Systems & Control Transactions

Research Article
Foundations of Computer Aided Process Design (FOCAPD 2024)
Breckenridge, Colorado, USA. July 14-18, 2024
Peer Reviewed Conference Proceeding

Cost-optimal Selection of pH Control for Mineral Scaling Prevention in High Recovery Reverse Osmosis Desalination

Oluwamayowa O. Amusat [a,*], Alexander V. Dudchenko [b], Adam A. Atia [c,d], and Timothy Bartholomew [c]

[a] Lawrence Berkeley National Laboratory (LBNL), 1 Cyclotron Rd, Berkeley, CA 94720, USA
[b] SLAC National Accelerator Laboratory, 2575 Sand Hill Rd, Menlo Park, CA 94025, USA
[c] National Energy Technology Laboratory (NETL), Pittsburgh, PA 15236, USA
[d] NETL Support Contractor, Pittsburgh, PA, 15236, USA
* Corresponding Author: ooamusat@lbl.gov

ABSTRACT

Explicitly incorporating the effects of chemical phenomena such as chemical pretreatment and mineral scaling during the design of treatment systems is critical; however, the complexity of these phenomena and limitations on data have historically hindered the incorporation of detailed water chemistry into the modeling and optimization of water desalination systems. Thus, while qualitative assessments and experimental studies on chemical pretreatment and scaling are abundant in the literature, very little has been done to assess the technoeconomic implications of different chemical pretreatment alternatives within the context of end-to-end water treatment train optimization. In this work, we begin to address this challenge by exploring the impact of pH control during pretreatment on the cost and operation of a high-recovery desalination train. We compare three pH control methods used in water treatment (H_2SO_4, HCl, and CO_2) and assess their impact on the operation of a desalination plant for brackish water and seawater. Our results show that the impact of the acid choice on the cost can vary widely depending on the water source, with CO_2 found to be up to 11% and 49% more expensive than HCl in the seawater and brackish cases, respectively. We also find that the acid chemistry can significantly influence upstream processes, with use of H_2SO_4 requiring more calcium removal in the softening step to prevent gypsum scaling in HPRO system. Our work highlights why incorporating water chemistry information is critical when evaluating the key cost and operational drivers for high-recovery desalination treatment trains.

Keywords: Technoeconomic Analysis, Optimization, Surrogate Model, Water, Pretreatment, Reverse Osmosis

INTRODUCTION

There is growing interest in transforming the linear water economy to a circular water economy, where wastewater is treated for reuse while contaminants are recovered as valuable products [1]. This paradigm shift would significantly reduce freshwater withdrawals and wastewater discharges to the environment and could enable distributed treatment, minimizing transportation costs and externalities. However, technological advances are needed to reduce the energy use and cost of high-recovery treatment trains, which are essential for circular water treatment and minimizing brine generation in inland water reuse applications.

Modeling high-recovery treatment trains is challenging due to complex water chemistry phenomena. As more water is recovered, the concentration of dissolved solids will eventually reach saturation, and the solids will precipitate out of solution. This precipitation can result in mineral scaling on the surfaces of equipment and damage them [2, 3]. While mineral scaling can be prevented or delayed through pretreatment, traditionally with chemical precipitation or the addition of antiscalants, it is critical to explicitly incorporate precipitation and mineral scaling predictions in technoeconomic assessments in order to relate the extent of pretreatment with the water recovery of the system. However, the complexity of these phenomena and limitations on data have historically hindered the incorporation of detailed chemistry into process-scale water treatment models, particularly for novel, high-recovery systems.

We previously developed a framework for integrating detailed water chemistry into the design of water treatment systems using data-driven surrogates [4]. We demonstrated that scaling mitigation using chemical addition is a substantial component of process cost and a requirement for achieving high recoveries in desalination treatment trains, and that chemical pretreatment must be explicitly accounted for in process design. However, despite a significant body of work on scaling and chemical pretreatment [5, 6], little has been done on assessing the technoeconomic implications of different chemical pretreatment alternatives within the context of end-to-end water treatment train optimization. This gap in the literature hinders the development of comprehensive optimization strategies that can effectively integrate chemical pretreatment with other treatment processes to achieve cost-effective desalination.

In this work, we begin to address this knowledge gap by exploring the technoeconomic implications of one important chemical pretreatment decision in high-recovery desalination: pH control. The pH of water entering a reverse osmosis (RO) treatment train impacts both mineral-scale formation and membrane longevity, making pH control critical. Using WaterTAP [7], an open-source tool for modeling desalination and water treatment systems, we conduct an in-depth operational and economic assessment of post-softening pH control using acidification in water treatment. We compare three commonly used acids, H_2SO_4, HCl, and CO_2, for pH control based on system cost, system operation, and safety for an emerging high-recovery desalination technology. Our results show that the choice of pH control acid can significantly impact costs and should account for the feedwater and acid chemistries, highlighting why water chemistry incorporation at the design stage of water treatment systems is critical. Through our analysis, we provide qualitative insights to guide decision-making on achieving high-recovery desalination.

METHODOLOGY

This section describes the desalination train, our modeling approach, and our optimization problem formulation for cost-optimal system design.

System Description

We investigate the impact of pH control choice on high-recovery treatment trains for brackish and seawater sources. We consider a medium-sized plant (5000 m^3/day); feedwater compositions are provided in Table 1.

Fig. 1 shows the schematic for our desalination train. Our proposed high-recovery treatment train uses high-pressure reverse osmosis (HPRO) technology, an emerging process for water desalination that allows RO systems to operate at significantly higher pressures than the 85-bar limit of traditional seawater RO, thus enabling higher recoveries [8, 9]. Recent work has shown that HPRO can be more energy efficient and cheaper than other high-recovery alternatives [8, 10]. For our case study, we explore the viability of HPRO technology with chemical pretreatment.

Current seawater RO systems are limited to 50% recovery [11]; pretreatment allows the desalination system to increase water recovery before mineral scaling occurs. Our chemical pretreatment is done in two steps: softening followed by acidification [5]. First, soda ash (Na_2CO_3) addition softens the water by removing calcium ions as $CaCO_3$. Next, acid addition lowers the pH. To assess the impact of pH control on HPRO performance, we consider three acidification alternatives: CO_2, H_2SO_4, and HCl.

The pretreated water goes through RO/HPRO, where clean water is produced. Energy is recovered from the high-pressure waste via an energy recovery device (ERD), improving the energy efficiency of the process.

Table 1: Plant feedwater conditions

	Brackish	Seawater
Capacity (m^3/d)	5000	5000
Temperature (°C)	25	25
Pressure (bar)	1.013	1.013
Na^+ (mg/L)	739	10556
K^+ (mg/L)	9	380
Ca^{2+} (mg/L)	258	400
Mg^{2+} (mg/L)	90	1262
Cl^- (mg/L)	870	18980
SO_4^{2-} (mg/L)	1011	2649
HCO_3^- (mg/L)	385	140
pH	7.07	7.56

HPRO Modeling

The HPRO system model was developed using WaterTAP, an open-source Python framework for the simulation and optimization of water treatment trains, built upon the Pyomo-based IDAES Integrated Platform [12]. We develop the HPRO system as a greybox model, combining mechanistic models for desalination components with surrogate models for water chemistry. The surrogates compute functions for the desired chemical phenomena that are added to the EO model formulation.

Physics-based models of the desalination components (RO, pumps, and ERD) are implemented using WaterTAP's model library which includes unit and costing models for the components. Detailed equations for each of the components may be found in Atia et. al. [13].

Detailed water chemistry and thermodynamic information are necessary to predict the impact of chemical

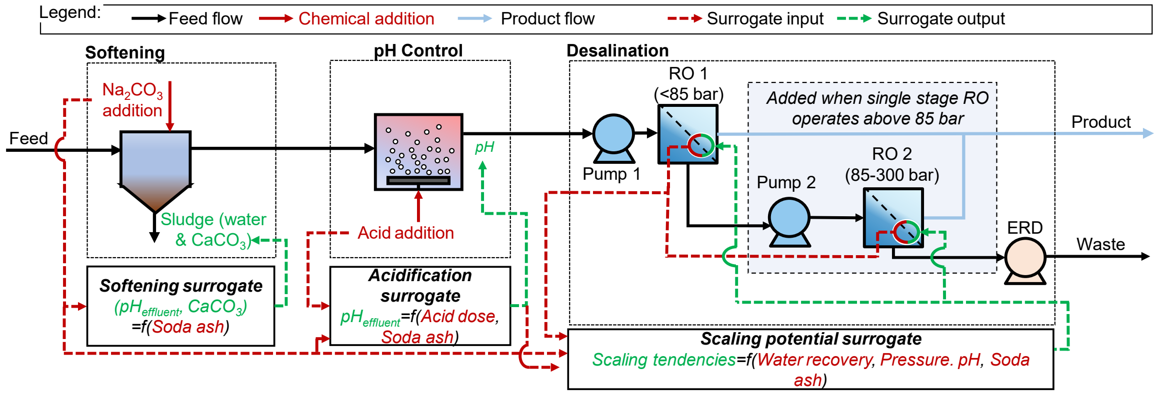


Figure 1: Schematic of the high-recovery treatment train showing surrogate insertion points. For softening and acidification, the surrogates predict the effluent pH and solids concentration directly from the decision variables (pretreatment chemical doses). For scaling, the surrogates predict scaling tendencies at the outlets of the RO units, with the inputs based on the upstream conditions and the RO operating conditions (pressure, recovery).

Table 3: Cost parameters for softening and acidification.

Chemical	Capital cost	Operating costs	Source(s)
Na_2CO_3	$12985x^{0.5901};\ x = lb/day$	Chemical cost: $\$0.19/kg$	[16, 17]
H_2SO_4	$-0.0029x^2 + 48.434x + 22{,}648;\ x = gpd$	Chemical cost: $\$0.12/kg$	[18-20]
HCl	$-0.0029x^2 + 48.434x + 22{,}648; x = gpd$	Chemical cost: $\$0.17/kg$	[18, 21]
CO_2	CO_2 liq. feed system: $9 \times 10^{-8}x^3 - 0.001x^2 + 42.578x + 130{,}812; x = lb/day$	Chemical cost: $\$0.24/kg$	[18-19, 22]
	CO_2 Basin: $4 \times 10^{-9}x^3 - 2 \times 10^{-4}x^2 + 10.027x + 19{,}287, \mathrm{x} = \mathrm{ft}^3$	Electricity: $0.11\ kWh/_{kg\ CO_2}$	

pretreatment in membrane systems. We incorporated the required water chemistry information into our WaterTAP model using surrogate models. As shown in Fig. 1, surrogates are used to represent three types of chemical phenomena in our process:

1. Softening – softening precipitates $CaCO_3$ from solution, changing the feedwater pH. The surrogate predicts the $CaCO_3$ concentration and pH as functions of the Na_2CO_3 concentration added to the feedwater. Distinct surrogates were developed for brackish water and seawater.
2. Acidification – the acidification process regulates the pH for desalination. For each acid (CO_2, H_2SO_4, HCl), we develop surrogates that predict post-acidification pH based on Na_2CO_3 and acid dose.
3. Mineral scaling – mineral scale formation limits the water recovery attainable in membrane systems. We develop surrogates to represent the scaling tendency (ST), which is the thermodynamic driving force for precipitation [2] and predicts whether scale formation will occur under specific conditions. A value of ST>1 indicates that scaling will occur. We monitor scaling at the RO outlet, with the scaling tendency dependent on the pretreatment conditions (Na_2CO_3 and acid doses) and RO operation (recovery, RO pressure). The scalants of interest are calcite ($CaCO_3$), gypsum ($CaSO_4.2H_2O$) and $CaSO_4$.

Water chemistry data is obtained from OLI [14], a water chemistry software that provides first-principles-based equilibrium calculations and chemistry models for electrolyte and non-electrolyte streams. To generate surrogate training data, we sweep across the decision variables for each acid; ranges for the decision variables for each acid and water source are shown in Table 2.

We used the PySMO software [15], part of the IDAES-IP, to generate surrogates for the chemical phenomena of interest. PySMO provides several surrogate methods, including radial basis functions (RBFs), Gaussian process models, and polynomial regression. For this application, we used RBFs because they had the best performance and are, in our experience, robust.

Optimization Problem

For each water source and acid choice, the objective is to minimize the levelized cost of water (LCOW) of the system:

$$\min_{d} LCOW = \frac{CRF * capital\ cost + annual\ operating\ cost\ [\$/yr]}{Treated\ water\ volume\ [m^3/yr]} \quad (1)$$

where d is the vector of decision variables (Na_2CO_3 dose, acid dose, water recovery, and RO pressure), and CRF is the capital recovery factor (set at 0.1).

Constraints on the optimization problem include:

- equality constraints representing the mechanistic models of the HPRO train components (pumps, RO, ERD).
- inequality constraints representing operational limitations of RO systems. The inlet crossflow velocity is limited to a maximum of 25 cm/s, the minimum allowable salt rejection in the RO is constrained to 98%, and maximum operating pressure of RO1 is limited to 85 bar.
- inequality constraints that ensure that no scale formation occurs based on the scaling tendency surrogates $\widehat{ST}_s$:

$$\widehat{ST}_s(d) \leq 1 \ \forall s \in [\mathrm{CaSO_4}, CaCO_3, CaSO_4.2H_2O] \quad (2)$$

The optimization problems are solved with IPOPT [26] using the MA27 linear solver in WaterTAP.

Table 2: Decision variable ranges and surrogate metrics. For the softening and acidification surrogates, we present the R^2 and maximum absolute errors.

	Range	
Variable	**Brackish**	**Seawater**
Na_2CO_3, mg/L	0-750	0-1200
Pressure, bar	10-110	50-300
Recovery	50-90%	50-87%
CO_2, mg/L	0-300	0-50
H_2SO_4, mg/L	0-150	0-50
HCl, mg/L	0-150	0-50
Surrogates	Metrics (R^2, MaxAE)	
Softening pH	1.00, 0.03	1.00, 0.02
Softening $CaCO_3$, mg/L	1.00, 7.59	1.00, 5.07
Acidification pH (CO_2)	0.99, 0.01	0.99, 0.05
Acidification pH (H_2SO_4)	0.99, 0.01	0.99, 0.04
Acidification pH (HCl)	0.99, 0.01	0.99, 0.03
Min ST classification accuracy (%)	>99.2	>99.2

Cost parameters for the different pretreatment options are shown in Table 3. The capital cost of CO_2 is made up of two components: the cost of the feed equipment and the cost of the recarbonation basin. All costs were converted to 2018 dollars using the CEPCI cost index. Acid purities of 99.5%, 93%, and 30% are considered for CO_2, H2SO4 and, HCl respectively [6, 16, 23], while the liquid CO_2 is assumed to be at –18°C and 20.4 atm [5]. It should be noted that the capacities in our optimization problem are treated in a continuous manner, with the installed capacities for pretreatment assumed to be equal to the minimum capacities required for daily operation.

RESULTS

Surrogate Performance

Table 2 summarizes our surrogate performance. For the softening process, RBF models with 13 terms were found to sufficiently capture the curvilinear relationship between the input (Na_2CO_3 dose) and outputs ($CaCO_3$ precipitation and pH), with $R^2 \approx 1$ and the mean absolute errors below 1 mg/L and 0.004 for both water sources. The maximum prediction error is 7.59 mg/L for precipitation and 0.03 for pH.

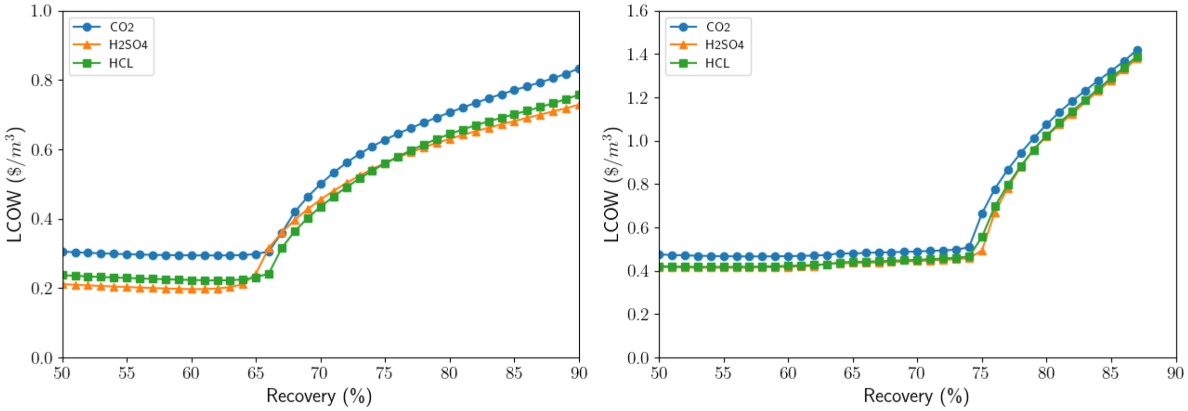
For post-acidification pH, the final RBF surrogates are trained on 100 training points, with the models predicting within ± 0.05 (less than 1%) of the true pH values observed from OLI. This level of accuracy makes the surrogates useful for comparing directly between the pH values of the different acids considered.

For mineral scaling, the most important factor is accurately determining whether or not scaling will occur. Thus, the critical performance metric for the scaling tendency surrogates is the accuracy in classifying potential operating scenarios into scaling or non-scaling. As shown in Table 2, our scaling tendency surrogates have >99% accuracy in discriminating between scaling/non-scaling cases. This means that our surrogates are accurate enough to provide the optimization model with accurate information about the operational feasibility.

Impact of Acid Choice on Cost

Figure 2 shows the optimal cost profiles for the different acids across a range of water recoveries for the two water sources. Our model results show that (a) there is a marked increase in cost beyond 66% and 74% recovery for brackish water and seawater, respectively; (b) the choice of acid for pH control has a greater impact on brackish water than seawater.

The cost profiles follow the same pattern: a regime where the cost profile is essentially flat, followed by a regime where the costs increase with recovery in a curvilinear manner. The flat regime corresponds to a region in which only pH control is required to prevent mineral scaling, and no softening is required (Na_2CO_3 dose=0). As recovery increases, however, pH control becomes insufficient to prevent mineral scaling, and Ca removal using softening becomes necessary. At this point, the LCOW increases rapidly, with softening costs dominating the



(a) Brackish

(b) Seawater

Figure 2: Cost profiles for (a) brackish (b) seawater with different pH control acid choices.

cost profile. Softening begins at about 64-66% and 74% for brackish and seawater, respectively.

CO_2 is the most expensive acid choice for both water cases. For brackish water, the cost difference between CO_2 and H_2SO_4 is as high as 49% in the no-softening region. For seawater, the difference between the costs of the three acids is much lower, particularly at the higher recoveries. CO_2 is still the most expensive, being almost 11.5% higher than H_2SO_4 in the no-softening regime and up to 5% higher in the high recovery, softening regime. The difference between the magnitudes of the effect of pH control on costs in our two water sources emphasizes the fact that feed water chemistry plays an important role in the acid choice for pH control.

Comparing the cost profiles for HCl and H_2SO_4 for the Brackish water case yields interesting results. We find that H_2SO_4 is cheaper than HCl at low recoveries (when softening is not needed) and high recoveries (> 76%). This finding agrees with the literature [6]. However, our results also show that in the mid-recovery regime of 66-76% (at low soda ash dosing requirements), pH control with HCl is cheaper. This results from sulfate-based scale formation that is promoted by the addition of H_2SO_4 and is discussed in detail in the section below.

It should be noted that while our results consistently show CO_2 as the most expensive of the three acidification options, we do not consider the cost of handling, monitoring, and extra maintenance costs necessary when using H_2SO_4 and HCl, which may be significant due to their corrosiveness. These additional costs, when combined with the uncertain nature of CO_2 costs [4], suggest that CO_2 may be cost-competitive with HCl and H_2SO_4 under best-case cost scenarios and thus should remain under consideration as an acidification option.

Impact on HPRO Operation

Softening

Fig. 3 shows the optimal Na_2CO_3 doses for the brackish water case. The softening profiles mirror the two-regime nature of the cost profiles – a flat regime with no softening, followed by a regime where more Na_2CO_3 is increasingly required to reach higher recoveries.

CO_2 and HCl require the same extent of water softening (same soda ash dose, resulting in the same amount of calcium removal), while use of H_2SO_4 requires a higher degree of softening. This is because H_2SO_4 increases the sulfate concentration of the stream, which favors sulfate-based scaling. Thus, additional calcium ion removal is required to counteract the sulfate ion increase and prevent gypsum scaling in the RO membrane. The additional calcium removal required when using H_2SO_4 depends on the recovery, varying from 2-41% across the recovery range. The challenge with gypsum scaling when using H_2SO_4 also means that Na_2CO_3 dosing for gypsum scaling control starts earlier than with the other acids. This finding agrees with the literature which suggests that using HCl may be preferred when calcium sulfate or barium sulfate scaling is a concern [6].

The increased soda ash consumption to prevent gypsum scaling when using H_2SO_4 for acid control is responsible for the high LCOW values (compared to HCl) observed with H_2SO_4 between 66-76% for the brackish water case. At low Na_2CO_3 doses, the additional softening costs incurred when using H_2SO_4 have a significant impact on the LCOW. However, past 76%, the cost impact of the additional softening required with H_2SO_4 is overshadowed by the overall cost of pH control pretreatment required to satisfy recovery targets, and H_2SO_4 becomes the cheapest option due to its higher purity and lower operating costs relative to HCl.

Our results show that softening is primarily required to control gypsum scaling: the recovery at which Na_2CO_3 dosing starts corresponds to when the gypsum scaling tendency constraint becomes active in the optimization problem ($\widehat{ST}_{gypsum} = 1.0$). Our results also show that the softening step cannot be designed independently of the downstream chemical operations (e.g. acidification). For the seawater case, softening begins at 74%, with Na_2CO_3 consumption levels the same for all acids.

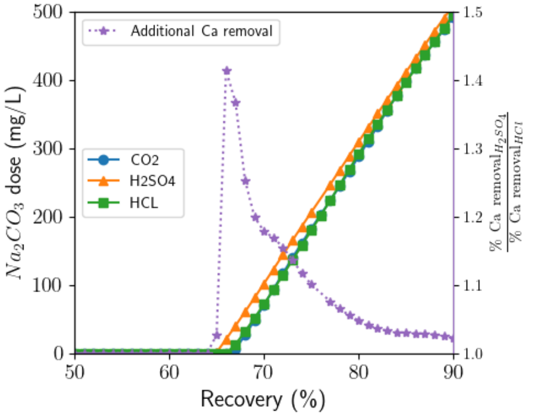


Figure 3. Na_2CO_3 concentration profile (left axis) and additional Ca removal required when using sulfuric acid (purple, right axis) for Brackish case.

pH control

Fig. 4 shows acid dose profiles for the two water sources. Seawater requires significantly less acid addition for pH control than brackish water despite its lower starting pH. The high acid requirement in the brackish case is due to its high bicarbonate concentration compared to the seawater source (see Table 1), which produces a buffering effect [24]. The cost-optimal acid doses required for the brackish water cases are between 4-6 times greater than that for seawater when using HCl/H_2SO_4, and 7-10 times greater with CO_2. The low acid consumption in the seawater case contributes to why the choice of acid has a smaller effect on the cost profiles.

For both water sources, control with CO_2 requires the highest acid dosing, requiring more than three times the HCl dosing at the highest recovery in the brackish case. The dosage requirements reflect the strengths of the acids: HCl and H_2SO_4 are strong acids ($K_a>1$) and thus require lower acid dosing, while the carbonic acid formed by CO_2 is a weak acid ($K_a<1$), meaning that higher concentrations are required. Our analysis of the scaling behavior indicates that pH adjustment is the preferred mechanism for controlling calcite scaling, with the calcite scaling tendency constraint active ($\widehat{ST}_{calcite} = 1.0$) in the optimization problem over the entire recovery range.

Fig 5. shows the pH exiting the pretreatment stage after acid addition for the Brackish case. Again, we find one acid behaving differently from the other two. HCl and H_2SO_4 drop the pH to similar values across the range. However, using CO_2 necessitates dropping the pH lower. We observed the same pattern in the seawater case (not shown). The reason for this is that CO_2 addition increases the carbonate ion concentration of the stream, favoring more calcite scaling. Since pH control is the mechanism for controlling calcite scaling in the system, the pH must be lowered more than in the HCl and H_2SO_4 cases to combat the effect of the higher carbonate concentration.

The results of our analysis of the pretreatment process show that while choosing H_2SO_4 for pH control impacts gypsum scaling and the operation of the softening step, choosing CO_2 impacts calcite scaling and the pH of the feedwater to the desalination train. These findings on CO_2 and H_2SO_4 underscore why water chemistry incorporation at the design stage in water treatment is critical.

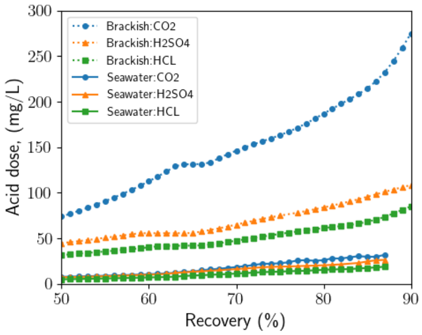


Figure 4. Optimal acid doses for brackish and seawater.

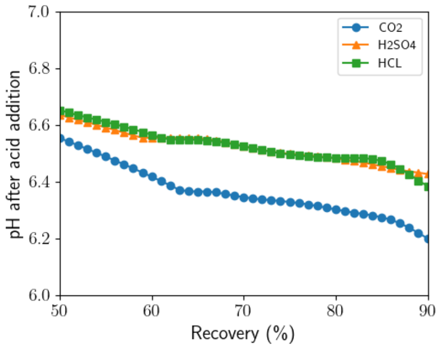


Figure 5. pH post-acidification for Brackish case.

Safety considerations

Safety is a critical factor to consider when dealing with acids in water treatment due to the requirements for onsite storage. Fig. 6 shows onsite acid storage requirements for ten days of plant operation (ten-day storage assumption adopted from [18]). Despite requiring the lowest acid dosing requirements (Fig. 4), HCl requires the highest storage capacity in the seawater case and the joint highest in the brackish case. This is due to its low purity compared to the other two alternatives. H_2SO_4 requires the lowest volume for onsite storage due to its high density and typical purity at 93%. H_2SO_4 also causes less fuming to the atmosphere than HCl, which results in less corrosion to surrounding metal components [6]. Thus, while the LCOW results are comparable, H_2SO_4 is safer than HCl due to its significantly lower storage requirements and lower corrosiveness. However, of the alternatives considered, CO_2 is the safest choice for pH control. Unlike H_2SO_4 and HCl, it is non-corrosive, reduces pipe clogging, and requires much lower handling and monitoring costs (not modeled in this work) [25].

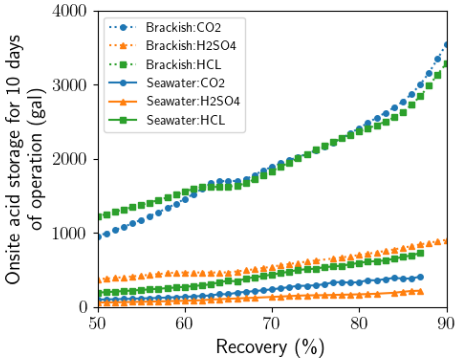


Figure 6. Onsite acid storage for 10 days of operation.

CONCLUSION

We present an assessment of the impact of pH control pretreatment choices on the cost and operation of a medium-sized high-recovery RO desalination plant by comparing three common acidification options (H_2SO_4, HCl, and CO_2). We find that the impact of the acid choice on the cost can vary widely depending on the water source, with the seawater LCOW being significantly less sensitive to the acid choice than our brackish water (11.5% vs 49%). Our results show that the choice of pH control acid should account for the properties of the feedwater (e.g., buffer capacity), the chemistry of the acids (e.g., sulfate vs. bicarbonate anions), and the scalants of concern. Water sources with calcite scaling as a primary concern may prefer to avoid CO_2 acidification, while H_2SO_4 may exacerbate sulfate scaling challenges. Our findings underscore why water chemistry incorporation at the design stage of water treatment systems is critical. The methodology used in this work can easily be applied to evaluate the benefits of process changes and innovations that allow higher maximum allowable scaling tendencies or reduce the cost of chemical precipitation pretreatment. This includes the effect of antiscalants, which can be incorporated into our methodology by increasing the tendency threshold (i.e., RHS of Eq. 2) beyond 1.0, as demonstrated in a previous work [4].

In the future, we will extend this analysis to include an assessment of alternative chemical softening options. We will also consider the impact of electrified pretreatment as an alternative to chemical pretreatment.

ACKNOWLEDGEMENTS

This material is based upon work supported by the National Alliance for Water Innovation (NAWI), funded by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy (EERE), Advanced Manufacturing Office, under Funding Opportunity Announcement Number DE-FOA-0001905. The version of IPOPT implemented in this work was compiled using HSL, a collection of Fortran codes for large-scale scientific computation. See http://www.hsl.rl.ac.uk.

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the U.S. Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or The Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the U.S. Government or any agency thereof or the Regents of the University of California.

REFERENCES

1. M.S. Mauter, P.S. Fiske. Desalination for a circular water economy. Energy Environ. Sci. 13:3180-3184 (2020). https://doi.org/10.1039/D0EE01653E
2. A. Matin, F. Rahman, H.Z. Shafi, S.M. Zubair. Scaling of reverse osmosis membranes used in water desalination: Phenomena, impact, and control; future directions. Desalination. 455: 135–157 (2019). https://doi.org/10.1016/j.desal.2018.12.009
3. T. Tong, A.F. Wallace, S. Zhao, Z. Wang. Mineral scaling in membrane desalination: Mechanisms, mitigation strategies, and feasibility of scaling-resistant membranes. J. Membr. Sci. (2019). https://doi.org/10.1016/j.memsci.2019.02.049
4. O. Amusat, A. Atia, A. Dudchenko, T. Bartholomew. Modeling framework for cost-optimization of process-scale desalination systems with mineral scaling and precipitation. ACS *ES&T Eng.* https://doi.org/10.1021/acsestengg.3c00537
5. L.K Wang, J. S. Wu, N.K. Shammas, K. Nazih D.A. Vaccari. Recarbonation and Softening. Physicochemical Treatment Processes. In: Physicochemical Treatment Processes. Handbook

of Environmental Engineering, vol 3. Ed: Wang, L.K., Hung, YT., Shammas, N.K. (eds) Humana Press (2005). https://doi.org/10.1385/1-59259-820-x:199

6. Nitto. Chemical pretreatment for RO and NF. Technical Application Bulletin , No. 111 (2022). https://membranes.com/wp-content/uploads/Documents/application-report/TAB111.pdf
7. WaterTAP contributors, WaterTAP: An open-source water treatment model library. Version 0.6. Sponsored by California Energy Commission, National Alliance for Water Innovation, and USDOE., (n.d.). https://github.com/watertap-org/watertap.
8. D.M. Davenport, A. Deshmukh, J.R. Werber, M. Elimelech. High-Pressure Reverse Osmosis for Energy-Efficient Hypersaline Brine Desalination: Current Status, Design Considerations, and Research Needs, Environ. Sci. Technol. Lett. 5: 467–475 (2018). https://doi.org/10.1021/acs.estlett.8b00274.
9. J. Wu, B. Jung, A. Anvari, S. Im, M. Anderson, X. Zheng, D. Jassby, R.B. Kaner, D. Dlamini, A. Edalat, E.M.V. Hoek. Reverse osmosis membrane compaction and embossing at ultra-high pressure operation, Desalination. 537: 115875 (2022). https://doi.org/10.1016/j.desal.2022.115875.
10. A.V. Dudchenko, T.V. Bartholomew, M.S. Mauter. High-impact innovations for high-salinity membrane desalination, Proceedings of the National Academy of Sciences. 118:e2022196118 (2021). https://doi.org/10.1073/pnas.2022196118
11. T. Tong, M. Elimelech. The global rise of zero liquid discharge for wastewater management: drivers, technologies, and future directions. Environ. Sci. Technol. 50: 6846–6855 (2016).
12. A. Lee, J.H. Ghouse, J.C. Eslick, C.D. Laird, J.D. Siirola, M.A. Zamarripa, D. Gunter, J.H. Shinn, A.W. Dowling, D. Bhattacharyya, L.T. Biegler, A.P. Burgard, D.C. Miller. The IDAES process modeling framework and model library—Flexibility for process simulation and optimization. J.Adv. Manuf 3: e10095 (2021). https://doi.org/10.1002/amp2.10095.
13. A.A. Atia, J. Allen, E. Young, B. Knueven, T.V. Bartholomew, Cost optimization of low-salt-rejection reverse osmosis. J. Desal. 551:116407 (2023). https://doi.org/10.1016/j.desal.2023.116407
14. P. Wang, A. Anderko, R.D. Young, A speciation-based model for mixed-solvent electrolyte systems, Fluid Phase Equilibria. 203: 141–176 (2002). https://doi.org/10.1016/S0378-3812(02)00178-4
15. PySMO: Python-based Surrogate Modelling Objects — IDAES v1.13.2, (n.d.). https://idaes-pse.readthedocs.io/en/stable/explanations/modeling_extensions/surrogate/api/pysmo/index.html. (Accessed November 16, 2023).
16. McGivney W, Kawamura S. Cost Estimating Manual for Water Treatment Facilities. J.Wiley&Sons (2008).
17. Miara A, Talmadge M, Sitterley K, Evans A, Huang Z, Macknick J, McCall J, Kurup P, Akar S, Van Allsburg K, Stokes-Draut J, Bartholomew T, Lee A, Gingerich D, WaterTAP3 (The Water Technoeconomic Assessment Pipe-Parity Platform), (2021). https://doi.org/10.11578/DC.20210709.1
18. Sharma JR. (2010). Use of cost equations and cost indexes for preliminary cost estimates of water treatment plants." M.S. thesis, Dept. of Civil Eng., Univ. of Texas at Arlington, Arlington, TX (2010).
19. Sharma, JR, Najafi M/ Qasim SR. Preliminary Cost Estimation Models for Construction, Operation, and Maintenance of Water Treatment Plants, *J. Infrastruct. Syst.* Vol. 19, No. 4 :451-464 (2013). 10.1061/(ASCE)IS.1943-555X.0000155
20. Intratec. https://www.intratec.us/chemical-markets/sulfuric-acid-price. Accessed 2 Aug. 2023.
21. Intratec. https://www.intratec.us/chemical-markets/hydrochloric-acid-price.
22. R.C. Gumerman, R.L. Culp, S.P. Hansen, Estimating water treatment costs: Volume 2. Cost curves applicable to 1 to 200 mgd treatment plants, Drinking Water Research Division, Municipal Environmental Research Laboratory, US EPA, EPA-600/2-79-162b. (1979).
23. Intratec. Intratec Primary Commodity Prices Commodities Specifications. https://cdn.intratec.us/docs/methodologies/ipcp-commodities-specifications.pdf.
24. L. Birnhack, N. Voutchkov, O. Lahav. Fundamental chemistry and engineering aspects of post-treatment processes for desalinated water—A review. Desalination 273: 6–22 (2011).
25. I.S. Al-Mutaz, M.A. Al-Ghunaimi, pH control in water treatment plant by the addition of carbon dioxide, in: The IDA World Congress on Desalination and Water Reuse, Bahrain, 2001: pp. 1–12.
26. A. Wachter, L.T. Biegler, L.T. On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming. Math. Prog. 106,25–57(2005).
