

Supporting Information for
Oxidation of Sulfides Following Anaerobic Municipal Wastewater
Treatment for Non-Potable Reuse Applications

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Contents

Table S1. Products of sulfide oxidation.	S3
Figure S1. SAF-MBR effluent sulfide concentrations.	S3
Figure S2. Titration of SAF-MBR effluent.	S4
Text S1. UV Calibration.	S4
Figure S3. NDMA photolysis in the lab and theoretical based on time.	S6
Figure S4. NDMA photolysis in the lab and theoretical based on fluence.	S7
Table S2. Incidence fluence using correction factors.	S8
Figure S5. UV fluence correlation to flowrate for pilot UV unit.	S9
Table S3. Gradient method parameters for detecting sulfite using HPLC/UV.	S9
Table S4. Ion chromatography gradient method parameters.	S10
Table S5. Comparison of elemental sulfur concentrations by the TSS and chloroform extraction/HPLC.	S10
Figure S6. Total chlorine residuals measured 90 min after dosing sodium hypochlorite into SAF-MBR effluent.	S11
Figure S7. Sulfide concentrations measured after dosing NaOCl into SAF-MBR effluent in the pipeline contactor.	S12
Table S6. TSS before and 60 minutes after NaOCl addition to SAF-MBR effluent.	S12
Table S7. TSS before and 60 minutes after H ₂ O ₂ addition to SAF-MBR effluent.	S13
Figure S8. Percent of sulfides remaining in SAF-MBR effluent 6 minutes after H ₂ O ₂ addition during pilot experiments.	S14
Figure S9. Sulfide concentrations measured after dosing H ₂ O ₂ into SAF-MBR effluent in the pipeline.	S15
Figure S10. Sulfur species measured 60 minutes after H ₂ O ₂ addition to SAF-MBR effluent during a laboratory experiment.	S16
Figure S11. Chlorine dose required to achieve a 5 mg-Cl ₂ /L residual after 90 minutes during pipeline contactor and laboratory experiments with sulfide oxidation by H ₂ O ₂ .	S17
Figure S12. Chlorine residuals 24 hours after NaOCl application to SAF-MBR effluent that had previously been treated with H ₂ O ₂ .	S18
Figure S13. Total coliform in pipeline contactor effluent after UV disinfection.	S19
Table S8. Total coliform in disinfected pipeline contactor effluent.	S20
Text S2. Initial cost comparison.	S20
Table S9. Cost of laboratory and pilot experiments.	S23
Table S10. Unit chemical reagent costs.	S24
Figure S14. Initial total cost estimates of pilot and laboratory experiments.	S24
References	S25

Table S1. Products of sulfide oxidation.

Sulfur Species	Oxidation Number of Sulfur	Molar Consumption for H ₂ O ₂ or HOCl to Oxidize 1 M Sulfides to Indicated Species
Hydrogen sulfide (H ₂ S) / Bisulfide (HS ⁻)	-2	N/A
Elemental sulfur (S)	0	1
Thiosulfate (S ₂ O ₃ ²⁻)	+2	2
Sulfite (SO ₃ ²⁻)	+4	3
Sulfate (SO ₄ ²⁻)	+6	4

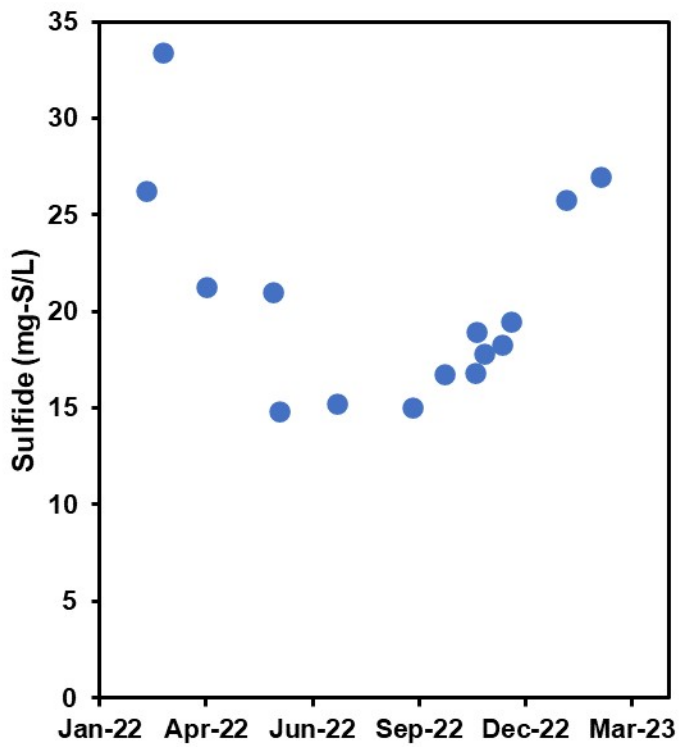


Figure S1. SAF-MBR effluent sulfide concentrations. Dates on the x-axis indicate the beginning of the indicated month.

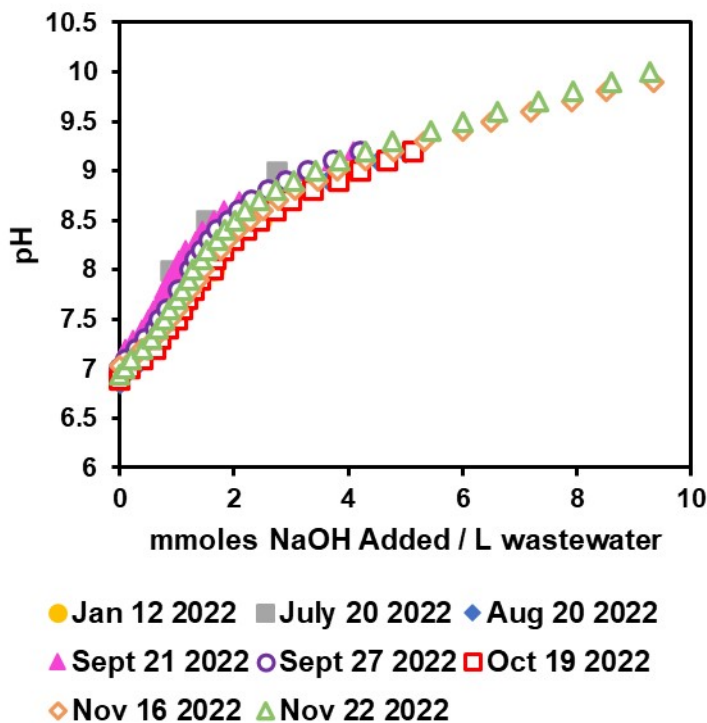


Figure S2. Titration of SAF-MBR effluent to pH ~10. The range reflects changes in buffer capacity for titrations conducted on different days.

Text S1. UV Calibration.

Overview: A low-pressure UV reactor (Trojan Technologies Viqua Pro 30; 254 nm) was installed on site after the pipeline contactor to provide UV disinfection for non-potable reuse applications. We calibrated the UV photoreactor by using NDMA as an actinometer, since its molar extinction coefficient and quantum yield are known. The UV fluence delivered to the water is controlled by varying the flowrate, and thus the residence time, of water within the reactor. The UV reactor was calibrated to determine the incident UV fluence (mJ/cm^2) delivered as a function of different flow rates through the reactor. The calibration first involved measuring the photodecomposition of NDMA within a lab-scale collimated beam apparatus (Szczuka et al., 2021) in which the UV fluence rate was well-characterized. Then, water spiked with NDMA was passed through the on-site UV reactor at different flow rates. When the percent degradation of the NDMA within the pilot reactor for a specific flow rate equals the percent degradation within the collimated beam apparatus for a specific delivered fluence, that indicates that the flowrate within the pilot reactor is associated with that specific incident UV fluence. The following paragraphs outline the procedure for the UV reactor calibration in more detail.

Equations: In general, Equation S1 describes the photolysis of a compound, C, over time.

$$[S1] \quad -\frac{dC}{dt} = 1000\phi_{\lambda}I_{o\lambda}\frac{\epsilon_{\lambda}C}{\alpha_{\lambda} + \epsilon_{\lambda}C} \frac{1 - 10^{-(\alpha + \epsilon C)l}}{z}$$

Where:

C = concentration of photolyzed compound (M)

ϕ_λ = quantum yield, percentage of photons absorbed at wavelength λ by NDMA that leads to its photolysis

α = attenuation coefficient at 254 nm; equivalent to the absorbance of the sample

$I_{o\lambda}$ = Incident fluence rate at wavelength λ (Ein cm⁻² s⁻¹)

ϵ_λ = molar extinction coefficient of compound C (M⁻¹ cm⁻¹)

l = path length of light (cm)

z = depth of sample (cm)

Note that ϕ_λ , α , $I_{o\lambda}$ and ϵ_λ all depend on wavelength, but here we are using a monochromatic light source (low pressure mercury lamp emitting at 254 nm). The incident fluence rate can be converted from Ein cm⁻² s⁻¹ units to mJ cm⁻² s⁻¹ units using the 470 kJ/Ein energy associated with 254 nm photons.

Step 1: Determine incident fluence rate of a lab-scale collimated beam low pressure UV lamp (254 nm)

The incident UV fluence rate delivered by the lab-scale collimated beam apparatus was determined using iodide/iodate actinometry, as described in Rahn (1997). The incident fluence rate of the UV lamp was determined to be 0.52 mJ/(cm²*s).

Step 2: Calculate the UV fluence of the lab-scale low-pressure UV lamp for different exposure times

The incident UV fluence at the air-water interface increases as the exposure time to the UV light increases. The UV fluence for different exposure times under the collimated UV lamp was calculated using:

Incident UV Fluence (mJ/cm²) = Incident Fluence rate (mJ cm⁻² s⁻¹)*(time spent under UV lamp in s)

For 30 min of exposure (1800 seconds), the incident fluence would be 931 mJ/cm².

Step 3: Determine theoretical photolysis of NDMA

For a solution containing only one compound (NDMA), $\epsilon C l$ is α and where $\epsilon C l < 0.02$, which occurs in very dilute solutions, Equation S1 reduces to Equation S2:

$$[S2] \quad -\frac{dC}{dt} = 2303\phi I_0 \epsilon C$$

Note here that for a collimated beam, the pathlength l equals the depth, z. Equation S2 also incorporates the factor of 1000 needed to convert from cm³ to L since I_0 is in units of Ein cm⁻² s⁻¹. Using Equation S2, we can predict the photolysis of NDMA in dilute solution by using the known molar extinction coefficient of NDMA at 254 nm (1650 M⁻¹ cm⁻¹) and the quantum yield at pH 7 under air-saturated conditions (0.3) (Lee et al., 2005). For 1 μ M NDMA, the UV absorbance at 254 would be 0.00165 cm⁻¹, satisfying the $\epsilon C l < 0.02$ requirements for Equation S2. Based on Equation S2, we would expect first-order decay with a pseudo first-order rate constant of 1.25×10^{-3} s⁻¹. The fraction of NDMA remaining for various exposure times (C/C_0) can be predicted for each exposure time and thus for each incident UV fluence. We compared this to the experimental data using the collimated beam apparatus in the

laboratory. Using 1 μM NDMA, Figure S3 below indicates that data from two experimental rounds in deionized water agreed with the predictions. This validates the use of NDMA as an actinometer.

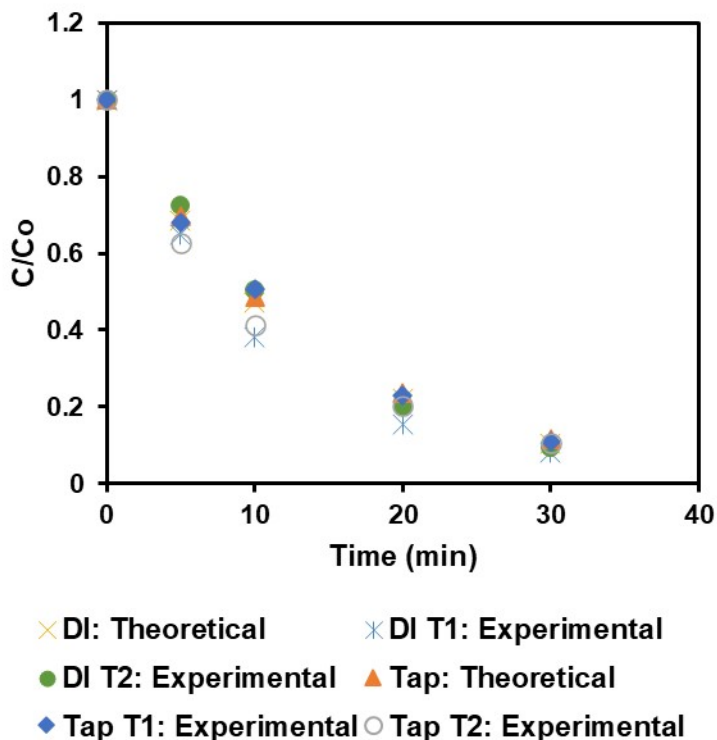


Figure S3. NDMA photolysis measured experimentally in the lab and predicted by Equation S2 (theoretical) for different UV exposure times.

Note that the fluence rate calculated by iodide/iodate actinometry provides the incident fluence rate (i.e., the fluence delivered to the air-water interface). The average fluence experienced by molecules in solution can be reduced because solution constituents absorb photons between the air-water interface and the molecule and the degree of absorbance increases with the pathlength, as indicated in Equation S1. For the $\epsilon Cl < 0.02$ conditions relevant to the NDMA in DI water experiment, the solution is essentially transparent and the fluence does not significantly decrease with increasing pathlength. However, in real waters, the degree of photodegradation will be decreased due to solution absorbance and we would want to report the average UV fluence experienced throughout the solution to predict contaminant degradation.

For example, at the pilot site, deionized water was not available and we spiked tap water with 1 μM NDMA. The tap water source at the pilot site and the lab was the same. The lab tap water absorbance at 254 nm was 0.04 cm^{-1} , and thus the $\epsilon Cl < 0.02$ condition appropriate to the use of Equation S2 is no longer met. Thus we used Equation S1, simplified by assuming that the contaminant (NDMA) is a minor contributor to the total solution absorbance (α), as in Equation S3. For tap water, the correction is minor and again the predicted and experimental degradation in Stanford tap water were about the same (Figure S3).

$$[S3] \quad -\frac{dC}{dt} = 1000\phi_{\lambda}I_{o\lambda}\frac{\epsilon_{\lambda}1 - 10^{-(\alpha)l}}{\alpha_{\lambda}z}C$$

For both the lab deionized water and tap water experiments, the C/C_0 values can also be plotted against UV fluence as shown in Figure S4, based on the conversion from exposure time to incident fluence in Step 2 above.

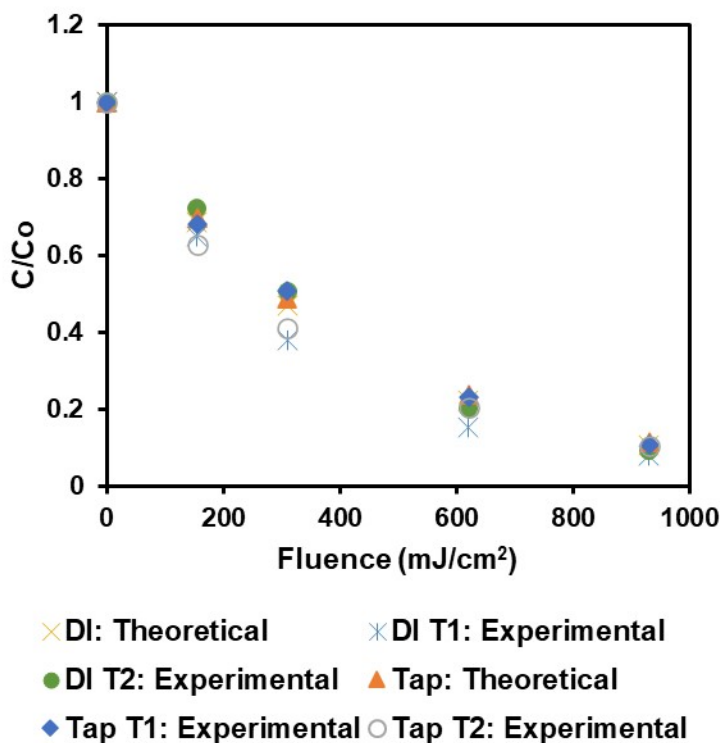


Figure S4. NDMA photolysis measured in the lab and predicted (theoretical) vs. average UV fluence.

Step 4: Measure C/C_0 for NDMA spiked into tap water within the pilot unit for different flowrates

At SVCW, buckets of tap water (pH 7) were spiked with 1 μM NDMA and passed through the pilot UV unit at different flowrates. Effluent samples were measured for residual NDMA to calculate C/C_0 (Table S2). Based on the predicted relationship between NDMA degradation in deionized water and incident UV fluence (which is approximately equal to the average UV fluence for deionized water), a fluence-based NDMA degradation rate constant can be derived as $0.0024 \text{ (mJ/cm}^2\text{)}^{-1}$. This value was used to convert the C/C_0 values for NDMA observed for different flowrates to the average UV fluence delivered to the tap water for these flowrates (Table S2).

Note that this is the average UV fluence experienced by the NDMA within the parcel of water, which is less than the incident UV fluence delivered to the water by the lamp, since there was significant UV absorbance at 254 nm within the tap water used for this field experiment (0.055 cm^{-1}). Ultimately, we want the incident UV fluence provided by the pilot unit as a function of flowrate. Then we can correct the incident UV fluence using the absorbance of specific waters (e.g., SAF-MBR effluent) to indicate the average UV fluence delivered to a specific water parcel for a specific flowrate.

To convert the average UV fluence delivered to the tap water to the incident UV fluence provided by the pilot-scale lamp, we can recognize that the first-order photodegradation rate constant for NDMA in deionized water would be provided by Equation S4:

$$[\text{S4}] \quad k_{obs} = 2.303 \times 1000 \phi \epsilon I_{DI}$$

Equation S3 predicts NDMA photodegradation within the tap water sample in the UV reactor using the absorbance ($\alpha = 0.055 \text{ cm}^{-1}$) and assuming a pathlength of 4 cm and solution depth of 4 cm for the pilot unit. Accordingly, the first-order NDMA photodegradation rate constant would be provided by Equation S5:

$$[S5] \quad k_{obs} = 1000\phi\epsilon I_{inc}(1 - 10^{-\alpha l})/(\alpha Z)$$

where I_{inc} represents the incident UV fluence delivered to the air-water interface.

Setting the two k_{obs} values equal, we can solve for I_{inc} in terms of I_{DI} :

$$[S6] \quad I_{inc} = 2.303\alpha Z I_{DI}/(1 - 10^{-\alpha l})$$

Table S2 below provides the I_{inc} values determined using this correction factor. Then, for a water containing a specific UV absorbance (e.g., SAF-MBR effluent), we can calculate the average UV fluence delivered for a specific flowrate based on this incident UV fluence associated with that specific flowrate and the UV absorbance of that water. We do that by inverting the equation above:

$$[S7] \quad I_{av} = I_{inc}(1 - 10^{-\alpha l})/(2.303\alpha Z)$$

The right-most column in the table below shows values calculated for a water with a UV absorbance of 0.3 cm^{-1} (similar to many SAF-MBR effluent samples) and a pathlength and depth of 4 cm.

Table S2. Incidence fluence using correction factors.

Q	Field-Tap	Average Fluence	Incident Fluence	SAF-MBR Fluence
gpm	C/C _o	I _{DI} in mJ/cm ²	I _{inc} in mJ/cm ²	mJ/cm ²
3.5	0.29	523	667	226
2.9	0.25	582	742	252
1.95	0.13	858	1094	371
1.15	0.10	944	1203	408

The correlation is provided in Figure S5 below for this hypothetical water.

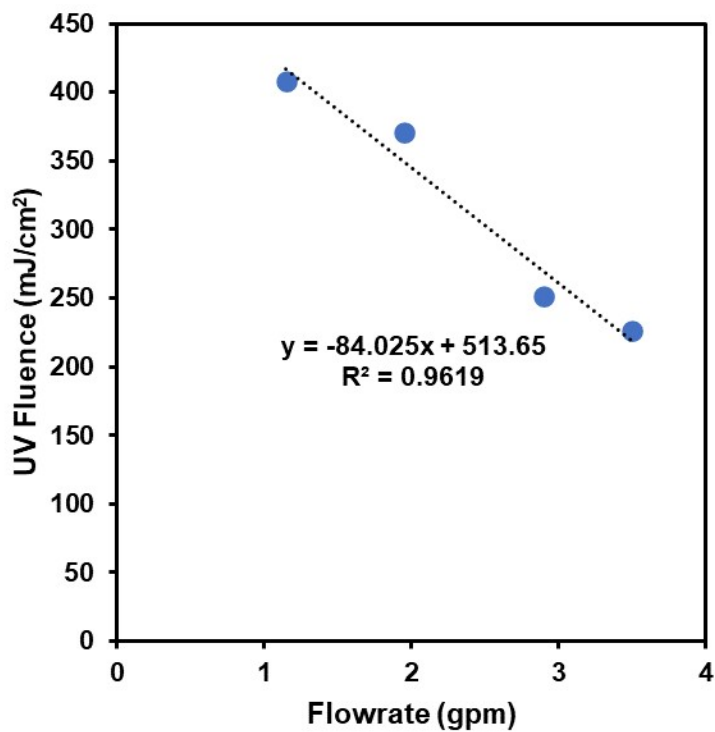


Figure S5. Average UV fluence correlation to flowrate for pilot UV unit.

Table S3. Gradient method parameters for detecting sulfite using HPLC/UV.

Time (min)	Flow (mL/min)	% Methanol	% 0.25% (v/v) Acetic Acid
0	0.73	12	88
1.064	0.73	12	88
2.280	0.73	30	70
2.889	0.73	30	70
3.496	0.73	50	50
4.560	0.73	100	0
5.016	0.73	100	0
5.031	0.73	88	12
5.500	0.73	88	12

Table S4. Ion chromatography gradient method parameters. Eluent flow was 1 mL/min.

Time (min)	Concentration (mM)
0	5
5	5
6	10
11	10
12	15
17	15
18	20
23	20
24	25
29	25
30	40
33	40
34	5
42	5

Table S5. Comparison of elemental sulfur concentrations by the TSS and chloroform extraction/HPLC analytical methods for a laboratory experiment involving NaOCl addition (Figure 3).

pH	HOCl:Sulfide Dose	Elemental sulfur according to TSS (μM)	Elemental sulfur according to chloroform extraction/HPLC (μM)
6.3	6.2	133 (± 39)	135 (± 9)
7.0	2.7	117 (± 23)	156 (± 30)

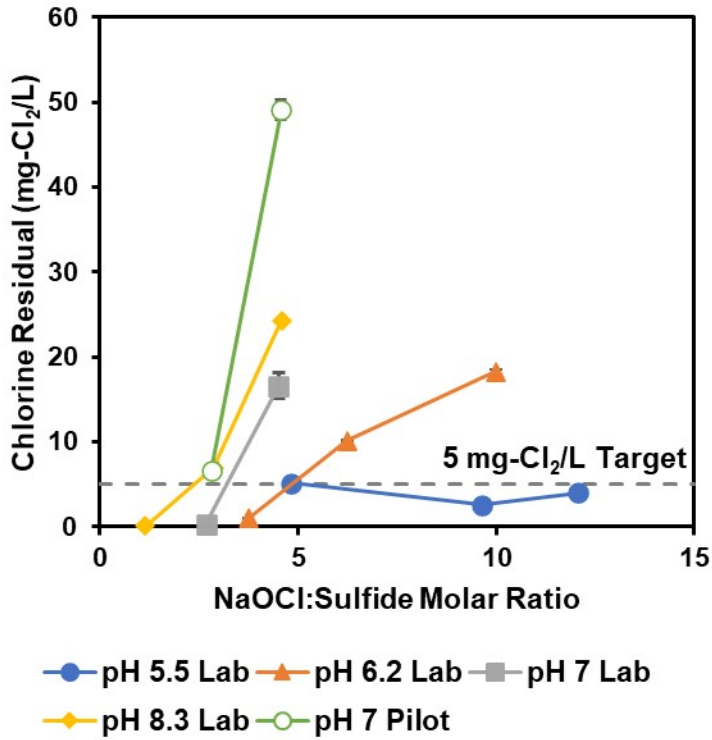


Figure S6. Total chlorine residuals measured 90 min after dosing sodium hypochlorite into SAF-MBR effluent as a function of NaOCl:sulfide molar ratios in laboratory and pilot-scale experiments. Error bars represent the range of experimental duplicates for laboratory data and analytical duplicates for pilot data. Note that a separate experiment with a similar initial sulfide concentration determined that a 3.4 NaOCl:sulfide ratio did not leave a chlorine residual at pH 5.5.

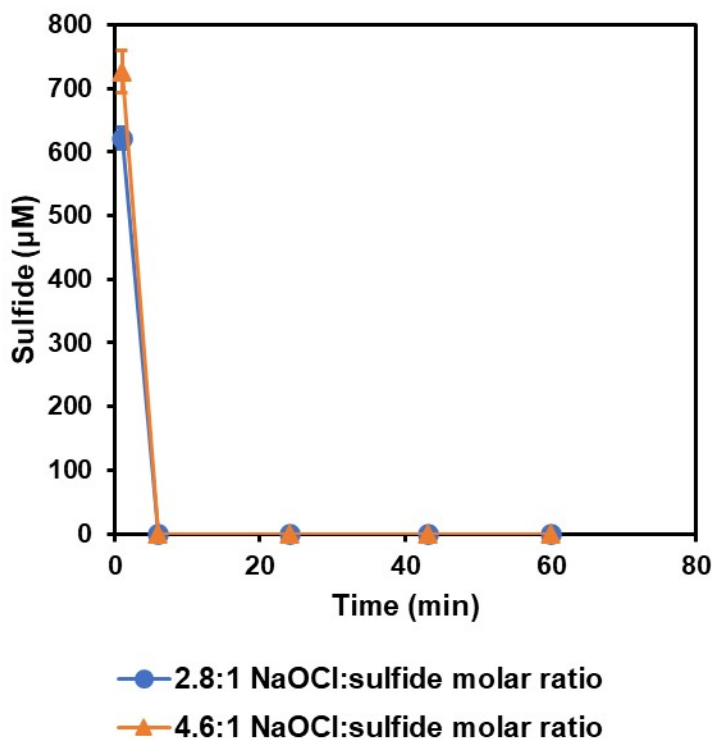


Figure S7. Sulfide concentrations measured after dosing NaOCl into SAF-MBR effluent in the pipeline contactor at pH 6.9 during two different pilot tests conducted at either a 2.8 NaOCl:sulfide molar ratio (620 µM sulfides) or a 4.6 NaOCl:sulfide molar ratio (720 µM sulfides). Error bars represent the range of analytical duplicates.

Table S6. TSS before and 60 minutes after NaOCl addition to SAF-MBR effluent during laboratory experiments at various pH conditions and NaOCl doses. Range between duplicates are indicated in brackets.

pH	NaOCl:Sulfide Molar Ratio	Pre-NaOCl TSS (mg/L)	Post-NaOCl TSS (mg/L)
5.5 (lab)	4.8	< 2	< 2
6.2 (lab)	6.2	< 2	4.3 (±1.3)
6.9 (pilot)	2.8	4.2 (±1.2)	8.9 (±4.0)
6.9 (pilot)	4.6	3.5 (±0.9)	6.2 (±0.1)
7.0 (lab)	2.7	< 2	3.8 (±0.8)
8.3 (lab)	2.9	< 2	5.3 (±3.8)

Table S7. TSS before and 60 minutes after H₂O₂ addition to SAF-MBR effluent. Range between analytical duplicates are indicated in brackets.

pH	H₂O₂:Sulfide Molar Ratio	Initial Sulfide (μM)	Influent TSS (mg/L)	Effluent TSS (mg/L)
7.1 (lab)	1.2	665	< 2	5.5 (±0.5)
7.1 (lab)	1.2	761	< 2	15.8 (±0.8)
7.0 (pilot)	1.3	476	< 2	4.8 (±1.8)
7.1 (pilot)	1.7	821	< 2	19.4 (±0.6)
7.1 (pilot)	1.8	805	< 2	17.4 (±1.4)
7.1 (lab)	1.8	665	< 2	9.0 (±0)
7.1 (lab)	2.5	665	< 2	10.5 (±1.0)
7.1 (pilot)	6.3	878	< 2	14.9 (±1.4)
7.1 (pilot)	6.4	862	< 2	16.3 (±0.5)
8.3 (pilot)	2.4	636	< 2	< 2
8.3 and 9 (lab)	2.5, 3.5, and 4.5	335	N/A ¹	N/A
8.3 (lab) ²	3.4	761	< 2	< 2
8.3 (pilot)	3.5	1,194	< 2	< 2
8.3 (pilot)	3.8	730	< 2	< 2
8.3 (pilot)	4.4	937	< 2	< 2
8.3 (pilot)	5.4	1,083	< 2	< 2

¹ TSS not measured

² from experiment in Figure S7

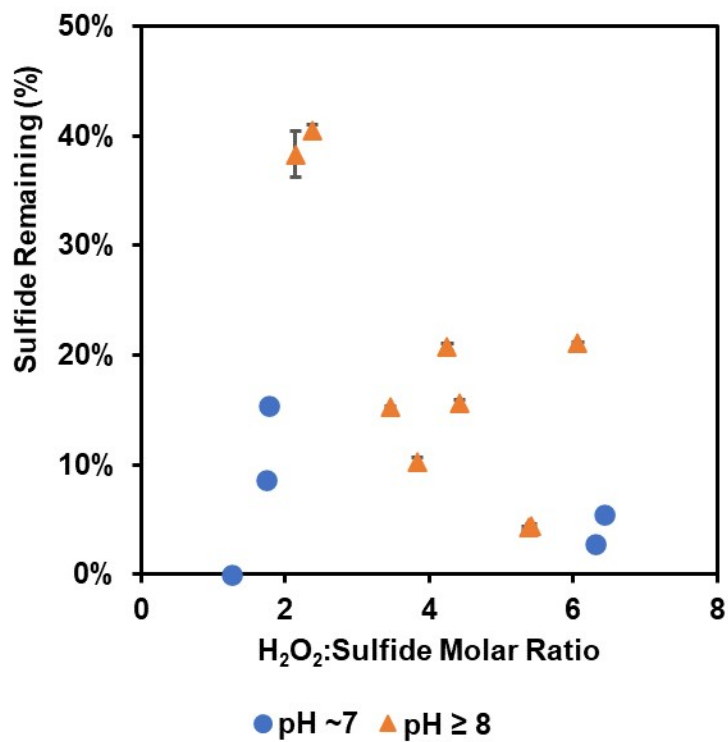


Figure S8. Percent of sulfides remaining in SAF-MBR effluent 6 minutes after H₂O₂ addition during pilot experiments. Error bars represent the range of analytical duplicates.

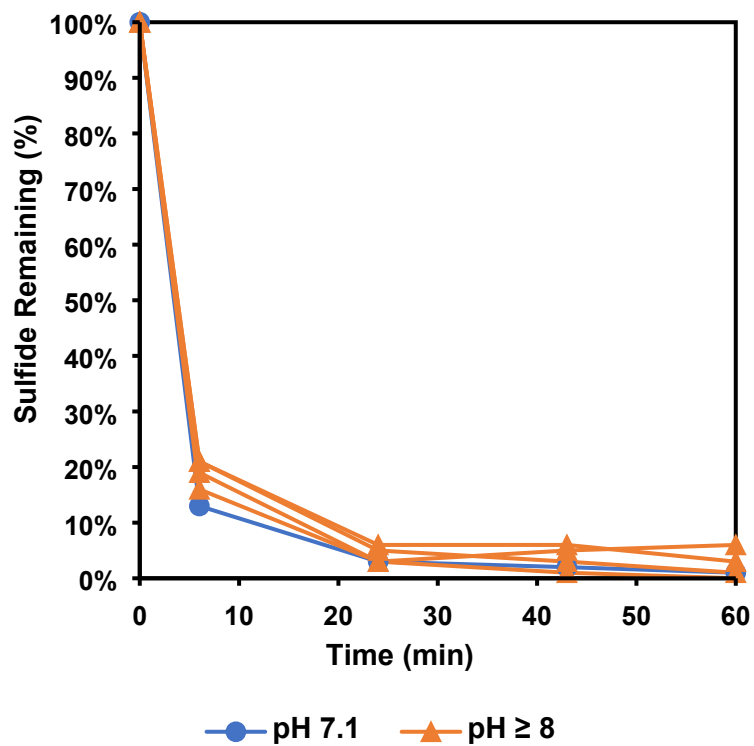


Figure S9. Sulfide concentrations measured after dosing H_2O_2 into SAF-MBR effluent in the pipeline contactor during pilot tests where >10% of sulfides remained after 6 minutes (first sample port) and the H_2O_2 :sulfide molar ratio was > 1 at native pH conditions (~7) and > 3 at pH > 8.2.

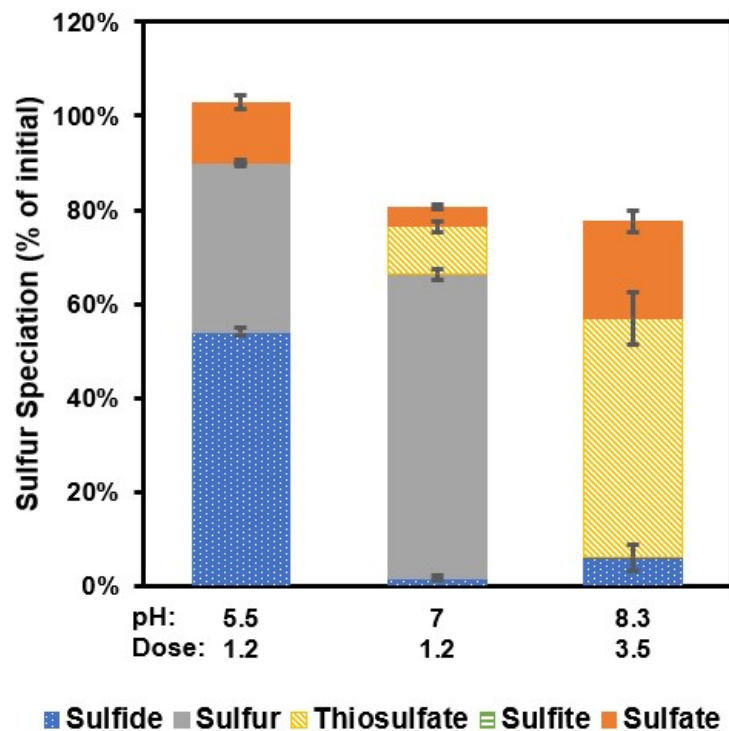


Figure S10. Sulfur species measured 60 minutes after H₂O₂ addition to SAF-MBR effluent during a laboratory experiment at various pH conditions. “Dose” = H₂O₂:sulfide molar ratio. Error bars represent the range of experimental duplicates. The initial sulfide concentration was 761 μM.

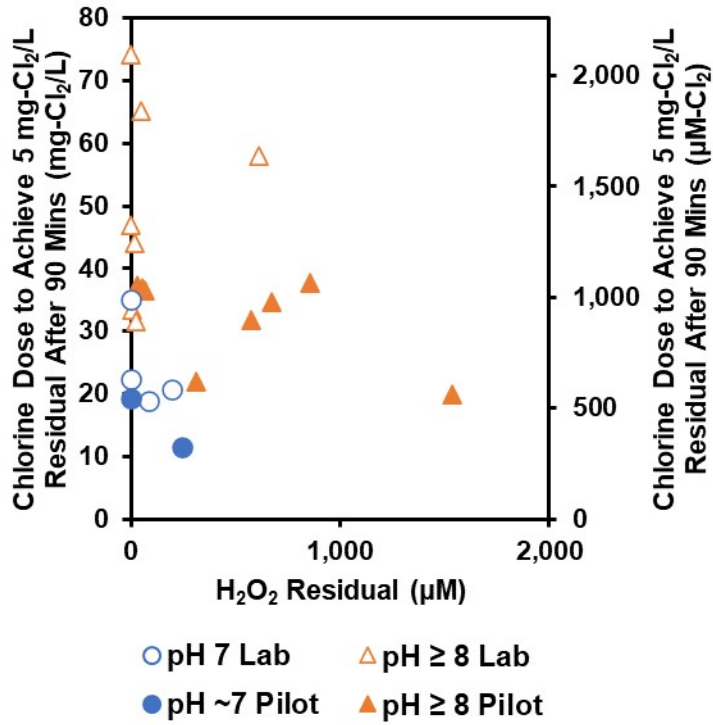


Figure S11. Chlorine dose required to achieve a 5 mg-Cl₂/L residual after 90 minutes during pipeline contactor and laboratory experiments with sulfide oxidation by H₂O₂.

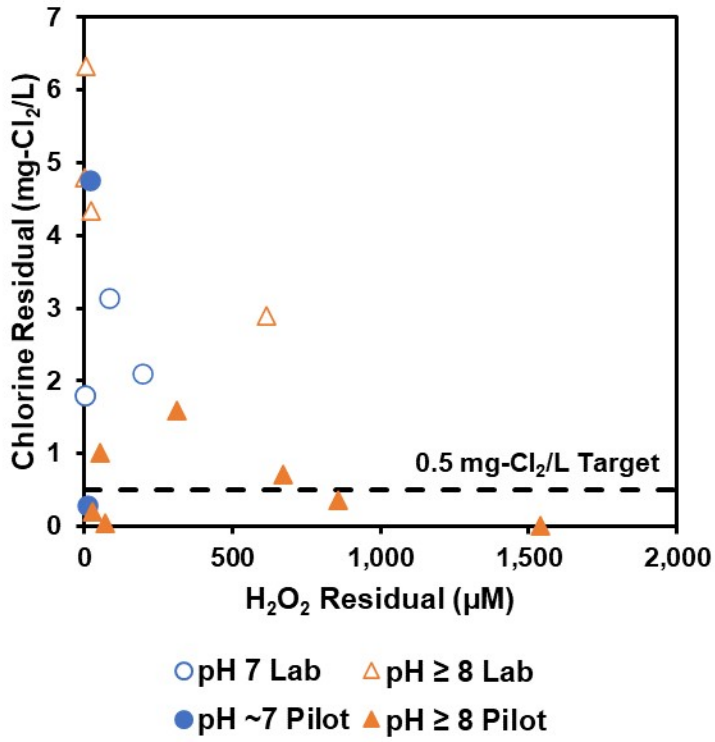


Figure S12. Chlorine residuals 24 hours after NaOCl application to SAF-MBR effluent that had previously been treated with H₂O₂.

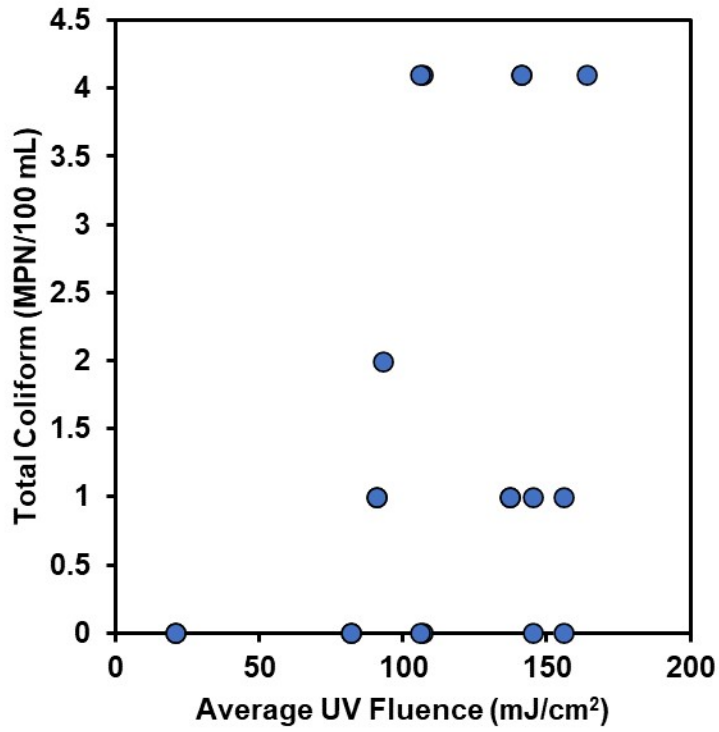


Figure S13. Total coliform in pipeline contactor effluent after UV disinfection including duplicate samples for each pilot run. Two of the pilot runs had only one data point (no duplicate) due to processing errors.

Table S8. Total coliform in disinfected pipeline contactor effluent.

	Units	Test #1 ¹	Test #2	Test #3	Test #4	Test #5
pH		9.1	8.4	8.2	8.5	9.0
H ₂ O ₂ :Sulfide Molar Ratio		3.6	3.4	3.3	3.4	4.5
UV ₂₅₄	cm ⁻¹	0.43	0.33	0.31	0.30	0.30
NaOCl Dose to provide 5 mg-Cl ₂ /L residual	mg-Cl ₂ /L	35	37	38	47	>53
<u>Total Coliform</u>						
SAF-MBR Effluent	MPN/100 mL	4.6	6.3	200	10	1.5
After H ₂ O ₂ but before Filtration	MPN/100 mL	14	7	13	2	0
After Cartridge Filtration	MPN/100 mL	244	N/A	N/A	N/A	N/A
UV Dose 1	MPN/100 mL	2.0 ²	1.0, 1.0	1.0, 0	0, 0	0, 0
I _{inc} , I _{avg} ³	mJ/cm ²	376, 93	258, 81	435, 145	238, 82	62, 21
UV Dose 2	MPN/100 mL	0, 4.1	0, 4.1	4.1 ²	0, 1.0	0, 0
I _{inc} , I _{avg}	mJ/cm ²	435, 107	337, 106	494, 164	454, 156	454, 155
UV Dose 3	MPN/100 mL	4.1, 4.1	1.0, 1.0	-	-	-
I _{inc} , I _{avg}	mJ/cm ²	572, 141	435, 137	-	-	-
Chlorine (Dose, mg Cl ₂ /L)	MPN/100 mL	0, 0 (39)	0, 0 (37)	0, 0 (40)	0, 0 (47)	0, 0 (47)

¹ Cartridge filter (100% polypropylene, Aquaboon; 5 µm prefilter and 1 µm main filter) before UV disinfection.

² No total coliform duplicate due to processing error.

³ I_{inc} = incident UV fluence (fluence emitted by UV reactor), I_{avg} = average incident fluence (incident fluence corrected for absorbance of wastewater)

Text S2. Initial cost comparison.

For a series of pilot and laboratory experiments reflecting a range of conditions (e.g., type of oxidant, pH), initial cost calculations were conducted as described below. Table S9 provides the conditions (initial sulfide concentration, oxidant:sulfide molar ratio, pH, etc.) for each experiment. These conditions reflect those needed to meet Title 22 guidelines. For example, ultrafiltration was included where the treated effluent featured high TSS. Chlorination to achieve a 5 mg-Cl₂/L total chlorine residual after 90 min was included. Moreover, UV disinfection at 200 mJ/cm² average UV fluence was included in all scenarios in order to achieve 5-log inactivation of MS2 bacteriophage. The procedures used to calculate each cost type are detailed below.

Unit costs for chemical reagents: Unit costs for H₂SO₄ (\$248/ton for a 93% by weight solution), NaOH (\$864/ton for a 50% by weight solution), H₂O₂ (\$545/ton for a 50% by weight solution), and NaOCl (\$0.57/L for a 12.5% by weight solution) were obtained from Orange County Water District (CA; communication with Dr. Megan Plumlee), reflecting full costs for delivered reagents in 2023. Using the densities of these technical grade solutions, the costs per mole (\$/mole) for each chemical reagent were calculated (Table S10).

Costs for pH adjustment: Experiments indicated that adjusting the SAF-MBR effluent to pH 6.2 and 5.5 required 4.4 mM and 7.8 mM hydrochloric acid, respectively. Adjusting pH with sulfuric acid would require half as much sulfuric acid (i.e., 2.2 mM and 3.9 mM H₂SO₄) since it is a diprotic acid. Using the \$0.03/mole cost for H₂SO₄ (Table S10) indicates that the cost of adjusting the SAF-MBR effluent to pH 6.2 and 5.5 would be \$0.06/m³ and \$0.11/m³, respectively.

Similarly, titration experiments (Figure S2) indicated that the average NaOH required adjust SAF-MBR effluent to pH 8.3 and 9.0 were 1.65 mM and 3.45 mM, respectively. Note that several of the experimental conditions involved pH between 8.2 and 9.1 (Table S9). Since the titration curves were linear in this range (Figure S2), the NaOH required to titrate SAF-MBR effluent to these pH values was calculated by linear interpolation. Using the \$0.08/mole cost for NaOH (Table S10) indicates that the cost of adjusting the SAF-MBR effluent to pH 8.3 and 9.1 would be \$0.12/m³ and \$0.28/m³, respectively.

H₂O₂ cost: The experiments involving H₂O₂ oxidation of sulfides evaluated the oxidation as a function of H₂O₂:sulfide molar ratio. The initial sulfide concentrations varied from 330-650 μM (Table S9). To compare different conditions (e.g., pH) on a common basis, calculations assumed that the initial sulfide concentration was 600 μM for each experiment. The H₂O₂ concentration needed to meet the H₂O₂:sulfide molar ratio used in the actual experiment was calculated in reference to the 600 μM assumed initial sulfide concentration. Capital costs for a H₂O₂ contactor were not considered. We expect these costs to be minor given that the contact time needed for sulfide oxidation was ≤ 24 min (Figure S9), suggesting that the oxidation could be conducted within piping between process units. Based on the \$0.04/mole cost for H₂O₂ (Table S10), the cost for H₂O₂ treatment ranged from \$0.03/m³ to \$0.15/m³ depending on the H₂O₂:sulfide molar ratio.

NaOCl cost: NaOCl costs were included both for experiments where NaOCl was used to oxidize sulfides and where NaOCl was used after sulfide oxidation by H₂O₂ to provide a total chlorine residual of 5 mg-Cl₂/L after a 90 min contact time. For experiments that used NaOCl to oxidize sulfides, a range of NaOCl:sulfide molar ratios were dosed to capture the optimal NaOCl:sulfide molar ratio that resulted in a 5 mg-Cl₂/L total chlorine residual after 90 minutes. This optimal NaOCl:sulfide molar ratio for each experiment was determined by linear interpolation of the total chlorine residuals measured experimentally after 90 minutes. Similar to H₂O₂ costs, the initial sulfide concentration was assumed to be 600 μM to place reagent costs for different pH and other experimental conditions on a common basis. Based on the \$0.29/mole cost for NaOCl (Table S10), the cost for NaOCl treatment ranged from \$0.42/m³ to \$0.83/m³ depending on the NaOCl:sulfide molar ratio.

For experiments that used H₂O₂ to oxidize sulfides and then added NaOCl to provide a total chlorine residual, it was assumed that the dose of NaOCl to provide a 5 mg-Cl₂/L residual after 90 minutes would not depend on the initial sulfide concentrations as the sulfides would already be oxidized by H₂O₂. We used the NaOCl dose needed to achieve a 5 mg-Cl₂/L total chlorine residual after 90 minutes determined during each experiment (Table S9). Based on the \$0.29/mole cost for NaOCl (Table S10), the cost for NaOCl treatment ranged from \$0.05/m³ to \$0.24/m³, except for the experiment conducted at pH 5.5, where the NaOCl cost was \$0.57/m³ (Table S9).

Capital costs for construction of a chlorine contact basin with a 90 minute modal contact time were not included. However, we expect this contact time and the associated capital cost to be consistent across all experimental conditions and so this cost would not differ between conditions.

Filtration cost: We considered that filtration would be required for all experiments where substantial TSS concentrations associated with elemental sulfur formation were noted. Filtration costs were not

considered for experiments involving sulfide oxidation by NaOCl treatment at pH 5.5 or H₂O₂ treatment at pH ≥ 8, where elemental sulfur formation was not observed. Here we assumed that membrane-based systems would be used. Giammar et al. (2022) reported levelized costs of water (LCOW; includes capital and operating and maintenance costs) for microfiltration at Orange County Water District, CA (\$0.18/m³) and Big Spring, TX (\$0.20/m³) as determined by the Water Techno-economic Assessment Pipe-Parity Platform (WaterTAP3). Using a value of \$0.19/m³ as an average value, this cost was adjusted upward by a factor of 1.16 to convert from January, 2021 to May, 2023 dollars using the US consumer price index (US DLS, 2023). The resulting cost for filtration (\$0.21/m³) was used for all scenarios where filtration would be needed; the cost of filtration was not expected to vary with varying sulfur concentrations.

UV disinfection cost: UV disinfection costs were based on data reported in Plumlee et al. (2014) for a UV/H₂O₂ advanced oxidation process (AOP). The annual O&M cost for AOP treatment was reported to be \$0.03 million/MGD in 2011 dollars, excluding the cost of H₂O₂. This cost was adjusted upward by a factor of 1.34 to convert from September, 2011 to May, 2023 dollars using the US consumer price index (US DLS, 2023). The authors used an electricity price of \$0.0988/kWh based on the U.S. Energy Information Administration (average retail price of all customer classes; US EIA, 2011). UV O&M costs were increased to account for an electricity price of \$0.110/kWh, which is the most current data in the US EIA data base (US EIA, 2022). Assuming a 10 MGD facility, the annual O&M cost of the UV portion of AOP would be \$0.03/m³. Assuming that the incident UV fluence of AOP is 1000 mJ/cm², the UV treatment cost was scaled for each experiment based on the incident UV fluence applied as reported in Table S9. Plumlee et al. (2014) reported the capital cost of AOP to be \$0.21 million/MGD. Assuming the full cost of a 10 MGD AOP facility with a 15-year service life, the capital cost of UV disinfection is \$0.01/m³. The total cost of UV disinfection ranged from \$0.03 to \$0.06/m³.

Table S9. Cost of laboratory and pilot experiments.

Experiment	Oxidant	Initial Sulfide (μM)	Oxidant to Sulfide Molar Ratio	pH	NaOCl Dose (mg-Cl ₂ /L)	I _{inc} ¹ (mJ/cm ²)	UV ₂₅₄	Cost (\$/m ³)						
								H ₂ O ₂	NaOCl	Filtration	H ₂ SO ₄	NaOH	UV	Total
Pilot	H ₂ O ₂	476	1.3	7.0	19	556	0.28 ²	0.03	0.08	0.21	-	-	0.03	0.35
Pilot	H ₂ O ₂	483	2.4	7.0	12	588	0.30	0.06	0.05	0.21	-	-	0.03	0.35
Pilot	H ₂ O ₂	537	6.1	8.8	20	694	0.36 ³	0.15	0.08	-	-	0.22	0.03	0.48
Pilot	H ₂ O ₂	509	2.1	9.1	37	694	0.36 ³	0.05	0.15	-	-	0.28	0.03	0.52
Pilot	H ₂ O ₂	470	4.3	8.7	32	694	0.36 ³	0.10	0.13	-	-	0.19	0.03	0.46
Pilot	H ₂ O ₂	540	4.0	9.0	35	597	0.30	0.10	0.14	-	-	0.26	0.03	0.53
Pilot	H ₂ O ₂	607	3.6	9.1	37	678	0.35	0.09	0.15	-	-	0.28	0.03	0.55
Pilot	H ₂ O ₂	571	3.4	8.4	36	636	0.33	0.08	0.15	-	-	0.15	0.03	0.41
Pilot	H ₂ O ₂	587	3.3	8.2	38	600	0.31	0.08	0.15	-	-	0.11	0.03	0.37
Pilot	H ₂ O ₂	626	3.4	8.5	22	592	0.30	0.08	0.09	-	-	0.16	0.03	0.37
Lab #1	H ₂ O ₂	330	1.2	7.0	22	556	0.28 ²	0.03	0.09	0.21	-	-	0.03	0.36
Lab #1	H ₂ O ₂	330	1.8	7.0	24	556	0.28 ²	0.04	0.10	0.21	-	-	0.03	0.38
Lab #1	H ₂ O ₂	330	2.5	7.0	27	556	0.28 ²	0.06	0.11	0.21	-	-	0.03	0.41
Lab #1	H ₂ O ₂	330	2.5	8.3	37	605	0.31	0.06	0.15	-	-	0.13	0.03	0.37
Lab #1	H ₂ O ₂	330	3.5	8.3	38	610	0.31	0.09	0.16	-	-	0.13	0.03	0.40
Lab #1	H ₂ O ₂	330	4.5	8.3	41	611	0.31	0.11	0.17	-	-	0.13	0.03	0.43
Lab #1	H ₂ O ₂	330	2.5	9.0	51	596	0.30	0.06	0.21	-	-	0.26	0.03	0.56
Lab #1	H ₂ O ₂	330	3.5	9.0	56	594	0.30	0.09	0.23	-	-	0.26	0.03	0.61
Lab #1	H ₂ O ₂	330	4.5	9.0	55	593	0.30	0.11	0.23	-	-	0.26	0.03	0.63
Lab #2	H ₂ O ₂	650	1.2	7.0	35	556	0.28	0.03	0.14	0.21	-	-	0.03	0.41
Lab #2	H ₂ O ₂	650	3.5	8.3	58	694	0.36	0.09	0.24	-	-	0.13	0.03	0.48
Lab #2	H ₂ O ₂	650	3.5	5.5	140	543	0.27	0.09	0.57	-	0.11	-	0.03	0.80
Lab #3	NaOCl	584	4.8	5.5	-	1,390	0.75	-	0.83	-	0.11	-	0.06	1.00
Lab #3	NaOCl	566	3.9	6.2	-	1,158	0.63	-	0.68	0.21	0.06	-	0.05	1.00
Lab #3	NaOCl	656	3.2	7.0	-	819	0.44	-	0.56	0.21	-	-	0.04	0.80
Lab #3	NaOCl	614	2.4	8.3	-	926	0.50	-	0.42	0.21	-	0.13	0.04	0.79
Pilot	NaOCl	674	2.7	6.9	-	819	0.44	-	0.47	0.21	-	-	0.04	0.72

¹ Incident UV fluence to deliver an average UV fluence of 200 mJ/cm²

² Not measured but assumed to be the same UV₂₅₄ as Lab #2 experiment at pH 7.

³ Not measured but assumed to be the same UV₂₅₄ as Lab #2 experiment at pH 8.3.

Table S10. Unit chemical reagent costs.

	NaOCl	H ₂ SO ₄	H ₂ O ₂	NaOH
% by weight solution	12.5	93	50	50
\$/ton for the solution	-	248	545	864
kg in a ton	-	907	907	907
\$/g _{solution}	-	0.00027	0.00060	0.00095
g/L density of solution	1170	1840	1197	1500
g _{chemical} /L _{solution}	146	1711	599	750
\$/L for solution	0.57	0.50	0.72	1.43
Molar concentration (M)	2.0	17.5	17.6	18.8
\$/mole	0.29	0.03	0.04	0.08

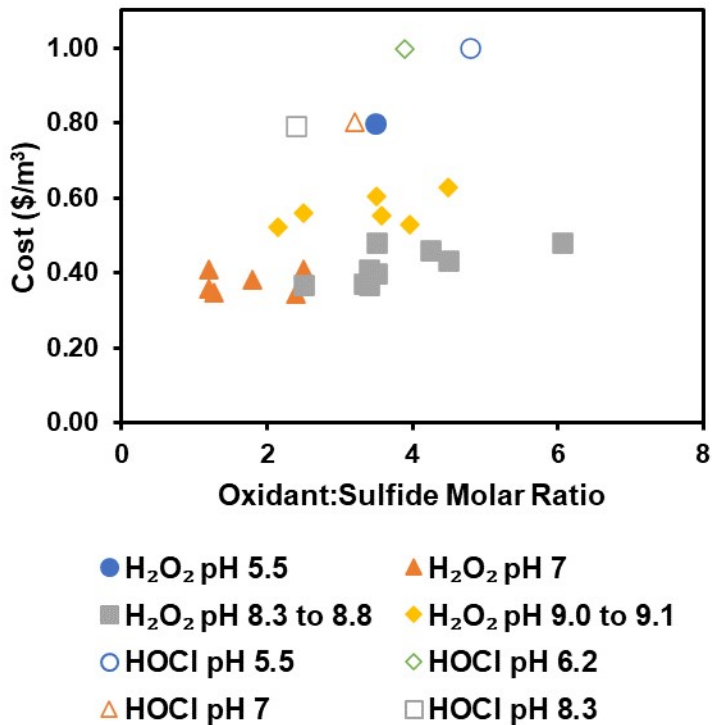


Figure S14. Initial total cost estimates of pilot and laboratory experiments. Costs include pH adjustment, hydrogen peroxide for sulfide oxidation, chlorine for sulfide oxidation, filtration, UV disinfection, and chlorine dosing for establishing a residual if hydrogen peroxide is used for sulfide oxidation.

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