WaterTAP Technical Brief: Ion Exchange Model Demonstration and Optimization

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Contract No. DE-AC36-08GO28308

Technical Report
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Suggested Citation
Sitterley, Kurban A., and Alexander Dudchenko. 2023. *WaterTAP Technical Brief: Ion Exchange Model Demonstration and Optimization*. Golden, CO: National Renewable Energy Laboratory. NREL/TP-5700-86512. https://www.nrel.gov/docs/fy23osti/86512.pdf.

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This work was authored in part by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Funding provided by U.S. Department of Energy Office of Energy Efficiency and Renewable Energy Industrial Efficiency and Decarbonization Office. The views expressed herein do not necessarily represent the views of the DOE or the U.S. Government.

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 Industrial Efficiency and Decarbonization Office under Funding Opportunity Announcement DE-FOA-0001905.

Executive Summary

Ion exchange is an important water treatment process for removing targeted contaminants, including those associated with hardness. In this report, we introduce the ion exchange model developed for the Water treatment Technoeconomic Assessment Platform (WaterTAP) and demonstrate an analysis of Ca^{2+} removal for 0.1 million gallons per day (MGD) and 10 MGD systems. The model is a single-component, steady-state implementation that enables process optimization based on the influent ion concentration, resin capacity, and resin selectivity. Based on a survey of costing references for ion exchange, the WaterTAP ion exchange model returns reasonable estimates for the levelized cost of water of an ion exchange process, and performs as expected when critical design parameters, such as the resin capacity and selectivity, are varied.

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1 Introduction

Ion exchange (IX) is a chemical separation process that has been used for selective contaminant removal in water treatment applications for decades. As the name suggests, IX involves the exchange of an undesired charged ion in the aqueous phase with an ion from the solid phase. The solid phase can be anything from a natural zeolite to a highly selective polymer-based resin that is typically packed into a column for the water to flow around (SenGupta 2017). The largest application of IX in water treatment today is for softening—the exchange of a divalent cation (e.g., calcium, barium) with a monovalent cation (typically sodium). IX can also play a role in selective contaminant removal, presenting an attractive alternative to bulk separation processes (Gottlieb and Watkins 2012).

The cost of IX, like many other water treatment processes, is dependent on several aspects of the overall system including the influent water quality, treatment objectives, and any local discharge regulations that must be considered for waste streams. Further, the accuracy of the cost estimate is impacted by the extent that the uncertainties and variables in a given project are understood, the stage of planning or operation for a given project, and the data available for the model (Sharma 2010). Accurate cost estimates for IX require (1) the optimization of process design for specific resin performance and feed composition, which impact capital costs, and (2) the estimation of regeneration cycles, backwashing, and rinsing requirements, which impact operating costs. Modeling different resin properties and regeneration approaches can help operators understand how their current process performance and cost are affected by resin choice or a change in breakthrough concentration threshold. For example, a higher breakthrough concentration threshold will result in a longer cycle and less frequent regenerations (Gottlieb and Watkins 2012), possibly resulting in lower costs. Similarly, effective IX models can help researchers focus on aspects of the process that can improve performance, reduce costs, or both.

Ion Exchange Overview

The IX process can be broken down into four distinct steps (Crittenden et al. 2012; Wachinski 2017; Inamuddin and Luqman 2012): (1) service, where IX absorbs ions of interest from the feed while releasing counter ions into the feed; (2) backwashing, where water is flowed in the opposite direction to remove remaining feed and accumulated particulates; (3) regeneration, where a concentrated solution is passed through the column to create a reverse exchange process, resulting in absorbed ions being released into the regenerate solution (eluent) and IX resin reabsorbing original counter ions (e.g., Na^+); (4) rinse, where remaining regenerate solution is flushed out and the resin is regenerated prior to the column entering the service step. The completion of all four steps represents one cycle of an IX process. The duration of each of these steps is a function of many aspects of the process, including the water matrix, resin properties, and regenerant choices.

During the service run, the effluent concentrations of any ions of interest (e.g., anions if using anion exchange resin) are effectively zero at first and increase until they break through the bed (Inamuddin and Luqman 2012). Operation continues until the effluent concentration reaches the breakthrough concentration threshold and the bed must begin the regeneration step. Regeneration is typically the most expensive aspect of the IX process and can render the IX process more expensive and difficult to operate than other comparable processes (Korak, Mungan, and Watts 2022).

The choice of regenerant is dictated by the design strategy and resin type, but typical regenerants include NaCl, HCl, H_2SO_4, and NaOH. Regeneration is chemically inefficient in that a higher concentration of regenerant must be used to remove an equivalent amount of the exchanged ion (Korak, Mungan, and Watts 2022). Thus, regardless of the regenerant used, proper and economic disposal of the concentrated regenerant stream is a critical consideration for process design. Table 1 provides a summary of key decision variables and metrics in IX. Notably, the cost of handling the spent regeneration brine is not considered in this analysis. Brine management for IX is typically done by a separate unit process (Korak, Mungan, and Watts 2022) and is thus outside the outside the scope of this analysis.

Table 1: Critical Decision Variables and Metrics for Ion Exchange Model

Variable(s)	Description	Cost Impact
Resin capacity	Mass of target ion the resin can sorb before regeneration is required.	Higher resin capacity results in longer breakthrough times, lower regeneration frequency, and lower costs.
Resin selectivity	Affinity of resin for target ion.	Higher resin selectivity results in a higher usable fraction of the resin capacity, longer breakthrough times, lower regeneration frequency, and lower costs.
Service flow rate	Sometimes referred to as “loading rate,” this is the linear flow of feed pushed through each column in bed volumes per hour.	Higher service flow rate results in lower resin volume needed and lower costs.
Regeneration type and concentration	The amount of regenerant required to regenerate resin each cycle.	Increased regeneration concentration results in higher demand for regenerant and higher costs.
Breakthrough time	The time until the breakthrough concentration is detected in the effluent stream.	Increased breakthrough time results in longer cycle times, lower regeneration frequency, and lower costs. *NOTE: Breakthrough time cannot be directly set by user of ion exchange model. Linked to breakthrough concentration.*
Breakthrough concentration	The constituent concentration at which the regeneration step of the cycle begins. In practice, this would be determined by the operator based on their level of comfort. In the WaterTAP model, this is determined/calculated by the model based on influent concentration and resin characteristics.	Higher breakthrough concentration results in longer breakthrough times, longer cycle times, lower regeneration frequency, and lower costs. *NOTE: Breakthrough concentration cannot be directly set by the user of ion exchange model.*

2 Methods

Model Overview

The model implemented in WaterTAP is an empirical-performance-based model for a fixed-bed IX process with the following criteria and assumptions: (1) single liquid phase, (2) single reactive solute and single solvent (water) only, (3) isothermal operation, (4) steady-state operation, (5) plug-flow regime, and (6) the resin has a constant separation factor with favorable Langmuir isotherm (LeVan, Carta, and Yon 2019). Additional details of the WaterTAP IX model, including process equations and variables, are available in the WaterTAP documentation (WaterTAP Contributors n.d.).

The model accounts for process equilibrium, kinetics, and hydrodynamics to predict performance, bed/column geometry, capital, and operating costs. The model is based around determining the conditions for a single cycle of the IX process. User-defined resin parameters are used to establish a breakthrough concentration and breakthrough time using the constant-pattern assumption (LeVan, Carta, and Yon 2019).

Capital cost calculations were adapted from the U.S. Environmental Protection Agency's (EPA's) IX model (EPA 2022) and include the total cost for the number of vessels (columns) required, total resin volume, and backwashing and regeneration tanks. Operating costs include the electricity needed to run booster pumps, regeneration chemical costs, resin replacement costs, and, if applicable, the cost for disposal of spent resin and regenerant that is deemed hazardous.

Figure 1 presents a process flow diagram showing all the major flows and equipment included in the model. Included is the booster pump for the service step, a backwash tank and pump for the combined backwashing/rinsing step, and a regeneration tank and pump for the regeneration step. A small fraction of the influent flow splits to fill the backwash tank, and a small portion of the treated flow splits to fill the regeneration tank. The regeneration and backwashing/rinsing streams combine to make the waste stream.

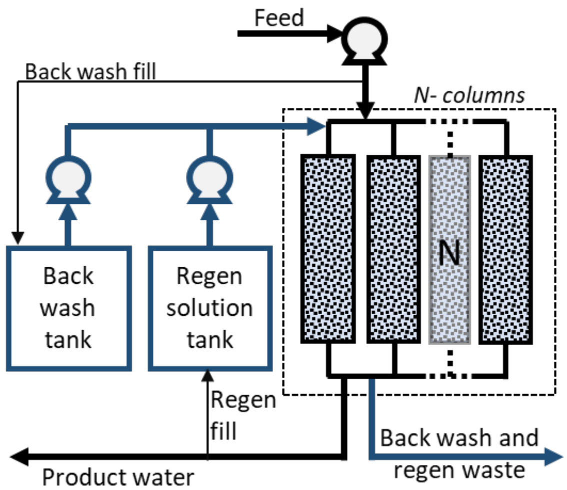

Figure 1: Process flow diagram of IX process modeled in WaterTAP. The process includes pumps for feed, regen, and backwashing steps and tanks for storing backwashing solution and regen solution. Additionally, *N* columns are modeled in parallel (shown in dashed box), based on column size limitations and system throughput.

3 Results

Here, we present how the developed WaterTAP model can be used to estimate levelized cost of water (LCOW) of IX as a function of resin cost, resin capacity, resin Langmuir constant (i.e., resin selectivity), influent ion concentration, and feed flow rate. For the analysis herein, we consider systems of two common scales—0.1 millions of gallons per day (MGD) and 10 MGD—targeting removal of Ca^{2+} ion from feed, which is a common target in water softening. We use 250 ppm of calcium as our base-case scenario, and an ion resin Langmuir constant of 0.9 (selectivity of 1.1).

3.1 Design and Cost of IX for Different Scenarios

The developed model enables analysis of IX cost breakdown and operational design changes as a function of IX resin performance metrics. Here, we select a base case of feed with 250 ppm calcium and vary selectivity and capacity to demonstrate the impact of IX resin properties on key IX design metrics and costs.

The LCOW for the IX process decreases with increases in capacity and decreases in Langmuir constant (correlating to an increase in selectivity). In general, increasing resin capacity will have a greater impact on LCOW than will decreasing the Langmuir constant (increasing selectivity) (Table 2). This uneven trade-off is due to a linear increase in usable resin capacity with an increase in maximum capacity, and a nonlinear increase in usable capacity of resin with a decrease in the Langmuir constant, as seen in Table 2. Tripling the maximum resin capacity leads to a tripling of usable capacity, whereas reducing the Langmuir constant by one-third increases the usable capacity by only 1.35 times. The higher usable resin capacity reduces required regeneration, which is a significant fraction of the overall cost of a regenerative IX process (nearly 50%), as shown in Table 2. When the resin capacity is increased by 3 times, the regeneration cost is reduced by nearly 48%, whereas decreasing the Langmuir constant (increasing selectivity) by 3 times only decreases the regeneration cost by ~21%. Higher usable capacity results in longer cycles and fewer regeneration steps for the IX process, thereby reducing the regenerant cost and overall LCOW. This trade-off between increasing selectivity and capacity is observed at all values of capacity and selectivity when treating 250 ppm calcium feed, as shown in Figure 2.

These results demonstrate that higher-capacity resins have the potential to decrease overall process costs, with typical resins today having a capacity range of 0.5–3 eq/kg, which varies significantly with specific operating conditions. The costs associated with this range of resin capacities in Figure 2 result in a LCOW that falls within the range of 0.39 ± 0.6 $/m^3, the average LCOW for IX as presented in various costing models (EPA 2022; Sharma 2010; Miara et al. 2021; FRTR n.d.).

An important aspect of IX operation that is not considered in this presented analysis is the impact of the regeneration dose required. Like previously mentioned, the regeneration step of the IX process (cost of the regenerant and disposal) is the most cost intensive part of the cycle and is why prediction of breakthrough time is critical for accurate IX costing. The dosing and chemical required for regeneration will be case-specific and, while the used for this analysis (125 kg NaCl per m^3 resin) is sufficient for a hardness application (EPA 2022), other applications may use a different regenerant and/or dose that could raise costs considerably. Further, in some applications (e.g., removal of perfluorinated substances) where regeneration is not possible or so inefficient as to be not cost-effective, the resin bed is entirely replaced with new resin rather than regenerated, adding additional operating costs (EPA 2022). Different approaches to reduce regeneration costs and disposal are presented in Korak, Mungan, and Watts (2022) and include regenerant reuse strategies, improving regeneration efficiency by incorporating it with downstream waste management, and partial regeneration approaches.

Table 2: Impact of Capacity and Selectivity Increase for Hardness Scenario

Parameter	Baseline Scenario	Scenario A (Capacity Increase)	Scenario B (Selectivity Increase)
Flow	0.1 MGD	0.1 MGD	0.1 MGD
Conc. In (Ca^{2+})	250 ppm	250 ppm	250 ppm
Resin Max. Capacity	1.50 eq/kg	4.50 eq/kg	1.50 eq/kg
Resin Usable Capacity	0.78 eq/kg	2.33 eq/kg	1.06 eq/kg
Langmuir Constant	0.9	0.9	0.3
Resin Selectivity	1.11	1.11	3.33
Resin Capacity Utilization	51.8%	51.8%	70.8%
Breakthrough Time	3 h	8.7 h	4 h
Resin Bed Cost (initial capital)	$2,840	$2,840	$2,840
Annual Regenerant Cost (NaCl @ 125 kg/m^3)	0.28 \$/m^3	0.17 \$/m^3	0.22 \$/m^3
LCOW	0.52 \$/m^3	0.35 \$/m^3	0.45 \$/m^3

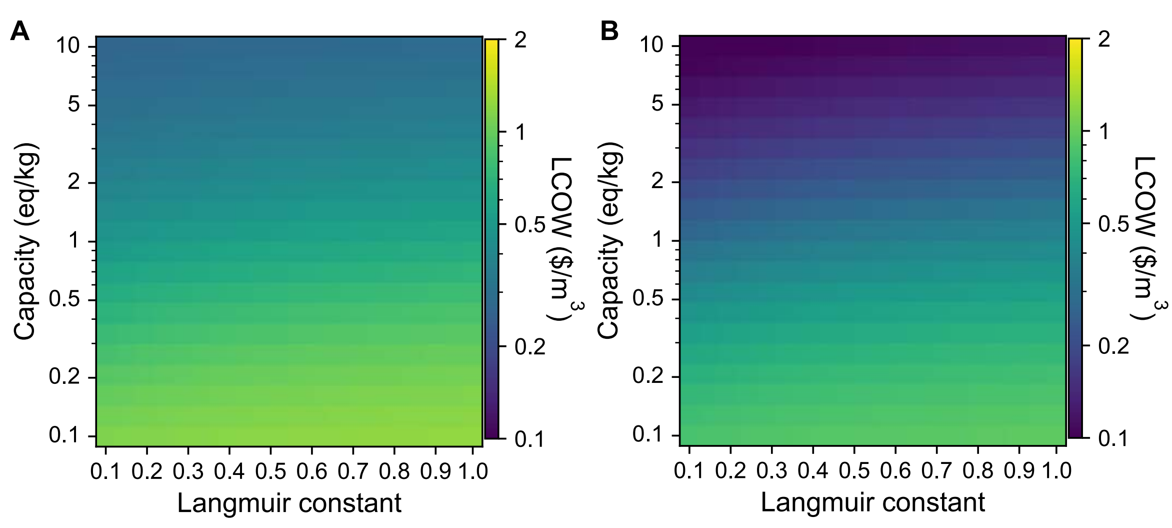

Figure 2: Impact of capacity and Langmuir constant on LCOW of IX treating 250 ppm calcium feed at (A) 0.1 MGD and (B) 10 MGD

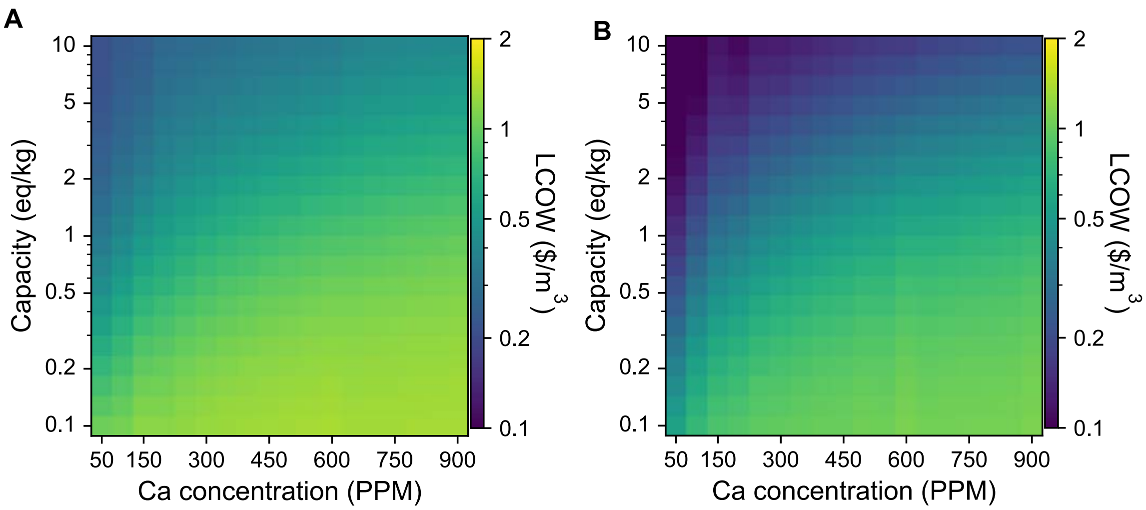

Figure 3: Impact of capacity and calcium concentration on LCOW of IX treating feed at (A) 0.1 MGD and (B) 10 MGD with Langmuir constant of 0.9 (selectivity of 1.1)

3.2 Impact of Constituent Concentration

The cost of IX increases with an increase in influent ion concentration and a decrease of capacity (Figure 3). This is an intuitive result for IX processes, as increasing capacity or decreasing influent ion concentration will increase the breakthrough time, leading to higher cycle times and lower regenerant required per cycle. Similarly, the operator could have a higher or lower breakthrough threshold that would impact costs in a similar fashion. The breakthrough threshold is the relative effluent concentration above which the service cycle is stopped, and regeneration begins (Inamuddin and Luqman 2012). Increasing or decreasing this threshold has the same effect as increasing or decreasing breakthrough time and would be reflected in the overall cost of the process.

3.3 Impact of Resin Cost

Resin cost plays an important role in determining overall process cost, because in general, pumps, tanks, and columns have a relatively lower cost than the IX resin. The cost for resin in current models is derived from the EPA model and ranges between $5,400/m^3$ and $7,300/m^3$ of resin ($150/ft^3$–$205/ft^3$). These costs depend on type of resin, supplier, and application. Using the IX model, Figure 4 presents how treatment costs change with respect to the cost of resin and changes in resin capacity. Increases in resin cost increase the LCOW; an increase in resin cost from the base case of ~$5,000/m^3$ to $100,000/m^3$ increases LCOW by nearly 10 times. However, an increase in resin cost with a similar increase in resin capacity can potentially decrease the overall processes LCOW. The results clearly demonstrate a nonlinear relationship between IX resin cost, capacity, and LCOW that can be analyzed with the developed WaterTAP model for a given application.

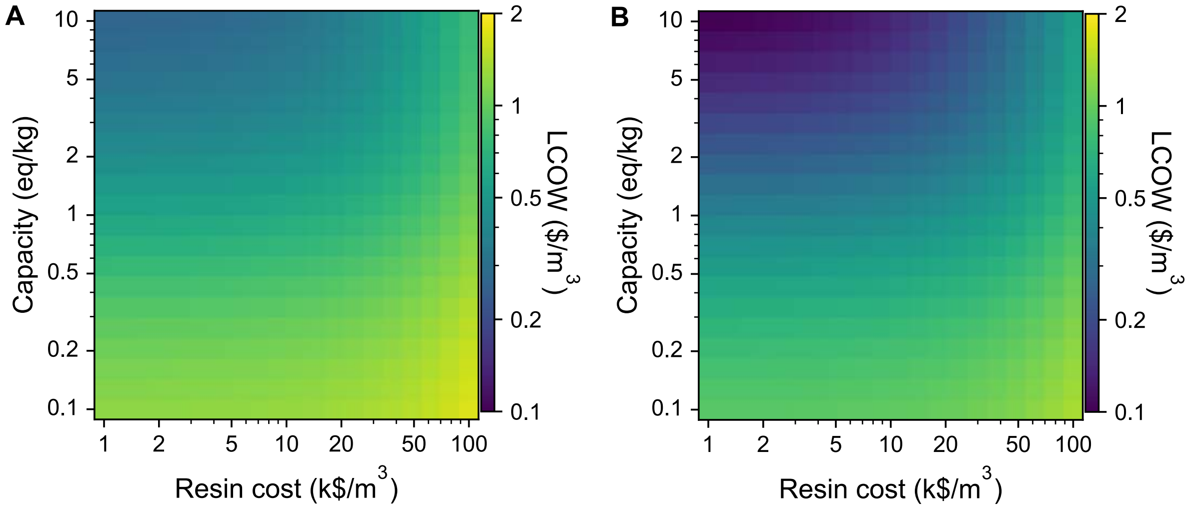

Figure 4: Impact of resin cost and capacity on cost of IX treating (A) 0.1 MGD and (B) 10 MGD feed with 250 ppm of calcium

4 Conclusion

This report presents an example of the analysis possible with the current implementation of the IX model in WaterTAP. We described key model assumptions and implementation, and presented a brief overview of the results and types of analysis that can be performed. We have further verified that the current implementation can produce LCOW estimates for the treatment of standard waters similar to those of prior models and cost estimations.

WaterTAP Resources

WaterTAP is an actively maintained and developed software package. The following is a permalink to the version of WaterTAP used for this report: https://github.com/watertap-org/watertap/tree/98aa405958. From that URL, navigate to watertap/examples/ion_exchange/ion_exchange_demo.py for a working demonstration of the IX model used for this report. The model's technical documentation, source code, and examples can be found on the WaterTAP documentation site (https://watertap.readthedocs.io/en/stable/) (WaterTAP Contributors n.d.).

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