Cost-optimal selection of pH control for mineral scaling prevention in high recovery reverse osmosis desalination

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Introduction

- Explicitly incorporating effects of chemical phenomena such as mineral scaling and pretreatment in water treatment system design is critical.
- Incorporation of detailed chemistry into process-scale water treatment models historically hindered by complexity of chemistry phenomena → our surrogates-based modeling framework makes this possible.
- **Research Gap:** Abundance of qualitative assessments and experimental studies on chemical pretreatment and scaling; very little on assessing the technoeconomic implications of chemical pretreatment alternatives within the context of end-to-end water treatment train optimization.
- **Goal:** Investigate impact of different pH control alternatives during pretreatment on the cost and operation of high-recovery desalination trains.
- **Why:** pH Control in reverse osmosis (RO) treatment trains critical to mineral-scale formation & membrane longevity.

Desalination Treatment Train

Proposed high-recovery treatment train: High-pressure reverse osmosis (HPRO) technology with chemical pretreatment (Figure 1).

High-pressure reverse osmosis (HPRO)

- **Innovation**: Membranes for higher operating pressures (> 200 bar) than currently possible with conventional reverse osmosis (≈ 85 bar).
  - Higher recoveries and efficiencies (with pretreatment)
  - Lower costs than other high-recovery alternatives

Chemical Pretreatment

- **Softening:** soda ash (Na_2CO_3) addition to remove calcium ions as $CaCO_3$.
- **Acidification:** Acid addition for pH control.
  - Three commonly-used alternatives evaluated: CO_2, HCl, H_2SO_4

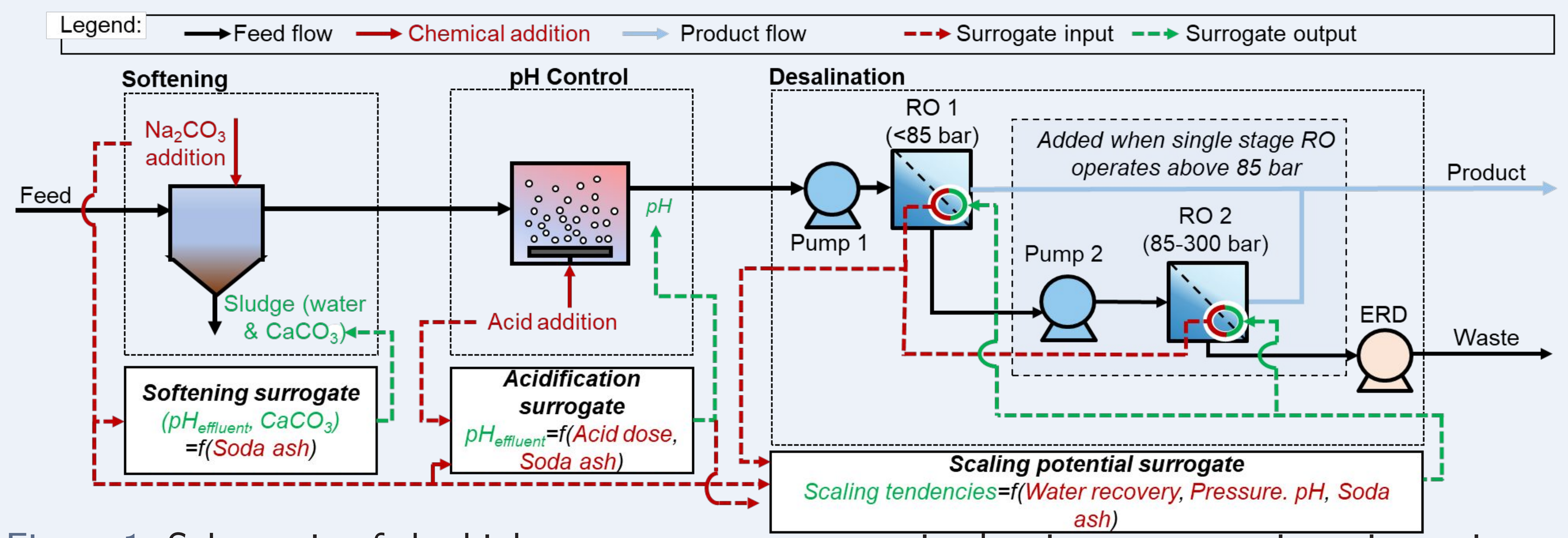


Figure 1: Schematic of the high-recovery treatment train showing surrogate insertion points.

System Modeling & Optimization Formulation

Given **Feedwater (FW)**,

$$\min_{d} LCOW = \frac{\text{CRF} \times \text{capital cost} + \text{annual operating cost},\ \$/\text{yr}}{\text{Treated water volume},\ \text{m}^3/\text{yr}}$$

s.t.

- **Pretreatment**
  - soda ash dose
  - Acid dose
- **RO parameters**
  - pressure
  - recovery
  - membrane area

- HPRO process models
- Operational constraints
- Pretreatment constraints
- Mineral scaling constraints (Scaling Tendency, $ST \leq 1$)

Equalities / Inequalities

Hybrid Modeling Approach

- First principles (mechanistic) models for desalination train components (RO, ERD, Pumps) from WaterTAP.
- **Surrogates for pretreatment & mineral scaling (RBF Models)**
  Chemistry data generated with OLI; surrogates trained with PySMO
  - Softening: $CaCO_3$ concentration, pH $= f\,(Na_2CO_3$ dose)
  - Acidification: pH $= g\,(Na_2CO_3$ dose, Acid dose)
  - Mineral scaling:
    - ST $= h\,(Na_2CO_3$ dose, Acid dose, RO Pressure, RO recovery)
    - Scalants: Calcite ($CaCO_3$), Gypsum($CaSO_4.2H_2O$), Anhydrite($CaSO_4$)

	Variable Range	
	Brackish	Seawater
Na_2CO_3, mg/L	0-750	0-1200
RO Pressure, bar	10-110	50-300
RO Recovery, %	50-90	50-87
CO_2, mg/L	0-300	0-50
HCl, mg/L	0-150	0-50
H_2SO_4, mg/L	0-150	0-50

	Metrics (R^2, MaxAE)	
	Brackish	Seawater
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

Approach: Integrate **detailed chemistry** into treatment train optimization with **surrogate models**

Key Result: Choice of **acid** largely depends on feedwater **composition** and the **primary scalants** of concern

Results: Process Economics

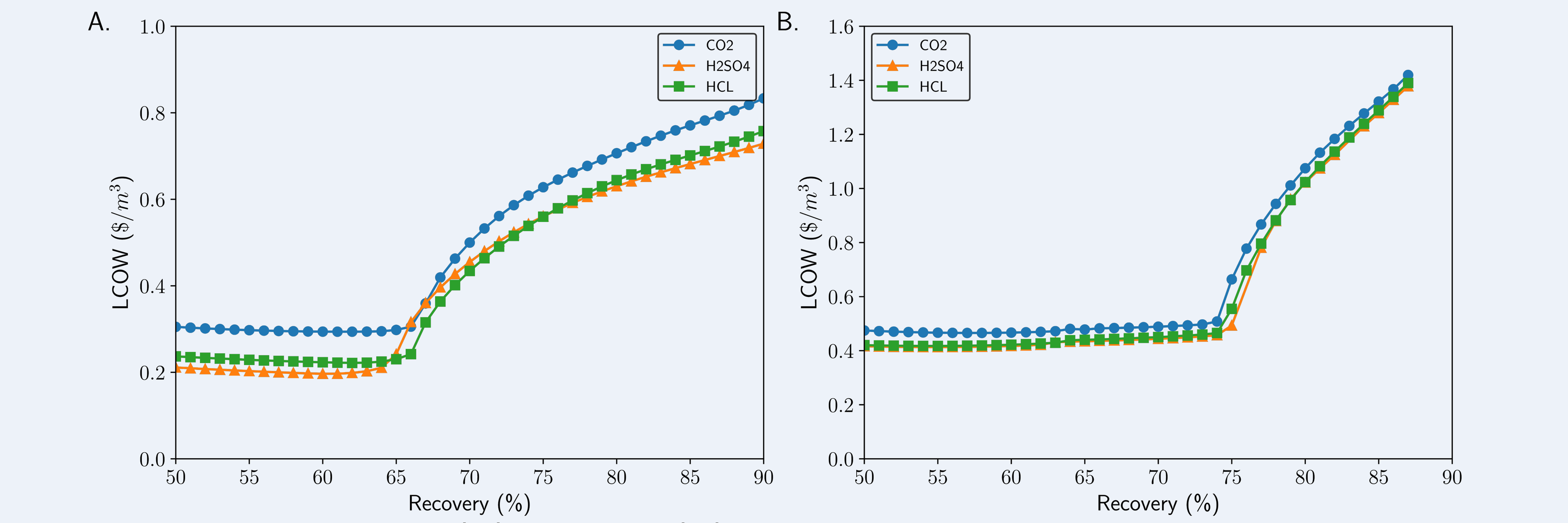
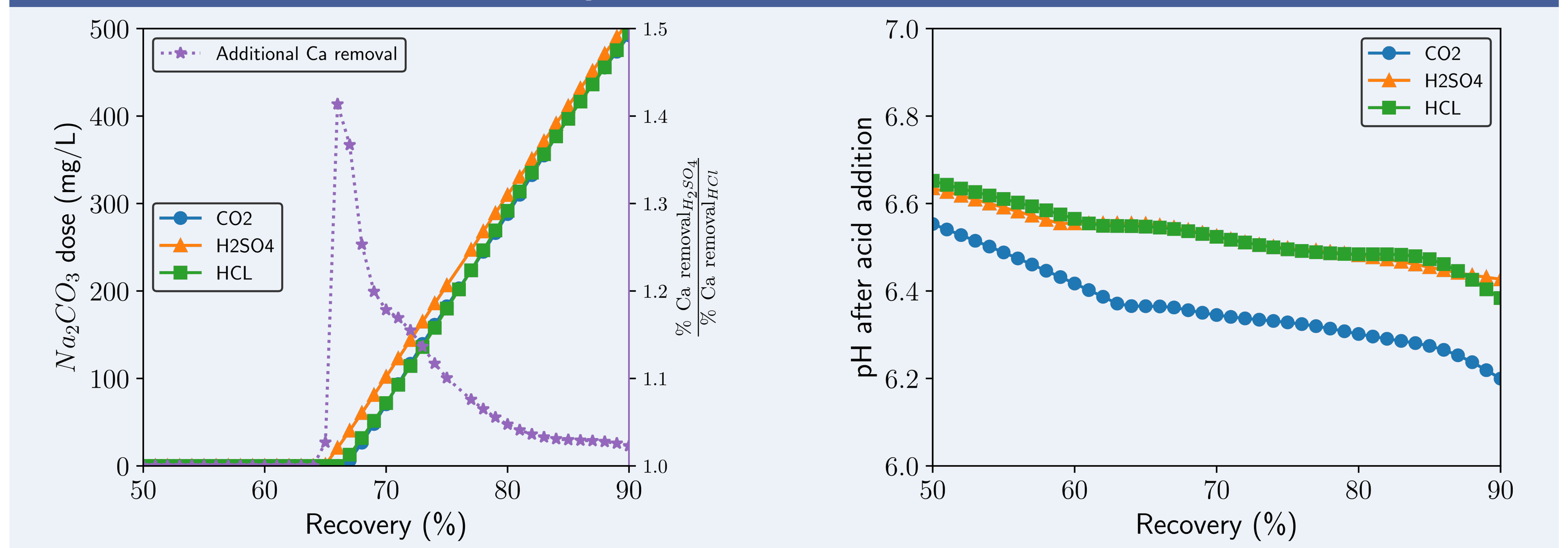


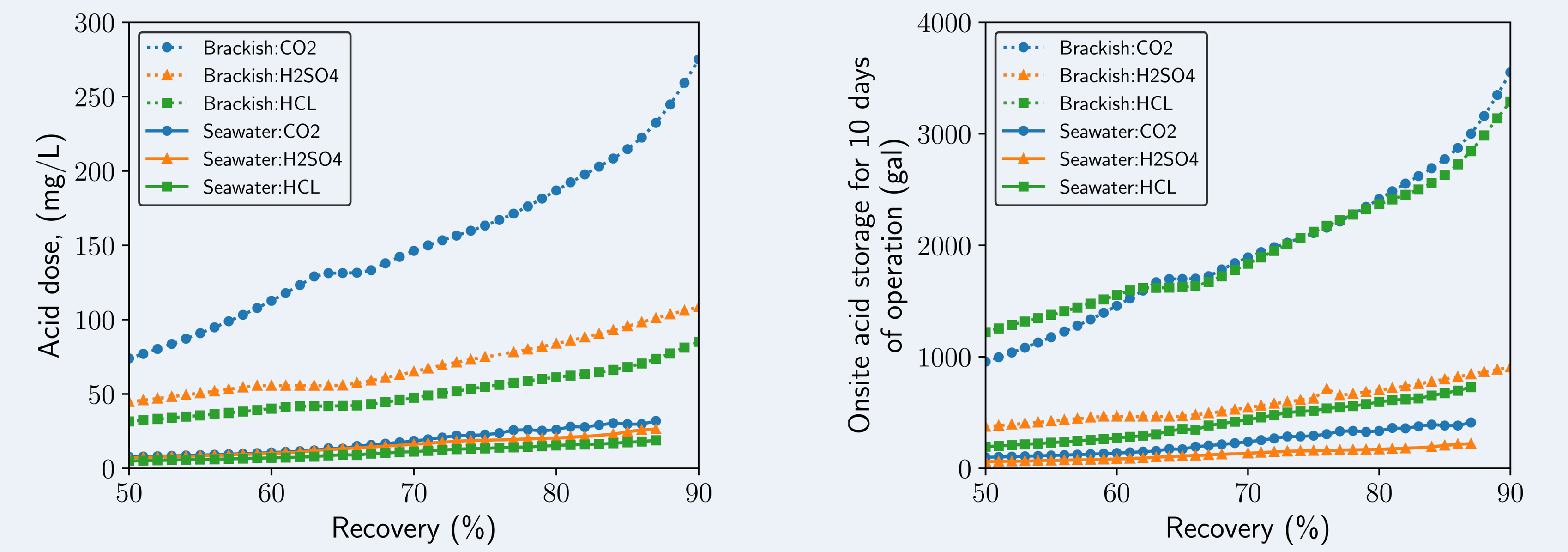
Figure 2: Cost profiles for (A) brackish (B) seawater with different pH control acid choices.

- CO_2 most expensive choice, HCl/H_2SO_4 similar.

Results: Process Operation



(a) Na_2CO_3 concentration profile - Brackish (b) pH profiles post-acidification - Brackish



(c) Optimal acid doses (d) Onsite acid storage - 10 days operation

Figure 3: Operational characteristics of HPRO system with different pH control options.

- Softening for gypsum scaling; pH adjustment for controlling calcite scaling.
- H_2SO_4 requires more softening than CO_2/HCl, favors gypsum scaling.
- CO_2 requires the highest concentration, needs lower pH for desalination.
  - CO_2 increases carbonate ion concentration, favoring calcite scaling.
- H_2SO_4 requires the lowest volume for onsite storage; CO_2 safest choice.

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