

Assessing Advances in Anti-fouling Membranes to Improve Process Economics and Sustainability of Water Treatment

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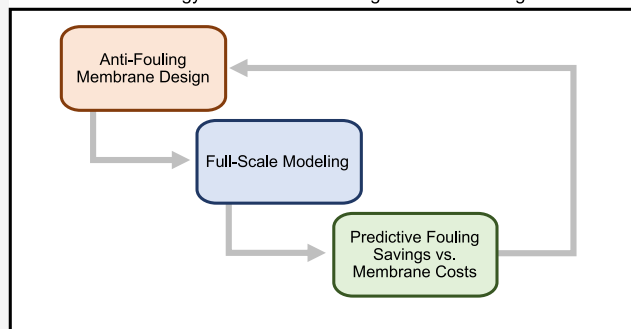
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Supporting Information

ABSTRACT: Membrane fouling in desalination and wastewater treatment increases operating costs and energy consumption. Accordingly, research efforts have focused on developing new membrane materials and surface treatments that can resist fouling. Due to the case-specific nature of fouling, there is limited quantification of the impacts these novel anti-fouling membranes can have on water treatment systems. To address this gap, we report results of high-level analyses that evaluated savings in cost, energy consumption, and life-cycle greenhouse gas emissions when membranes with improved fouling resistance are used in brackish water desalination with reverse osmosis and wastewater treatment with anaerobic membrane bioreactors. To carry out these analyses, we used models Water-TAP³ and GPS-X for desalination and wastewater treatment, respectively. We considered the influence of the membrane replacement rate and clean-in-place frequency in both scenarios. In the case of desalination, we also considered the influence of fouling factor and antiscalant dosage. In both scenarios, we determined that increasing membrane lifetime was the most influential factor in reducing operating expenses. Less influential factors included energy associated with increased pumping pressure to maintain a constant flux in the face of fouling and the frequency of clean-in-place events. Overall, desalination energy consumption was insensitive to the parameters we evaluated. Reducing energy associated with sparging in anaerobic membrane bioreactors offered the best opportunity to reduce AnMBR energy consumption in the wastewater treatment plant configuration we modeled. Greenhouse gas emissions were largely unaffected by the adoption of fouling-resistant membranes. Membranes made with new anti-fouling materials could be more expensive than current membranes. For the case studies we evaluate, depending on key variables such as membrane lifetime, the cost of desalination membranes could increase by 1.2–2.9 times, and the cost of anaerobic membrane bioreactor membranes could increase by up to 43% without operating costs increasing above our calculated baseline. This analysis highlights the promise of fouling-resistant membrane materials to reduce costs and energy consumption in water treatment systems. It also underscores a significant need for improved empirical data and multi-scale modeling to improve estimates of these savings.

KEYWORDS: desalination, wastewater, fouling, techno-economic analysis, life cycle assessment

Predictive Methodology to Inform Anti-Fouling Membrane Design



1. INTRODUCTION

The UN's Sustainable Development Goal 6 (SDG 6) aims to "ensure availability and sustainable management of water and sanitation for all by 2030".¹ Unfortunately, achieving this goal remains well out of reach.¹ As of 2021, two billion people lack access to safe drinking water services, 2.3 billion live in water-stressed countries, and 44% of municipal wastewater is handled unsafely.¹ As urbanization² and aging infrastructure³ push the boundaries of today's water treatment systems and climate change further exacerbates water stress, it is critical that water systems maintain resilience by adopting or expanding the technical capabilities to supply water from unconventional water resources (e.g., desalinated water and treated wastewater). To support sustainable development, technologies should be able to supply water with minimal energy demand

and maximum nutrient recovery. Desalination and wastewater treatment both play important roles in maintaining and/or increasing water supplies, and membrane operations play an important role within these processes. Reverse osmosis (RO) is a crucial component of desalination that can increase water supplies in regions lacking conventional water sources, and anaerobic membrane bioreactors (AnMBRs) are a promising technology for recovering energy and facilitating nutrient

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recovery from organic matter during wastewater treatment. One common technical challenge that spans these technologies is membrane fouling, which can significantly reduce membrane lifetimes and thus increase the plant's operating expenses (OPEX). Accordingly, many are developing novel anti-fouling membranes and surface treatments for membranes used in RO desalination and for the ultrafiltration (UF) membranes used in AnMBRs.^{4–11}

Several reviews summarize advances in anti-fouling membrane technology and provide qualitative information on how anti-fouling membranes could reduce costs through pre-treatment adjustments, energy consumption reductions, decreases in cleaning frequency, and extended membrane lifetimes.^{4,12–14} Others have worked on indices and models to describe fouling effects, described in later sections, including efforts that use neural networks to predict changes in flux and permeability due to fouling.^{15,16} These models, however, tend to be highly complex and do not include the costs associated with such changes, making them difficult to apply to full-scale OPEX calculations. On the other hand, operating costs have been studied and tabulated at various water treatment facilities, and anti-fouling membrane benefits have been qualitatively evaluated (see Section 3 and Table S1). Operating costs include membrane cleaning and replacement that are directly associated with fouling, but operating costs as a whole encompass more than fouling alone. It is possible to determine the costs of fouling as a subset of total operating costs at a specific facility in retrospect using large amounts of empirical operating data, but evaluations of such costs are rare in the peer-reviewed literature.¹⁷ Moreover, the existing literature does not quantitatively predict the potential of anti-fouling membranes to reduce OPEX. Anti-fouling membranes will not wholly eliminate fouling-associated costs and may be more expensive than conventional membranes. Accordingly, this gap in the literature impedes the design of cost-effective membranes that reduce fouling.

Our work here generates a range of potential cost savings based on various scenarios of fouling reduction effects on the operation. Such ranges enable technologists developing anti-fouling membranes to better quantify anti-fouling benefits and prioritize membrane improvements with the greatest impact. Predicting a range of potential cost and sustainability advantages of anti-fouling membranes is critical to guiding bench-scale scientists. These researchers develop membranes without a specific facility in mind and generally without access to facility-level empirical data. It is important to assess, even in the absence of full-scale fouling correlations and modeling capabilities, whether the benefits of less fouling (e.g., longer membrane lifetime, less energy intensity, and lower maintenance requirements) exceed the potentially higher costs of new membranes. Given this need, after briefly reviewing fouling mechanisms and influences on operating costs at desalination and wastewater treatment facilities, we develop and apply a method to estimate the range of cost and sustainability benefits of anti-fouling membranes for brackish water RO (BWRO) and AnMBR systems using two case studies.

The first case study involves the Kay Bailey Hutchison Desalination Plant (the KBHDP) in El Paso, Texas, U.S.A., and the second involves municipal wastewater treatment with an AnMBR. We note that many factors from feed water composition and pre-treatments to membrane characteristics and operating conditions influence fouling. The cost and

sustainability benefits of adopting low-fouling membranes will fluctuate based on the conditions of any single water treatment facility; therefore, the specific results from the case studies are not indicative of the exact potential savings any plant may see. Rather, we seek to address a gap in the open, peer-reviewed literature regarding quantitative predictions of the potential for anti-fouling membranes that are the subject of intense research^{4,12,14} to cut costs and energy consumption in water treatment facilities. We conclude by summarizing a research framework that involves membrane developers, users, and analysts that will enhance the development, cost, and sustainability assessments of anti-fouling membranes.

2. FOULING IN RO AND ANMBR PROCESSES

Considering the large and increasing use of membranes in water treatment systems, developing technologies to reduce fouling is critical. Membrane-based processes as a whole comprise 64–65% of global desalination installed capacity, with RO representing the most prevalent desalination technology.^{18–20} RO is often the principal desalination step, making it a foundational water treatment technique in areas lacking freshwater sources. The use of RO in desalination may be widespread, but the exact details of RO operation vary on a case-by-case basis. For instance, the energy intensity of RO desalination depends greatly on the water source, with brackish water desalination requiring anywhere from 0.25 to 2 kW h/m³ of treated water^{21–24} and seawater desalination requiring 2.6–8.5 kW h/m³ of treated water.^{25–28} In contrast to RO, AnMBRs in wastewater treatment are not yet as widely used in full-scale operation but could play a key role in energy and nutrient recovery strategies that aim to render self-sustainable wastewater treatment processes.²⁹ AnMBRs use UF membranes and offer greater energy and nutrient recovery potential than conventional wastewater treatment systems. Widely used conventional activated sludge (CAS) systems require 0.3–0.6 kW h/m³,³⁰ with nutrient removal and sludge treatment consuming additional energy. CAS treatment also emits greenhouse gases (GHGs) (~0.3 kg eCO₂/m³) from energy consumption and aerobic processes while underusing the energy, nutrients, and carbon resources recoverable from the wastewater itself. In contrast, AnMBRs aid in water treatment by combining anaerobic digestion of organic matter with porous membranes for solid/liquid separation. AnMBR operations produce a more nutrient-dense effluent that is better suited for nutrient recovery compared to CAS processes. Additionally, the biogas produced from anaerobic digestion provides an opportunity for enough energy recovery to yield a net-zero or even a positive energy balance.³¹ One study evaluating a range of AnMBR configurations and operating conditions found that net energy requirements ranged from –0.15 to 0.43 kW h/m³, indicating that methane recovery could potentially more than offset energy requirements for AnMBR operation.³² Currently, however, the energy balances of AnMBRs remain negative, largely due to the energy required for membrane fouling control, including backwash, membrane chemical cleaning, and, most significantly, gas sparging.

In both of these technologies, fouling imposes limits on water treatment effectiveness and efficiency. Organic fouling, biofouling, inorganic fouling (scaling), and colloidal fouling represent the primary categories of membrane fouling in water treatment, with the severity of each dependent on the influent composition, operating conditions, and the type of membrane used. Common organic foulants include proteins, lipids, humic

substances, and polysaccharides.^{33–35} Biofouling occurs as biofilms form from extracellular polymeric substances (EPSs) excreted by adhered bacteria, with common bacteria including *Mycobacterium*, *Flavobacterium*, *Acinetobacter*, *Pseudomonas*, *Cyanobacteria*, *Anthrobacter*, *Aeromonas*, and others.^{33,35} Inorganic fouling, or scaling, primarily occurs as inorganic compounds, such as silica (SiO_2), hydroxides, sulfates (such as CaSO_4 and BaSO_4), and carbonates (such as CaCO_3), exceed saturation levels and subsequently precipitate and deposit onto the membrane surface.^{33,35} Colloidal fouling can result from suspended organic (proteins, polysaccharides, etc.), inorganic (aluminosilicates, ferric oxide, etc.), and biological particles 1–1000 nm in size interacting with the membrane surface.^{33,36} These colloids can generally pass through non-membrane pre-treatments but are large enough to accumulate on membrane surfaces and within their pores while remaining difficult to remove via flow and diffusion patterns.^{33,36} The different fouling mechanisms are interconnected; for instance, biofouling is exacerbated by organic foulant accumulation that promotes biofilm growth,³³ and fouling is also interconnected with concentration polarization. Concentration polarization is a phenomenon that arises when the concentration of solutes increases significantly near the membrane's surface, increasing the osmotic pressure and impairing membrane performance.^{37,38} Fouling worsens concentration polarization, with colloidal fouling and biofouling especially limiting the back diffusion of solutes away from the membrane.^{33,35,37,39} Combined, these fouling mechanisms, along with concentration polarization, create extra hydraulic resistance to water permeation, deteriorating the water production efficiency.⁴⁰

These multiple forms of fouling, each with numerous individual foulants that could be present in the influent water, limit the ability of full-scale models to predict fouling impacts. Fouling is a highly case-specific, complex phenomenon dependent on the specific foulants present, their concentrations, any inter-foulant interactions that arise, the interactions between the foulants and the specific membrane in use, operating temperature and pressure, and other operational factors. Membrane properties such as hydrophilicity, surface charge, and surface roughness impact the fouling propensity of the membrane, and many are working to develop novel anti-fouling membranes using a diverse array of techniques to adjust these characteristics.^{12,41–47} What the literature lacks, however, are quantitative predictions of the reductions in OPEX that a desalination or wastewater treatment facility may gain from the use of new anti-fouling membranes. Ideally, large-scale water treatment facilities should be able to rely on models that can account for the relationships between fouling and operating parameters to help them predict the changes in OPEX if fouling-resistant membranes, which may be more expensive than conventional membranes, are installed. Comprehensive models that address both fouling and large-scale operations [including OPEX and capital expenditures (CAPEX)] are generally absent from the literature, necessitating the development of a method for predicting these changes. Figure S1 in the Supporting Information illustrates an ideal modeling scenario based on predictive fouling models that, as far as these authors are aware, do not exist, and the alternative framework utilized in this study that enables fouling impact predictions even in the absence of such models. The first step in developing a predictive framework that quantitatively evaluates the utility of anti-fouling membranes is under-

standing the aspects of plant OPEX that fouling most directly impacts.

3. FOULING IMPACTS ON OPERATION

The primary effects of fouling on the cost of membrane operations are seen through pre-treatment requirements, higher energy intensities, cleaning requirements, and eventual membrane replacement. In desalination, pre-treatment technologies range from the use of sand filtration to UF or nanofiltration (NF) membranes to reduce the intensity of the subsequent, principal RO treatment step. One such pre-treatment technique that is dedicated specifically to reducing fouling is the use of antiscalants—a technique employed by the KBHDP featured in the BWRO case study in this article. Antiscalant dosing is a type of pre-treatment that obstructs inorganic fouling processes by disrupting or delaying scalant crystallization.^{48,49} Antiscalants that reduce the rate of salt crystal nucleation on membrane surfaces include polyphosphates, polyelectrolytes (acidic acrylates and methacrylates), or polycarboxylic acids (molecular weight between 1000 and 3500 Da).^{48,50} Shih et al. and Kim et al. both demonstrated that antiscalants can significantly reduce fouling, limiting flux decline during lab-scale tests from ~30% in the absence of antiscalants to 1.5, 3.5%, or no flux decline at all depending on the antiscalant used (summarized in Table S1).^{51,52} The results of both studies suggest that the selection of the antiscalant is critical to minimizing the effect of membrane scaling. However, antiscalant dosing can exacerbate biofouling, and some antiscalants may increase eutrophication risks, incentivizing the use of anti-fouling membranes that could reduce the need for antiscalant dosage.⁵³ In wastewater treatment, pre-treatment options are often primarily centered on water treatment and are not necessarily focused on fouling reductions explicitly. However, pre-treatments can still prove to reduce fouling and the corresponding energy requirements. For instance, one study found that the use of primary sedimentation to remove organic solids before AnMBR treatment decreases the net energy requirements from 0.02–0.43 to –0.08–0.28 kW h/m³.³² It is not clear if these energy reductions resulted mainly from reductions in fouling or from other operational aspects such as the increased production of methane seen with the use of primary sedimentation in combination with mesophilic digestion,³² so different pre-treatment configurations were not assessed in the AnMBR case study presented in this article.

Pre-treatments, however, cannot completely prevent fouling, and over time, as fouling occurs, greater hydraulic pressure needs to be applied to achieve target water productivity, increasing energy consumption.⁵⁴ For example, in desalination, it has been estimated that a 10% increment in the applied hydraulic pressure due to RO membrane fouling results in the specific energy consumption of seawater desalination increasing by >0.2 kW/m³ over typical values of ~2.4 kW/m³ without fouling.⁵⁵ Wilf and Bartels also note that ~80% of the energy required to operate RO desalination plants goes to primary feed pumps,^{56,57} and any fouling that occurs directly influences these energy needs. Fouling's impact on wastewater treatment energy intensity arises primarily from the need for physical cleaning processes. As fouling worsens and energy demands increase, various cleaning methods are employed to reverse the fouling as much as possible. During the early fouling stages, it is feasible to remove the foulants by physical processes such as forward/back-pressure cleaning, vibration, rotation, and gas sparging. In wastewater treatment especially, these processes

result in increased energy intensities. Robles et al., for instance, reported that gas sparging to clean an AnMBR made up 79.7% of the AnMBR energy demand,⁵⁸ while Harclerode et al. found that pumping and gas sparging comprise 35–76% of an AnMBR's energy consumption.³²

Eventually, the flux cannot be recovered by mere hydraulic cleaning. At that point, harsh chemical cleaning is required.^{59–61} Common cleaning chemicals include HCl, NaOH, sodium hypochlorite (NaOCl), and ethylenediamine tetraacetic acid (EDTA),³³ and although these chemicals can mitigate some fouling impacts, this mitigation comes at a cost. For AnMBR treatment of municipal wastewater, some claim that cleaning comprises 2–7% of OPEX.³² Lin and Chen et al. found that the cost of chemicals to clean the AnMBR represented approximately 32.5% of OPEX,^{62,63} while a different AnMBR study found the costs of cleaning chemicals to be 17% of OPEX,⁵⁸ although it should be noted that both of these studies only evaluated costs of the AnMBR unit operation, not of an entire wastewater treatment plant (WWTP). Membrane cleaning disrupts operations and decreases efficiency and performance.^{53,64} In the case of RO processes, Patil et al. state that RO membrane cleaning comprised ~33% of OPEX,⁶⁵ while a different analysis suggests that cleaning chemical costs normally contribute about 10% to OPEX.⁶⁶ In one of the world's largest desalination plants in Ashkelon, Israel, the overall operating cost was estimated to be \$0.214/m³, wherein the cost of chemicals was \$0.021/m³, that is, ~10% of OPEX.⁶⁷ Moreover, while periodic membrane cleaning temporarily alleviates membrane fouling, chemical cleaning increases operating costs and shortens membrane lifetime. Currently, polyamide (PA) thin-film composite (TFC) membranes are the state-of-the-art RO membranes,⁶⁸ and while chlorine features in many cleaning processes and is commonly used to suppress biofilm growth, it damages the amide bonds of the PA composite RO membranes.⁶⁸ Such damage necessitates more frequent membrane replacements and increases operating costs. One study states that chlorine additions, increased pressure, and cleaning can represent about 30% of the total OPEX of an RO plant.⁶⁹

Careful cleaning and flux management can extend membrane lifetimes via the reduction of fouling, but ultimately, membranes will require replacement. Some estimate that AnMBR membrane replacement costs comprise 3–22% of OPEX depending on the system design and various operating factors,³² while others found that 23.4% of OPEX was from AnMBR membrane replacement requirements.⁵⁸ The membranes themselves can also be significant contributors to capital costs of WWTPs and desalination plants. Lin et al. found that membrane costs constituted 56% of the capital costs for an AnMBR.⁶² In a unique study that offered detailed full-scale analyses on the specific costs of fouling, membrane replacement costs for RO treatment of surface waters and municipal wastewater effluents represented 38–66% of the cost of fouling, indicating that these replacement costs may be the most expensive consequence of fouling.¹⁷ Different studies carried out for specific facilities reported that RO membrane replacement contributes between 13 and 33% of operating costs and could outweigh the benefits of restoring performance with fresh membranes, making it critical to quantitatively compare the potential benefits of anti-fouling membranes with the membrane cost.^{17,66,67,70} At the Ashkelon facility, membrane replacement costs were reported as \$0.028/m³ out of an OPEX of \$0.214/m³.⁶⁷ A review on RO desalination

noted that membranes constitute ~4% of the total plant cost, including amortized capital costs.⁷¹ Overall, a comprehensive analysis of the cost of fouling reported that total fouling costs comprised ~24% of OPEX for RO plants.¹⁷ Thus, fouling mitigation and reduction of irreversible fouling through the development of advanced materials and membranes are key to lowering the energy consumption, membrane replacement, and OPEX requirements of membrane-based water technologies.^{17,61,72,73}

Within the literature, there is an understanding of how fouling impacts OPEX at individual facilities, and some have even quantified these impacts using several years of empirical data (see Table S1 for a summary).¹⁷ While very useful, these methods do not provide a means for predicting fouling impacts in the absence of empirical data, and estimates of fouling costs do not, on their own, illustrate how anti-fouling membranes impact plant costs. Novel anti-fouling membranes that are in development, by definition, will not have years of full-scale use with which to assess their economic impacts. As a result, it is difficult to predict the range of cost savings that might be expected from developing and deploying anti-fouling membranes in a way that can guide the design of new membranes and even in decision making regarding investments in new membranes at water treatment facilities. We note that many have worked to model, index, and predict fouling. Several have detailed these efforts (see Table S2 for a high-level overview of existing models and indices).^{35,37,39,74} Existing models represent important advancements in predicting fouling impacts, but many require years of empirical data and/or highly complex calculations—making it difficult for a facility to anticipate the value of advanced materials that limit fouling or for a bench-scale researcher to quickly make choices about material design. The model produced by Tong et al. is an example of a significant step toward simplifying the number and type of parameters involved in fouling modeling.³⁴ This model, however, was tested using model wastewater containing only 1–2 fouling substances.³⁴ Existing models are also often designed to determine flux changes and/or water permeability changes. They generally do not address how reducing fouling will influence pressure gradients, cleaning frequency and protocols, and membrane replacement (see Figure S1 for an illustration of modeling needs). To improve the models' utility, they must go beyond the *effects* of fouling to the *cost* of these effects. The following case studies quantify a range of potential benefits from anti-fouling membranes in two case studies that can provide bench-scale researchers some guidance for predicting cost targets.

4. RO AND ANMBR CASE STUDIES

4.1. Modeling Methodologies. We used two models to estimate cost and energy changes from adopting fouling-resistant membranes in representative BWRO-based desalination and in wastewater treatment processes that use an AnMBR. In the case of desalination, we used the Excel-based version of the National Alliance for Water Innovation's (NAWI) Water Techno-economic Assessment Pipe-Parity Platform (Water-TAP³) to estimate OPEX and energy consumption changes stemming from RO membranes that have improved fouling resistance.²¹ This model, used in similar analyses,^{75,76} is based on the International Atomic Energy Agency's (IAEA) well-established Desalination Economic Evaluation Program (DEEP) model.⁷⁷ The model evaluates both CAPEX over the plant's lifetime and OPEX to determine

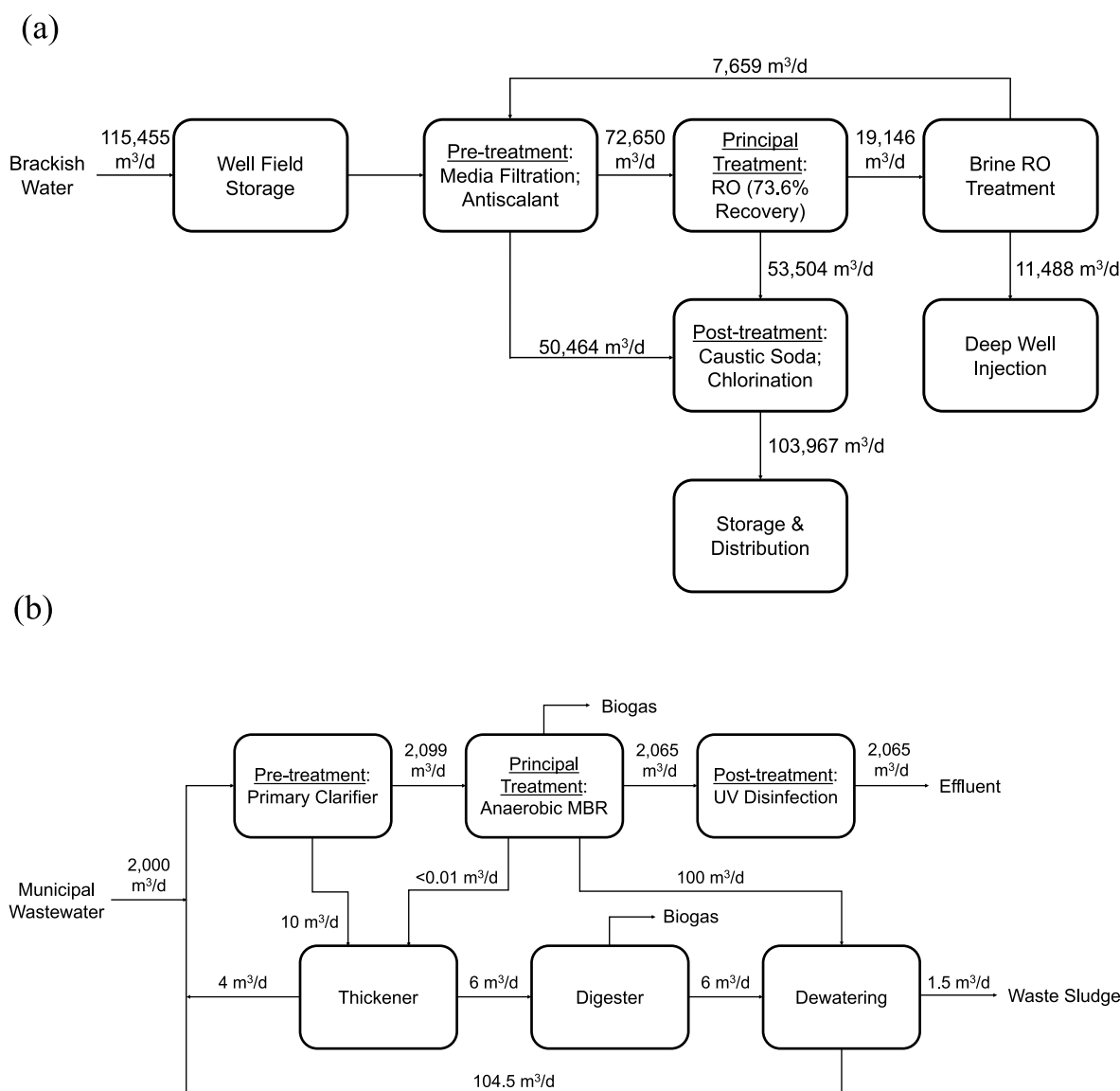


Figure 1. Process configurations for (a) brackish water desalination modeled after KBHDP using Water-TAP³ (b) municipal wastewater treatment with AnMBR in GPS-X. Note that the AnMBR was modeled using an anaerobic digester + MBR combination due to software constraints (see Supporting Information), and the separation of solids, liquids, and gases results in changing densities throughout the process. A total of 20 m³/d of biogas is produced in the wastewater treatment process.

the cost per m³ of produced water (i.e., the levelized cost of water) for different desalination process trains with representative data for different facilities (see Section S4 for more in-depth model discussion). Facility-specific data include water composition, capacity, location-specific costs (labor, electricity, etc.), and process train details. Water-TAP³ is a model that performs calculations assuming steady-state operation for the selected full-scale operation. This assumption means the model is not readily equipped for fouling cost calculations as fouling is inherently dynamic. Several calculations were therefore performed outside of the model based on the analysis conducted by Jafari et al.¹⁷ and incorporated into Water-TAP³ calculations, as detailed in Section S4. Existing models dedicated specifically to membrane fouling (discussed in Section S3) do not, to our knowledge, have full-scale costing calculations, but there are more dynamic full-scale modeling tools in the making that aim to better capture fouling effects. With increased dynamic capabilities, however, comes increased

complexity, and one goal of this analysis is to demonstrate that fouling costs can be estimated using readily available tools, data, and reasonable assumptions accessible to membrane developers, material scientists, plant operators, and others who can utilize such estimates for membrane development and investment choices.

For this project, we used Water-TAP³'s parameters for the KBHDP, which treats brackish water and is the largest inland desalination plant in the world. Our analysis of desalination focused on improvements in principal treatment RO membranes, so improvements in membranes used in the brine treatment RO step were not considered. To analyze a wastewater treatment case study, we used the software GPS-X.⁷⁸ GPS-X is dynamic software used by the industry that focuses on wastewater treatment processes, again allowing for full-scale cost analyses among other features. While certain unit operations in GPS-X [such as membrane bioreactors (MBRs)] feature relatively in-depth calculations related to fouling, the

AnMBR unit currently does not. We therefore utilized a combination of an MBR and an anaerobic digester to capture the dynamic changes in transmembrane pressure (TMP) due to fouling (a feature of the MBR unit operation but not the AnMBR) while also accounting for the biogas production and energy recovery that would be seen with AnMBR use. Biological aeration energy requirements for the MBR were neglected. Please see Figure 1a,b for process diagrams and Tables 1 and 2 for water characteristics in the BWRO and AnMBR case studies, respectively, as well as Sections S4 and S5 for detailed process modeling information.

Table 1. KBHDP Water Characteristics in Water-TAP³

constituent	units	KBHDP influent	KBHDP effluent
total flow	m ³ /d	115,455	103,967 ^a
calcium, dissolved	mg/L	145.0	66.9
chloride	mg/L	1315.0	606.3 ^b
magnesium, dissolved	mg/L	40.0	18.4
pH	pH	7.6	4.1 ^c
potassium	mg/L	19.0	8.8
sodium, dissolved	mg/L	825.0	380.4 ^b
sulfate, dissolved	mg/L	290.0	133.7
total dissolved solids (TDSs)	mg/L	2750.0	1268

^aTotal product water flow, not including brine. ^bHigher than the designated specification based on the California Water Board standard used by Water-TAP³ for this parameter—note that this study uses a pre-modeled design of the KBHDP to predict fouling impacts; resolving disparities in the specifications of effluent water from the previous modeling of KBHDP is not within the scope of this study. ^cLower than the designated specification based on the California Water Board standard used by Water-TAP³ for this parameter—note that this study uses a pre-modeled design of the KBHDP to predict fouling impacts; resolving disparities in the specifications of effluent water from the previous modeling of KBHDP is not within the scope of this study.

Table 2. Influent and Effluent Water Characteristics for a Full WWTP Treatment Train in GPS-X

constituent	units	GPS-X influent	GPS-X effluent
total flow	m ³ /d	2000	2065 ^a
total suspended solids (TSSs)	mg/L	229.2	1.0
chemical oxygen demand (COD)	mg/L	431.0	23.7
total nitrogen (TN)	mg/L	40.0	16.4
total phosphorus (TP)	mg/L	10.0	0.7

^aThis effluent represents only the flow rate of treated water exiting the system. The flow rate is higher than the influent flow rate due to density changes as solids are removed throughout the treatment train.

In our modeling, we accounted for the following effects of reduced membrane fouling: less frequent cleaning-in-place (CIP) (which reduces the cost of chemicals and downtime), lower TMP (which translates into less pumping energy consumption), and less frequent membrane replacement. We also accounted for changes in antiscalant pre-treatment requirements in the desalination case, and in the case of wastewater treatment with an AnMBR, we evaluated the influence of reducing the energy consumed in sparging the membrane with biogas when less fouling occurs. In both cases, we considered the influence of membrane cost since new membrane materials could be more expensive in exchange for enhanced membrane lifetimes. No additional labor was added

for CIP events, although in reality, depending on the type of CIP procedure (automatic or manual), there could be added labor costs.¹⁷ Decreases in fouling could increase the water recovery ratio in these processes, which could result in a reduced levelized cost of water; however, our focus here is on anti-fouling membrane impacts on OPEX, so we did not include the effects of increased recovery ratios. Furthermore, given the highly case-specific nature of irreversible fouling and the lack of predictive tools to anticipate irreversibility, we felt unable to defensibly account for irreversible fouling and neglected it, choosing to generate conservative estimates of anti-fouling benefits in the face of high uncertainty. Accordingly, we assume that TMP returns to its original value after each cleaning. Sections S4.2 and S5.2 detail additional calculations on how irreversible fouling could be accounted for in future analyses. Because our analysis includes only reversible fouling, the changes in energy demand that we estimate are therefore minimum values. We extracted purchased energy (e.g., kW h electricity) and cleaning chemical consumption from Water-TAP³ and GPS-X and calculated GHG emissions associated with the desalination and wastewater treatment processes using emission factors from the Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET) model.⁷⁹

Note that the listed water constituents are those utilized by the respective modeling software packages. In reality, the influent water to both the KBHDP and municipal WWTPs is highly complex, featuring many other components that often vary seasonally throughout the year.

4.2. Brackish Water Desalination with RO. Table 3 presents the main parameters we adopted to model brackish water desalination in our case study. Section S4 of the Supporting Information contains detailed information regarding parameter selection and calculation, when necessary. Importantly, quantitative relationships between the improved fouling factor, cleaning requirements, pumping power, antiscalant requirements, membrane replacement rate, and other effects of fouling are not available. As a result, we have selected reasonable ranges for each of these variables to bound the cost and sustainability benefits of anti-fouling membranes in BWRO systems based on several scenarios of different combined benefits.

4.3. Wastewater Treatment with AnMBR. Table 4 presents the main parameters we adopted to model wastewater treatment with AnMBR. Section S5 of the Supporting Information contains additional details regarding this modeling in GPS-X.

5. RESULTS AND DISCUSSION

In this section, we describe the potential influence of developing new membrane materials that have improved resistance to fouling for specific cases of brackish water desalination processes with RO and wastewater treatment with an AnMBR. As with fouling in general, these results are case-specific, but the methodology used to produce them (despite the absence of detailed fouling representation in system-level models and the lack of correlations between various fouling-impacted parameters) can be widely employed. It should be noted that while membrane improvements are considered only for the principal BWRO step in the KBHDP case and the AnMBR in the wastewater treatment case, the calculated OPEX, energy intensities, and GHG emissions reflect the entire treatment plant process train.

Table 3. Key Parameters (Baseline and Range) Used in the Brackish Water Desalination Case

variable	baseline	range	source
fouling factor ^a	0.85	0.85–0.925	Water-TAP ³ ; DEEP; EPA ^{21,77,80}
membrane replacement rate	0.0002 units/m ³	0.0001–0.0002 units/m ³	Water-TAP ³²¹
membrane price	\$350/unit		DEEP ⁷⁷
antiscalant dosage	0.005 kg/m ³	0–0.005 kg/m ³	Water-TAP ³²¹
antiscalant price	\$3.49/kg hydrazine		Water-TAP ³²¹
CIP frequency ^b	10 events/yr	5–10 events/yr	Jafari et al. ¹⁷
CIP duration ^b	7 h		Jafari et al. ¹⁷
acid price	\$0.17/kg HCl		Water-TAP ³²¹
base price	\$2.14/kg NaOH		Water-TAP ³²¹
product margin	\$0.12/m ³ product flow		Jafari et al. ¹⁷

^aChanges in fouling factor alter the design net driving pressure. For instance, a fouling factor of 0.85 represents anticipation that water permeability will decrease by 15%.⁸⁰ A higher fouling factor means the permeability is expected to decrease less and therefore translates to lower pumping energy consumption. ^bNot originally included in Water-TAP³. Calculations involving extra pumping power required between CIP events, CIP chemical costs, CIP chemical heating costs, downtime costs, and CIP waste disposal costs performed exogenously based on calculations performed in Jafari et al.¹⁷

Table 4. Key Parameters (Baseline and Range) Used in the Municipal Wastewater Treatment Case

parameter	units	baseline value	endpoints	source
chemical cleaning frequency	year ⁻¹	5		assumption
membrane lifetime	years	5	3, 7	Ang et al., Garg and Joshi, and Goon et al. ^{81–83}
CIP downtime cost	\$/m ³	0.12		Jafari et al. ¹⁷
CIP downtime	hours	5	2, 10	Jafari et al. and Wei et al. ^{17,84}
total plant life	years	30		assumption
total membrane area	m ²	4000		GPS-X default ⁷⁸
membrane cost	\$/m ²	20	15, 30	Metzger et al., Ling et al., and Cohen ^{85–87}
NaOH cost	\$/kg	2.14		Water-TAP ³²¹
HCl cost	\$/kg	0.17		Water-TAP ³²¹
NaOCl cost	\$/kg	1.5		USP Technologies ⁸⁸
sparging energy as % of the energy consumed in the AnMBR	%	80		Robles et al. ⁵⁸

5.1. Brackish Water Desalination with RO. In Figure 2, we record the results of our analysis with Water-TAP³ using KBHDP as a case study. We evaluated changes in OPEX by varying the antiscalant dosage and the change in membrane replacement rate, the two most influential variables (Section S4), along with CIP frequency (which accounts for costs associated with chemicals and downtime) and fouling factor, which proved less influential. The OPEX in the baseline scenario was 10.28 million dollars per year (MM\$/yr). The benefits we quantified from the adoption of anti-fouling membranes in the parameter space of our analysis (Table 3) yielded OPEX savings ranging from 0.26–1.75 MM\$/yr. As would be expected, the highest savings occurred when fouling was reduced to the greatest extent (50% reduced membrane replacement rate, no antiscalant addition, a CIP frequency of 5 times/yr, and a fouling factor of 0.925). The best-case scenario we explored demonstrates that if a novel anti-fouling membrane were capable of yielding those benefits, the cost savings experienced by the KBHDP could be on the order of ~1.75 MM\$/yr, which is a notable amount given that it represents ~17% of the baseline OPEX.

Energy consumption remained effectively constant regardless of parameter choice (Table S6); although as detailed in Section S4.2, Table S12, a further evaluation of the effects of irreversible fouling indicated that membranes offering reductions in both reversible and irreversible fouling could further reduce energy consumption. From Figure 2, it is evident that extended membrane lifetime is the primary benefit of enhancing membrane fouling resistance. Importantly, this finding is consistent with Jafari et al., who used several years of operational data to analyze the cost of fouling, indicating that the methodology presented here using steady-state process modeling can replicate key empirical trends even in the absence of detailed fouling models/data.¹⁷ Although in this case study, cleaning impacts were small relative to membrane lifetime impacts, future work can aim to incorporate advances in cleaning techniques that may impact membrane life. Efforts to optimize cleaning events using real-time decision making can yield efficient cleanings that reduce the number of cleanings required and/or keep membrane resistance minimal.⁸⁹ This optimization could result in decreased cleaning costs, and any reductions in cleaning frequency could extend membrane lifetimes as well, since chemical cleanings can damage RO membranes.⁸⁹ By assessing additional combinations of CIP frequencies and membrane lifetimes, the methodology utilized in this analysis could estimate how such improvements in cleaning optimization may impact plant OPEX as a whole.

In this scenario, improved membranes could yield millions of dollars in savings over a plant's lifetime; although, it is important to note that the results presented here are case-specific and represent conservative estimates limited by a lack of empirical data and detailed relationships between fouling parameters such as water quality, irreversible fouling, chemical CIP frequency, membrane life, and other parameters. Further analyses that incorporate data reflecting decreases in irreversible fouling, effects of lower CIP frequency on membrane lifetime, and potential improvements in selectivity could elevate cost and energy saving estimates beyond those we calculated. Being highly case-specific, these data are currently scarce. For instance, although it is qualitatively understood that CIP procedures, especially those involving acids, such as HCl, damage RO membranes, there are little to no quantitative data in the public domain on how these cleaning procedures impact membrane life in full-scale

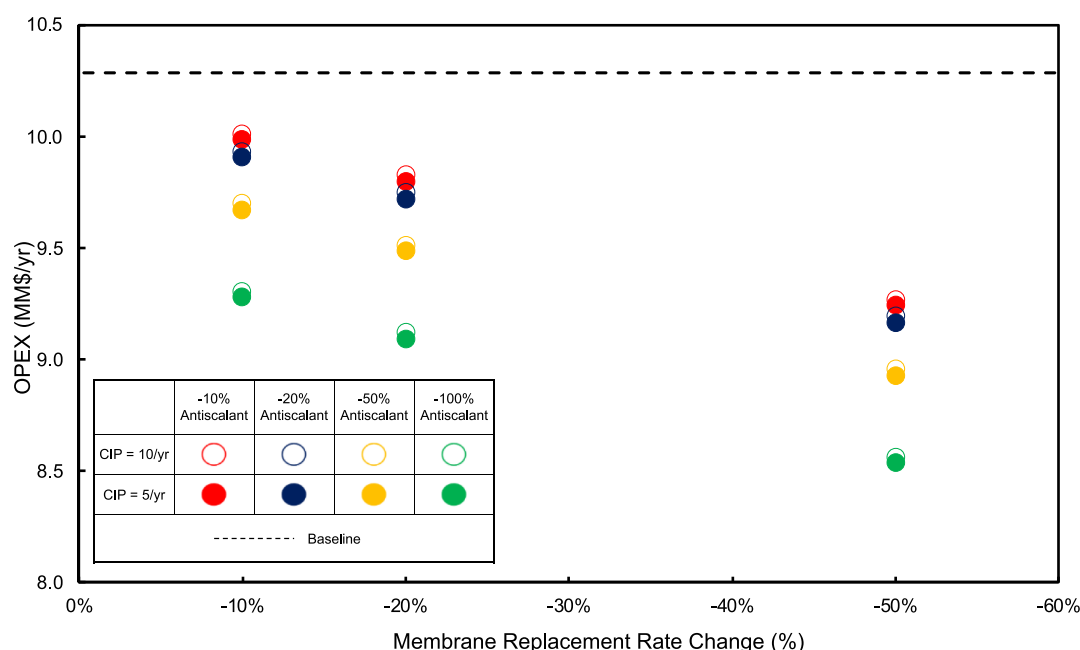


Figure 2. Impact of combined adjustments made to antiscalant addition, membrane replacement rate, and CIP frequency on total plant OPEX for KBHDP using Water-TAP³. Baseline OPEX is 10.28 MM\$/yr. Tabulated results are included in Section S4, as well as results from varying parameters independently, which demonstrated that changes in the membrane replacement rate and antiscalant additions were the most impactful. Note that the y-axis begins at 8.0 MM\$/yr to better illustrate the results, which demonstrate a maximum OPEX reduction of 1.75 MM\$/yr for this case study. We display results for the best-case fouling factor (0.925) in this figure because the choice of fouling factor had a very minimal role in modeling total plant OPEX. Results with both fouling factor scenarios are tabulated in Tables S4 and S5.

operations. The more empirical data are available regarding the effects of fouling on full-scale operations under a multitude of case-specific conditions, the more analyses such as those performed here can comprehensively account for all of fouling's effects under given operating circumstances.

New membrane materials may be more expensive, but our high-level analysis method can aid in the selection of novel membranes based on weighing the anticipated anti-fouling benefits against any added cost for the new membrane. Using the scenarios that yielded the least and most significant reductions in OPEX, our results suggest that overall OPEX could still be lower than the baseline scenario if the price of the new membrane does not increase more than 1.2 to 2.9 times that of the conventional membrane (Section S4.1). This methodology, therefore, enables the estimation of potential cost reductions for membrane users. This estimation of cost reductions, combined with the identification of the most impactful parameter (i.e., membrane lifetime), enables membrane developers to strategize membrane development to focus improvements on these high-impact areas and set targets for membrane costs.

5.2. Wastewater Treatment with AnMBR. In our evaluation of anti-fouling membranes in AnMBR systems, parameters relevant to fouling are varied independently from their baseline. This independent variation allows for the relatively quick identification of the variables likely to have the greatest impact on OPEX. In our modeling of wastewater treatment with AnMBR, we identified that, as with RO-based desalination of brackish water, the membrane lifetime is the parameter that most influences the baseline OPEX (\$27,150/yr) (Figure 3). Note that this baseline OPEX does not include labor or the consumption of chemicals that are used for purposes other than to control fouling; for example, we do not include the cost of chemicals used to manage or to remove

sulfide and phosphorus. Labor costs may change depending on the number of cleanings and membrane replacements per year, but we do not anticipate labor costs drastically changing from the baseline labor required for the plant if anti-fouling membranes are used. We would recommend that future work explore this aspect in greater detail; however, each plant likely has different policies governing the labor associated with plant operations that may or may not be influenced by changes in fouling.

Increasing the membrane lifetime from 3 to 5 years decreases OPEX by 39% (Figure 3d). The membrane cost and the number of cleaning events per year are the next most influential parameters. Cutting chemical cleaning events to 2 per year from 5 decreases OPEX by only 1% (Figure 3b). Energy consumption increases as TMP rises (see Section S5), but the cost of this additional energy does not notably influence OPEX. The main factor influencing energy use associated with lower-fouling membranes was a decrease in energy consumed for sparging in the AnMBR (Figure 3a). One estimate puts the share of energy used in an AnMBR for sparging at 80%.⁵⁸ When this parameter was decreased to 70%, process-level energy consumption dropped by 2%.

The membrane lifetime mostly influenced plant OPEX changes. The number of CIP events per year was the second most influential variable, and as mentioned previously, enhanced cleaning optimization using real-time feedback could further decrease the costs associated with cleanings and potentially improve membrane lifetimes.⁸⁹ This preliminary analysis also demonstrated the importance of the membrane cost (Figure 3c). As a result, we looked at these variables in more detail (Figure 4). If CIP events do not occur more than twice annually, OPEX remains below the baseline conditions only if the membrane lifetime is at least 7 years. In this case, membrane costs could increase by 43%. Hence, it is

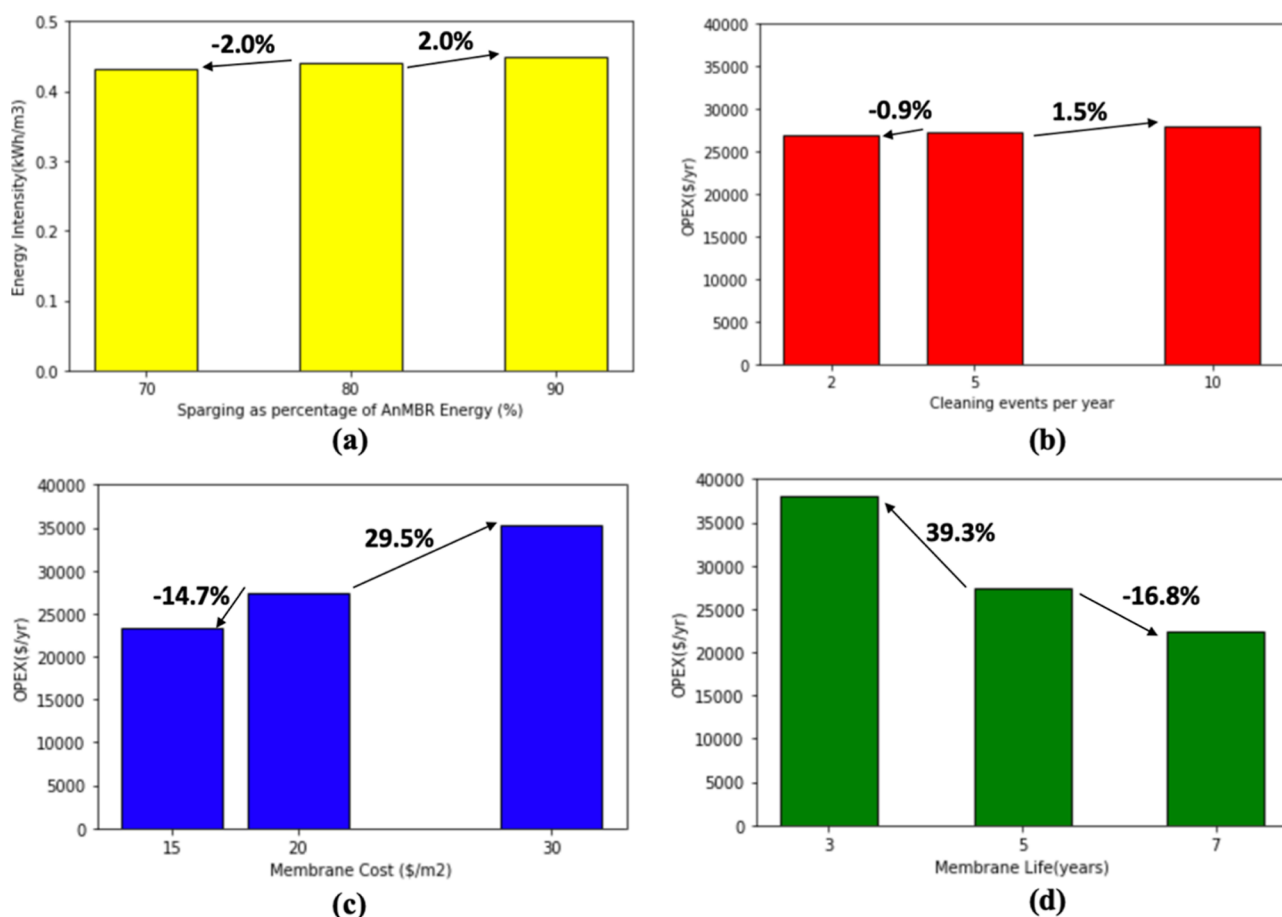


Figure 3. Influence of the amount of energy consumed in sparging the AnMBR on process-level energy intensity (a) and the influence of number of cleaning events per year (b), membrane cost (c), and membrane life (d) on OPEX. Baseline OPEX is \$27,150/yr and does not include labor or the consumption of all chemicals used in the facility.

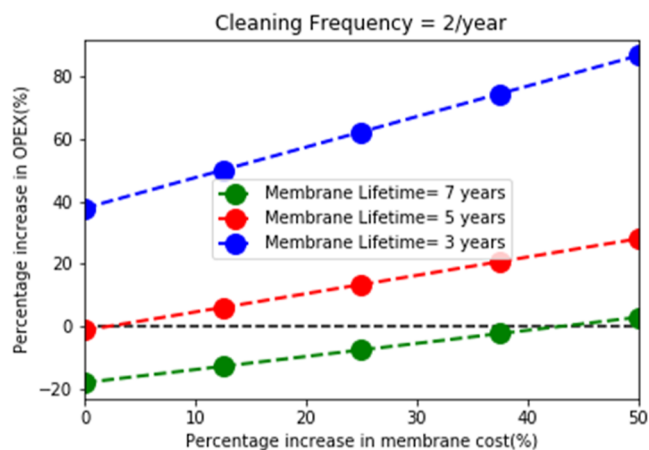


Figure 4. OPEX increases at a cleaning frequency of 2 times per year with variable membrane lifetimes. The dashed black line reflects baseline conditions. See Figure S5 for results with cleaning frequencies of 5 times per year and 10 times per year.

critical that novel anti-fouling membranes extend the life of membranes, and in this specific case, the membrane's cost could increase by 43% from the baseline to maintain economic viability.

As with modeling the benefits of enhancing membrane fouling resistance in desalination, we faced data limitations. Currently, there are limited data to characterize the inter-

relationships among cleaning frequency, membrane life, sparging energy, and increasing pressure to retain flux across the AnMBR membrane. These limitations can be addressed through improved empirical models that, once integrated into system-level models like GPS-X, capture these relationships and the process economic benefits fouling-resistant membranes can bring. NAWI, for example, is expanding WaterTAP³ into a Python-based model called WaterTAP that aims to provide more dynamic modeling capabilities that can better capture fouling influences on the operation. This tool is still in development, but eventually, the use of dynamic models in combination with empirically derived relations between factors like cleaning frequency and membrane life would enable far greater accuracy in anticipating anti-fouling membrane impacts on OPEX. Until such models and correlations are developed, analyses conducted with the above method can guide decisions on anti-fouling membrane development and its use in full-scale applications.

Ideally, a framework could be utilized across multiple disciplines in parallel, as illustrated in Figure 5 where large-scale needs influence membrane research and development, which subsequently informs analysis and future membrane decisions. Figure 5 represents a framework of data flow between membrane developers, membrane users, and analysts. As emphasized throughout this article, fouling is a very case-specific phenomenon dependent on water composition, operational variables, and the membrane itself. However,

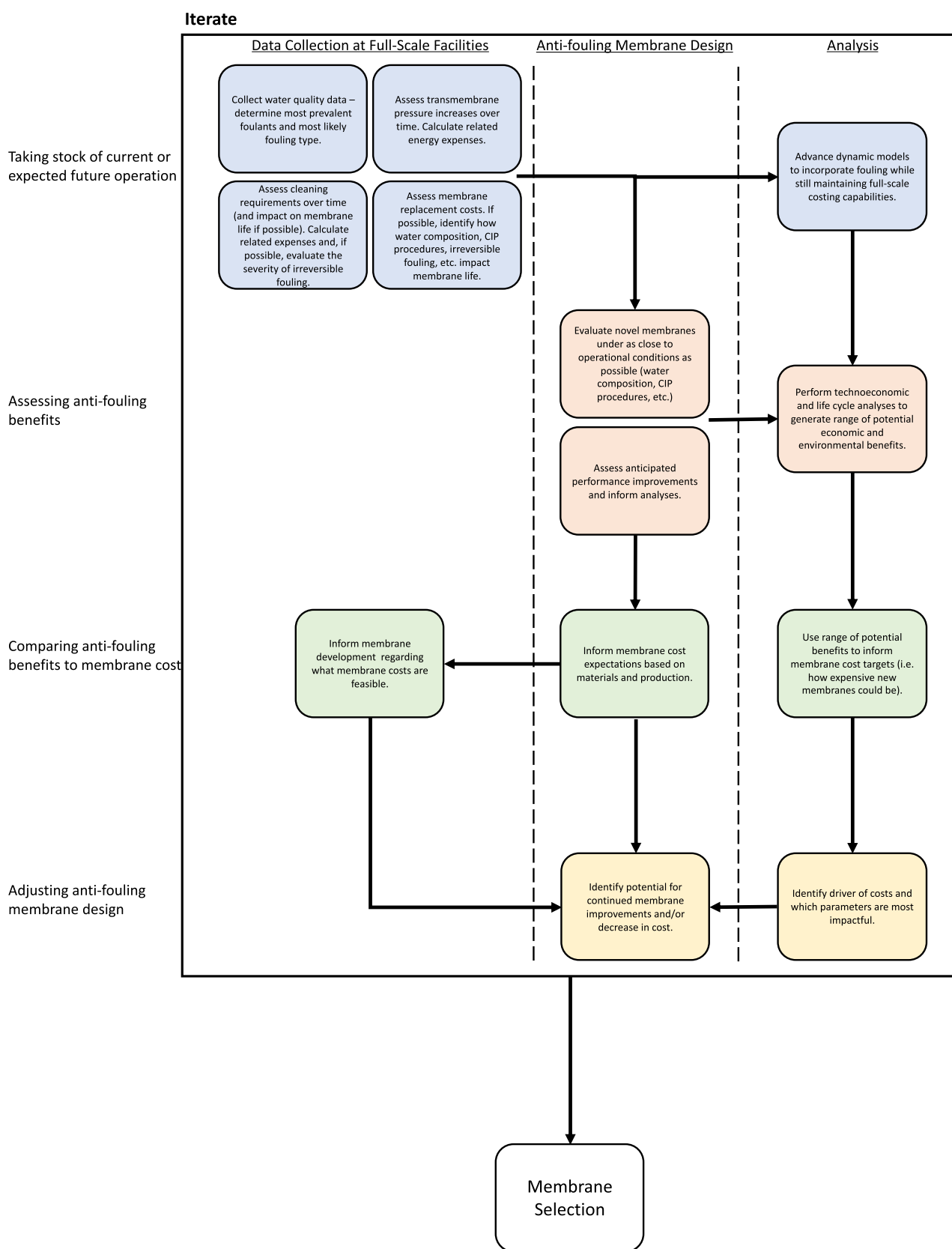


Figure 5. Data sharing between membrane designers, analysis teams, and full-scale operations is essential to evaluate novel anti-fouling membranes. Arrows crossing the dashed lines highlight areas of high collaboration importance.

existing models do not capture these phenomena in a way that relates them to plant-level OPEX and CAPEX. To bridge this gap requires direct collaboration between membrane devel-

opers and water treatment plant operators (desalination and wastewater). For example, access to plant-scale temperature and TMP data, cleaning protocol descriptions, and samples of

the actual influent water to the plant's membrane operation would inform model development and, correspondingly, membrane design. Essentially, full-scale operation data can inform the design and testing of novel anti-fouling membranes, with these results enabling predictions as to how operation (TMP, cleaning frequency, replacement frequency, etc.) may change. Full-scale data can also aid in the development of dynamic models capable of evaluating full-scale plant costs with the incorporation of fouling effects.

These models, in conjunction with data from membrane designers on the performance of new membranes under realistic operating conditions, would allow analysts to assess the economic and environmental impacts of novel anti-fouling membranes to a greater degree of certainty. These analyses would identify both how expensive novel anti-fouling membranes could be, while still maintaining economic viability, and which parameters are most impactful. For instance, the case studies performed here bounded how expensive anti-fouling membranes could be while maintaining or reducing baseline OPEX and found membrane lifetime to be the most significant driver of savings. These results, combined with full-scale information on feasible membrane costs and the estimated cost of the new membranes based on the materials, fabrication, and required production processes would supply membrane designers with information on how to best alter novel membranes to achieve a balance of anti-fouling results and low membrane cost. This process can then iterate until a suitable membrane is fabricated and selected.

5.3. GHG Emissions. We also considered the potential for reduced life cycle GHG emissions when new materials and surface treatments are used in membranes for brackish water desalination with RO and AnMBRs used in wastewater treatment. GHG emissions resulting from energy intensity changes were evaluated in GREET based on the U.S. grid (including energy resource collection/logistics, power generation, and distribution).⁷⁹ GHG changes resulting from chemical usage accounted for both the manufacturing and transport of the chemicals.⁷⁹ In the case of desalination, we did not see a change in GHG emissions per m³ of treated water, which held constant at approximately 450 g of CO₂ e/m³, regardless of changes in cleaning chemicals or energy consumption. GHG emissions from energy consumption contributed to 88% of the total GHG emissions. In the case of wastewater treatment with AnMBRs, the GHGs ranged from ~209 to 217 g CO₂e/m³, depending on the sparging energy intensity. The GHG emissions from energy consumption accounted for almost all GHGs (~91%), with only a negligible contribution from chemical consumption. Overall, the changes in energy and chemical consumption were minor in both case studies; the life cycle results, accordingly, did not show sensitivity to these changes. We might expect this result based on techno-economic results, which were most sensitive to membrane replacement rate and cost; although, it should be noted that neglecting irreversible fouling limited the impact on energy requirements in this study. In reality, changes in energy requirements may be more significant if irreversible fouling is reduced as well (see Sections S4.2 and S5.2), leading to a greater reduction in emissions. We also did not incorporate the effect of membrane manufacturing or disposal in the GHG emissions of desalination or wastewater treatment because previous analyses have noted that these effects are generally negligible relative to those of energy use.^{90–92} Additionally, a lack of data on manufacturing processes for novel anti-fouling

membranes that are not yet used in full-scale operation limits our ability to include membrane manufacturing and disposal impacts in the present study. We do recommend that any future work assessing a specific membrane with known manufacturing and disposal processes incorporates these impacts.

Additionally, we only evaluated the impact of anti-fouling membranes on the principal unit operation involved—not on pre-treatment, post-treatment, or waste disposal steps. The energy and the corresponding GHG impacts may be more impactful for membrane-based desalination pre-treatments and brine disposal techniques that are more prone to fouling in the first place. In desalination, pre-treatment membranes can remove much of the foulants, which reduces the fouling experienced by the RO unit operation, but it would likely mean that these membranes would foul significantly. Similarly, the brine produced from desalination would likely have increased concentrations of foulants that were rejected by the principal treatment steps, resulting in higher fouling tendencies for any subsequent membrane operations (such as the brine RO step at the KBHDP). Wastewater treatment can feature other membrane-based operations as well, including RO steps to polish the treated wastewater, and these steps would also be impacted by fouling. This study, however, is focused on the principal treatment steps only. Future work could explore the effect of these membrane life cycle stages on overall energy consumption and GHG emissions and cumulatively incorporate the changes anti-fouling membranes could yield in all membrane-based unit operations.

6. CONCLUSIONS

In general, membranes' ability to interact with foulants merits study from the molecular to process-level scales to realize the benefits we observed in our analysis of fouling-resistant membranes in BWRO and AnMBR processes. In addition, system-level models for desalination and wastewater treatment require improved treatment of membrane fouling, which is a dynamic process entailing both reversible and irreversible processes. More dynamic models would enable future work to especially consider the effects of irreversible fouling on energy consumption in greater detail than what was feasible with the models used in this analysis. Additionally, there is a need for empirical data to inform the relationships among process conditions (e.g., feedwater composition), cleaning regimens, membrane composition/structures, and membrane lifetimes that can support improved modeling of the benefits of new anti-fouling materials. These models will improve decision making in the industry and can inform early-stage research by setting cost and performance targets. One potential modeling tool that could benefit from these advances is the above-described, emerging WaterTAP model. Overall, from the case studies analyzed here, it is possible with a publicly accessible, open-source model to develop an understanding of potential savings that could result from anti-fouling membranes at full scale. Our results found membrane lifetime to be the driver behind fouling-related costs, and with the illustrated information-sharing framework, we proposed a collaborative framework among membrane users, developers, and analysts to improve our understanding of how anti-fouling membranes save cost and energy. With expected cost savings often a requirement for inclusion in proposals to funding agencies for the development of energy-saving technologies, such collaborations and the modeling they can support are a necessity for

bench-scale researchers. We note again that the results reflect our chosen case studies. This analysis exemplifies how to determine the extent of cost and sustainability benefits that might motivate investments in new membrane materials and can guide the development of new membrane materials toward performance and cost targets.

■ ASSOCIATED CONTENT

SI Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acsestengg.2c00184>.

A literature review of the costs of fouling, existing fouling models, and indices; conceptualization of fouling predictions for full-scale analyses; process modeling parameters; process modeling sensitivity analyses; irreversible fouling discussion; Water-TAP³; and GPS-X modeling documentation (PDF)

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Notes

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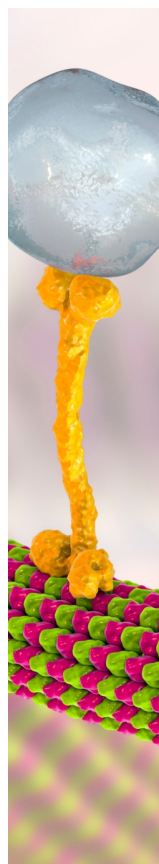
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