Making Techno-Economic Assessments Work For You

Tim Bartholomew

August 7th, 2025

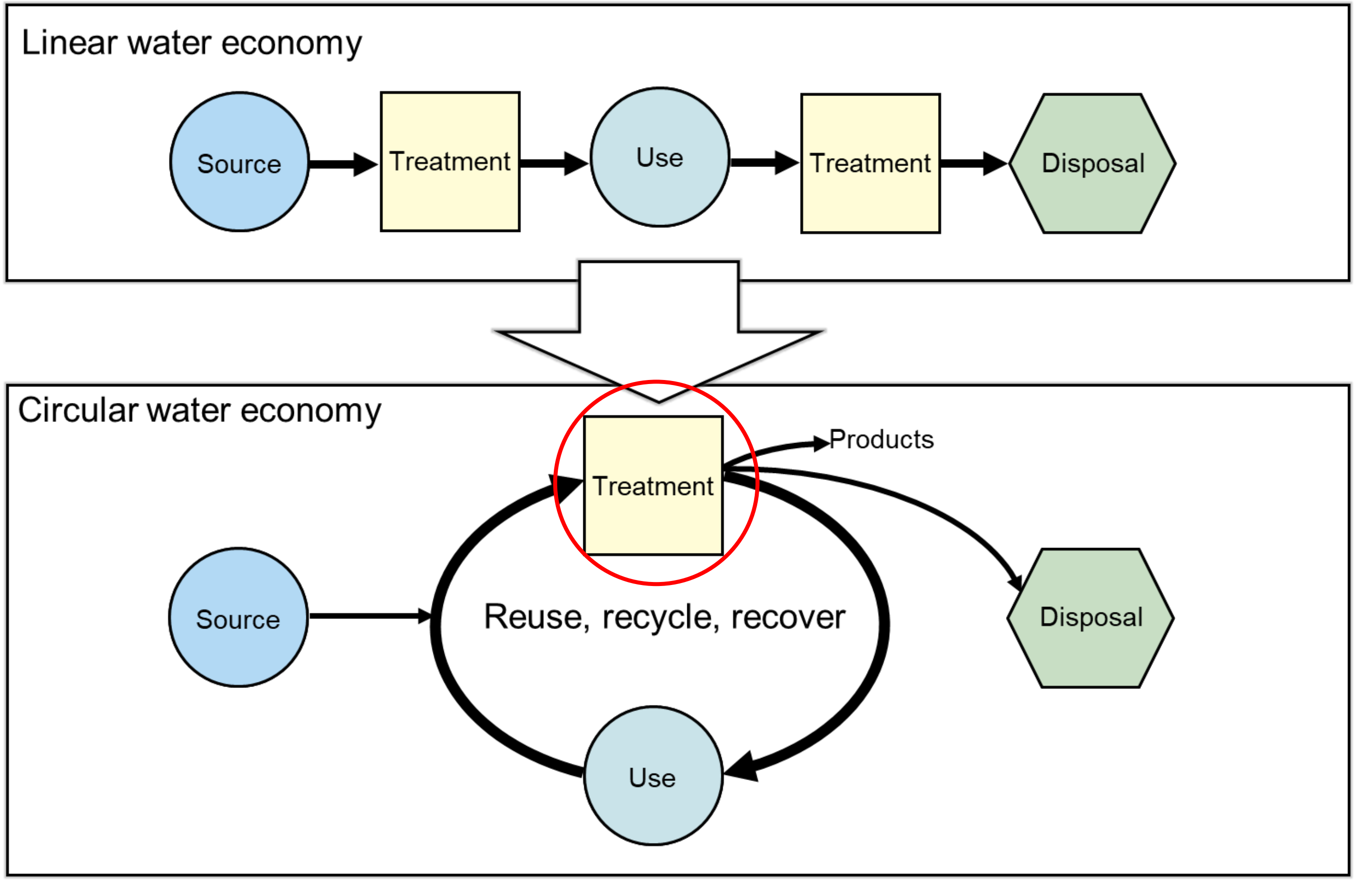
Process systems engineer supporting R&D

- Expertise:
  - Detailed process modeling, techno-economic assessment, and mathematical optimization
  - Emerging water treatment and desalination technologies

- Education background:
  - Ph.D. Civil and Environmental Engineering from Carnegie Mellon University
  - B.S. Chemical Engineering from Washington University in St. Louis

- Employment background:
  - National Energy Technology Laboratory (NETL), led development of a National Alliance for Water Innovation (NAWI) funded open-source software tool called **WaterTAP**
  - Horizon Modeling Solutions, cofounded a consulting company for supporting R&D

A paradigm shift for water management requires advances in treatment technologies



Circular water economy is currently perceived as non-viable because of the **insufficient performance** or **high cost** of treatment technologies

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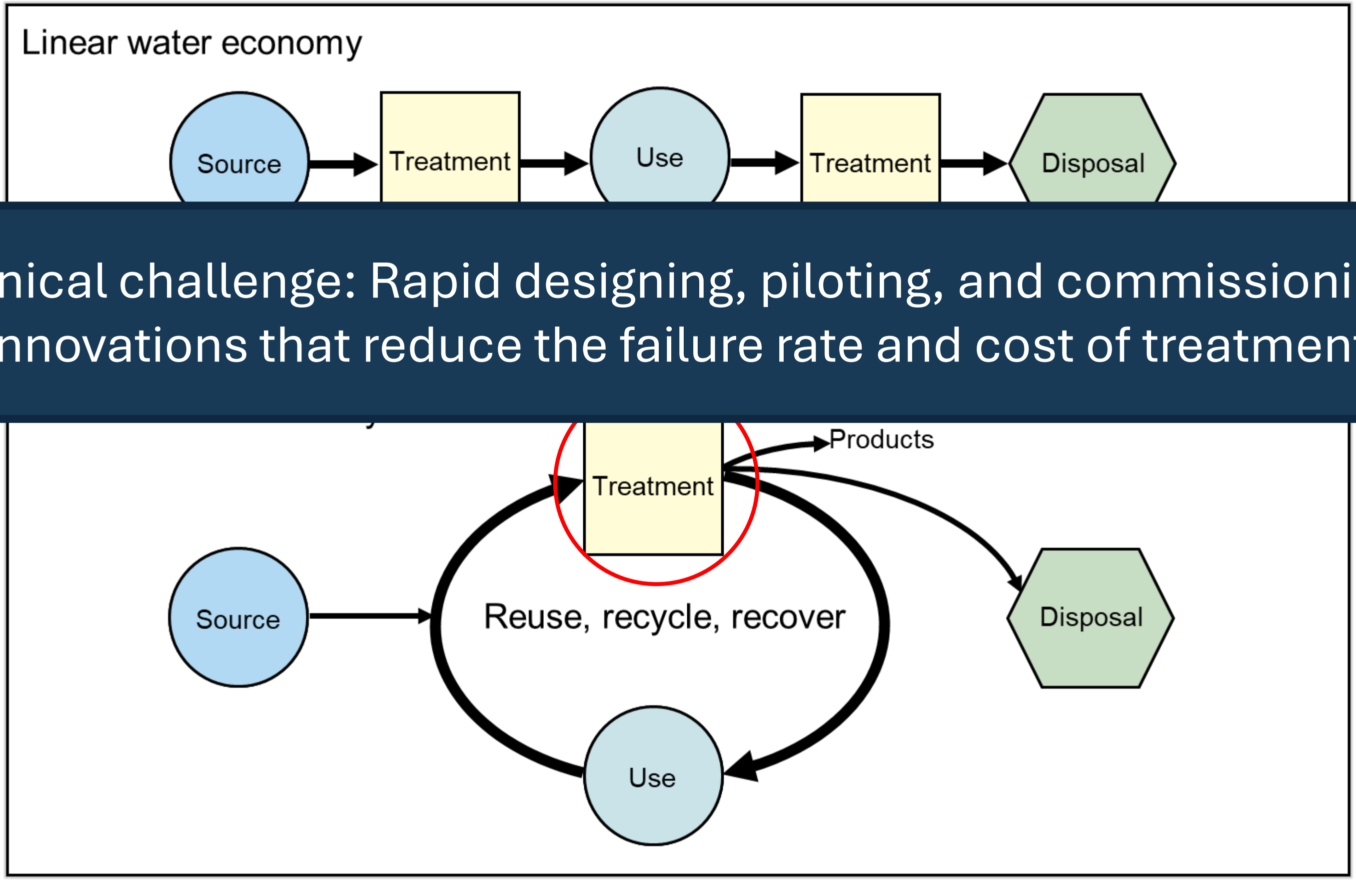
A paradigm shift for water management requires advances in treatment technologies



Technical challenge: Rapid designing, piloting, and commissioning of innovations that reduce the failure rate and cost of treatment

Circular water economy is currently perceived as non-viable because of the **insufficient performance** or **high cost** of treatment technologies

TEAs estimate performance and financial metrics

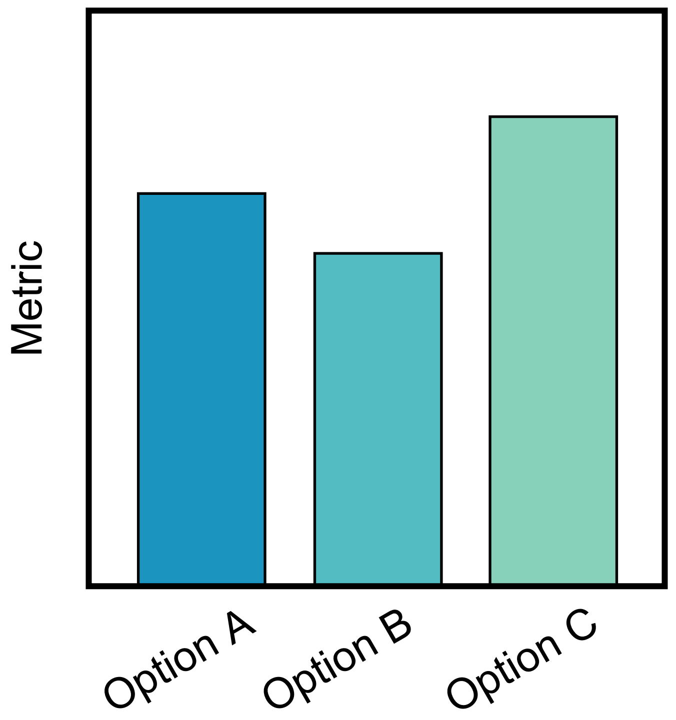
Performance metrics:

- Production or recovery
- Efficiency
- Energy and material consumption
- Waste generation

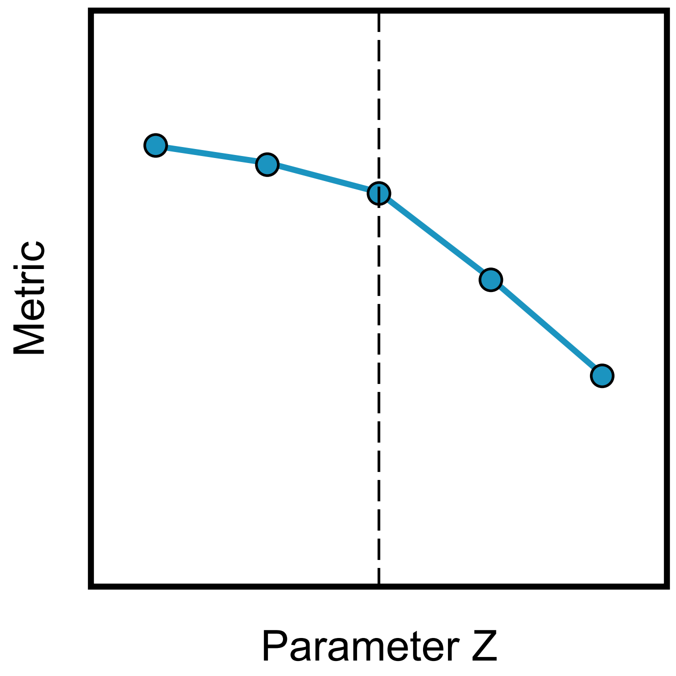
Financial metrics:

- Specific operating cost
- Specific capital cost
- Levelized cost of product or waste
- Net present value
- Internal rate of return

Compare metrics



Quantify the effect of a modeling parameter



Horizon Modeling Solutions

There is a wide range of value and detail in TEAs

"All models are wrong, but some are useful"

- George Box, British Statistician 1919-2013

Increasing detail

Process model	Assumed performance	Simple conceptual	Data driven surrogate	Mechanistic	Hybrid mechanistic
Cost model	Back of envelope	Simple direct	Simple with indirect factors	Detailed	Detailed site-specific
Process data	Analogy	Bench	Small pilot	Large pilot	Commercial
Cost data	Analogy	Textbooks Literature	Expert elicitation	Specific online quotes	Complete vendor quotes

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Analyses with the lowest detail

- Provide value by identifying promising opportunities
- Limited insight into what is possible or how to get there

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Analyses for established technologies

- Primarily use simple models backed by validated data
- Focused on execution and operations, rather than improved design

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Analyses for new technologies

- Provide value by projecting costs from performance assumptions
- Limited insight into best applications or best design/operations

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Detailed analyses for new technologies

- Identify most promising applications, best design and operation for different scenarios, pinpoint technical and financial bottlenecks
- Support in bench and pilot design, operation, and evaluation

Conducting a TEA for new technologies can be challenging

Time and skill intensive steps:

1. Scope out relevant system to cover technology benefits and costs
2. Implement or develop predictive models linking decision variables to performance and cost
3. Obtain process and financial parameter values when data is typically limited
4. Determine design and operation without established heuristics

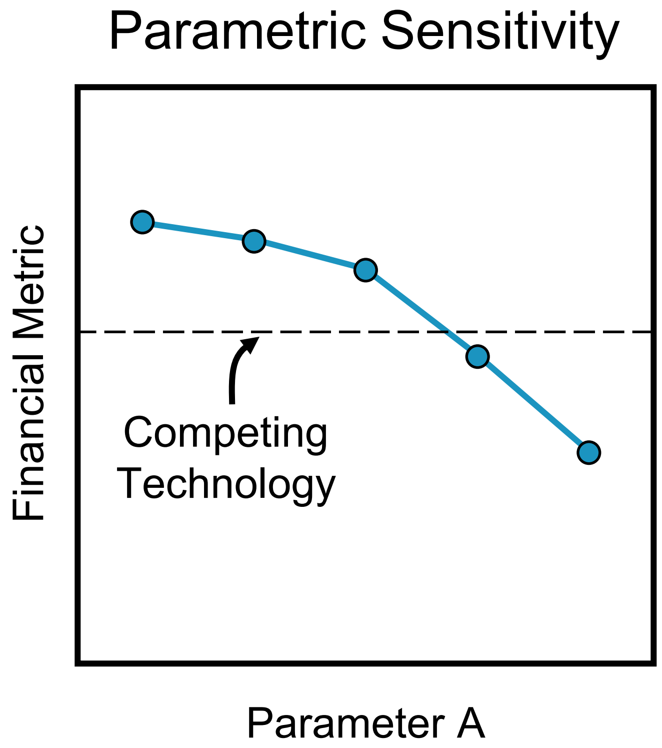
Two overall approaches:

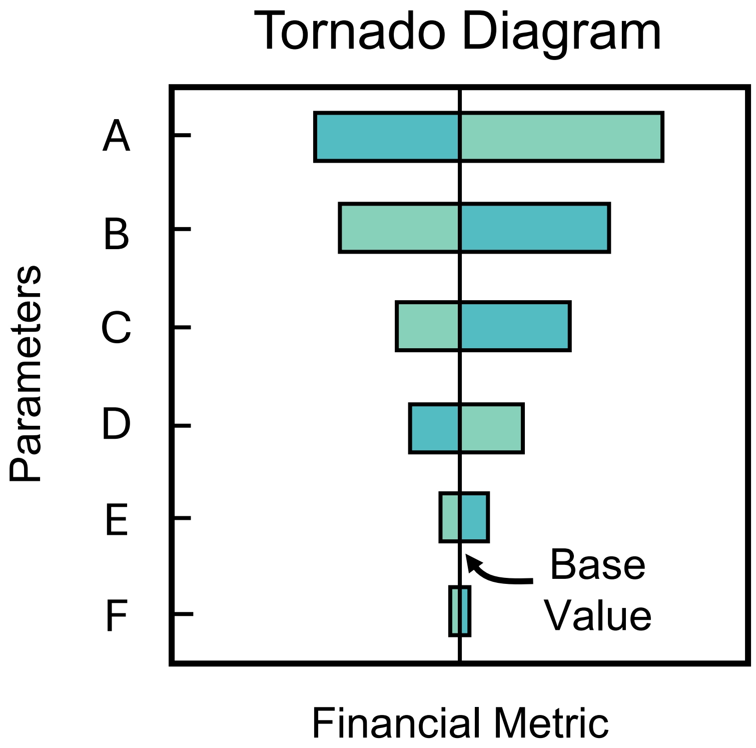
1. Engineers in industry
    - Cobble together available software tools and in-house spreadsheets
    - Inherent limitations for modeling new technologies and incompatibilities due to interfacing between tools
2. Researchers in academia
    - Build models from scratch
    - TEAs have variable quality and can take several months to two years to complete

Start guiding R&D with a cost model and process data

Cost models are required, but predictive process models are optional

- Use an assumed performance process model based on your data or understanding
- Vary the financial and performance parameters to set research goals and priorities





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Cost model can combine engineering handbooks and online resources

- Use costing frameworks in chemical engineering handbooks (Towler & Sinnott, Seider et al.)
  - Tables for generic equipment costs, factors for estimating indirect costs (engineering, siting, etc.)
  - Update to today's dollars with the chemical engineering plant cost index (CEPCI), blog description
  - Curate online equipment cost quotes and establish a range and/or simple relationship
- Leverage the Activate Technomics course: https://www.activate.org/techonomics
  - Educational videos, downloadable Excel models with costing framework and parameter ranges
  - Developed by Chris Burk from Burk Techno-Economics with more resources at his site

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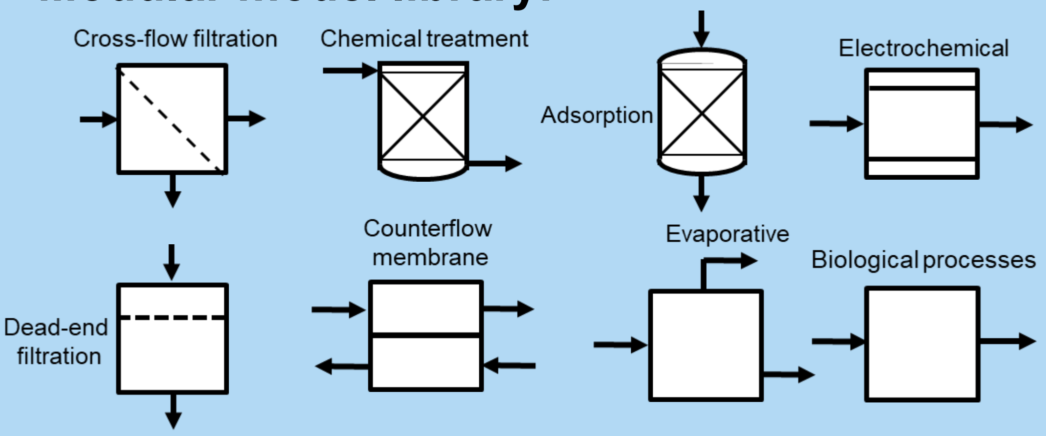
- Assumed process models can help set research goals and priorities
- But they lack insight into whether targets are realistic or how to reach them

WaterTAP provides a platform for improving the quality and decreasing the effort of TEAs

NAWI $15M+ of funding

Unified

Modular model library:



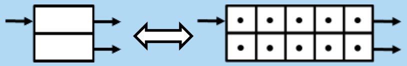
Flexible

Powerful

Core attributes:

- Open-source
- Multi-hierarchical
- Customizable
- Equation oriented
- IDAES compatible

python



$$f(x) = 0$$

PYOMO

IDAES
Institute for the Design of Advanced Energy Systems

Software release:

- Publicly accessible on GitHub
- Released every quarter

GitHub

```
pip install watertap
```

https://github.com/watertap-org/watertap

https://watertap.readthedocs.io/en/latest/

Core capabilities:

- Simulation to evaluate new device integration
- Optimization to explore complex systems
- Sensitivity analyses to consider uncertainty
- Parameter estimation to fit real-world data
- Data-driven models for complex phenomena

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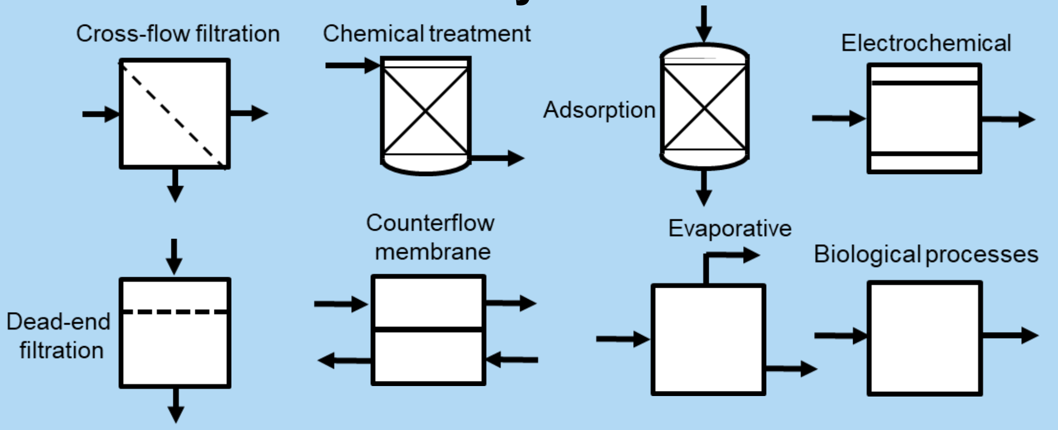

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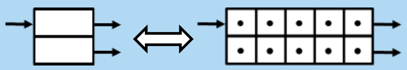

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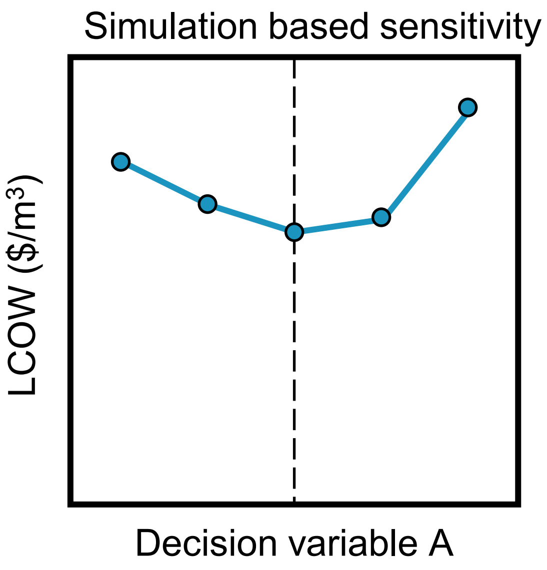
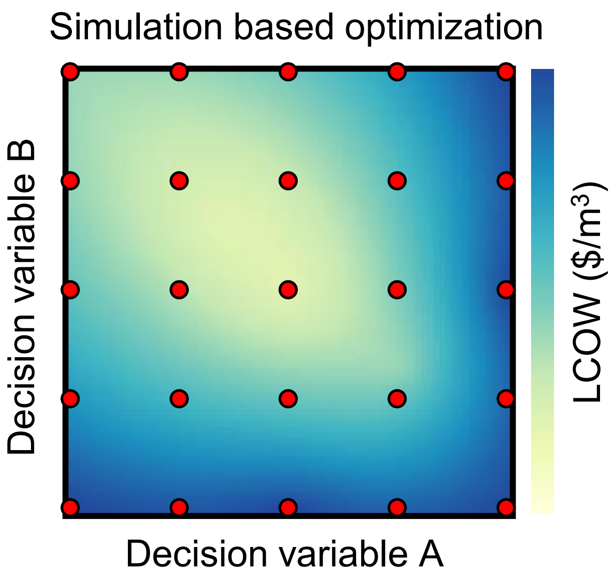
WaterTAP was developed to provide a centralized platform that makes TEAs more transparent, reproducible, comparable, and extendable

Horizon Modeling Solutions

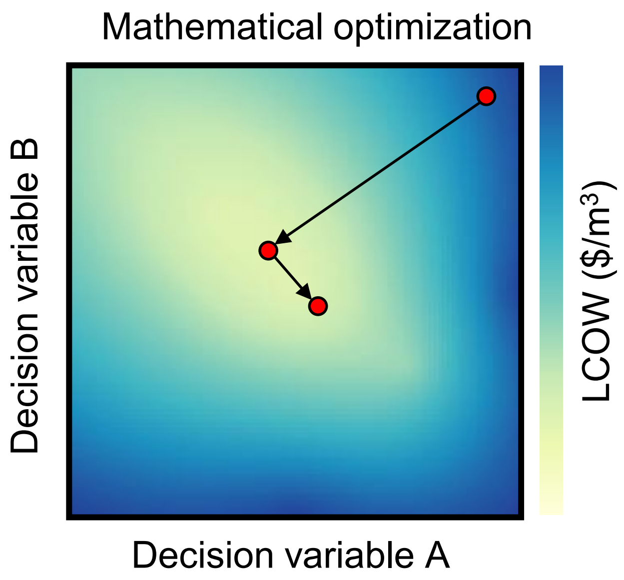
Mathematical optimization greatly expands TEAs

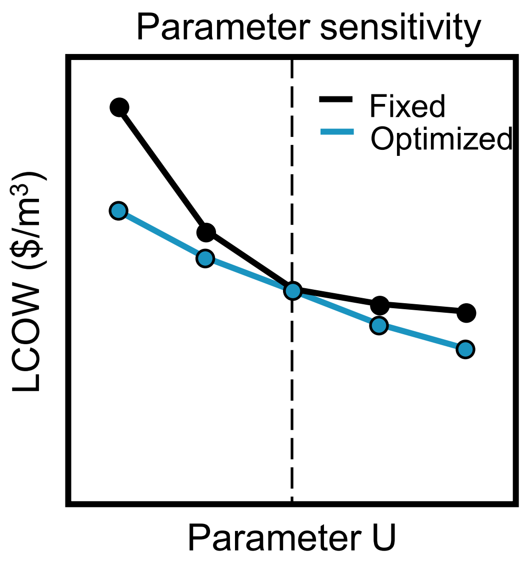
Simulation based modeling focuses on **decision variables**





Optimization based modeling focuses on **parameters** (model assumptions)





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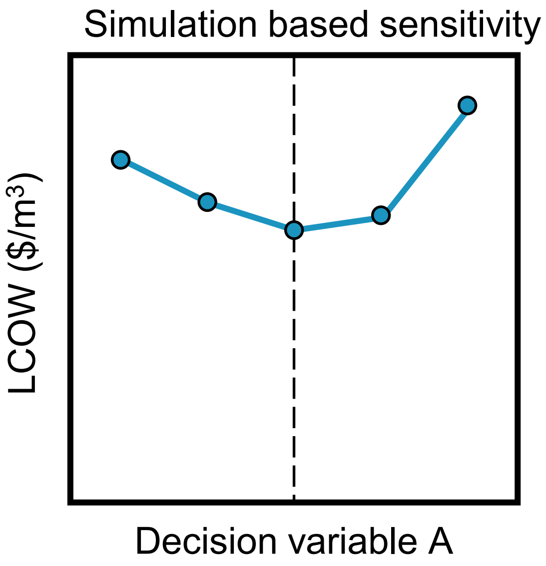

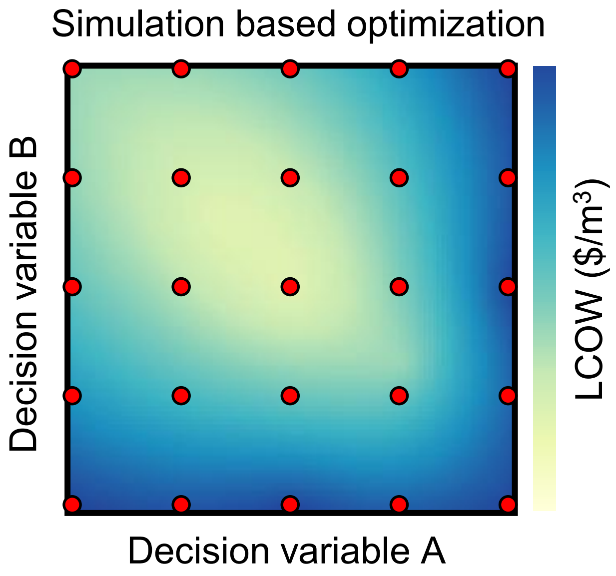

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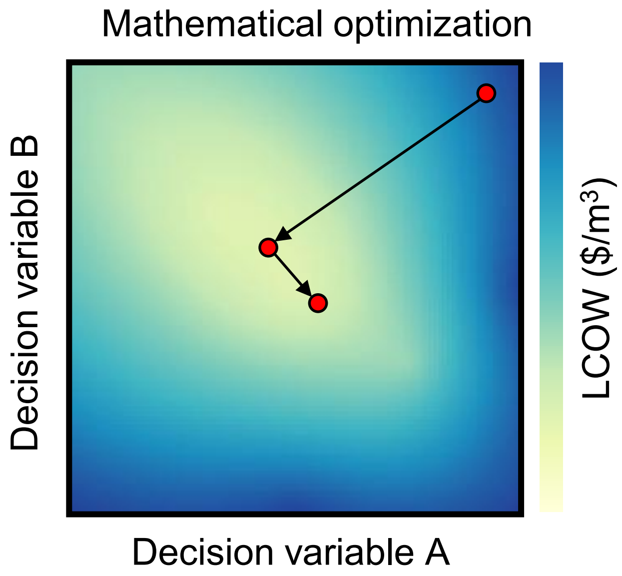
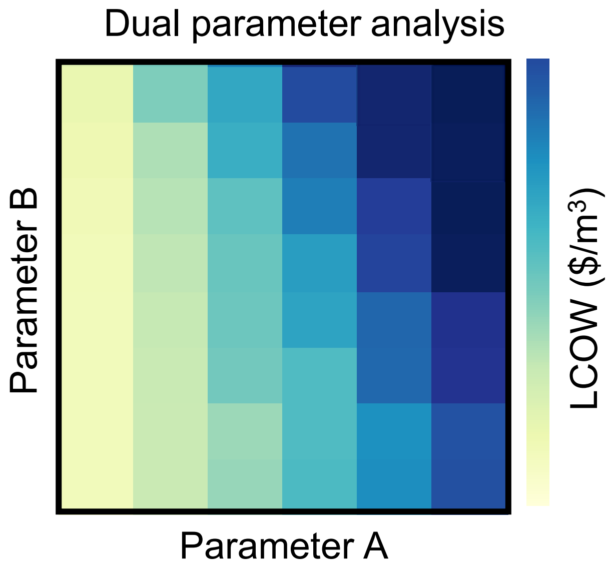
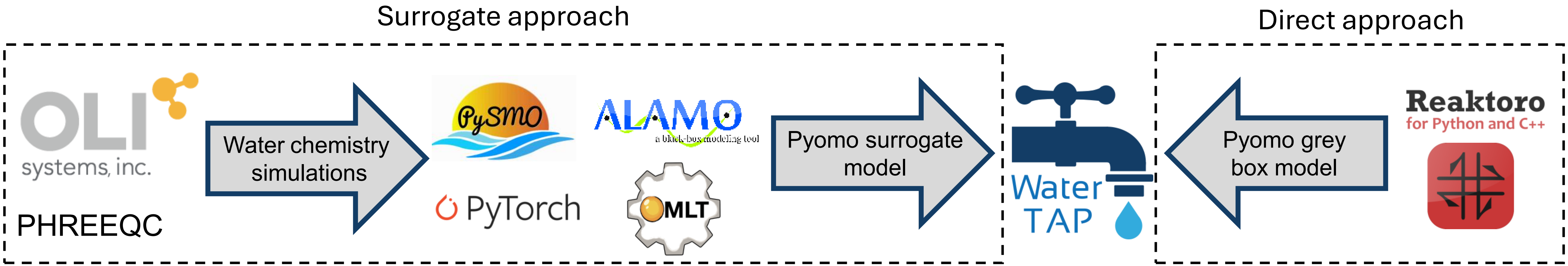




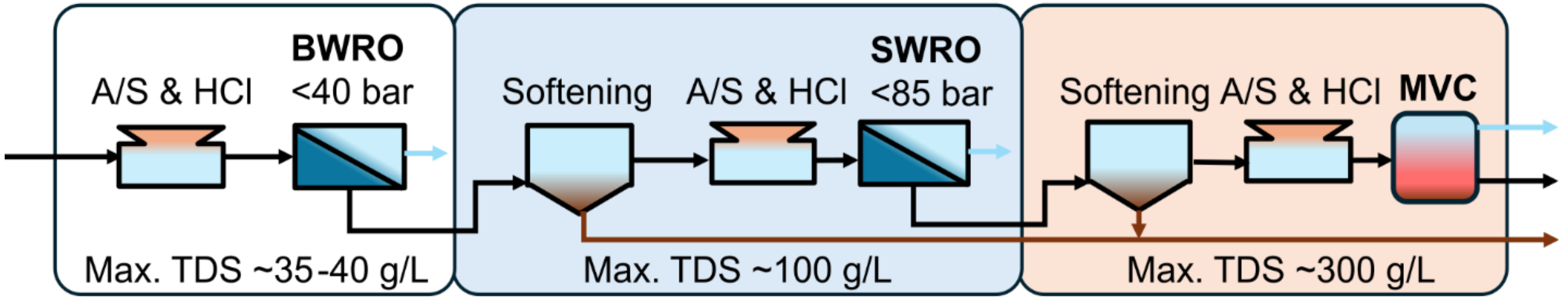
Detailed water chemistry is supported on WaterTAP

- Modeling complex water chemistry is challenging and data intensive
  - Numerous reactions and interactions across aqueous, vapor, and solid species
  - Dependent on concentrations of all species (even very small values)
  - pH, temperature, pressure can all be significant
- Electrolyte theoretical models can be built on the platform (e.g., eNRTL, MSE, Pitzer)
  - Data availability limits the species than can be considered
  - WaterTAP does not currently support a database for these models
- WaterTAP leverages external water chemistry software



Evaluating the potential of a conceptual process

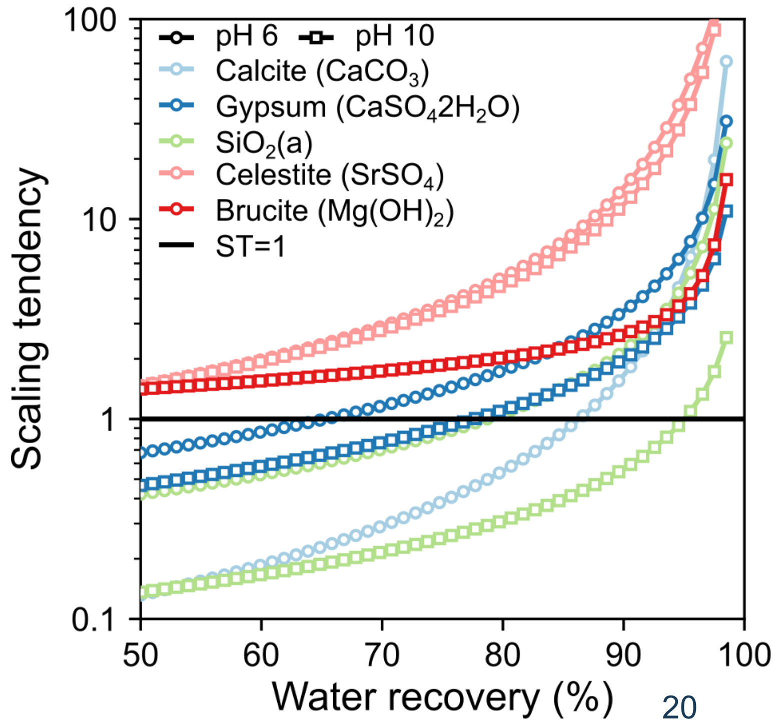
Objective: Model a novel high recovery system using conventional technologies



Description:

- 2 membrane and 1 evaporative process
- Constrained by mineral scaling
- Antiscalants, pH control, and softening for interstage percipitation

Ion	Conc. (mg/L)
Na	739
Cl	870
K	9
Ca	258
Mg	90
SO4	1011
HCO3	385
Sr	3
SiO2	25
TDS	3397



Approach

- Mechanistic model for desalination processes
- ML model for water chemistry from PHREEQC
- Hypothetical model for antiscalant efficacy

Horizon Modeling Solutions

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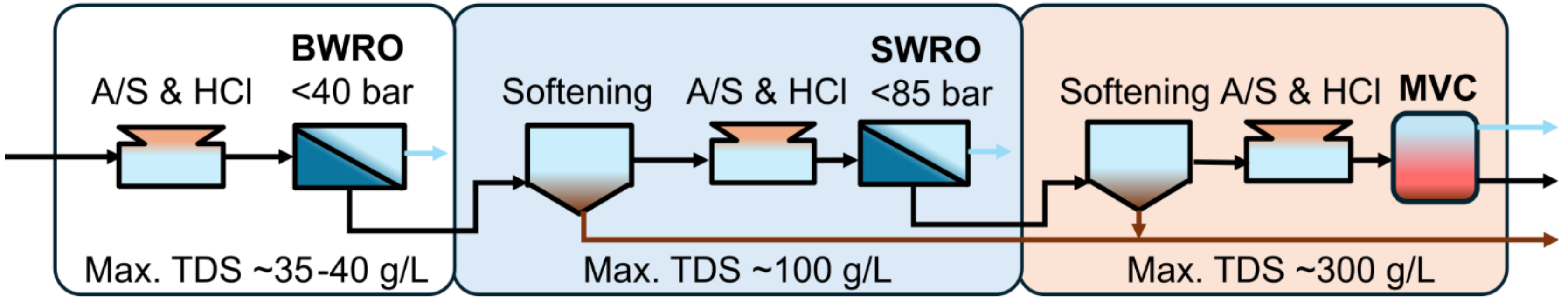
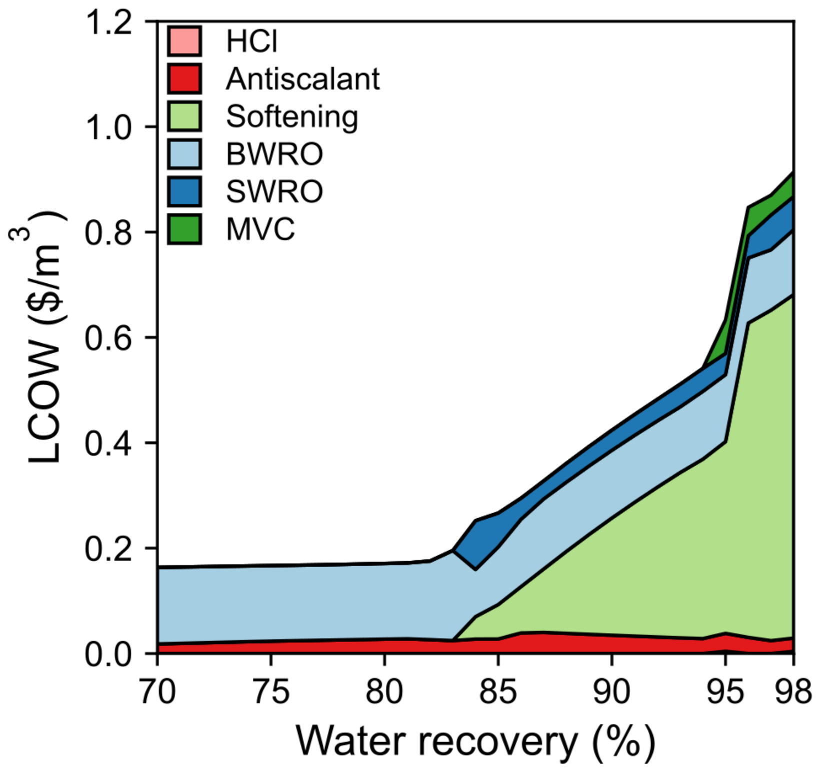


Surprising results:

- Costs are below \$1/m^3
- Recoveries up to 98% recovery

Other results:

- Mineral scaling dictates extent of recovery in each stage
- Higher salinity desalination technologies contribute a small amount to the cost
- Softening cost becomes dominant



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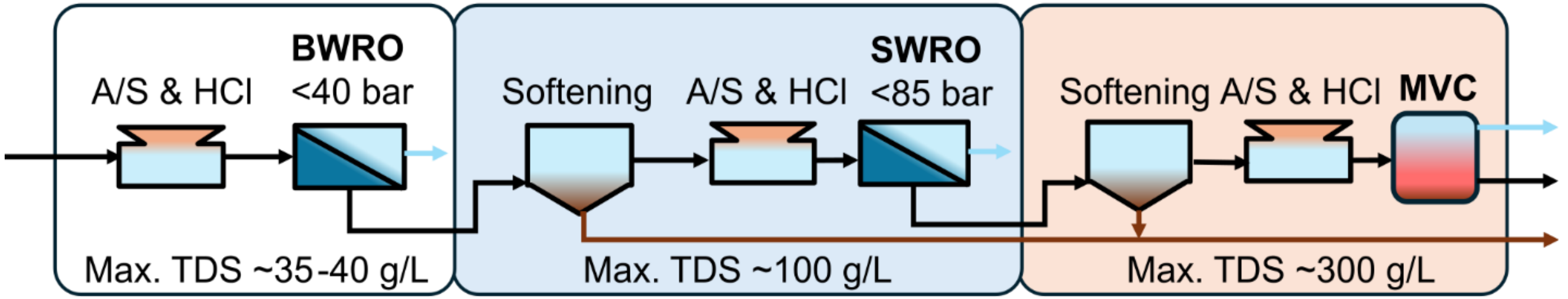

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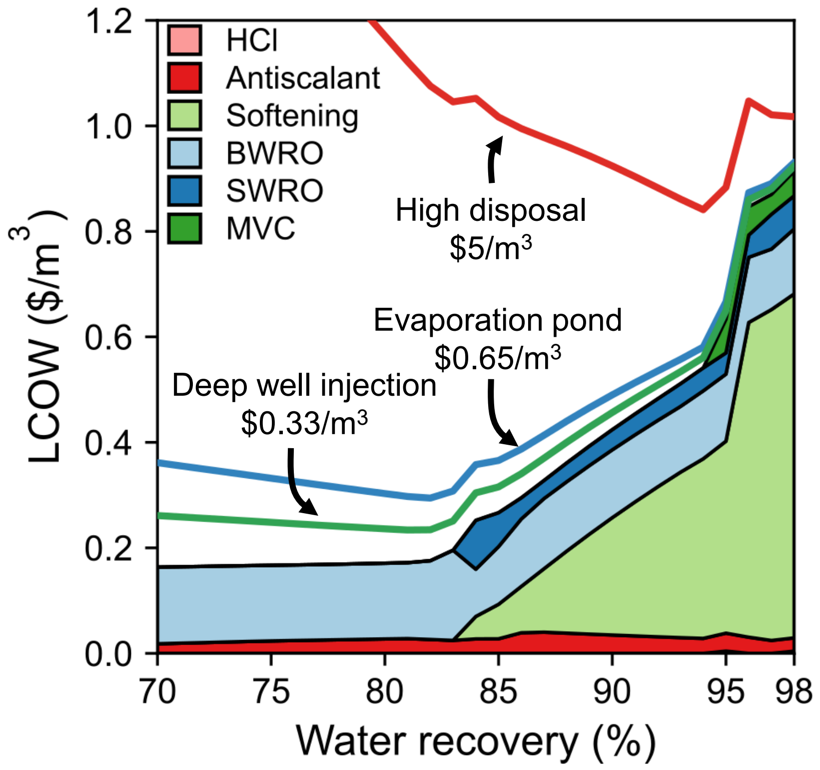
- Disposal does not raise overall cost significantly, typical disposal costs -> BWRO
  high disposal costs -> BWRO and SWRO



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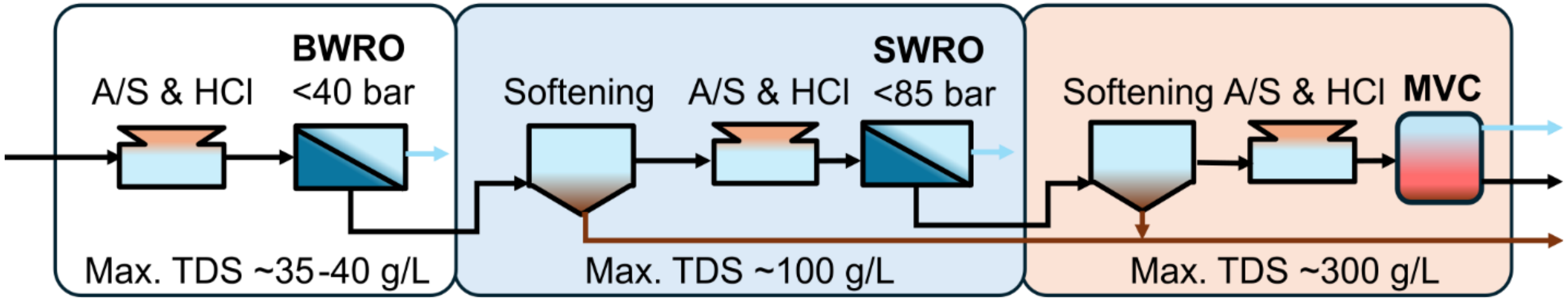

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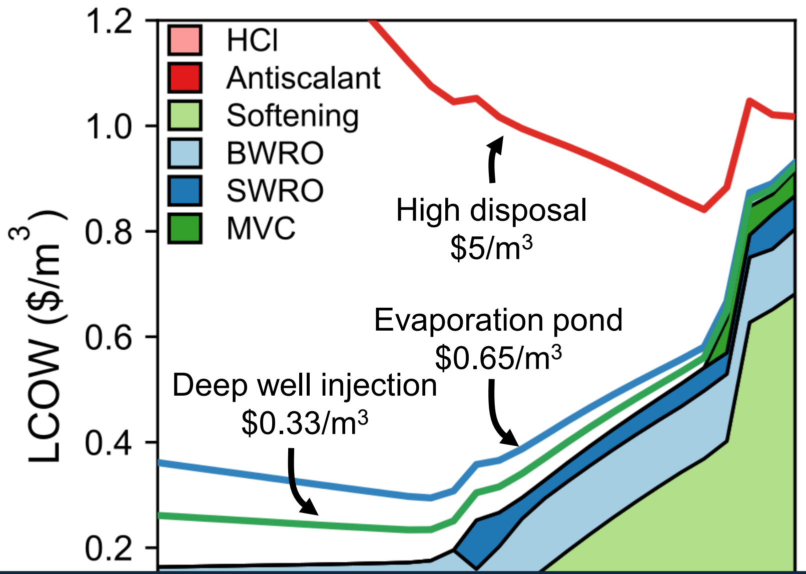

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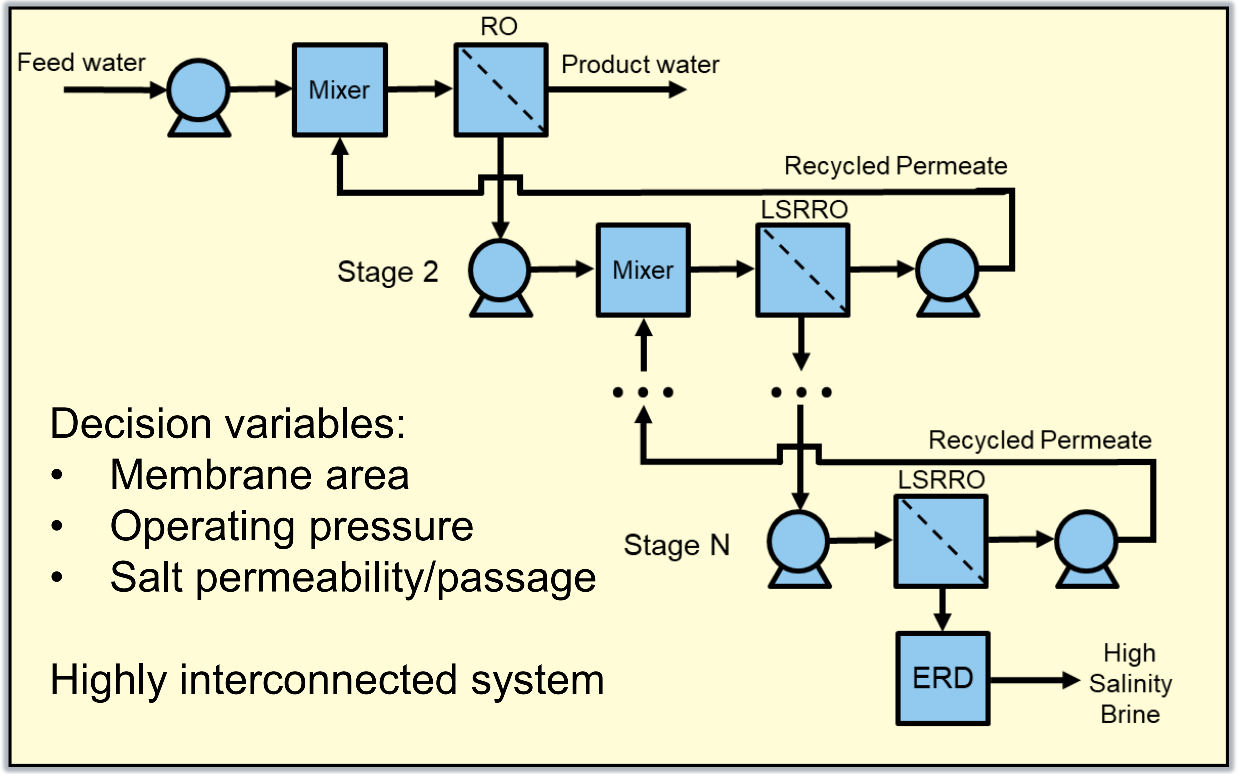
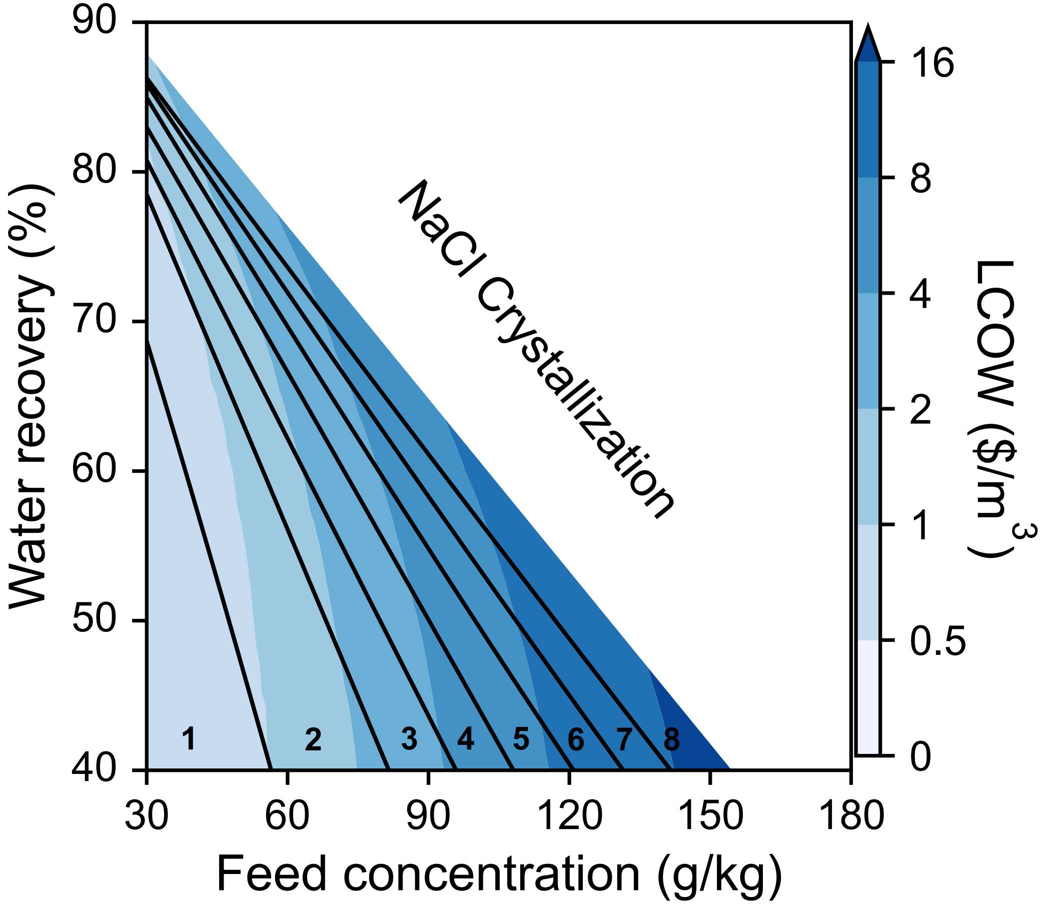
- Antiscalants, acid addition, and softening can likely achieve high recoveries
- Improvements in high concentration desal technologies has limited value

Horizon Modeling Solutions

Exploring the potential of a novel membrane process

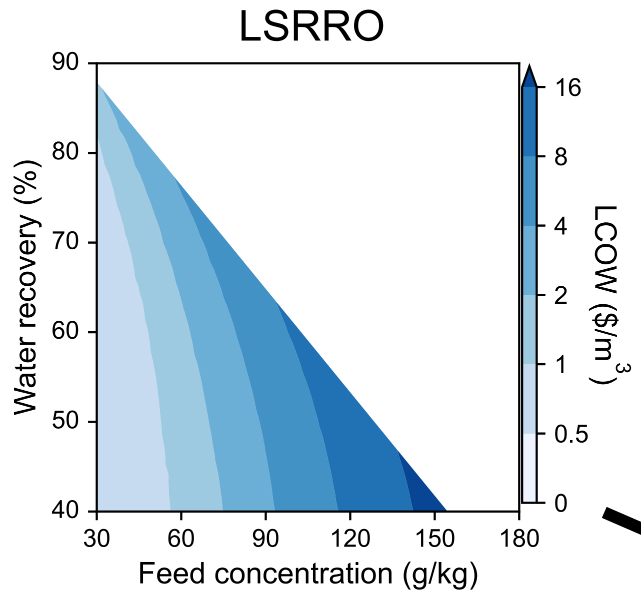
Low salt rejection reverse osmosis (LSRRO)

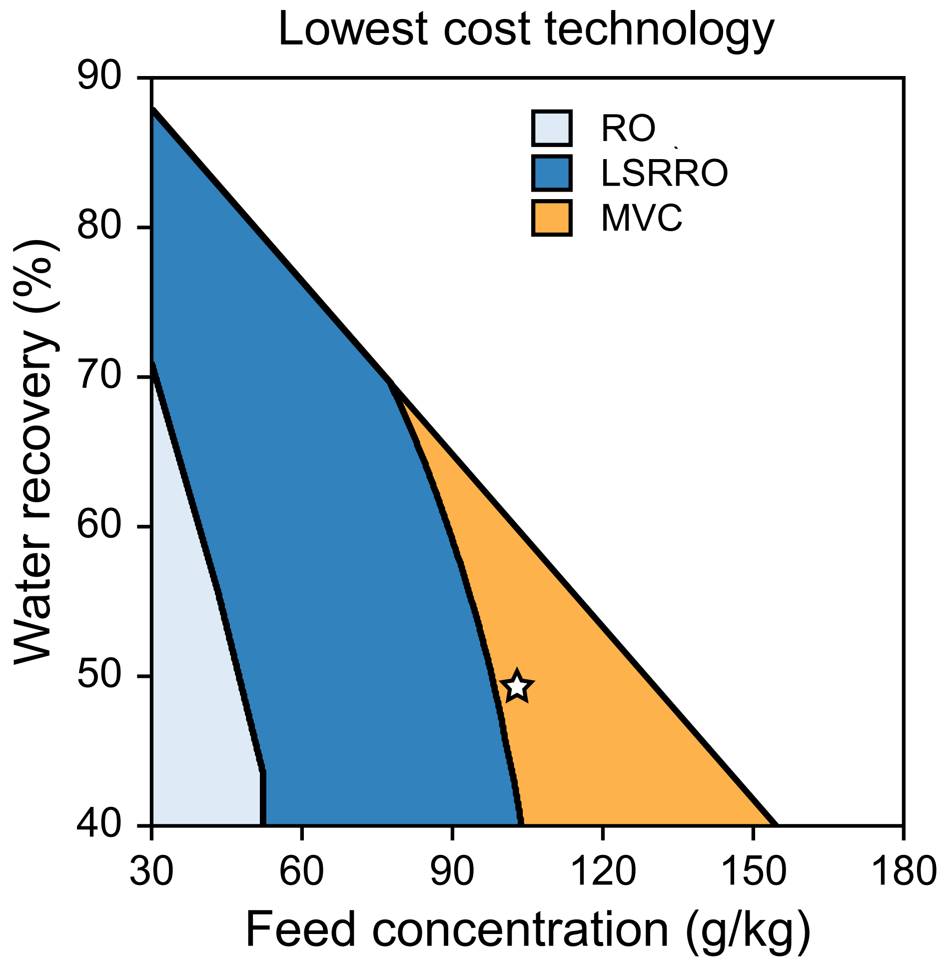


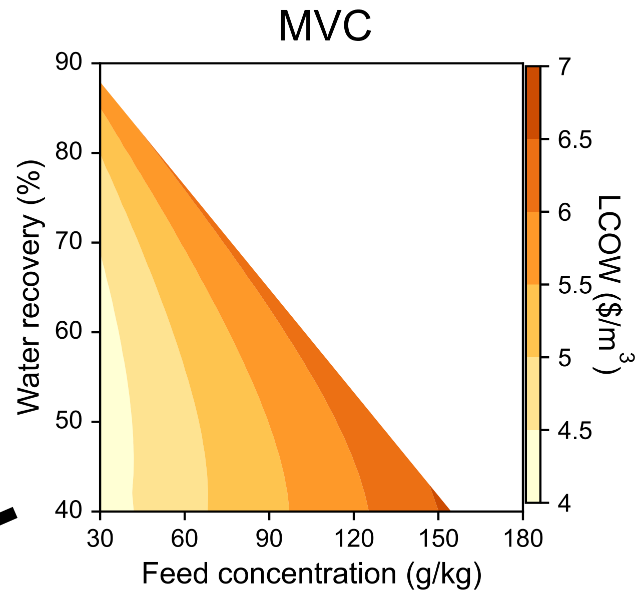


Quantifying technoeconomic viability through comparison

Case: 100 g/kg and 50% water recovery







Tucker et al. *Water Research.* 2024, 260, 121950

Using sensitivity analysis to prioritize development

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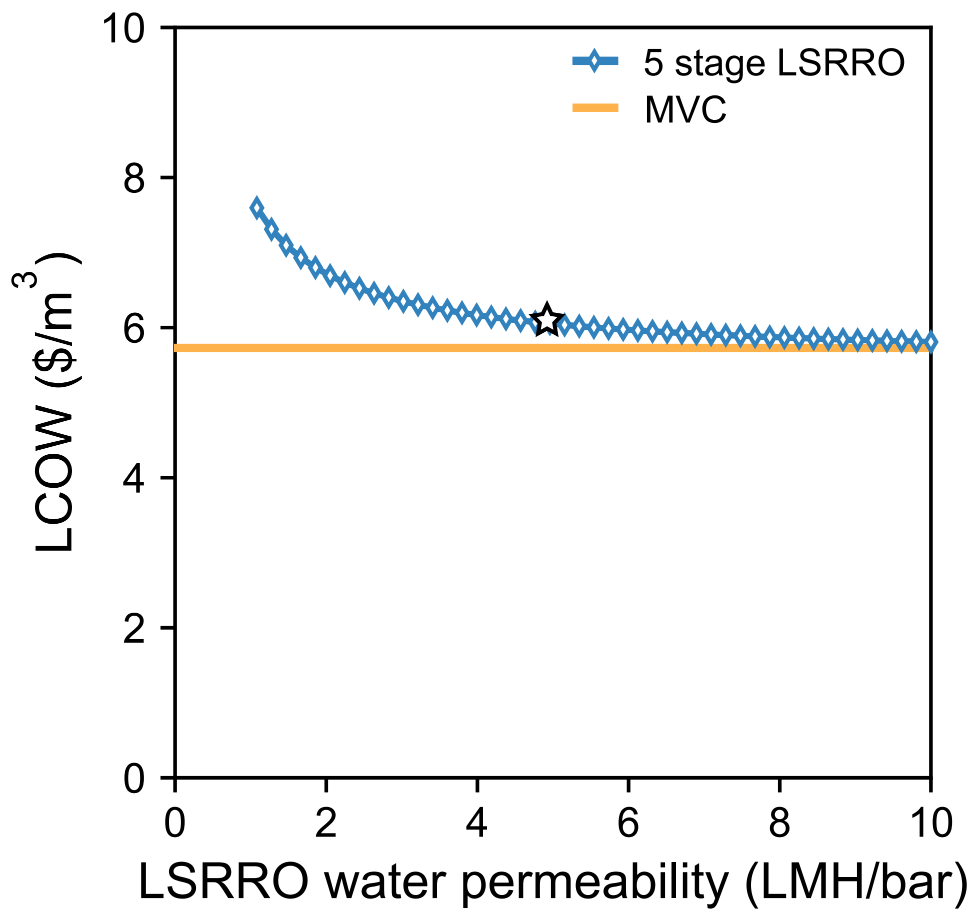

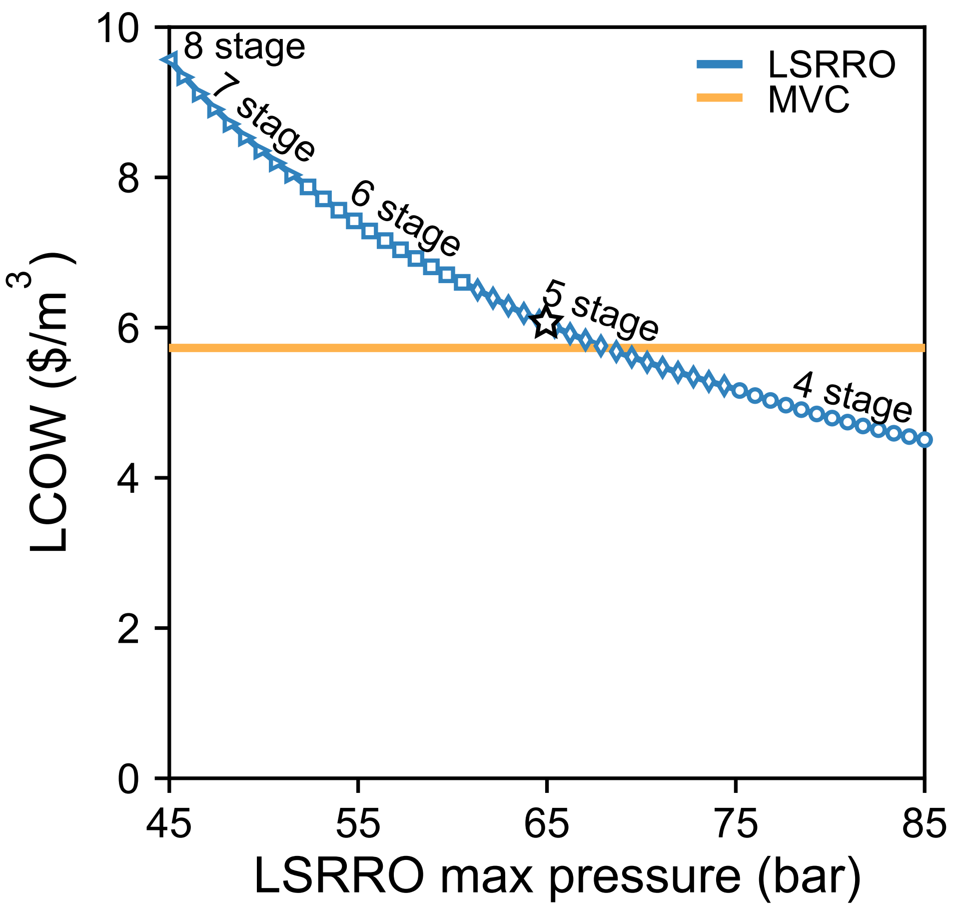

Horizon Modeling Solutions

Atia et al. *Desalination.* 2023, 551, 116407

Identifying impactful and viable research targets

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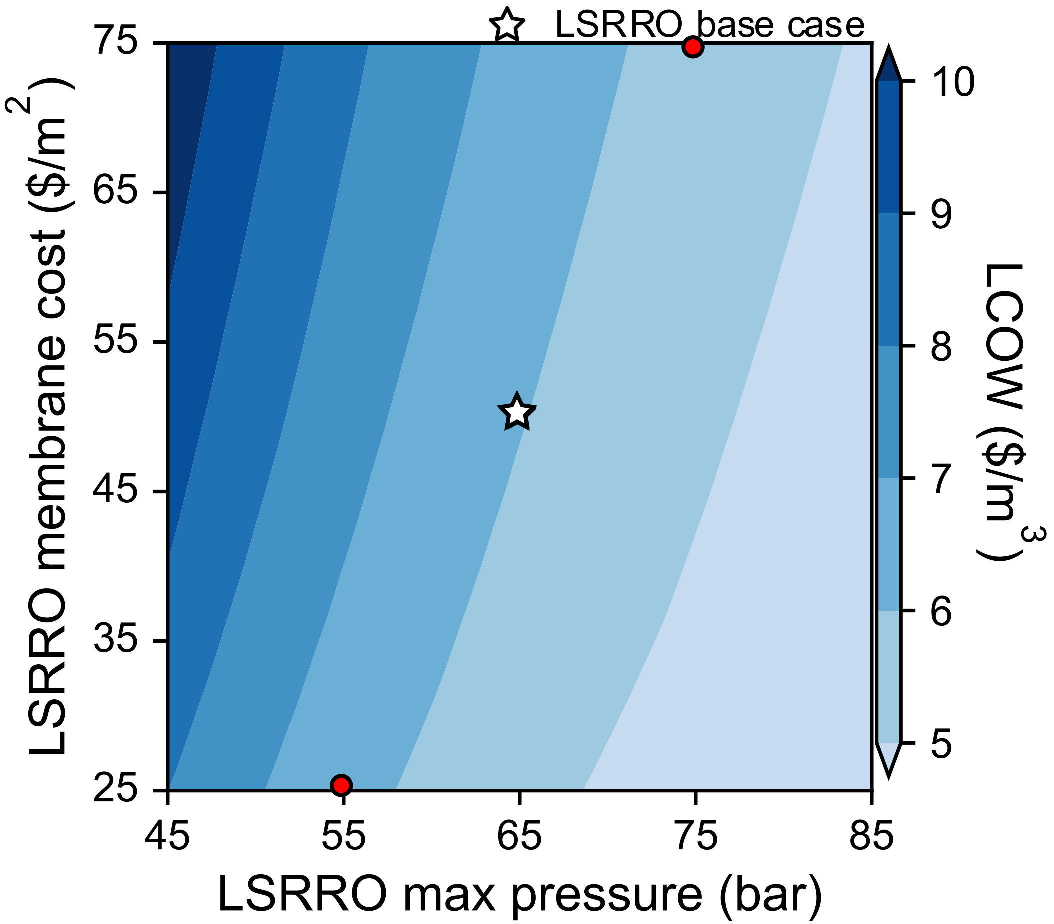

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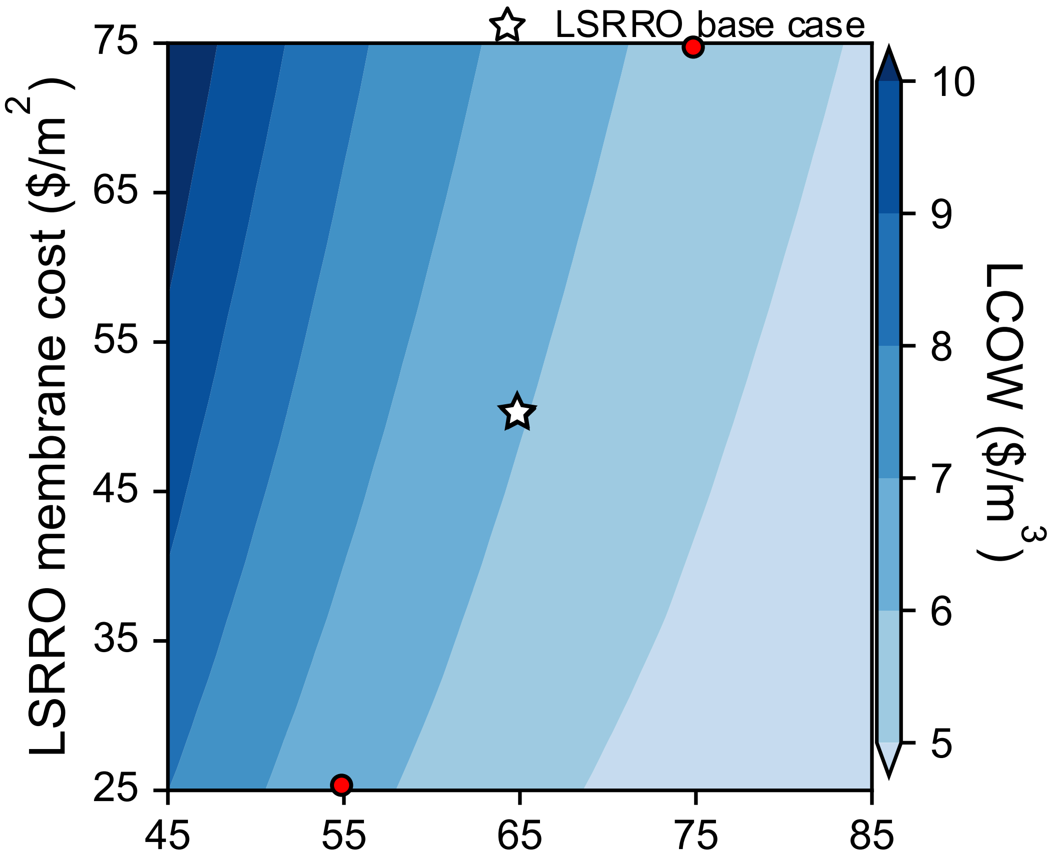
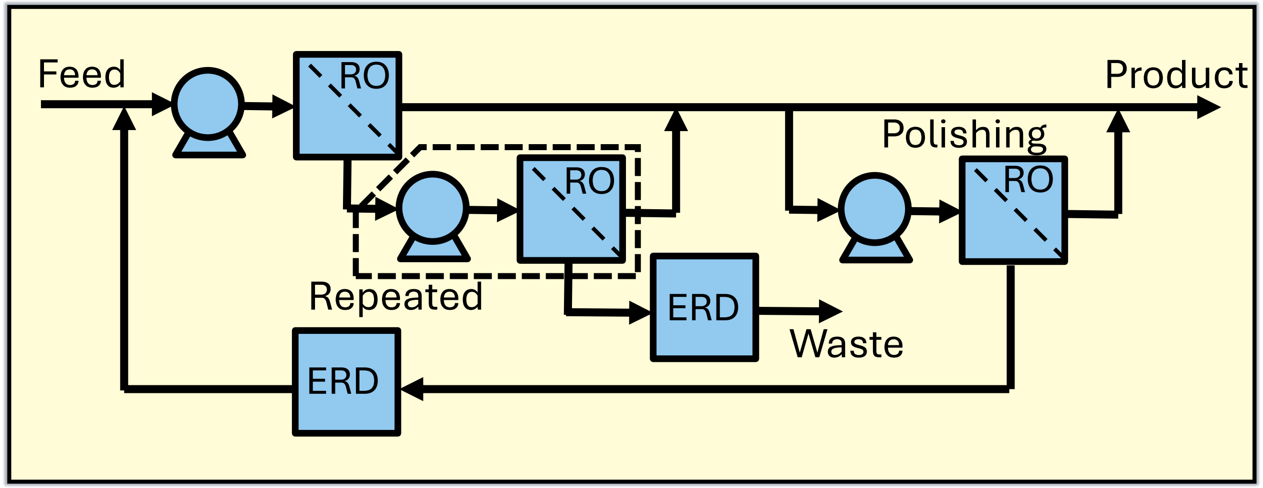


- LSRRO is a promising technology for feed salinities between 35-150 g/L TDS
- R&D should focus on increasing the maximum allowable pressure
- Mathematical optimization expands the analysis for the whole application space

Horizon Modeling Solutions

Projecting the implications of bench-scale data

High pressure reverse osmosis (HPRO)



Prof. Eric Hoek

Two known challenges:

- Membrane compaction at high pressures decreases water permeability and increases salt permeability
- Equipment that operates at higher pressures are more expensive

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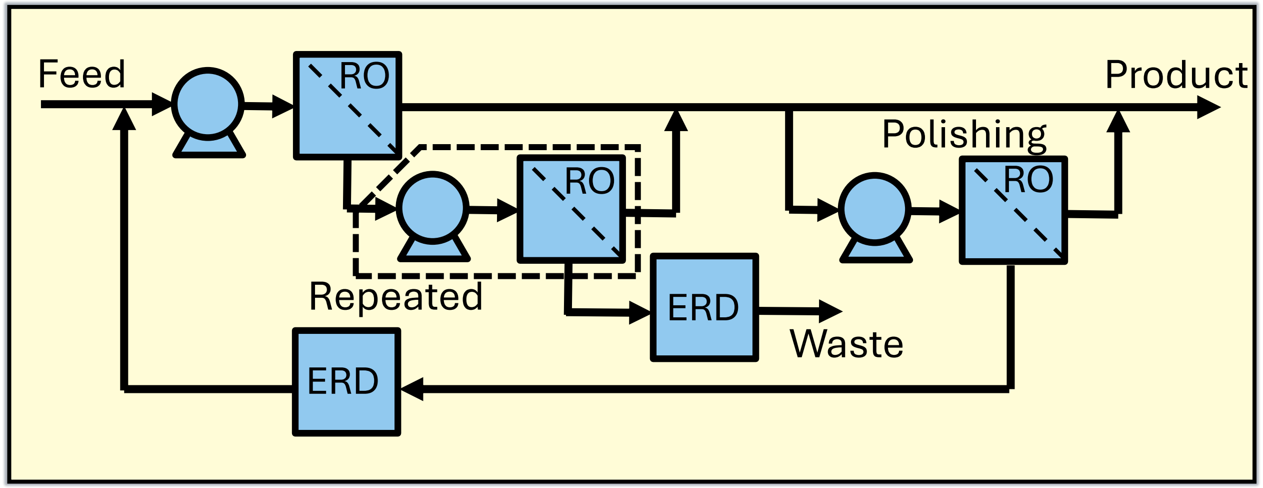

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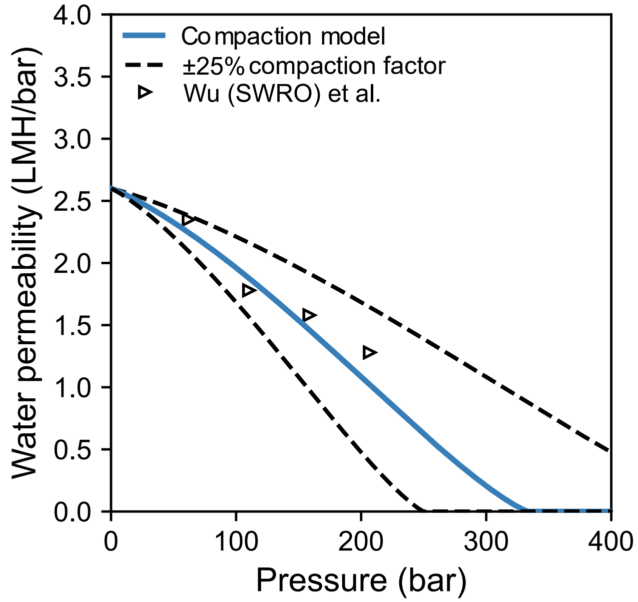

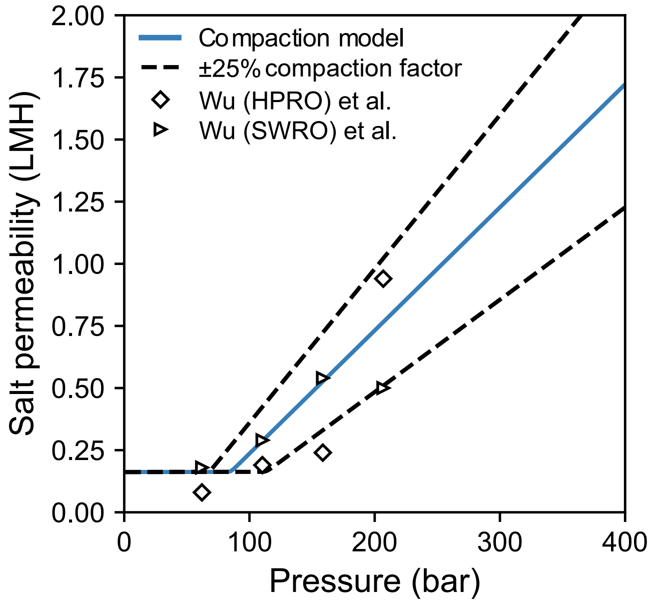

Wu et al. *Desalination.* 2022, 537, 115875

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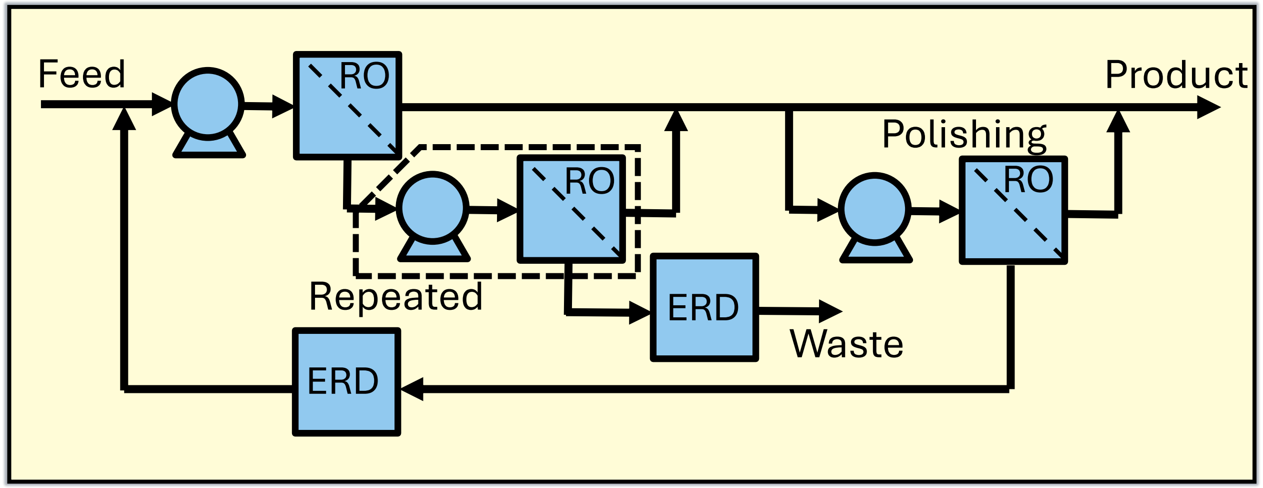

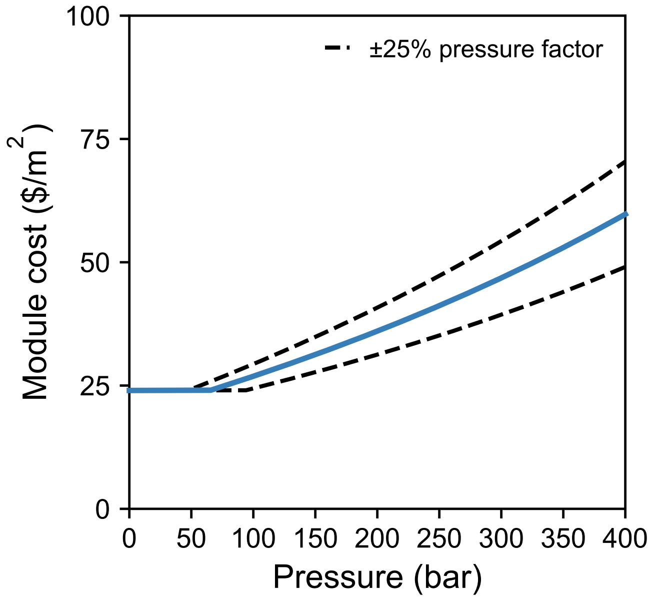

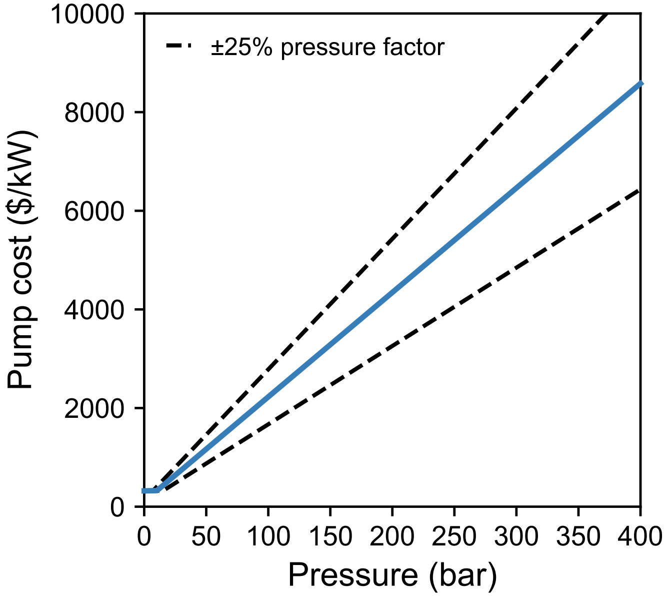

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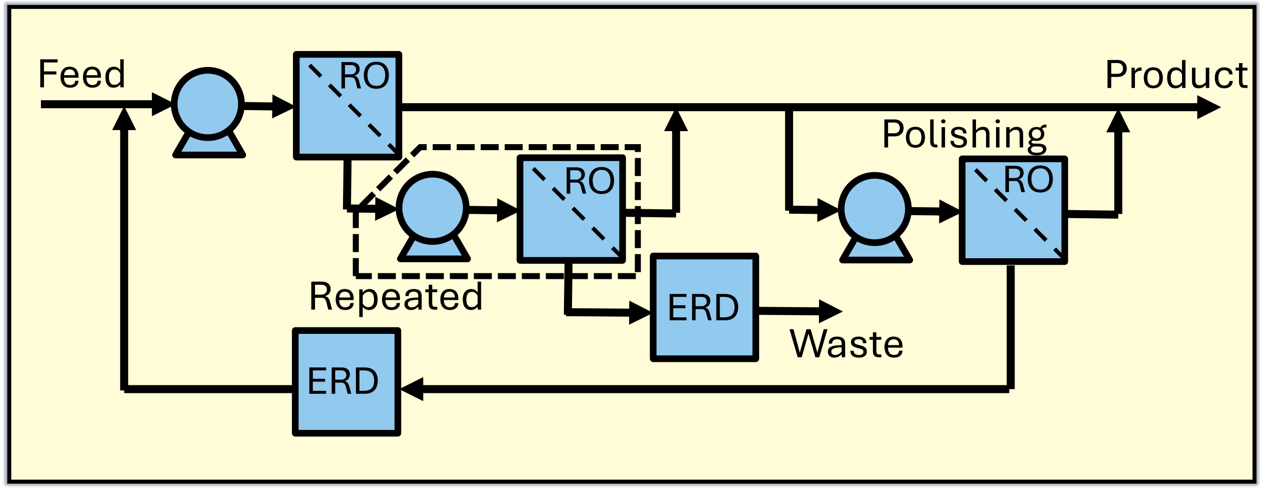
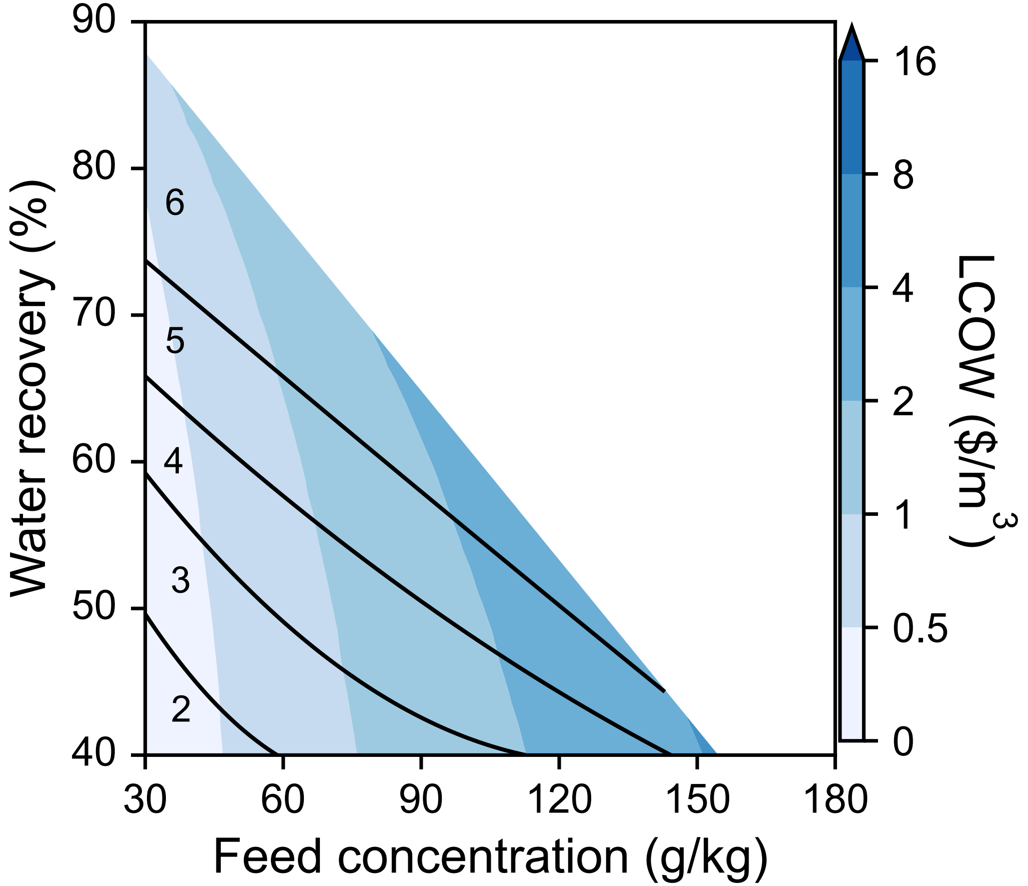


Two known challenges:

- Membrane compaction at high pressures decreases water permeability and increases salt permeability
- Equipment that operates at higher pressures are more expensive



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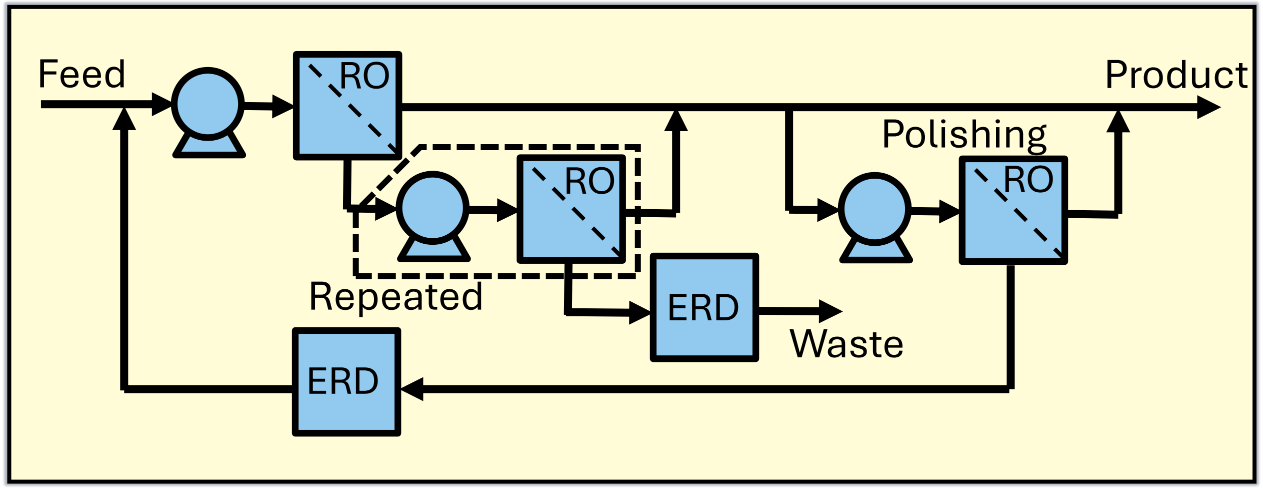
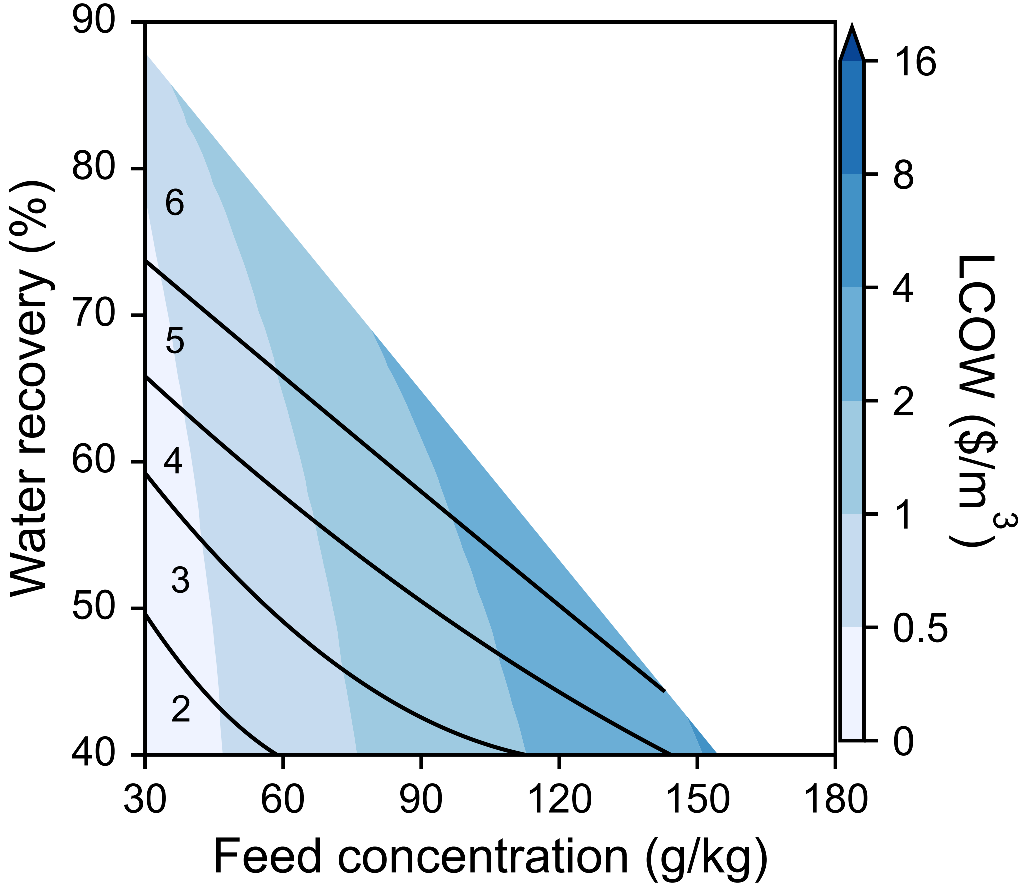




Two known challenges:

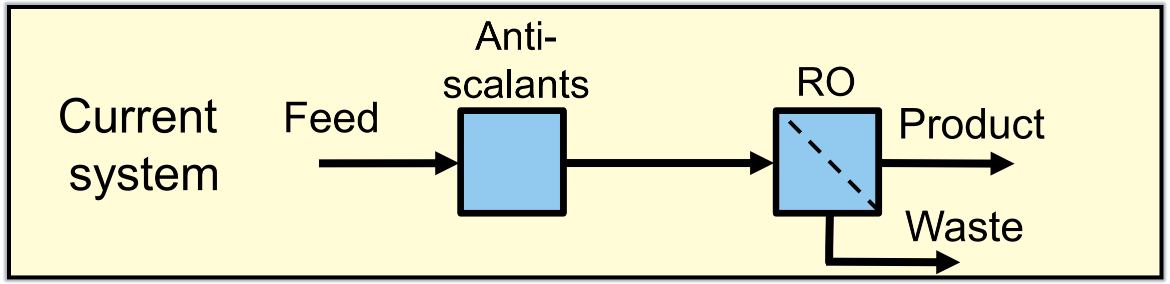
- Membrane compaction at high pressures decreases water permeability and increases salt permeability
- Equipment that operates at higher pressures are more expensive

- HPRO is promising despite membrane compaction and higher component costs
- Modular models enable rapid assembly of different systems (LSRRO and HPRO)

Horizon Modeling Solutions

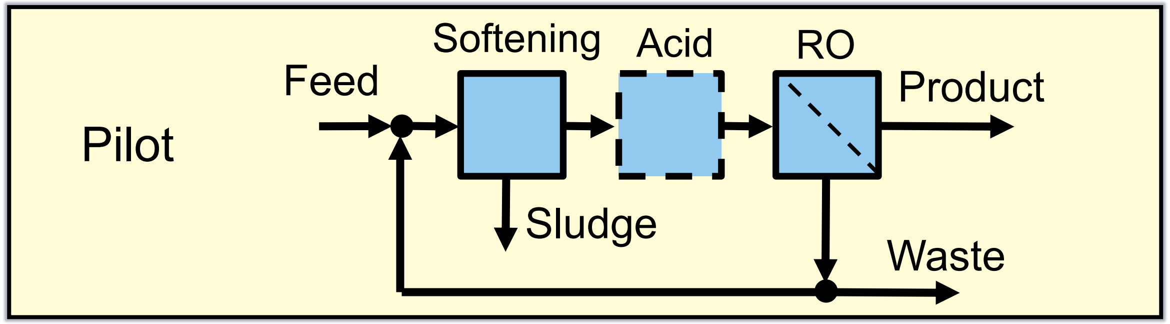
Assisting pilot design and operation

Distributed brackish water desalination in Kenya (off grid and driven by solar power)



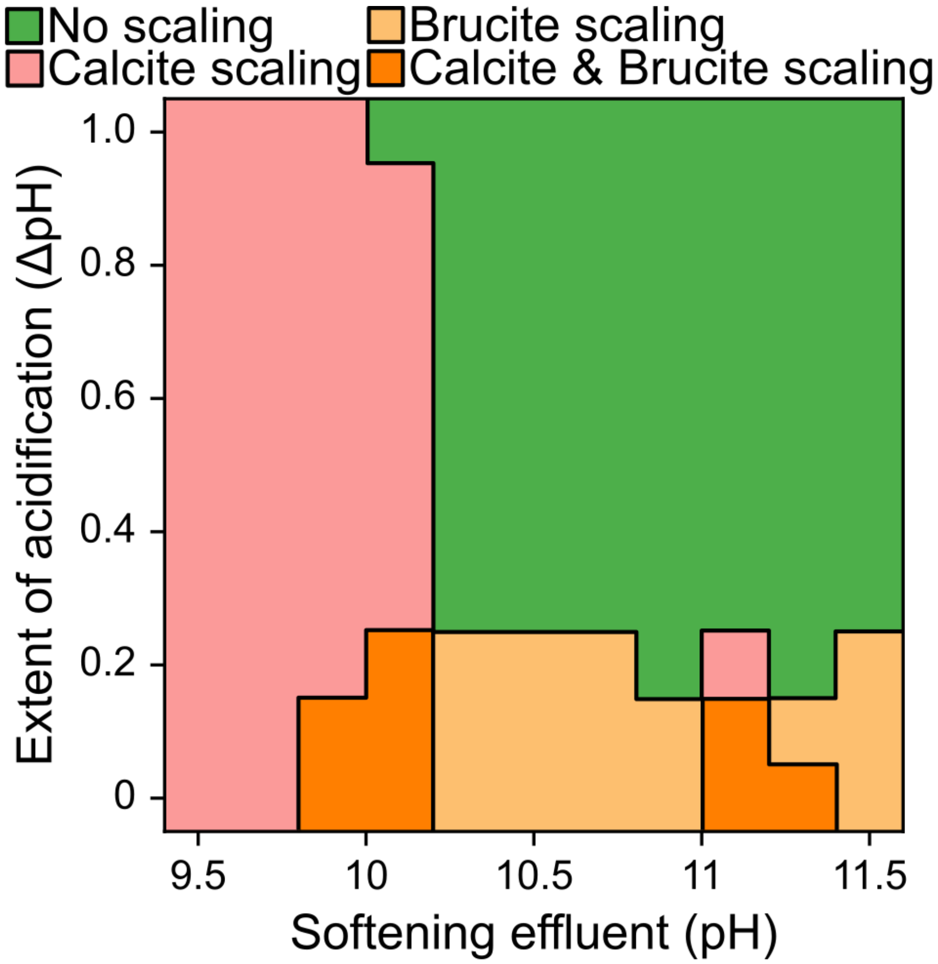
Pilot seeks to address two issues:

- Mineral scaling even with significant antiscalant dosing (at a high cost)
- High disposal volumes with only 50% water recovery



TEXAS
The University of Texas at Austin

Prof. Manish Kumar



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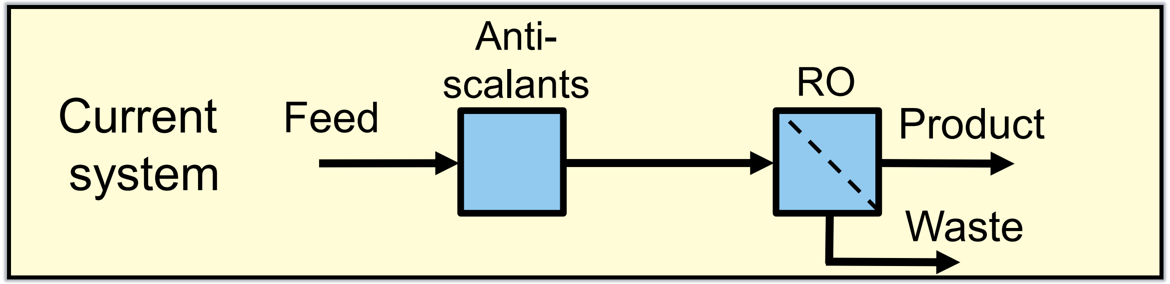

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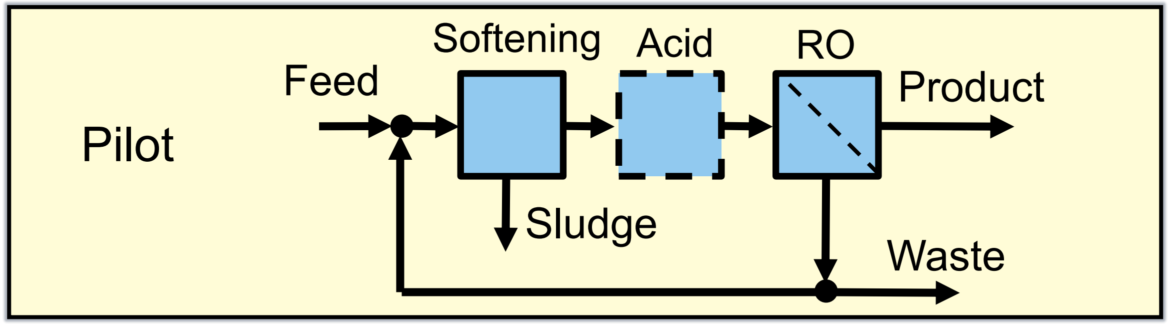


Before

After

Benefits:

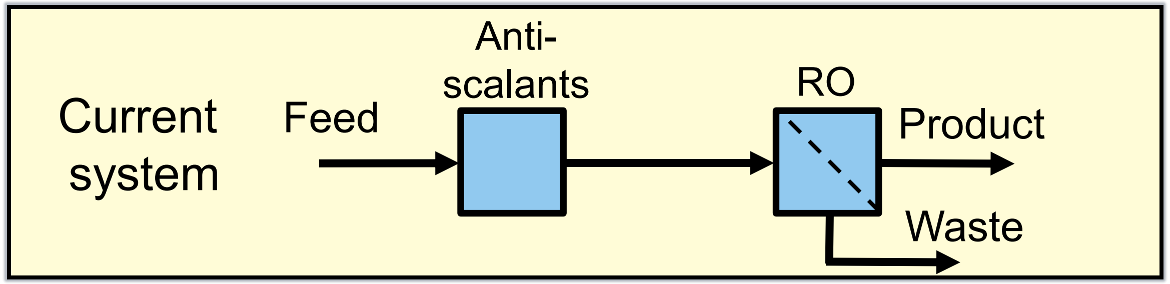
- Reduce brine production by 67.5%
- No use of antiscalants

Cons:

- Lime softening and waste sludge generation

Assisting pilot design and operation

Distributed brackish water desalination in Kenya (off grid and driven by solar power)



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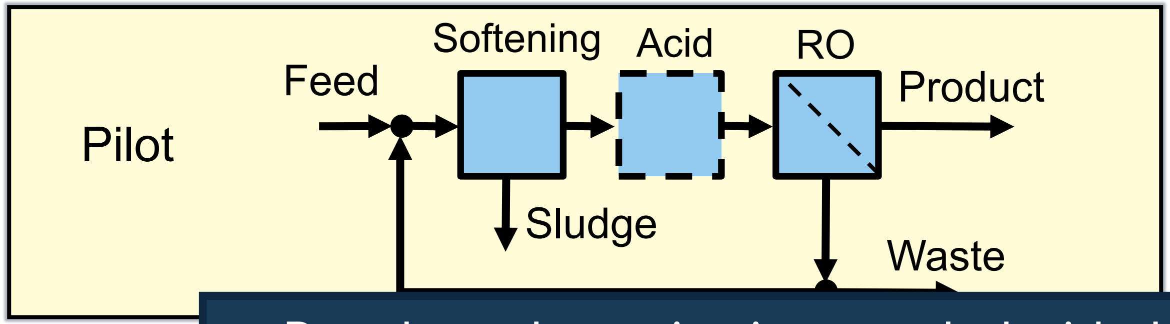

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ion

- Bench-scale testing is extended with detailed process-scale modeling
- Analysis identified a risk for pilot failure and suggested the fix

Evaluating a potential commercial-scale retrofit

Large groundwater desalination plant

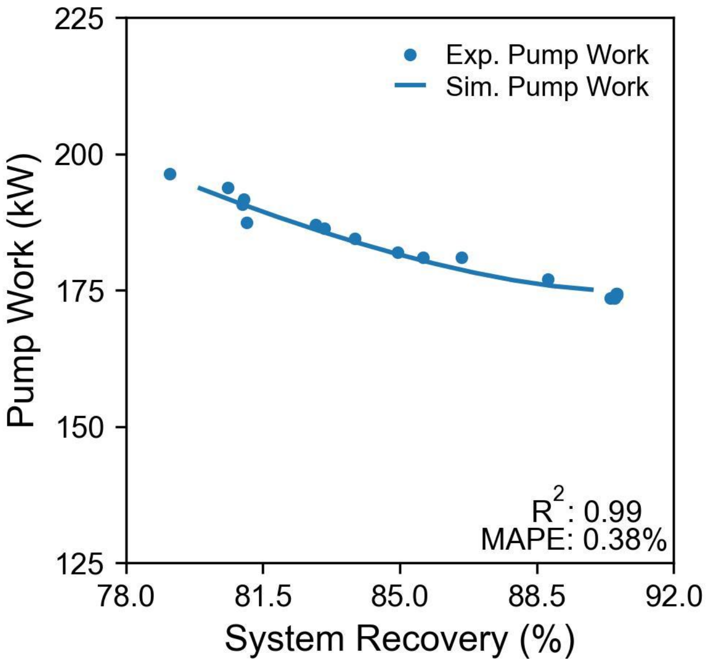
Analysis seeks to evaluate a potential retrofit:

- Reduce disposal costs by increasing recovery
- Potentially add third stage RO with feed flow reversal to mitigate mineral scaling

CalPolyPomona

Chino Basin Desalter

Prof. Mingheng Li



Evaluating a potential commercial-scale retrofit

Large groundwater desalination plant

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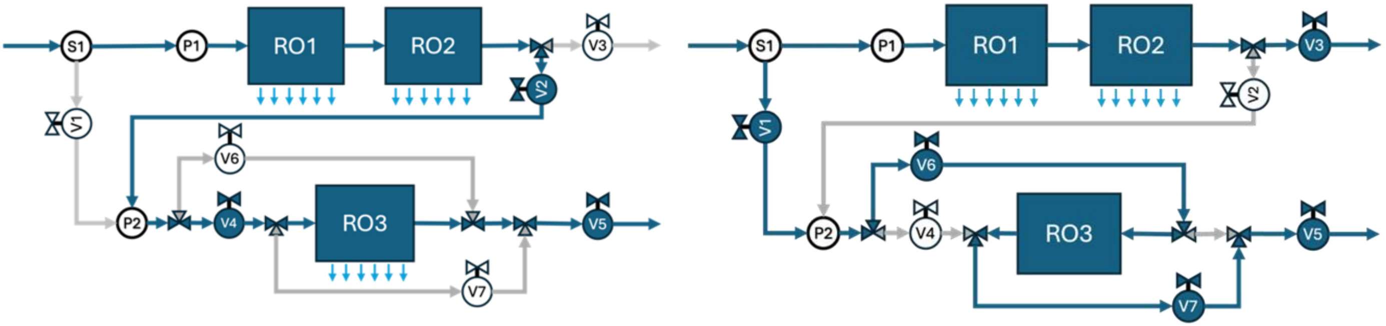
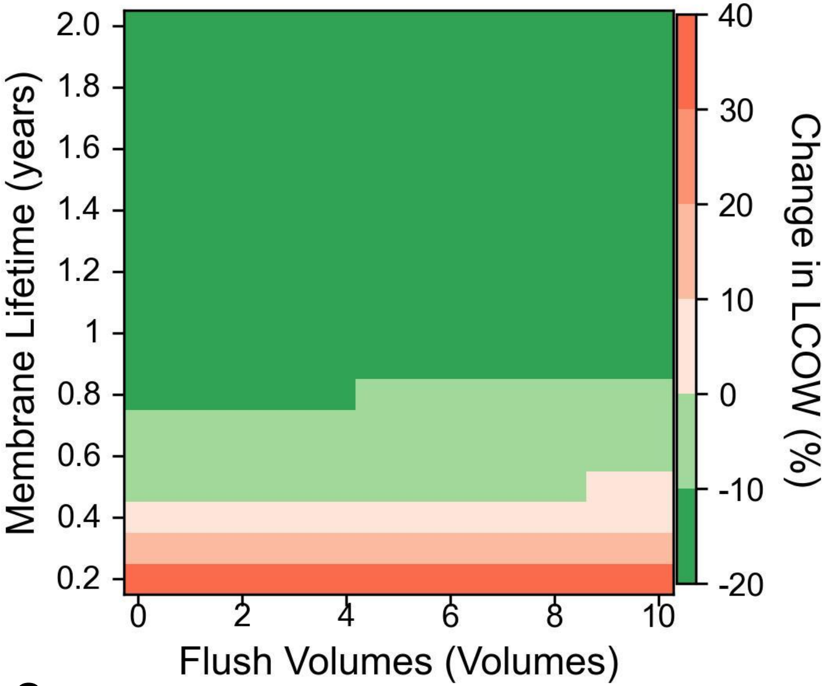
Normal operation (RO3 switch's flow direction)

Flushing of RO3 during flow switch, wastes part of feed





What impact does membrane life and flush volumes have on viability?

Horizon Modeling Solutions

Evaluating a potential commercial-scale retrofit

Large groundwater desalination plant

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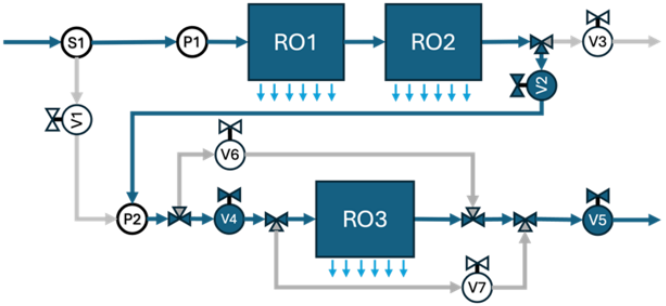

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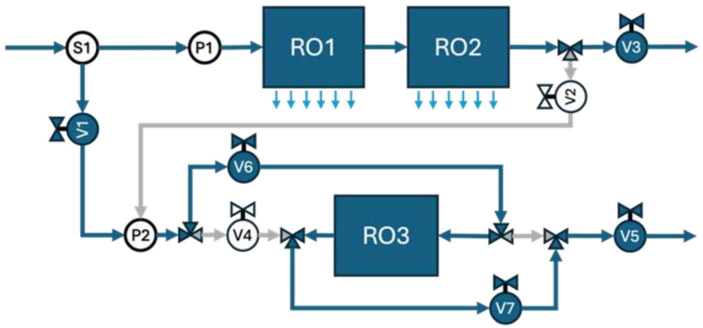
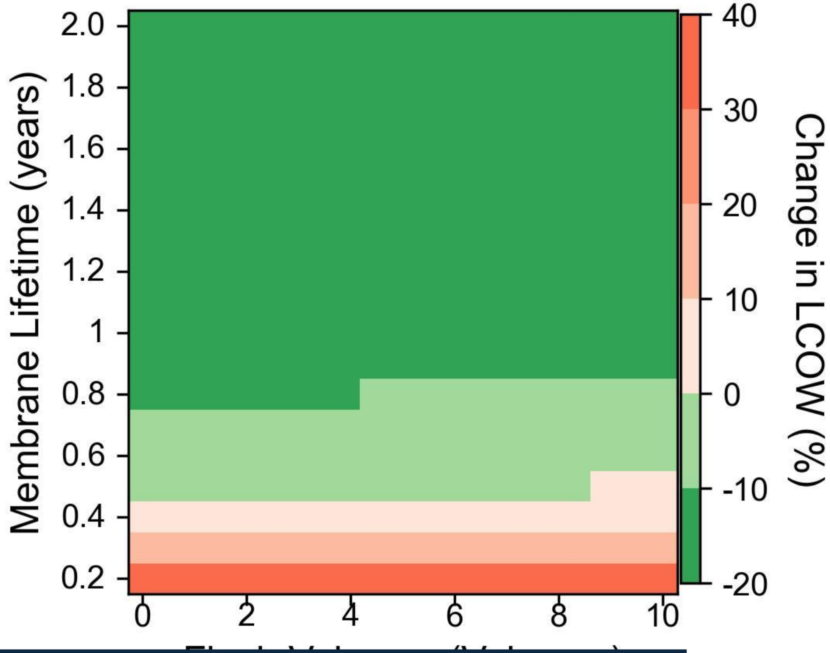




What impact

- Significant insight with varying two assumed performance parameters
- Suggests further investigation into membrane lifetime (not necessarily flushing)

Horizon Modeling Solutions

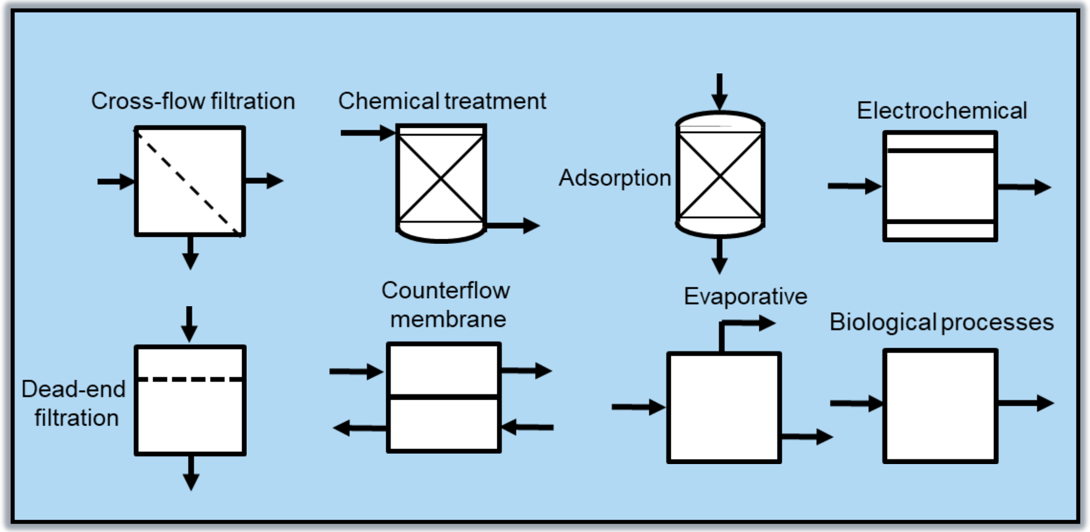
WaterTAP has a broad water treatment library

Membrane:
- Reverse osmosis
- Osmotically assisted reverse osmosis
- Nanofiltration
- Membrane distillation

Evaporative:
- Mechanical vapor compression
- Multi-effect distillation
- Crystallizer

Electrochemical:
- Electrodialysis
- Electrolyzer
- Electrocoagulation

Chemical:
- Stoichiometric and equilibrium reactors



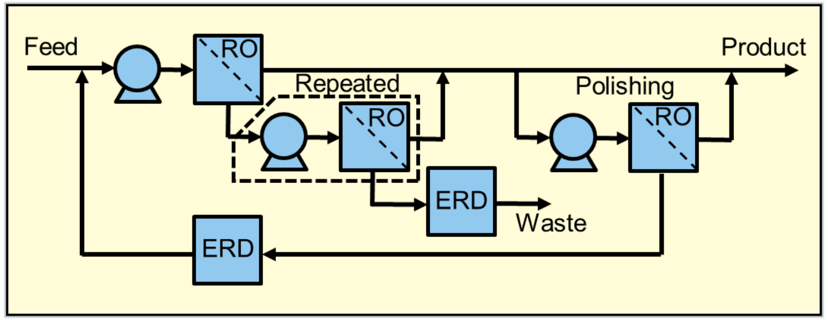
Ad/absorption:
- Ion exchange
- Granular activated carbon
- Solvent extraction

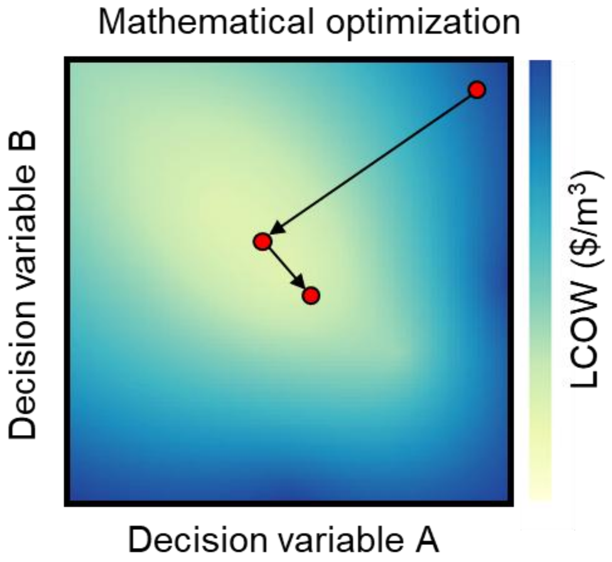
Biological:
- Activated sludge
- Anaerobic digestor

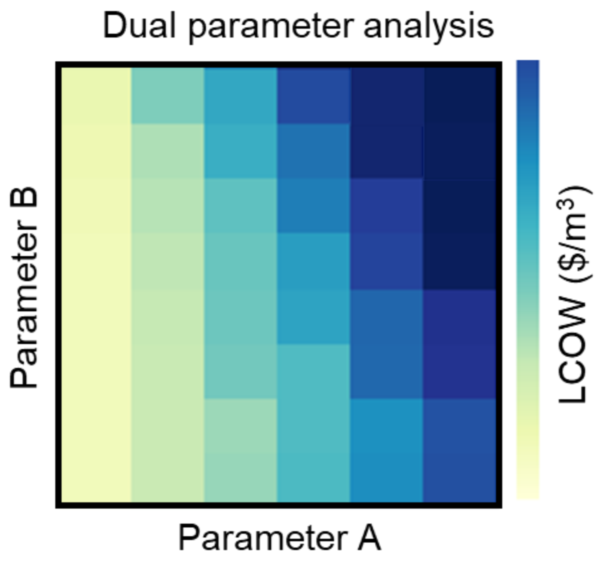
Auxiliary equipment:
- pumps, heat exchangers, mixers, splitters

Process scale modeling provides value in TEAs

- Use process and cost models that:
  - Link key design and operating variables to the performance and cost
  - Represent the system, not just the technology
- Use mathematical optimization to handle the design and operating variables
- Consider uncertainty through deterministic and stochastic sensitivity analyses
- Incorporate real world data through:
  - Parameter estimation with mechanistic models
  - Hybrid models with data-driven surrogate models







TEA provides quantitative decision support for R&D

Predictive process modeling with optimization transforms TEAs:

- Evaluate full application space and identify most promising ones
- Determine best design and operation for a model and specified parameters
- Focus analysis on modeling assumptions and parameters, not decision variables
- Pinpoint technical and financial bottlenecks and determine priority for development
- If model predictions are shown to be inaccurate, they can be updated with implications assessed quickly

Process systems engineering and TEA can support bench and piloting efforts:

- Plan – support system design and experimental campaign to achieve objectives
- Operate – fault detection and attribution, suggest modifications
- Evaluate – project the implications of the data for commercial scale deployment

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Questions?