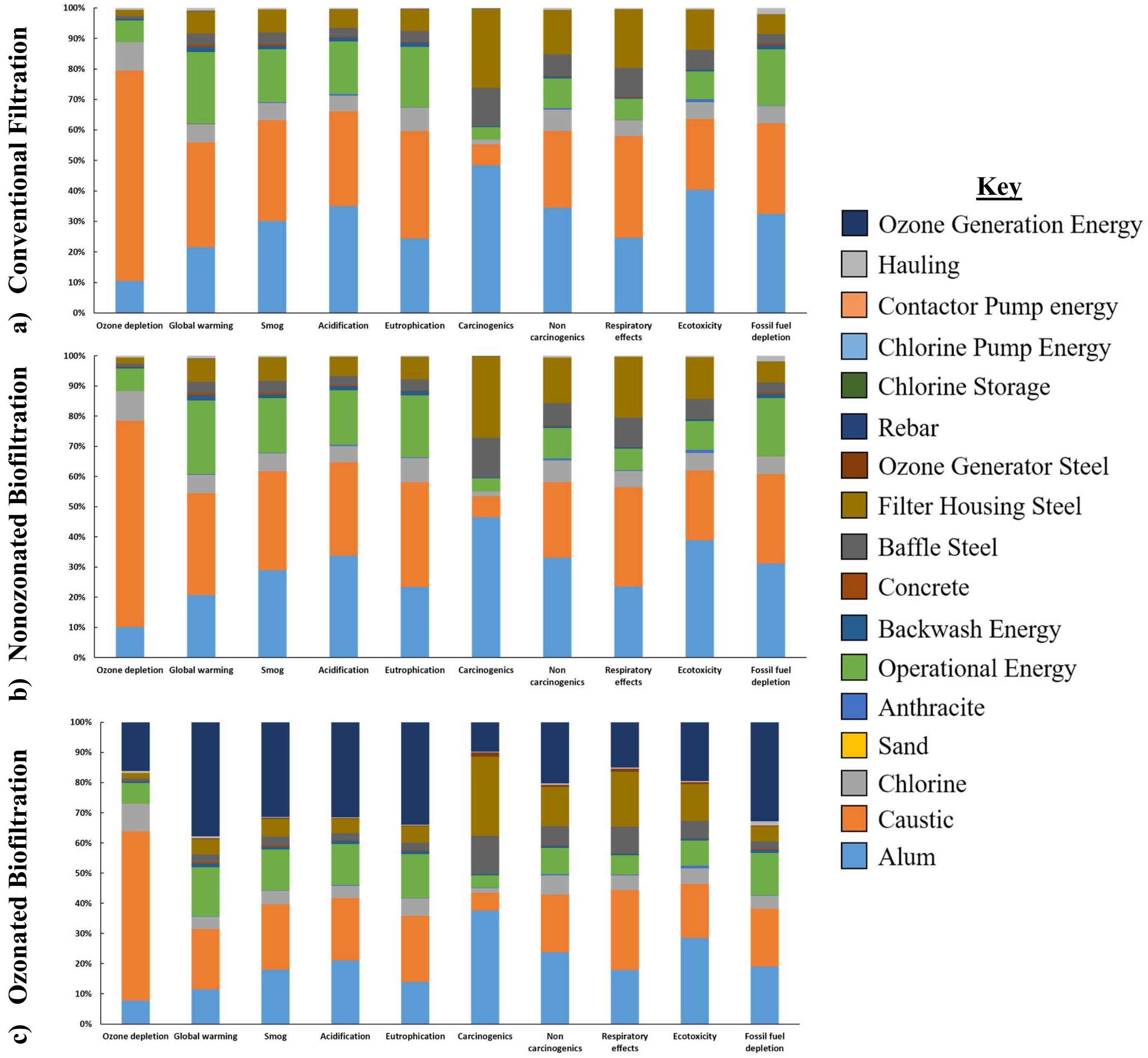

Figure S7. Impact breakdown in relation to total impacts for (a) conventional filtration, (b) nonozonated biofiltration, and c) ozonated biofiltration for the typical source water scenario (from Figure 3).

S7.3 Alternative Chemical Analysis

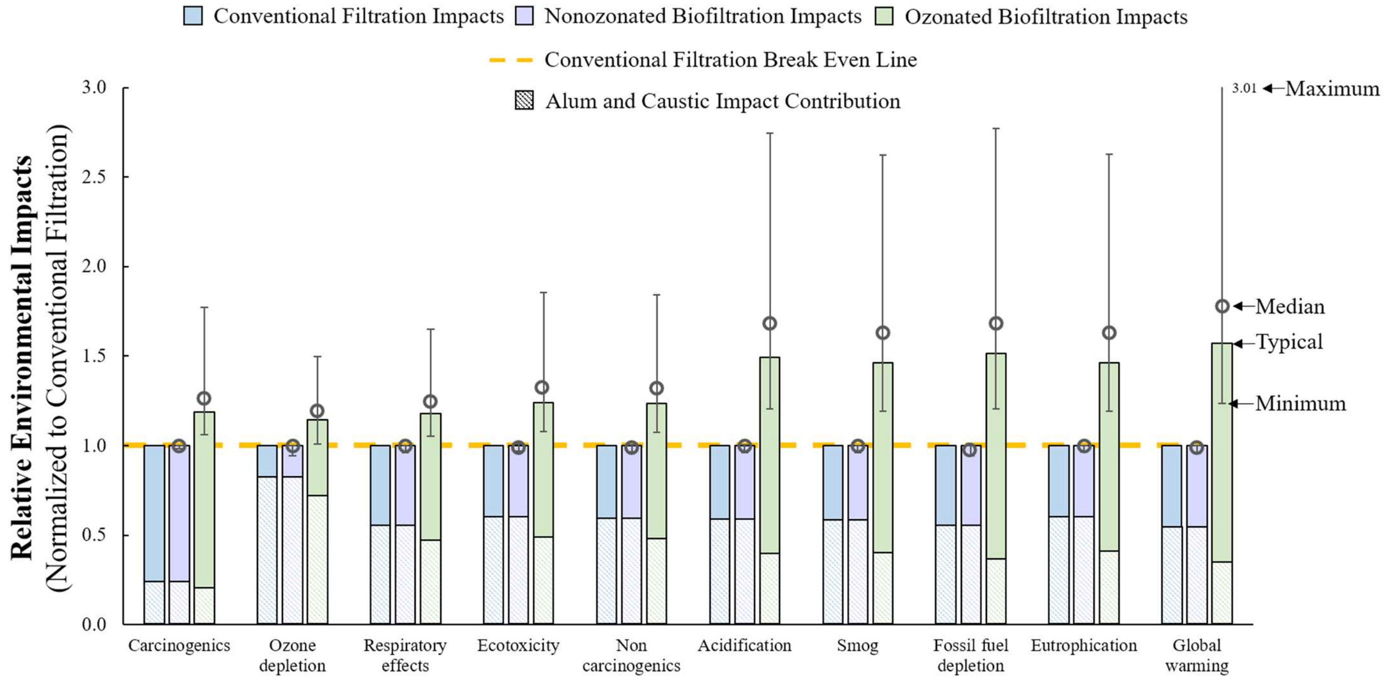

Figure S8. Same as Figure 3 in the main paper, except the coagulant used was ferric chloride. The distribution selections had no notable changes in results.

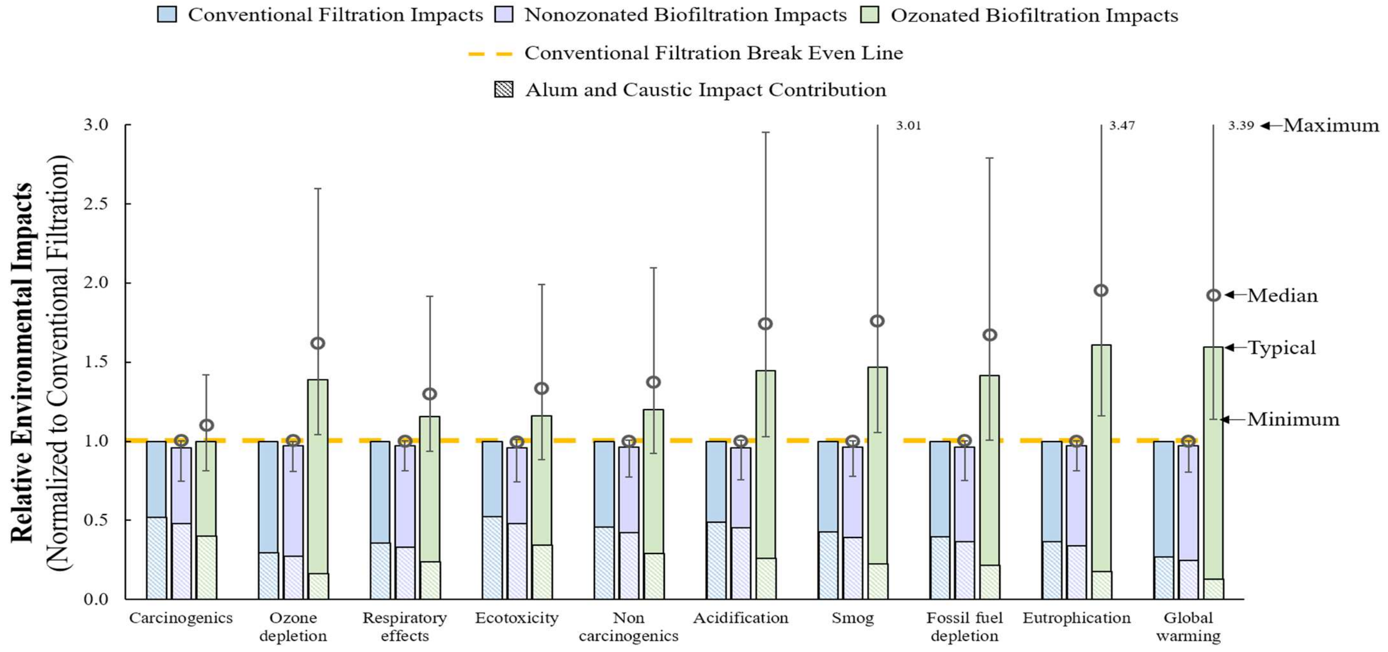

Figure S9. Same as Figure 3 in the main paper, except the pH adjustment chemical used was lime. The distribution selections had no notable changes in results.

S7.4 Ozone Uncertainty due to Source Water

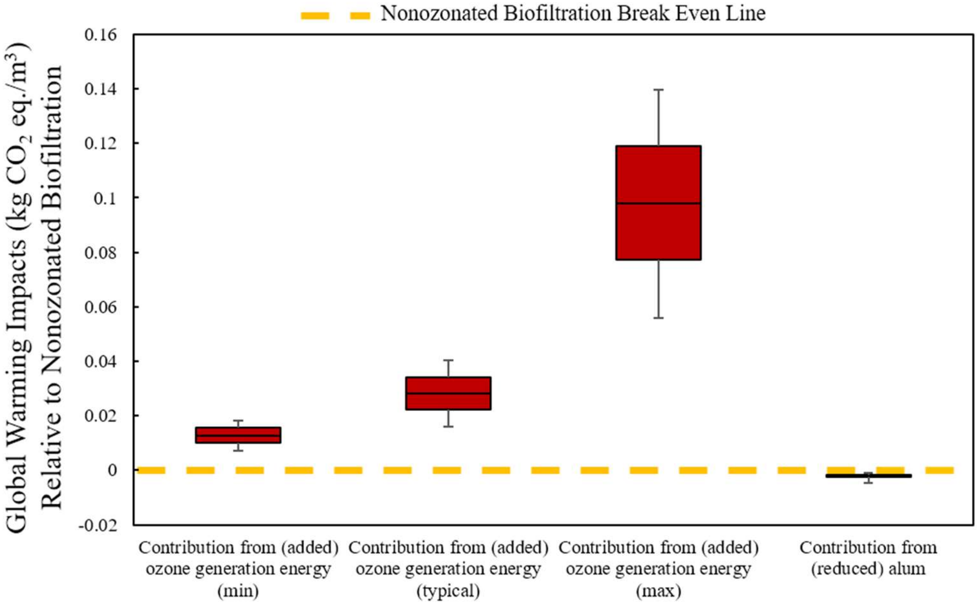

Figure S10. Results for ozone energy and alum offset impacts from using ozonation where error is due to source water quality as opposed to design uncertainty. Ozone energy results were discretely separated into low typical and high ozone energy impact scenarios. Comprehensive source water analysis (20,000 source waters at 15°C) evaluated under the enhanced coagulation treatment scenario.

S8. Comprehensive Source Waters Analysis

S8.1 Additional Source Water Analysis

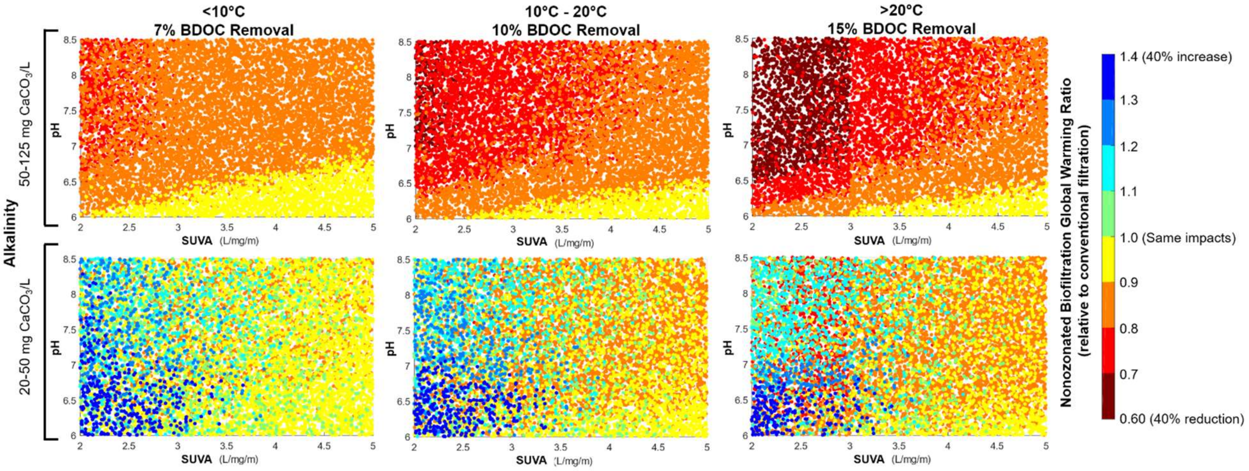

Figure S11. 15% biofilter TOC removal corresponded to performance expected above 20°C or above, 10% between 10°C and 20°C (typical), and 7% biofilter TOC removal corresponded to performance expected below 10°C. Comprehensive source water analysis (20,000 source waters at 15°C) evaluated under the 50% treatment scenario.

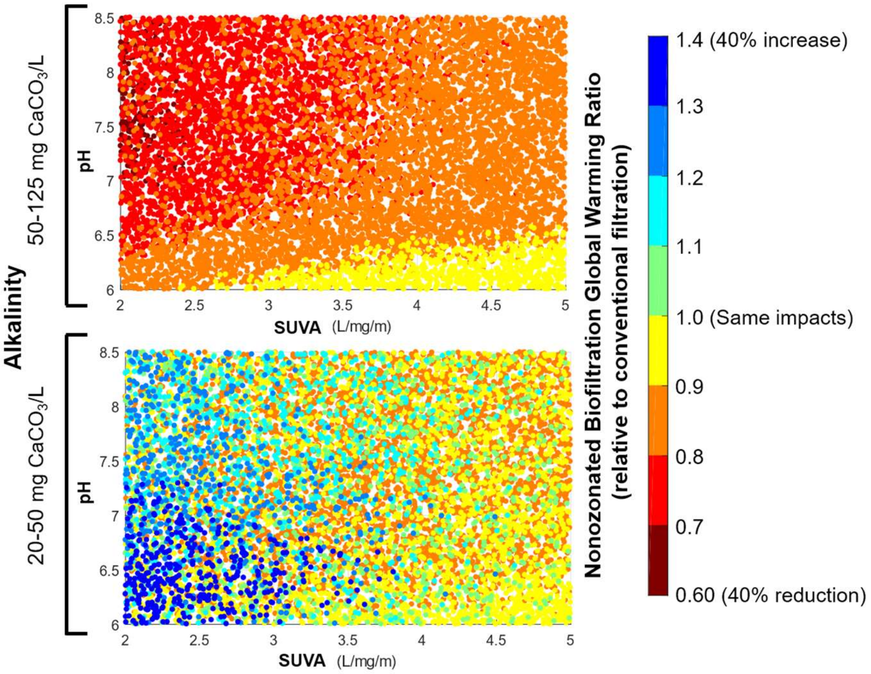

Figure S12. High TOC range (5 to 8 mg/L TOC) bins (excluded from Figure 5). Comprehensive source water analysis (20,000 source waters at 15°C) evaluated under the 50% treatment scenario.

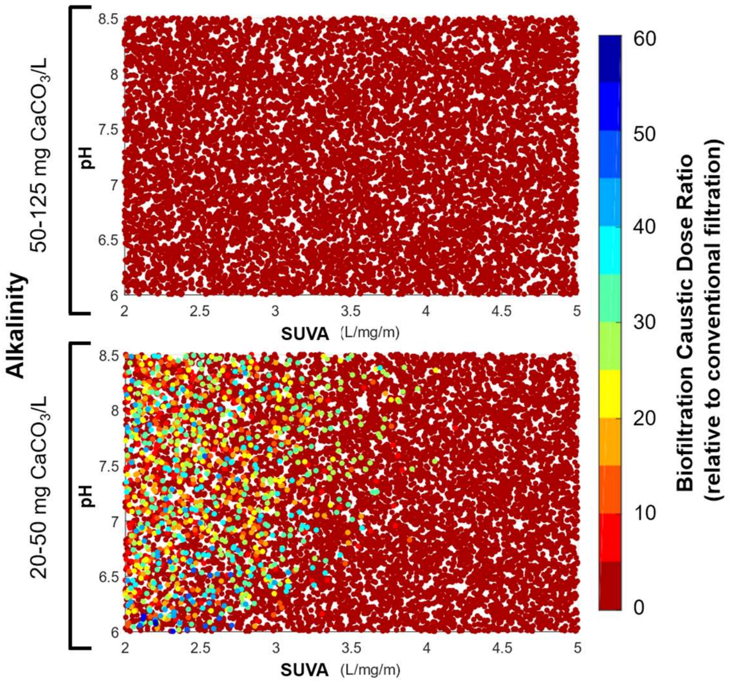

Figure S13. Biofiltration caustic soda dose compared to conventional filtration caustic dose for all 15°C scenarios. Comprehensive source water analysis (20,000 source waters at 15°C) evaluated under the 50% treatment scenario.

S8.2 pH Trend Analysis

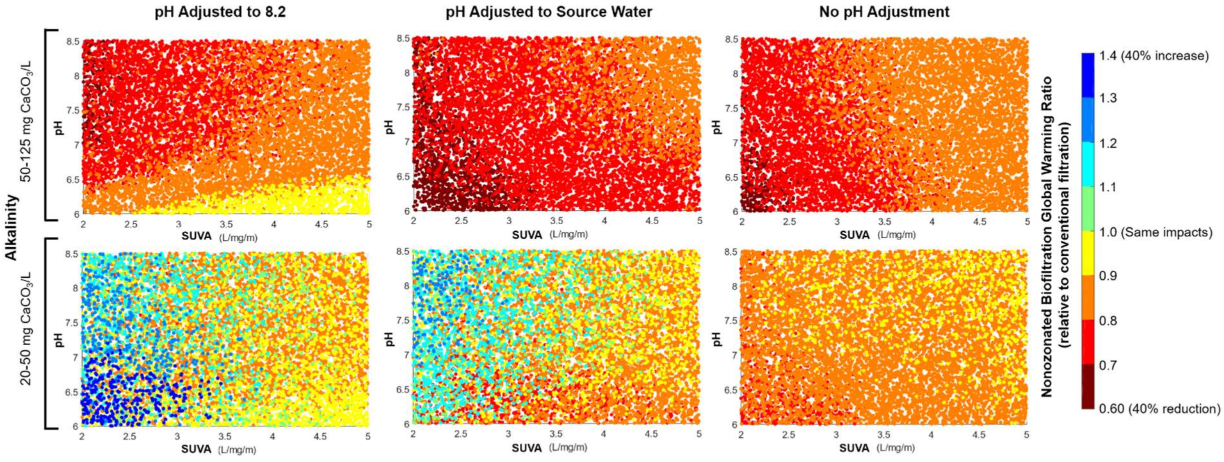

Figure S14. Trends when the caustic pH adjustment at the end of the plant is bringing the pH up to 8.2, pH back to the source water pH, and no pH adjustment. Comprehensive source water analysis (20,000 source waters at 15°C) evaluated under the 50% treatment scenario.

S8.3 Sensitive Parameters

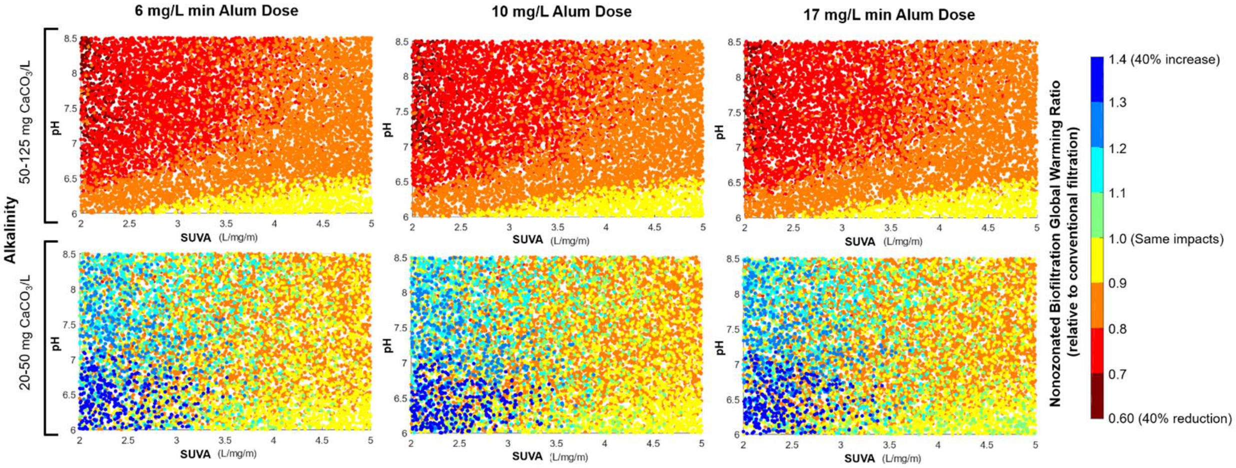

Figure S15. Figure 5 from main paper with a 6 mg/L, 10mg/L (typical), and 17 mg/L minimum allowable alum dose. Comprehensive source water analysis (20,000 source waters at 15°C) evaluated under the 50% treatment scenario.

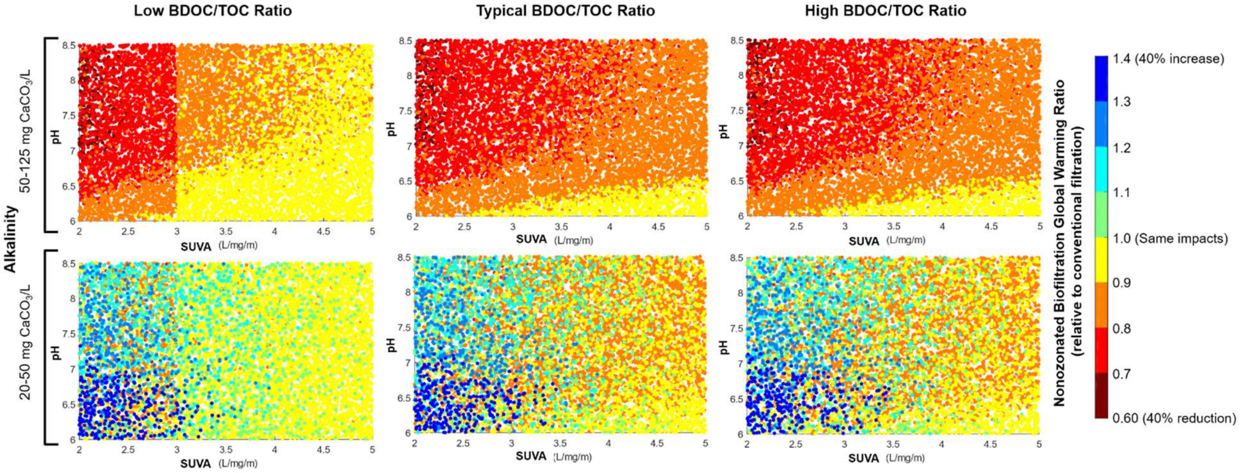

Figure S16. Figure 5 from the main paper with a source water BDOC/TOC ratio of 0.14, 0.20 (typical), and 0.27. Comprehensive source water analysis (20,000 source waters at 15°C) evaluated under the 50% treatment scenario.

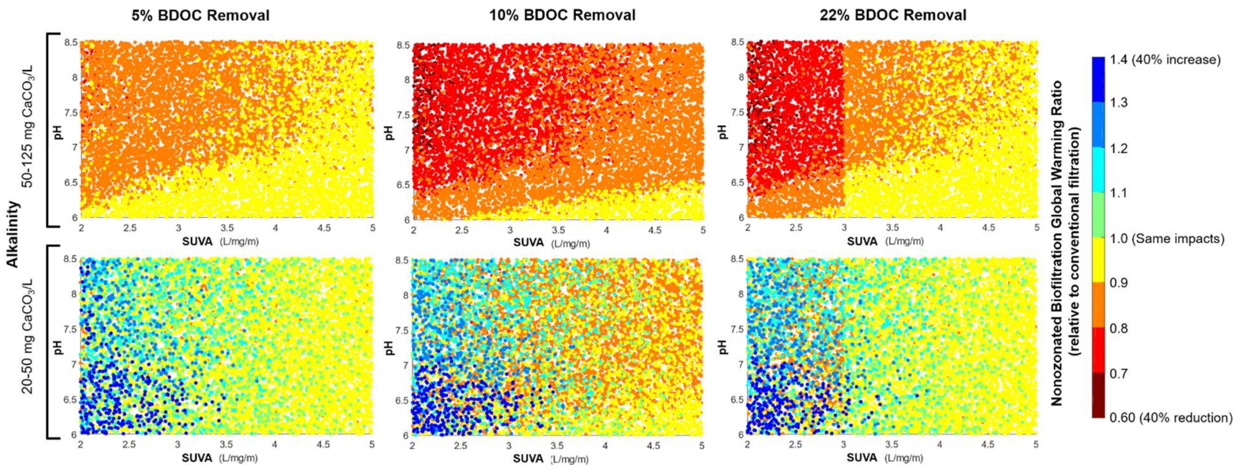

Figure S17. Figure 5 from the main paper with 5%, 10% (typical), and 22% BDOC removal through nonozonated biofiltration. Comprehensive source water analysis (20,000 source waters at 15°C) evaluated under the 50% treatment scenario.

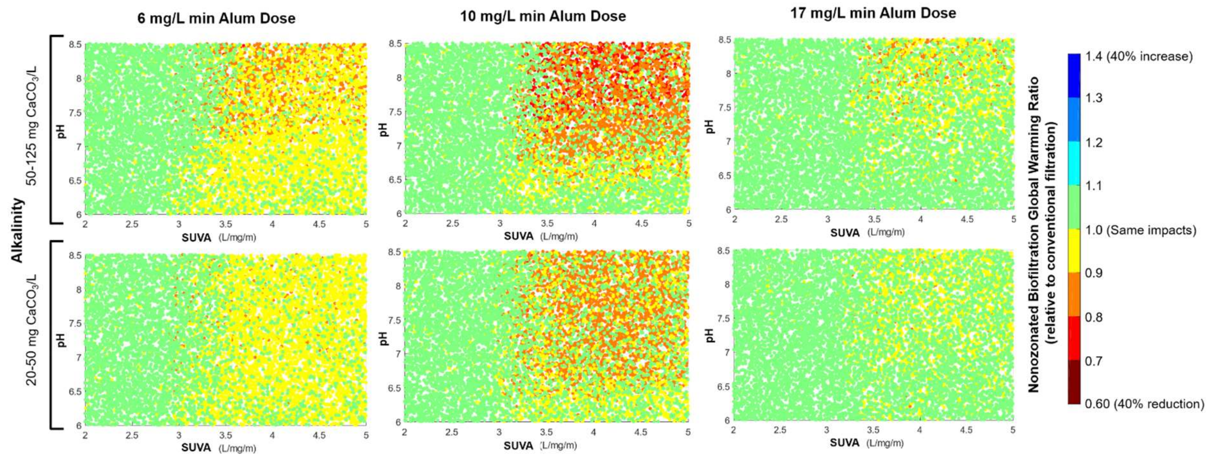

Figure S18. Figure 5 from main paper with a 6 mg/L, 10 mg/L (typical), and 17 mg/L minimum allowable alum dose. Comprehensive source water analysis (20,000 source waters at 15°C) evaluated under the enhanced coagulation treatment scenario.

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