NAWI National Alliance for Water Innovation

# WaterTAP Overview

## Water treatment Technoeconomic Assessment Platform (WaterTAP)

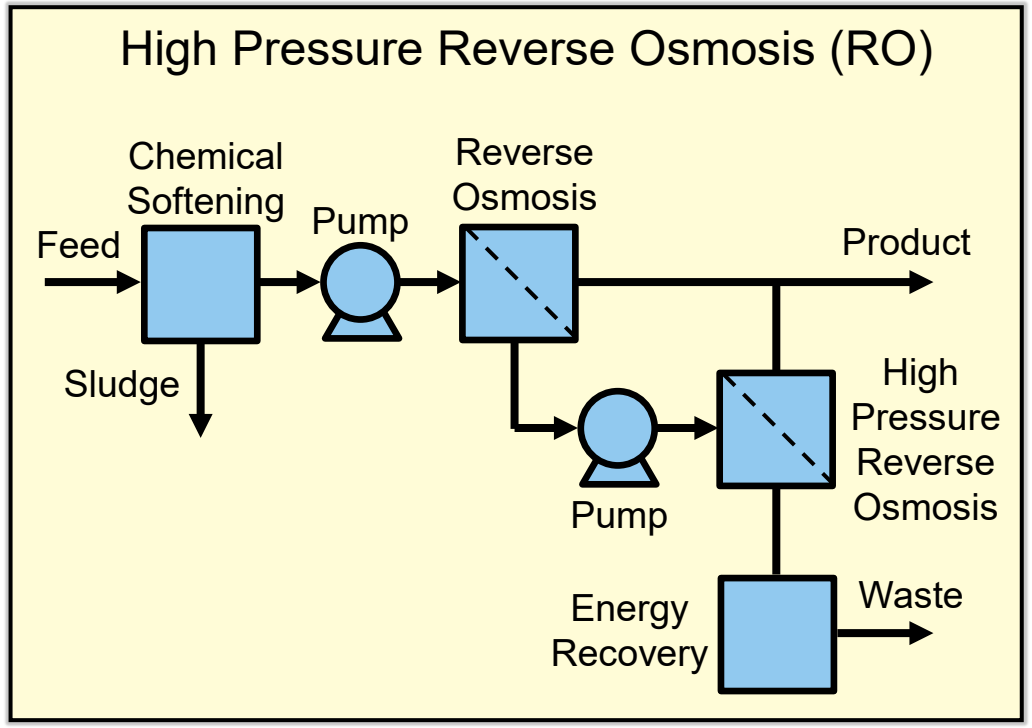
**Tim Bartholomew**

**Wednesday October 11th, 2023**

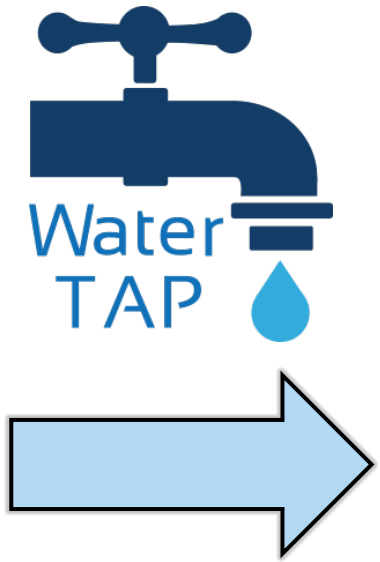
# WaterTAP is a software tool for water treatment technoeconomic assessments

**Objective:** Develop a modeling platform to evaluate water treatment options and identify high impact opportunities for innovation within materials, processes, and systems

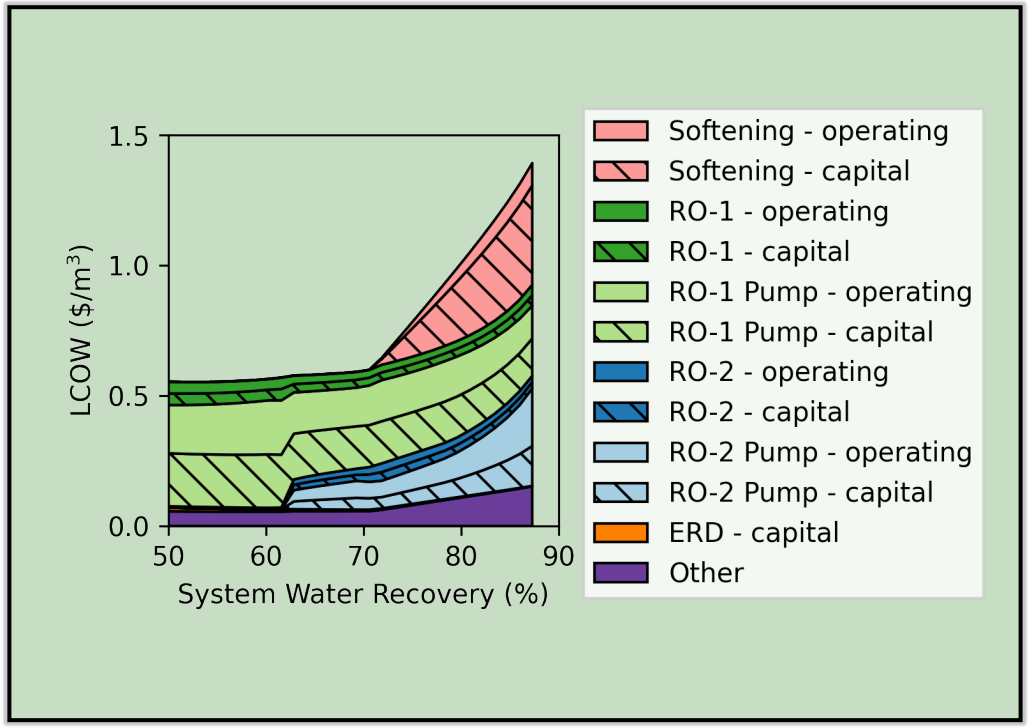
Emerging water treatment technology




Software tool




Technoeconomic assessment



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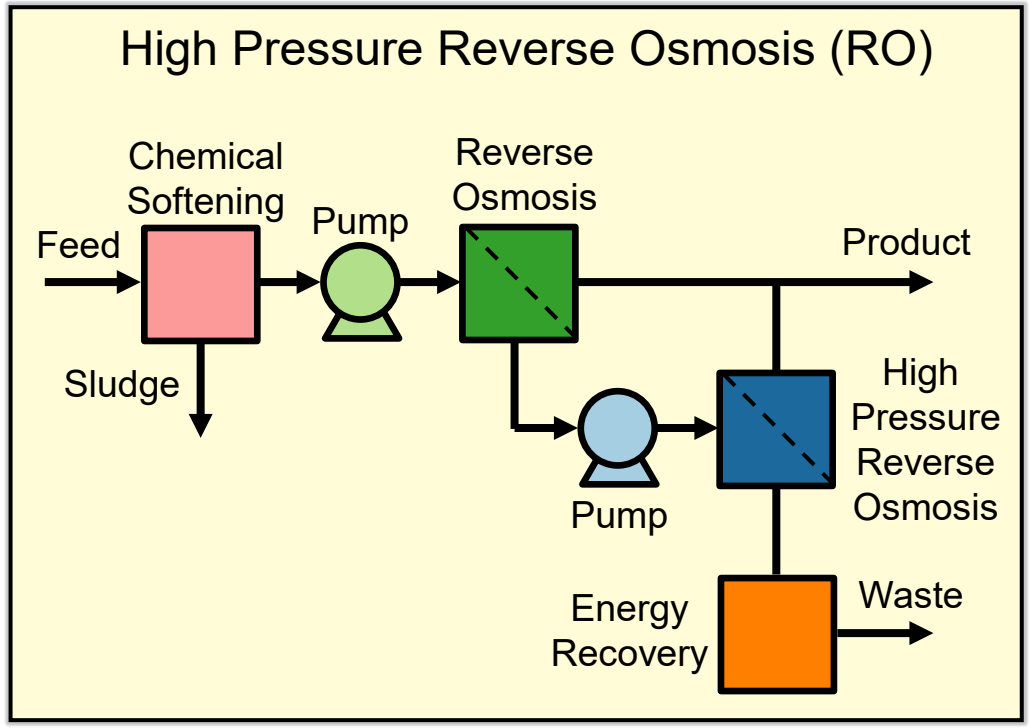
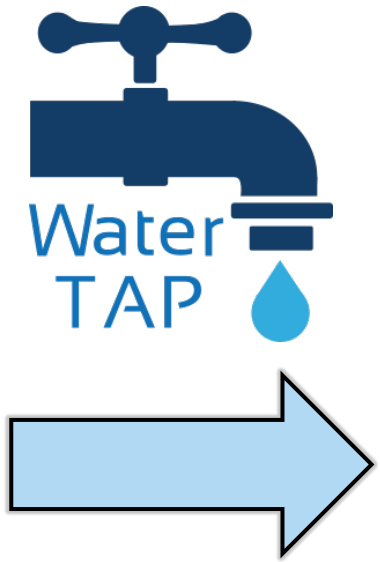
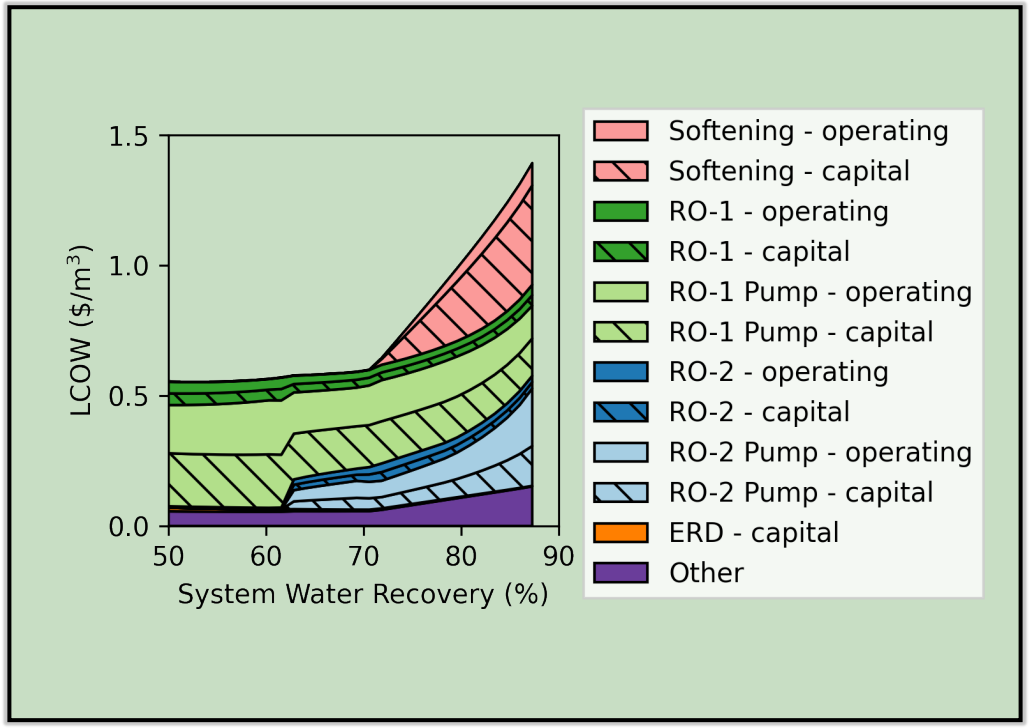



Software tool




Technoeconomic assessment



# Multiple research programs are funding WaterTAP

NAWI National Alliance for Water Innovation

- DOE's water desalination hub
- $110M over 5 years across multiple national labs, universities, and industry partners
- Advance early-stage desalination technologies

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

**Industrial Efficiency & Decarbonization Office (IEDO)**

- Advance water resource recovery systems
- $27M over 3 years across 15 research projects
- Biological wastewater treatment technologies

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

**Solar Energy Technology Office (SETO)**

- Advance solar driven high salinity desalination technologies

# Multiple research programs are funding WaterTAP

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- Advance e

U.S. DEPARTMENT OF ENERGY | Energy Efficiency &

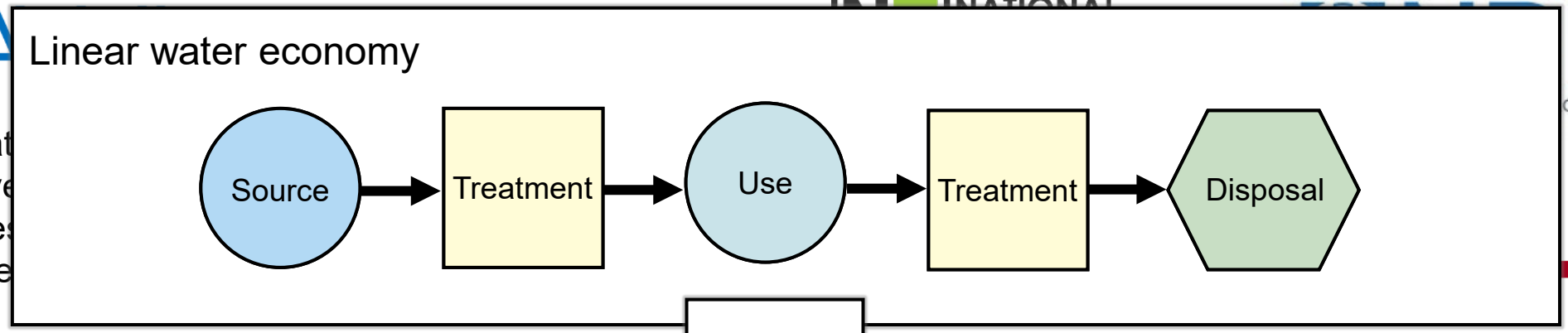
**Industrial Eff**

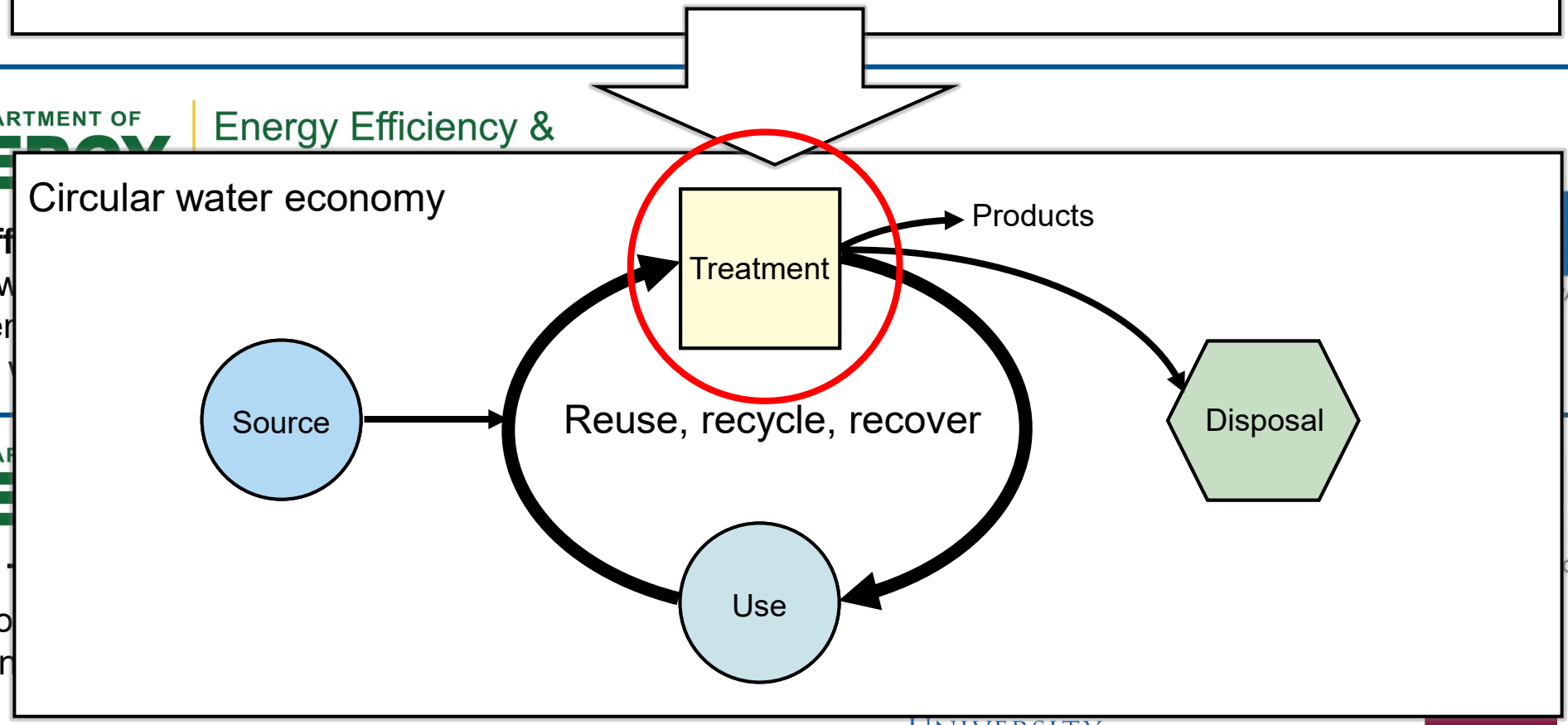
- Advance w
- $27M over
- Biological

U.S. DEPAR ENE

**Solar Energy**

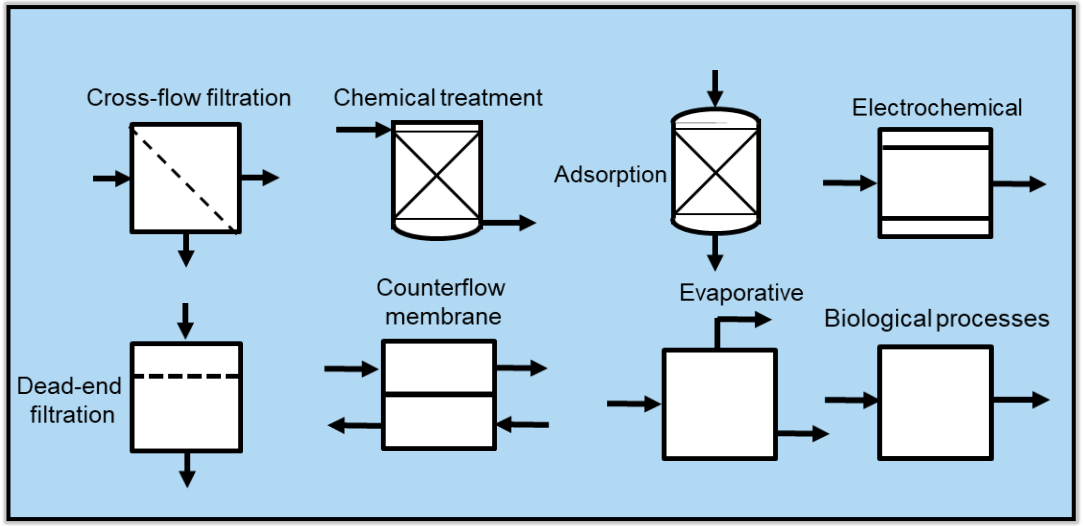
- Advance so
  desalination



# WaterTAP is a process systems engineering tool built on other DOE investments

Unified




Flexible

- Open-source
- Multi-hierarchical
- Customizable

Powerful

- 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
- https://github.com/watertap-org/watertap
- One-click code-signed downloads for GUI https://watertap-org.github.io/

GitHub

**Software engineering:**

- Industry standard development practices
- Every code change must pass peer review, code standards, and automatic tests
- Online documentation updated for each release
- Modular packaging system supports many users & contributions

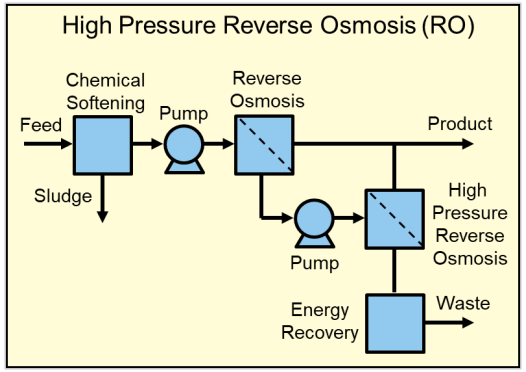
Scan QR code for documentation and tutorials

NAWI

# IDAES provides core capabilities for WaterTAP

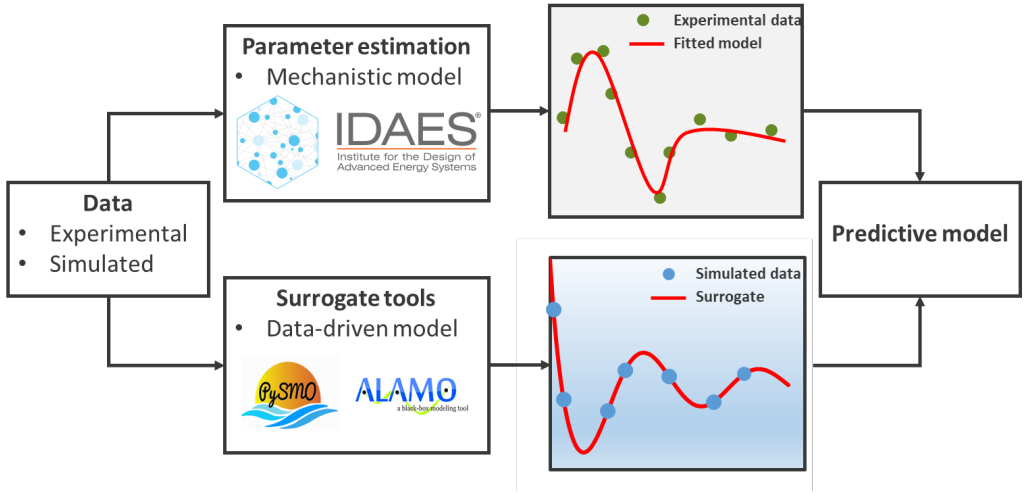
**Assessing technoeconomic performance:**

- Simulation and optimization of treatment trains assembled from modular model library
- Parametric and stochastic sensitivity analyses



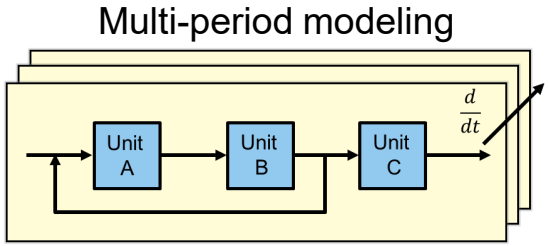

**Interfacing experimental data and models:**

- Parameter estimation tools - fitting mechanistic models to data
- Surrogate modeling tools – developing empirical models from data with PySMO and ALAMO



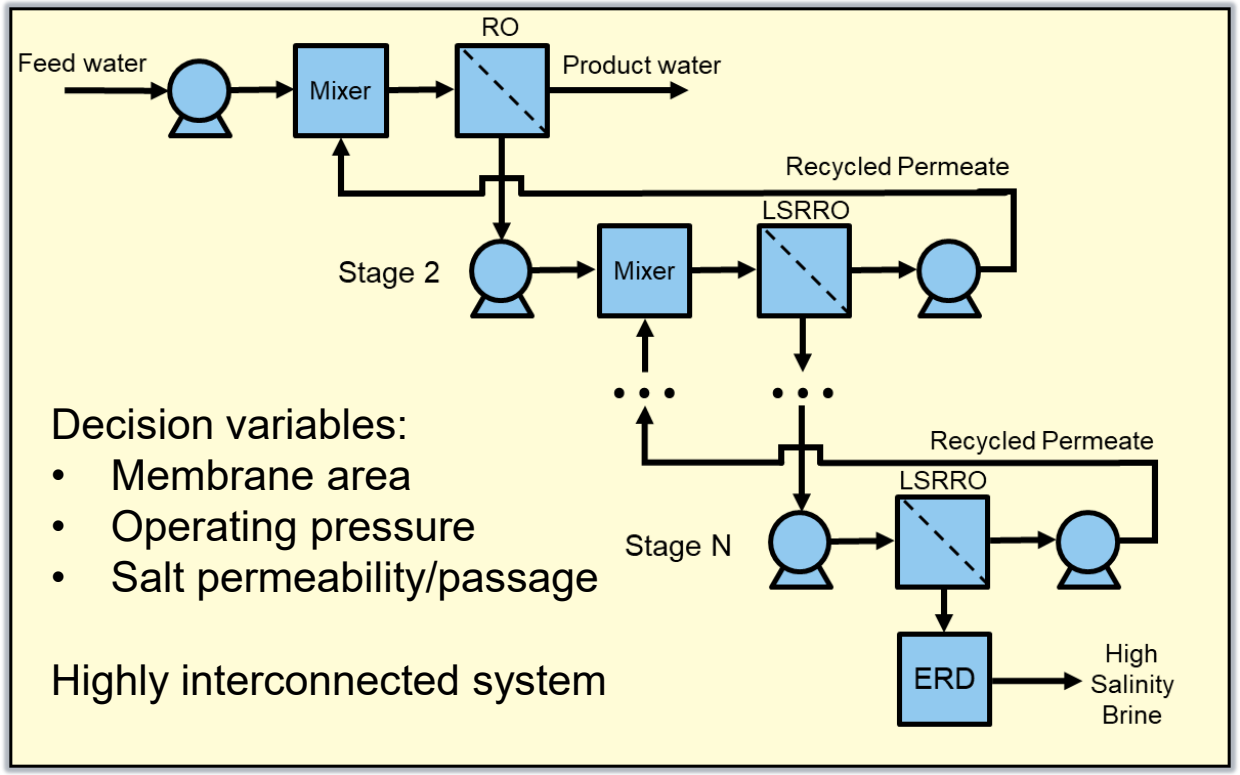

**Representing systems over time:**

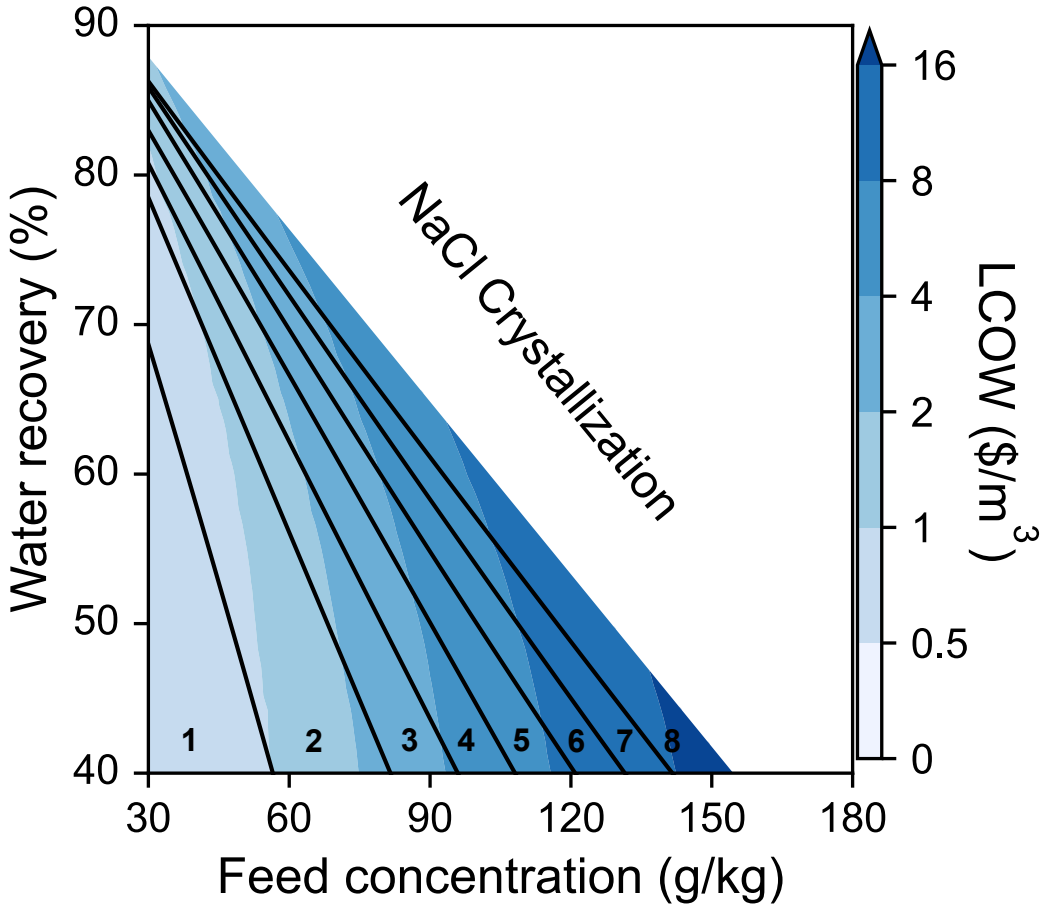
- Multi-period modeling tools from DISPATCHES



# WaterTAP supports the analysis of emerging water treatment technologies

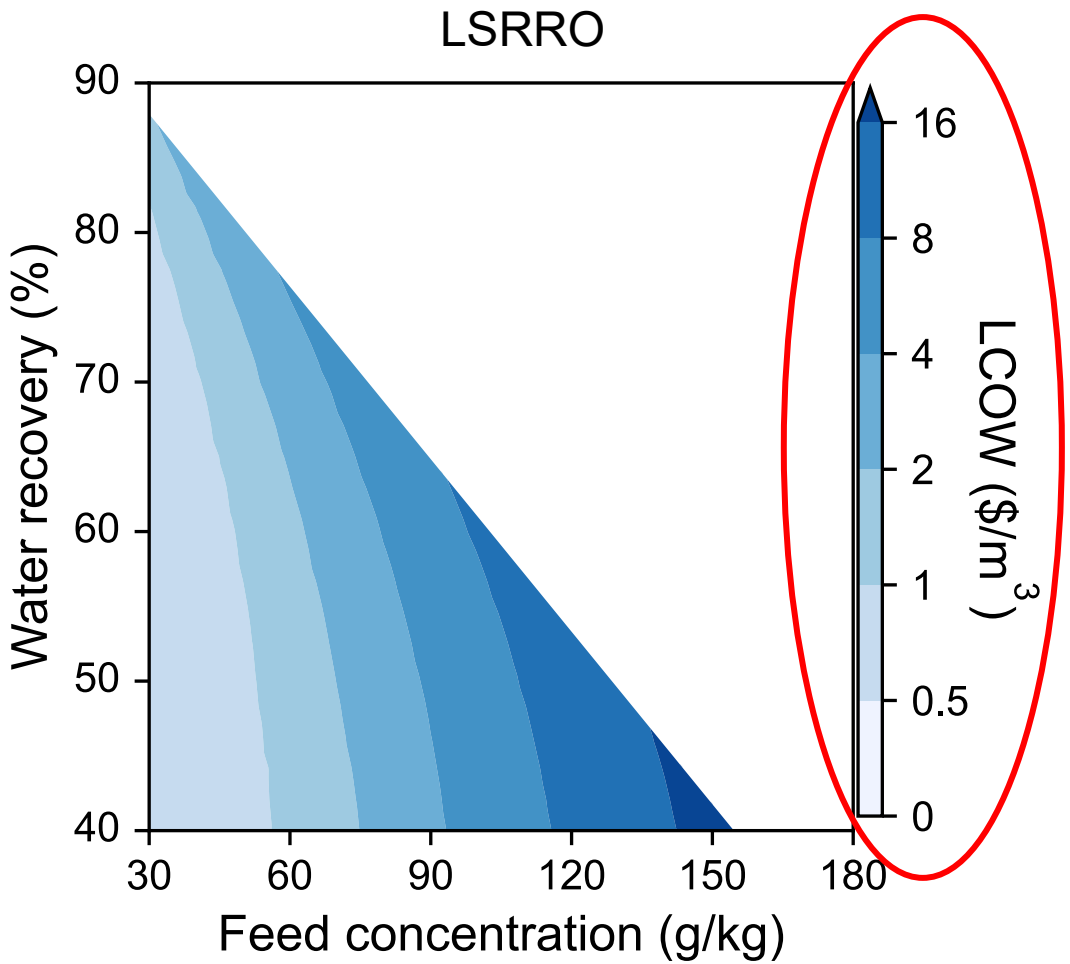
Low salt rejection reverse osmosis (LSRRO)

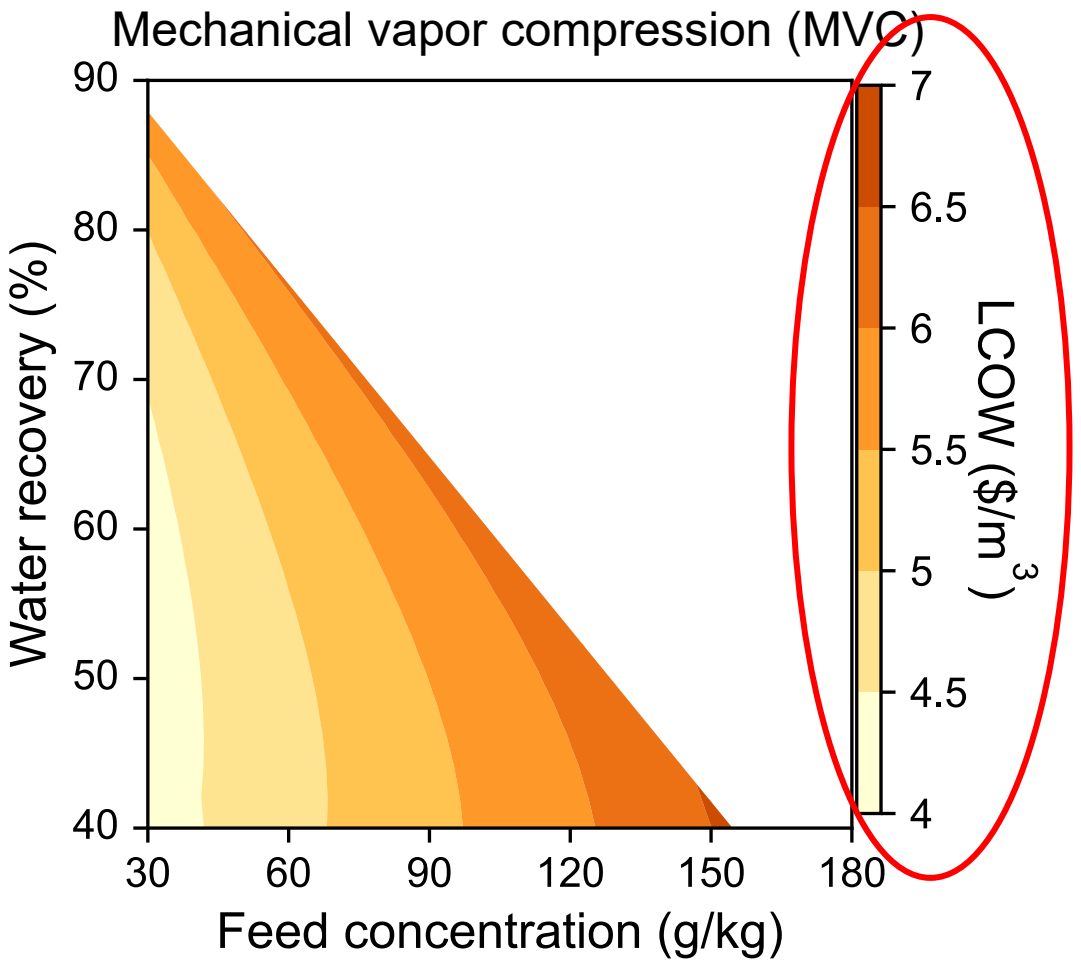



Atia et al. *Desalination.* 2023, 551, 116407

# Quantifying technoeconomic viability through comparison






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

Tucker et al. *Under Review at Desalination*

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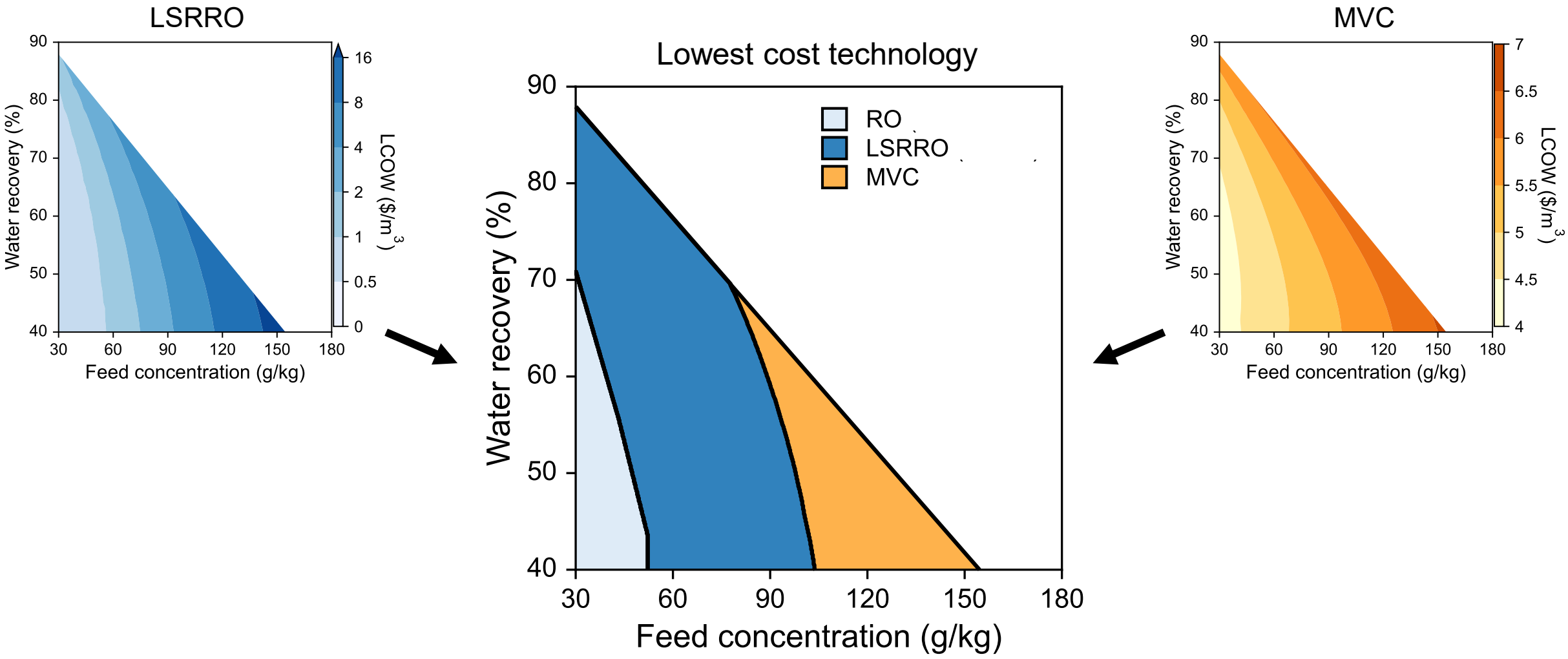
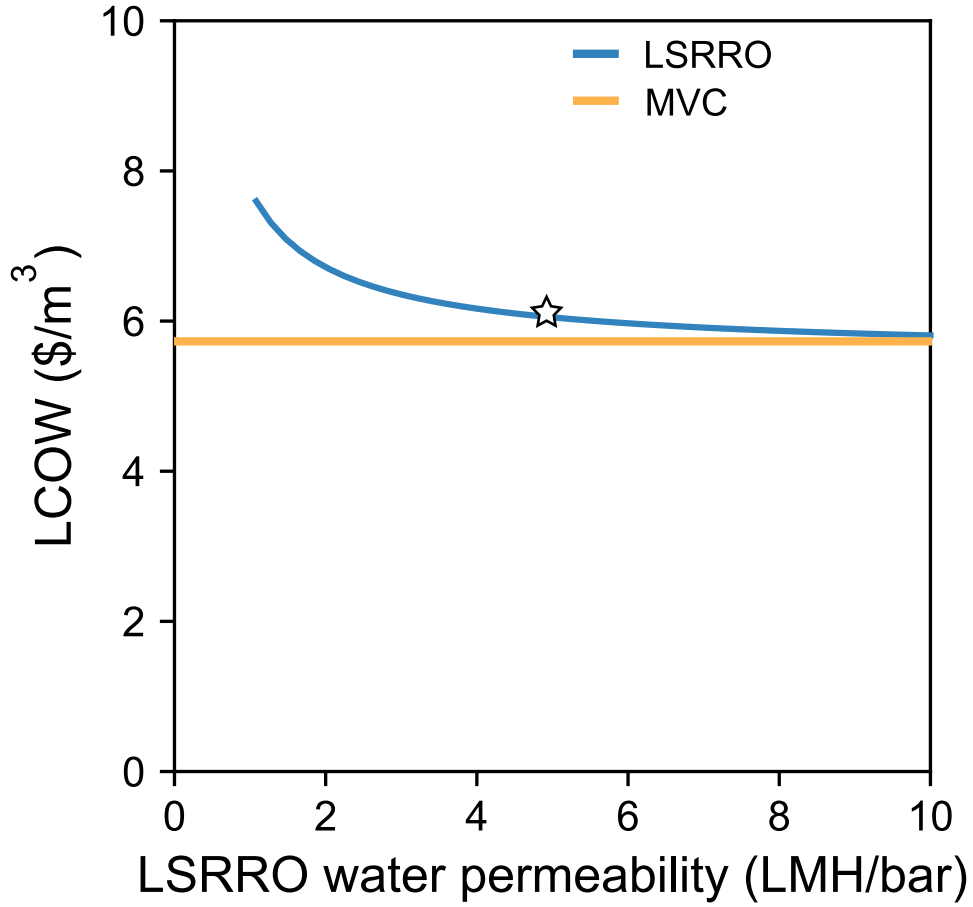
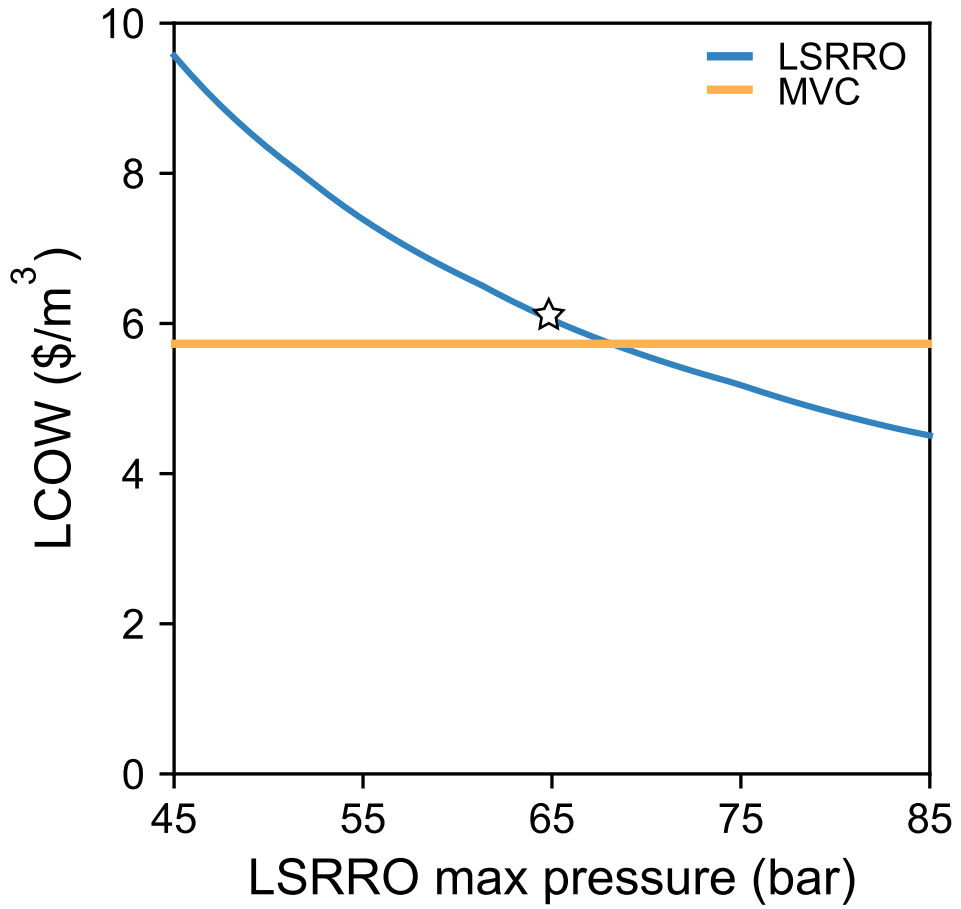


# Parameter sensitivity can be used to prioritize development

Case: 100 g/kg and 50% water recovery

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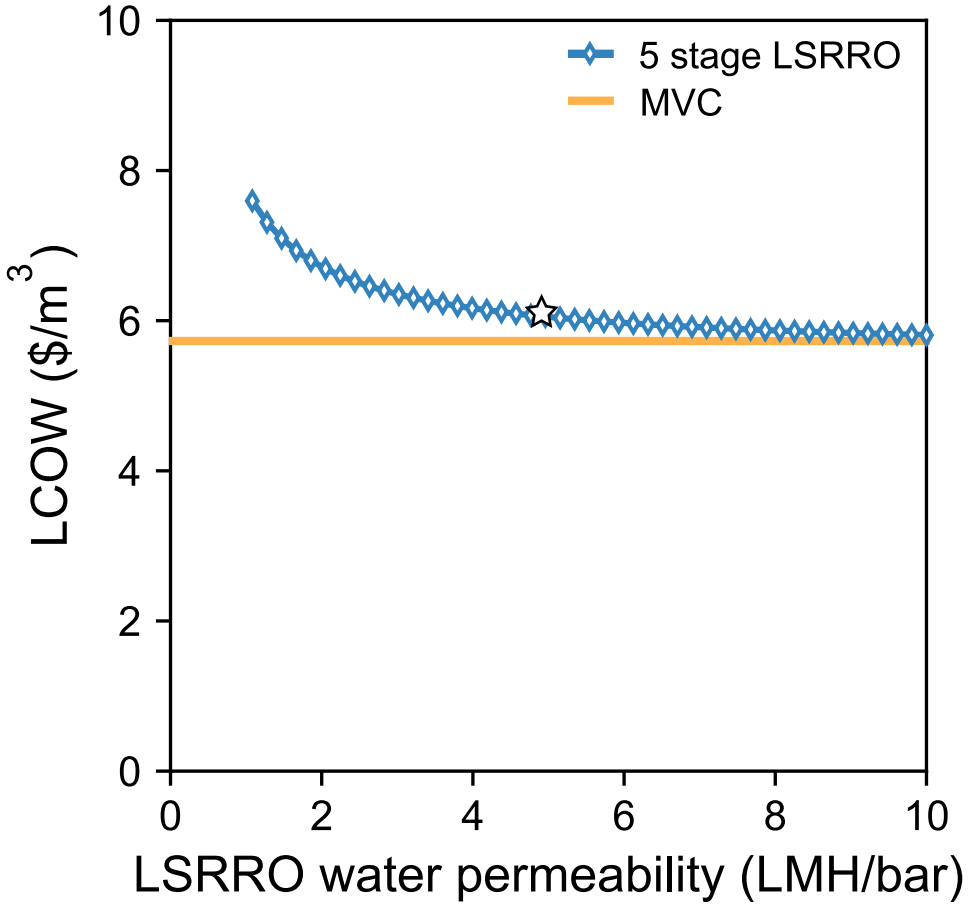
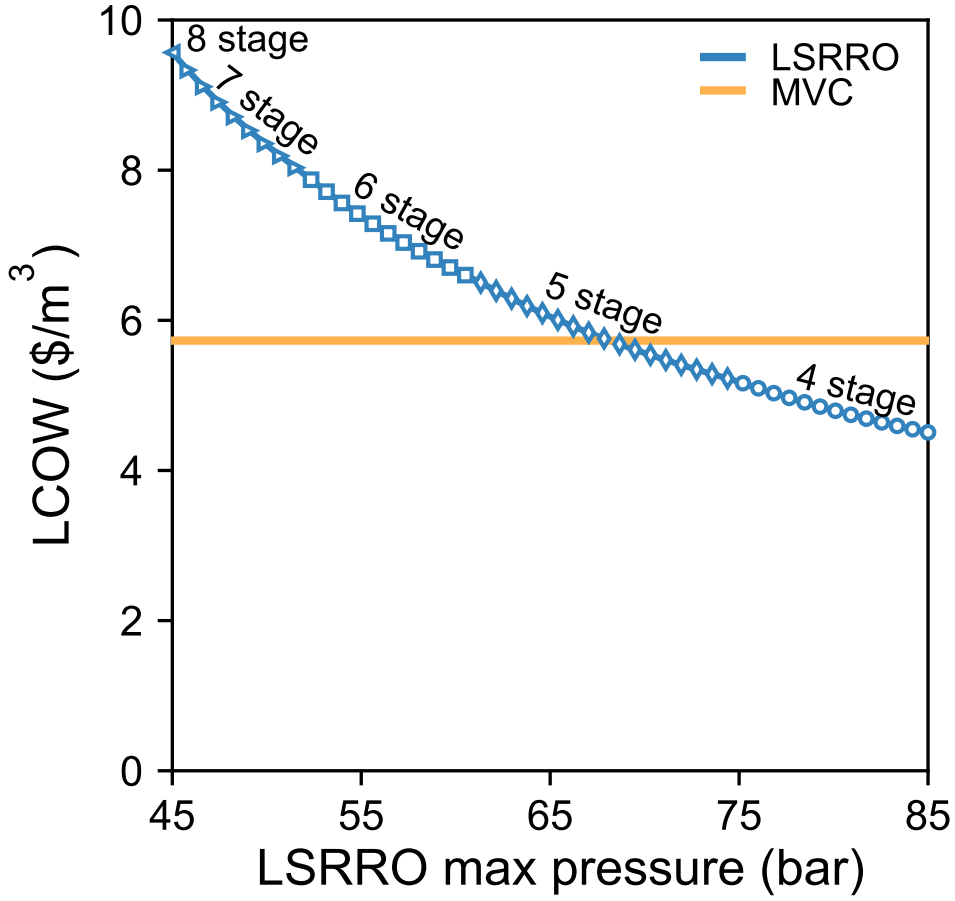


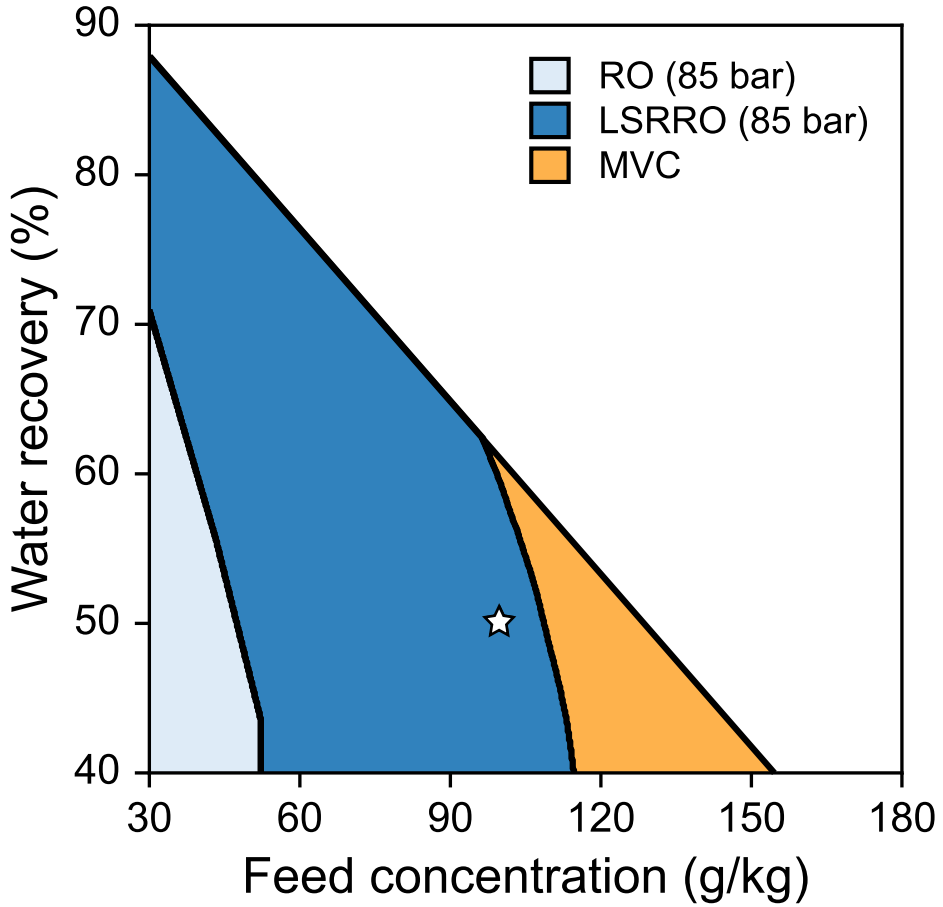



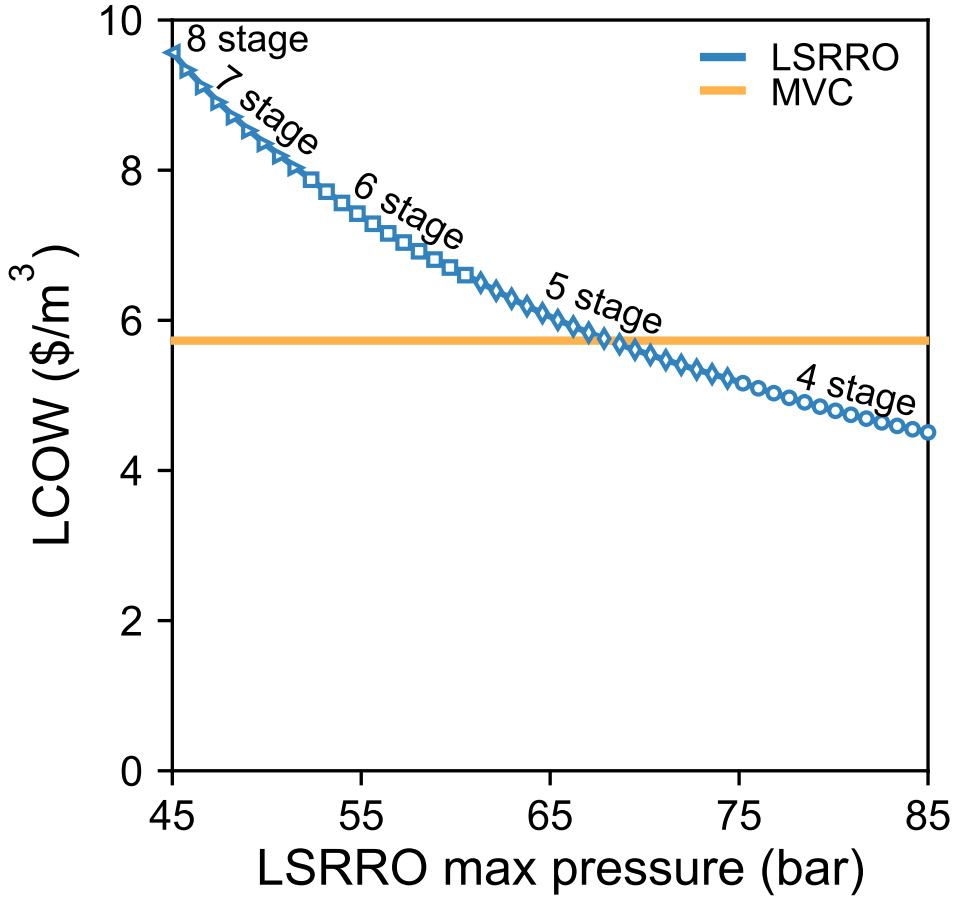



Atia et al. *Desalination.* 2023, 551, 116407

# Multi-dimensional analyses are enabled by comprehensive modeling capabilities

Case: 100 g/kg and 50% water recovery



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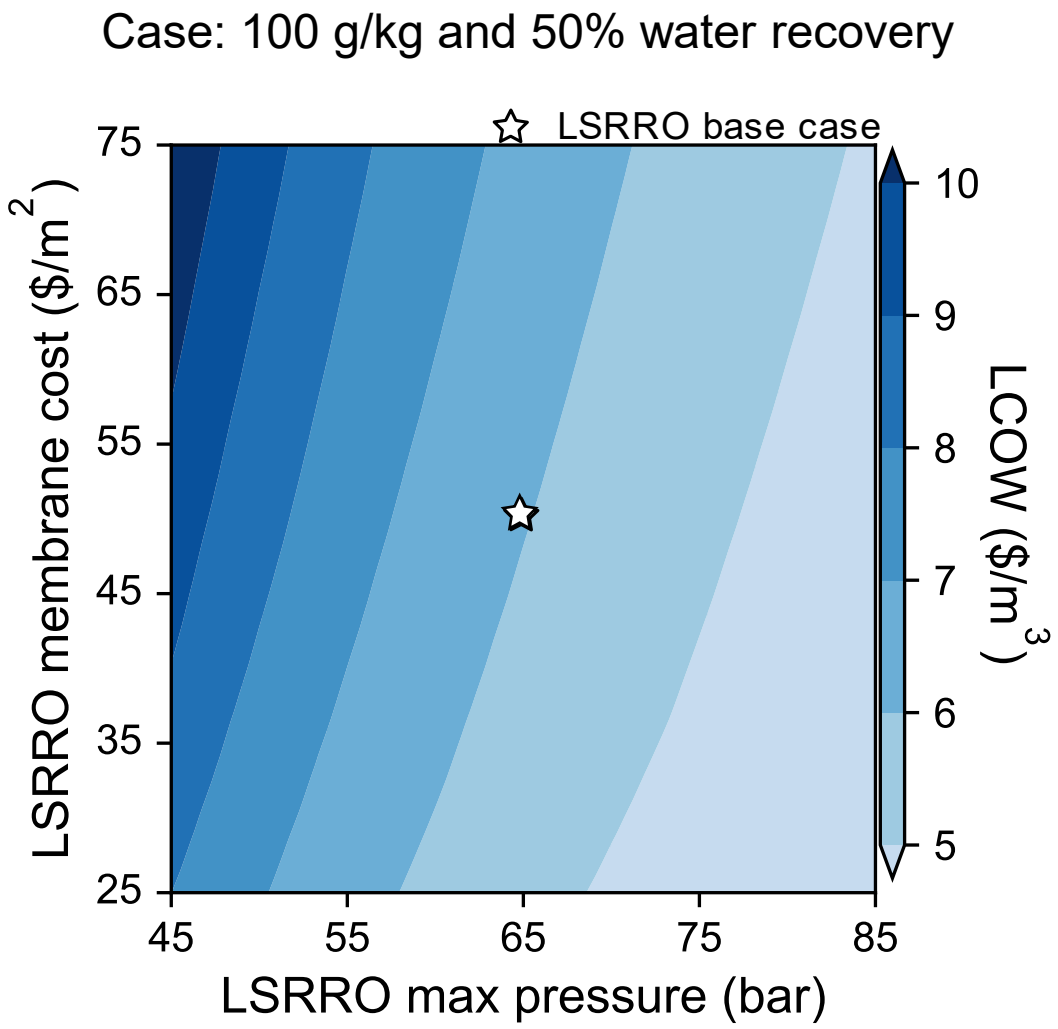
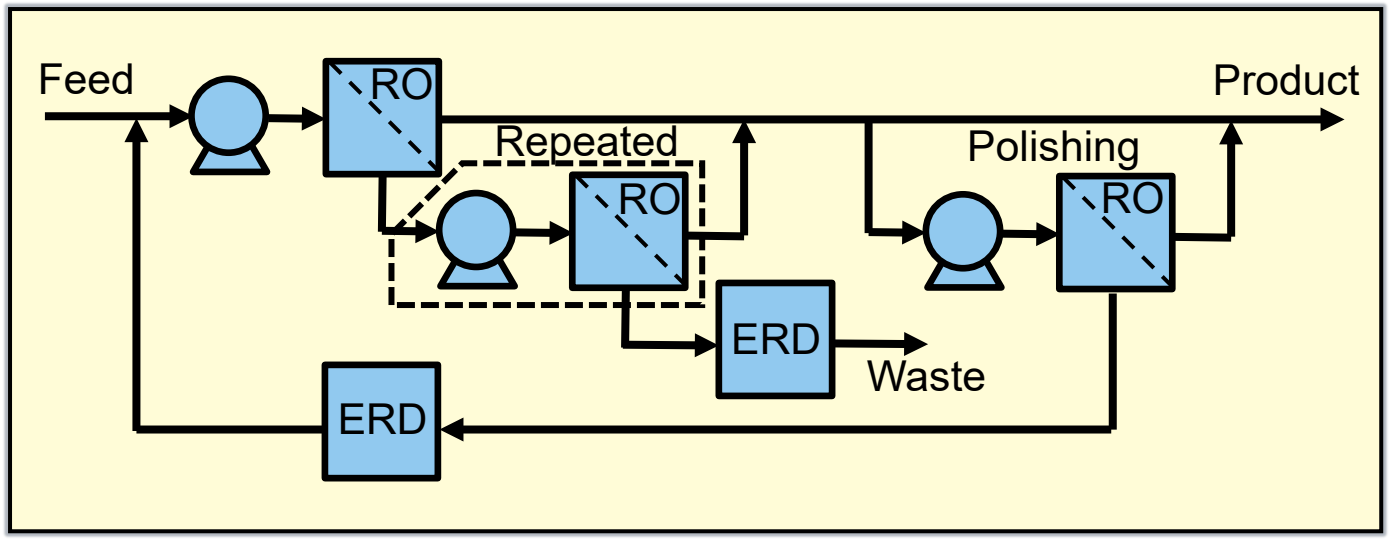
# Varying performance and cost parameters establishes research targets

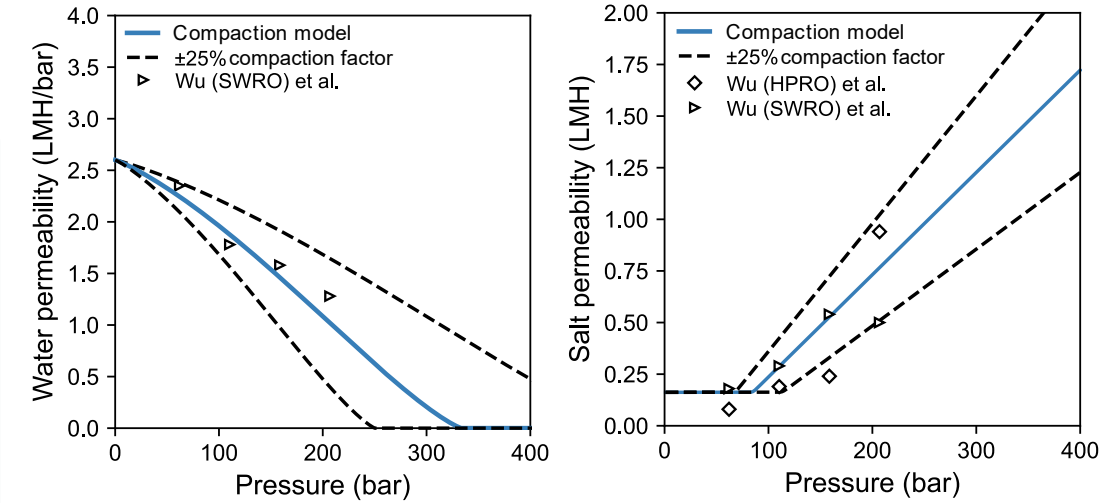


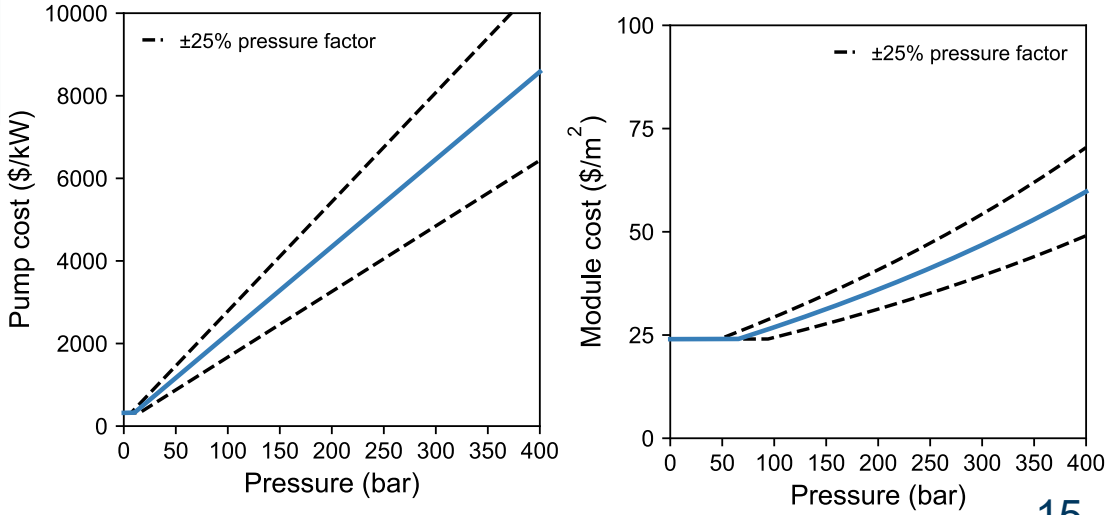

Atia et al. *Desalination.* 2023, 551, 116407

# Understanding the impact of membrane compaction and increasing costs for high pressures

Multistage high pressure reverse osmosis (HPRO)




Dudchenko et al. *In preparation*

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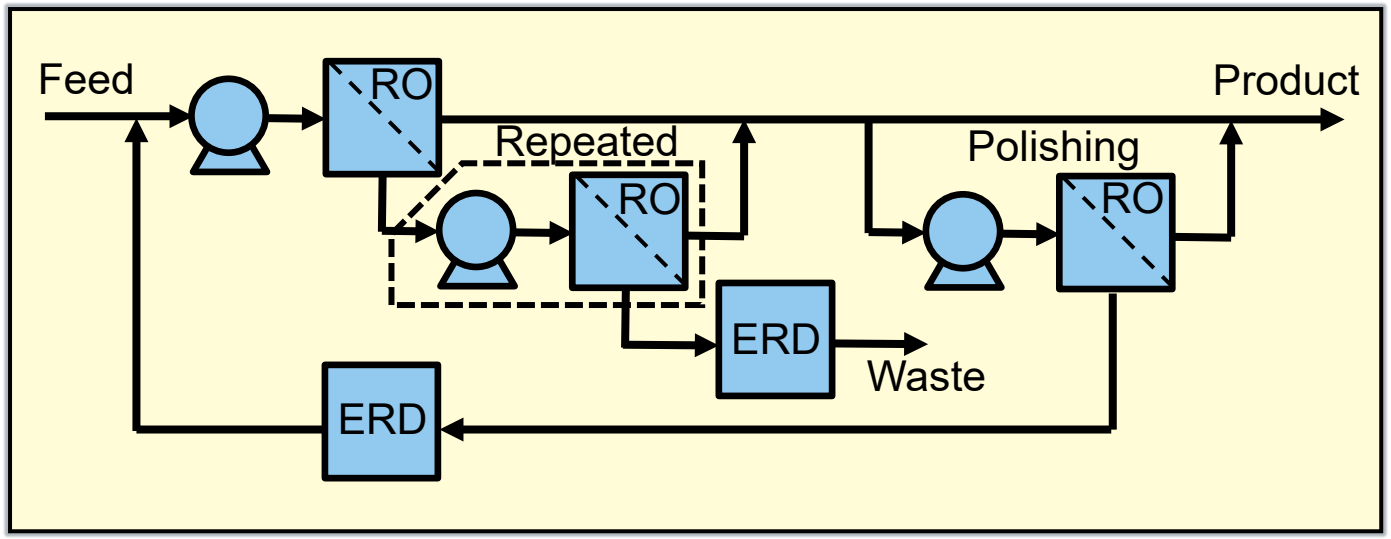
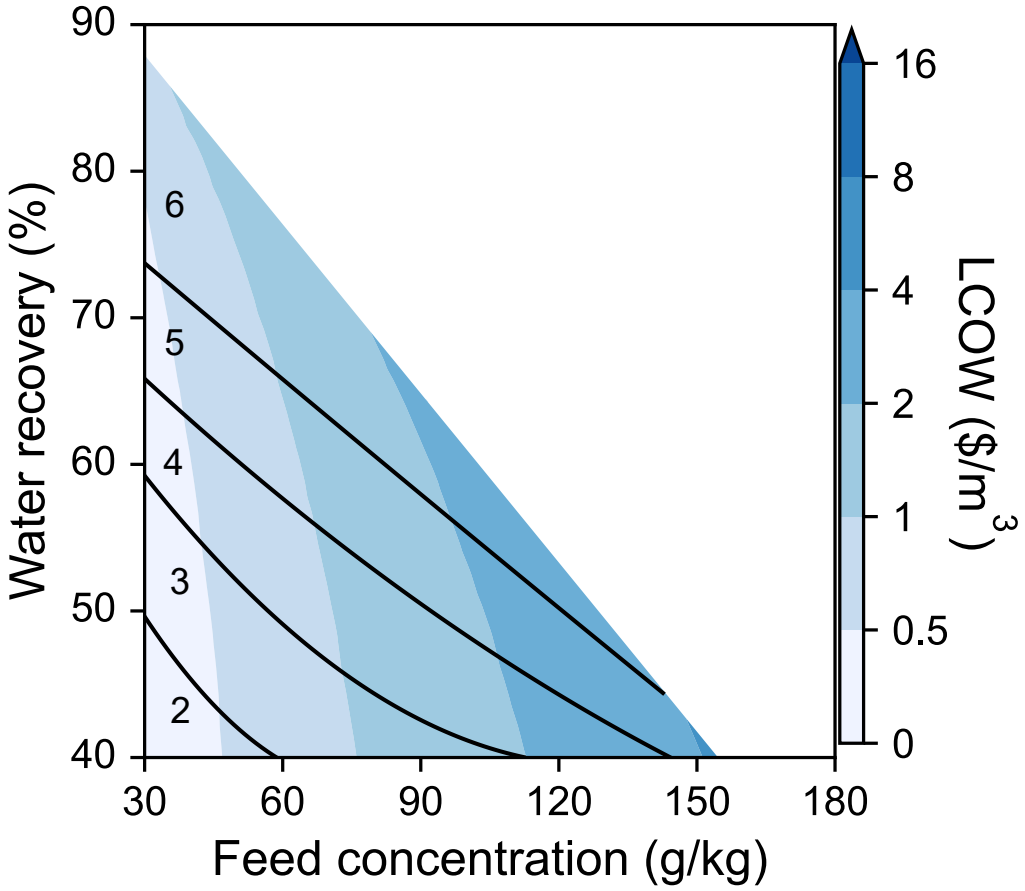





Dudchenko et al. *In preparation*

# Stochastic analyses help prioritize the most impactful innovations

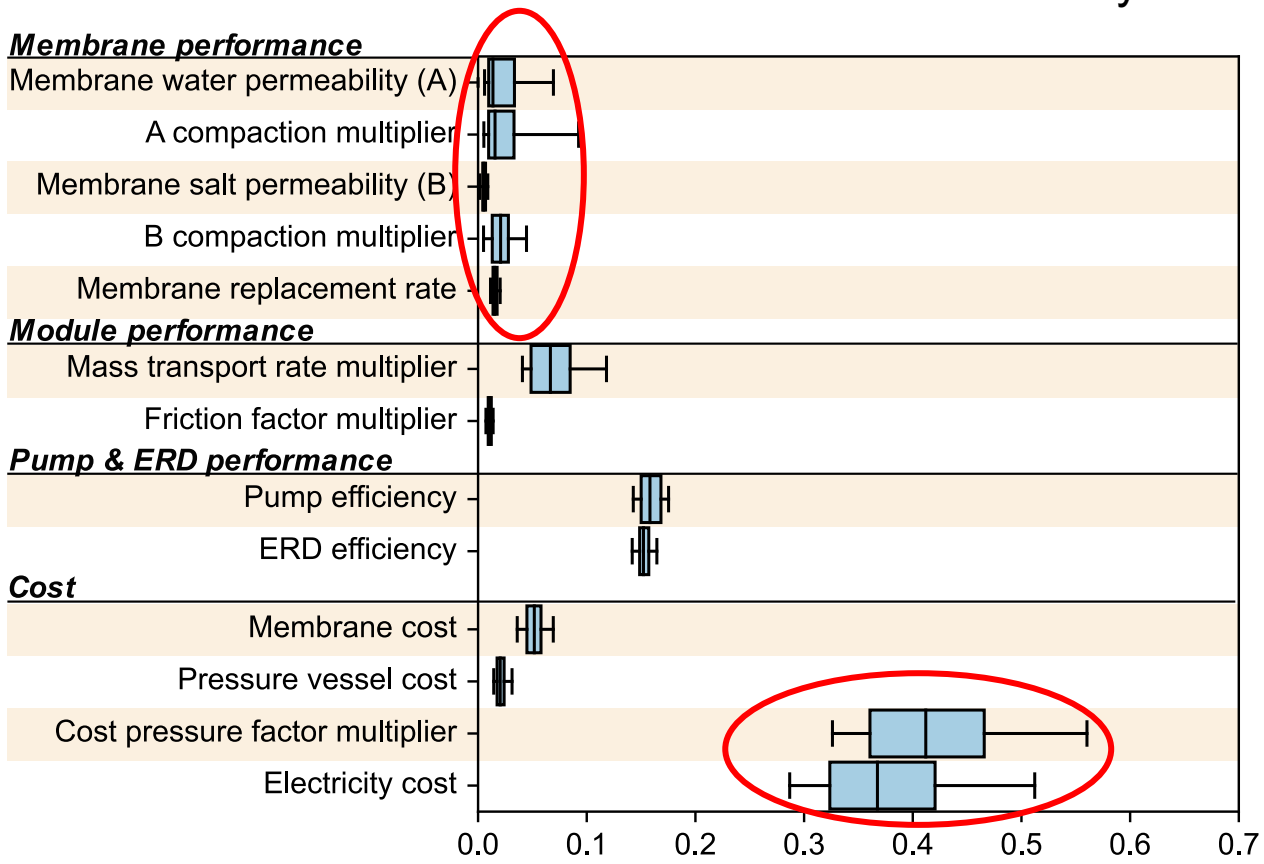
[1]Dudchenko et al. *PNAS.* 2021, 118 (37)

| Parameters | Base | Improved |
|---|---|---|
| **Membrane performance** | | |
| Water permeability (LMH/bar) | 2.5 (4x) | 10 |
| Salt permeability (LMH) | 0.16 (¼ x) | 0.04 |
| A compaction multiplier* | 1 | 0.5 |
| B compaction multiplier* | 1 (½ x) | 0.5 |
| Annual membrane replacement | 20 | 10 |
| **Module performance** | | |
| Mass transport rate multiplier | 1 | 2 |
| Friction factor multiplier | 1 | 0.5 |
| **Pump & ERD performance** | | |
| Pump efficiency | 75 (1.2x) | 90 |
| ERD efficiency | 75 | 95 |
| **Cost** | | |
| Membrane cost ($/m2) | 17 | 8.5 |
| Pressure vessel cost ($/m2) | 7 | 3.5 |
| Cost pressure factor multiplier* | 1 | 0.5 |
| Electricity cost ($/kWh) | 0.07 | 0.02 |

*theoretical relationships proposed in this work

Stochastic value of innovation (VOI)[1]

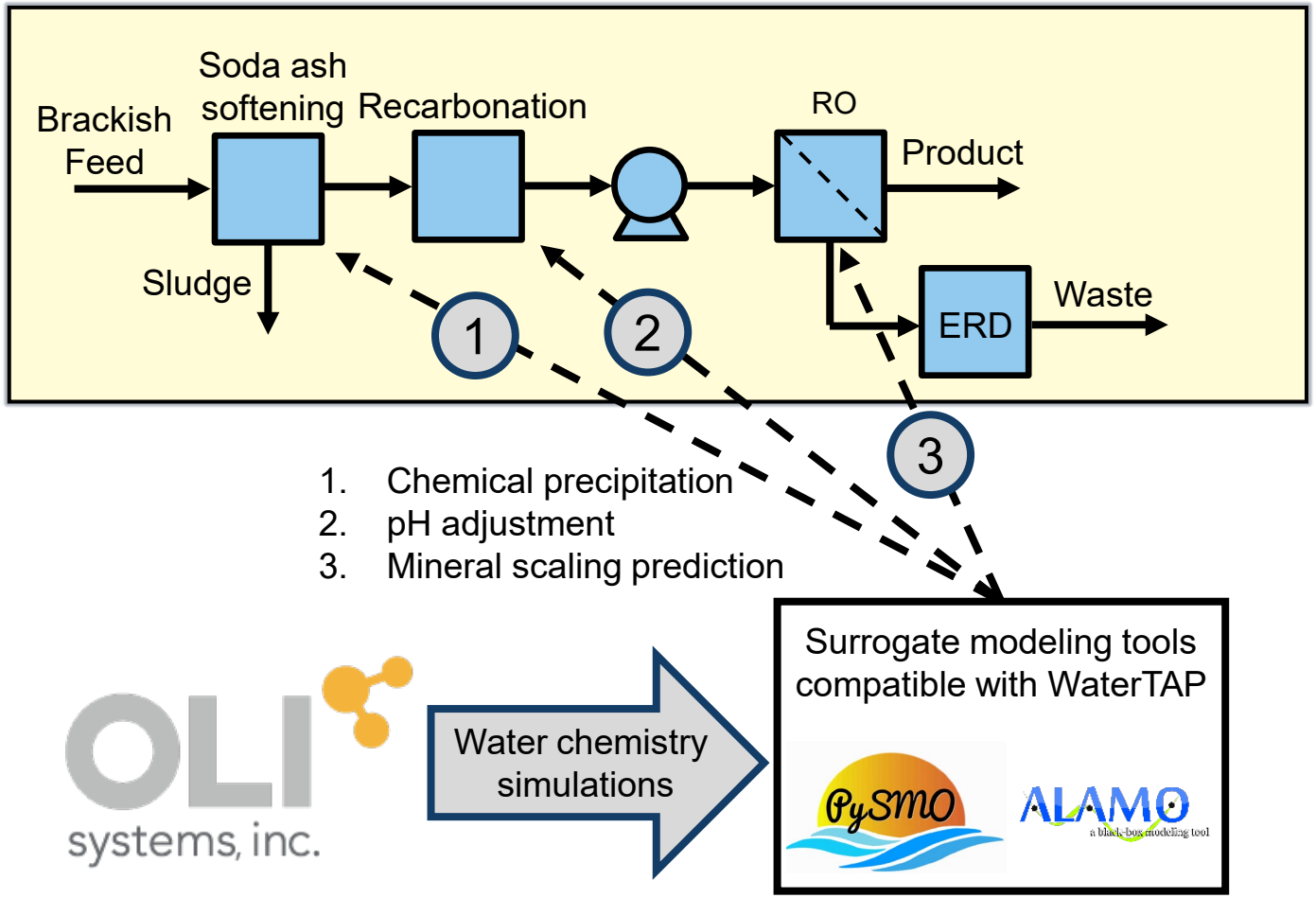
- Monte Carlo scenario generation
- Finite difference sensitivity

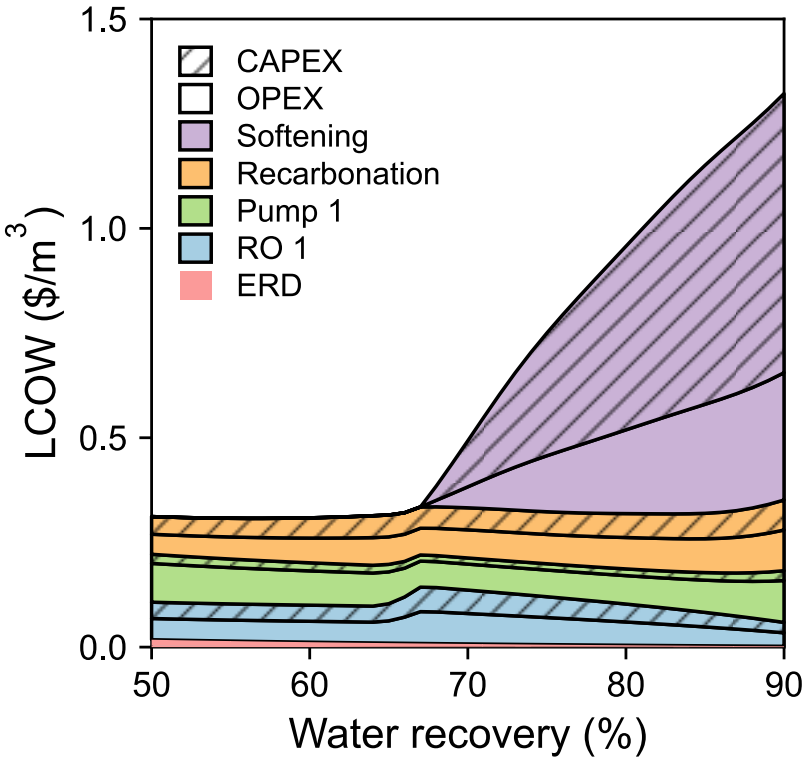



$$\text{VoI} = \frac{\%_{\Delta\text{LCOW}}}{\Delta_{\text{percentile}}}$$

Dudchenko et al. *In preparation*

# Incorporating detailed water chemistry for process scale cost optimization



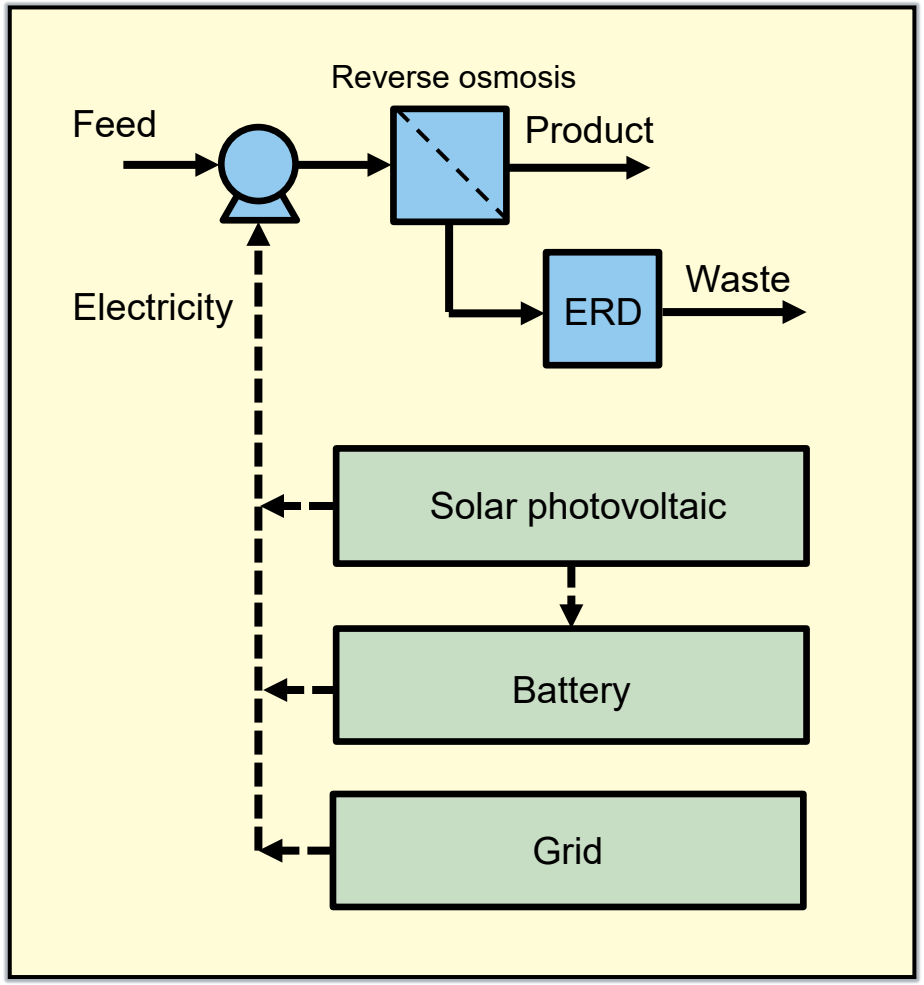




Amusat et al. *In preparation*

# WaterTAP can represent solar driven desalination

WaterTAP-REFLO

Renewable energy and flexible load operation (REFLO)




WaterTAP

- Water treatment models

System Advisor Model (SAM)

- Solar energy models
- Weather data

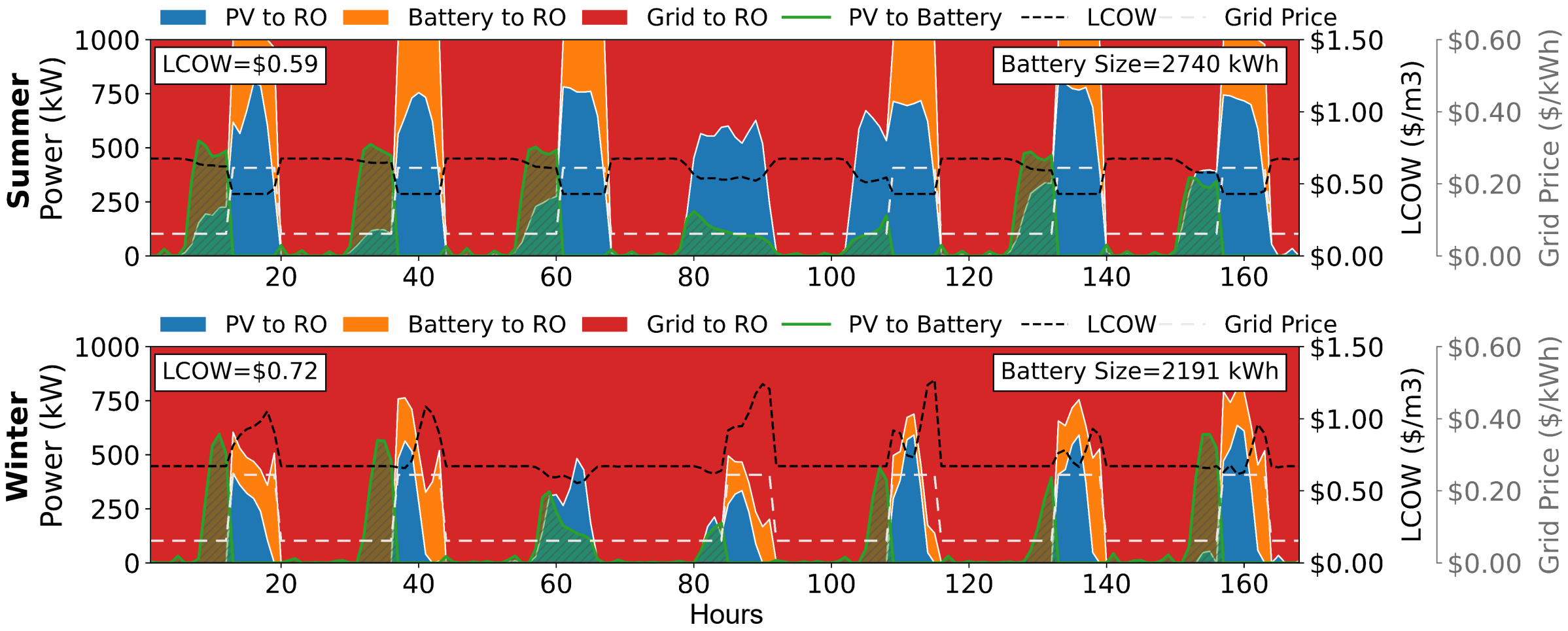
IDAES
Institute for the Design of Advanced Energy Systems

- PSE platform for simulation and optimization
- Surrogate modeling from PySMO and ALAMO

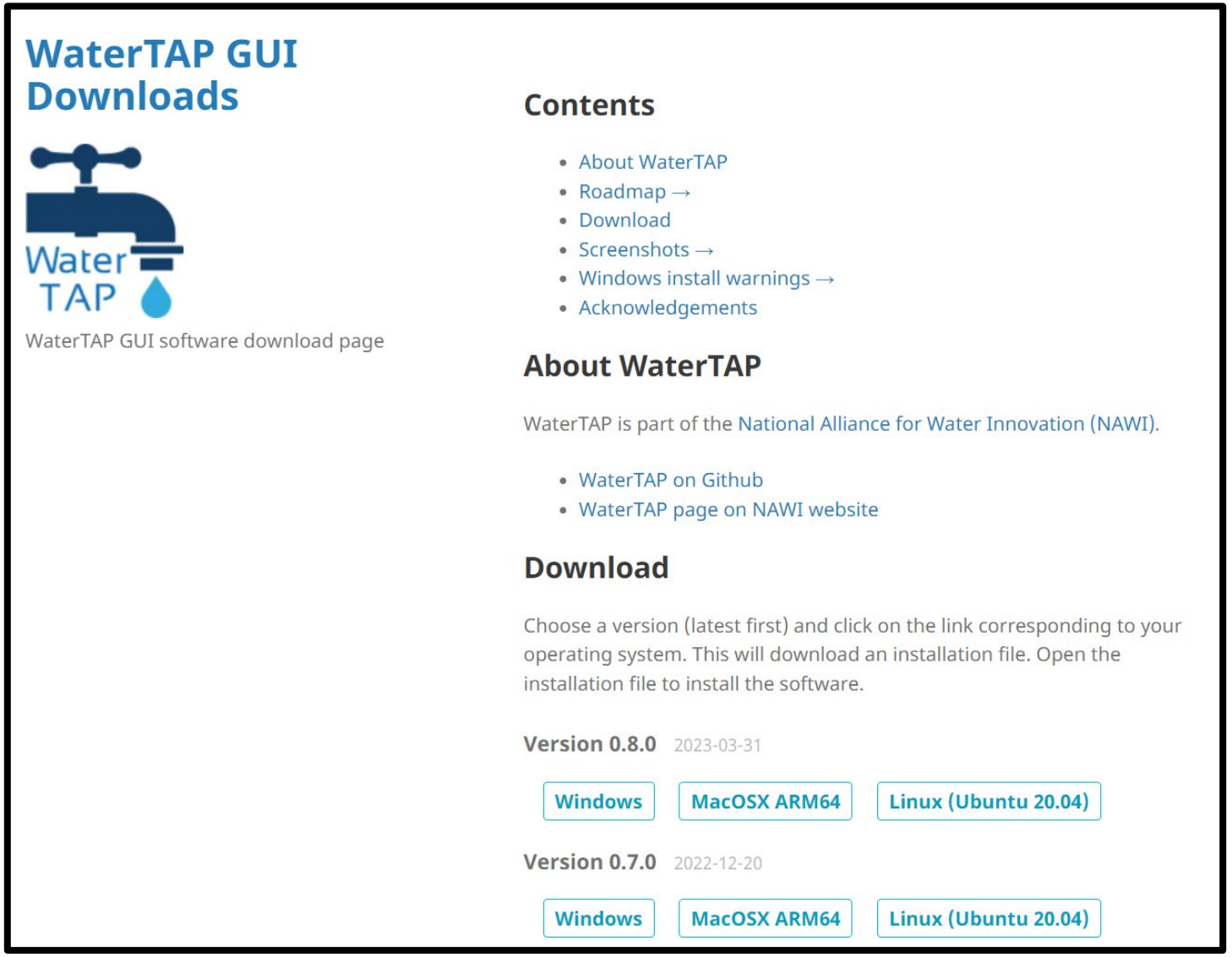
DISPATCHES
Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems

- Multiperiod modeling for IDAES compatible models

# Multiperiod modeling enables time dependent analyses



# WaterTAP has developed a GUI for non-coders



## WaterTAP GUI Downloads

WaterTAP GUI software download page

### Contents



### About WaterTAP

WaterTAP is part of the National Alliance for Water Innovation (NAWI).

- WaterTAP on Github
- WaterTAP page on NAWI website

### Download

Choose a version (latest first) and click on the link corresponding to your operating system. This will download an installation file. Open the installation file to install the software.

**Version 0.8.0** 2023-03-31

Windows | MacOSX ARM64 | Linux (Ubuntu 20.04)

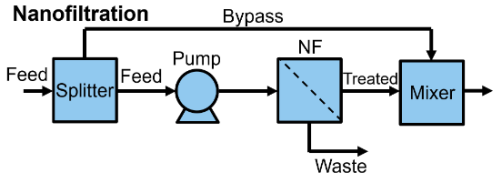
**Version 0.7.0** 2022-12-20

Windows | MacOSX ARM64 | Linux (Ubuntu 20.04)

# Users can modify inputs, solve, see results and save

NAWI WaterTAP — RETURN TO LIST PAGE

**NF-DSPM-DE with bypass** — DEGREES OF FREEDOM: 3




INPUT | OUTPUT | COMPARE

Previous Configurations: [ ]  RESET FLOWSHEET | SOLVE | SWEEP

**Feed**

| | | |
|---|---|---|
| Volumetric flow rate | 3600 L/h | Fixed |
| Ca_2+ concentration | 257.99 mg/L | Fixed |
| SO4_2- concentration | 1010.98 mg/L | Fixed |
| HCO3_- concentration | 384.99 mg/L | Fixed |
| Na_+ concentration | 738.98 mg/L | Fixed |
| Cl_- concentration | 890.93 mg/L | Fixed |
| K_+ concentration | 9 mg/L | Fixed |
| Mg_2+ concentration | 90 mg/L | Fixed |

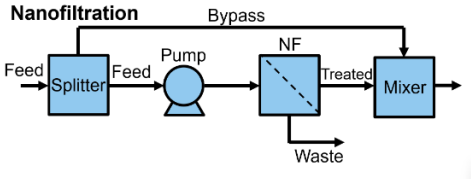
**NF design**

| | | | |
|---|---|---|---|
| NF pump pressure | 3 bar | | Free |
| | Lower 1 | Upper | |
| NF area | 50 m^2 | | Free |
| | Lower 0 | Upper 1000 | |
| NF water recovery | 0.089 fraction | | Free |
| | Lower 0 | Upper 0.95 | |

NF membrane props. | NF CAPEX | NF OPEX | System constraints | Bypass design

NAWI WaterTAP — RETURN TO LIST PAGE

**NF-DSPM-DE with bypass** — DEGREES OF FREEDOM: 3




INPUT | OUTPUT | COMPARE

**NF design**
- NF pump pressure 5.85 bar
- NF area 455.73 m^2
- NF water recovery 0.95 fraction
- NF product volume flow 2977.27 L/h
- NF water flux 6.54 LMH

**NF membrane props.**
- Pore size 0.5 nm
- Effective membrane thickness 859.89 nm
- Charge -680 mol/m^3
- Dielectric constant for pore 41.3 dimensionless

**NF CAPEX**
- Membrane cost 15 $/m^2
- Membrane replacment rate 0.2 fraction/year

**NF OPEX**
- Electricity price 0.07 $/kWhr
- Plant capacity utilization 0.9 fraction of uptime
- Maintenance-labor-chemical factor 0.03 fraction of investment cost/year

**System constraints**
- Disposal cost 10 $/m^3

**Bypass design**
- NF bypass 0.1295 fraction

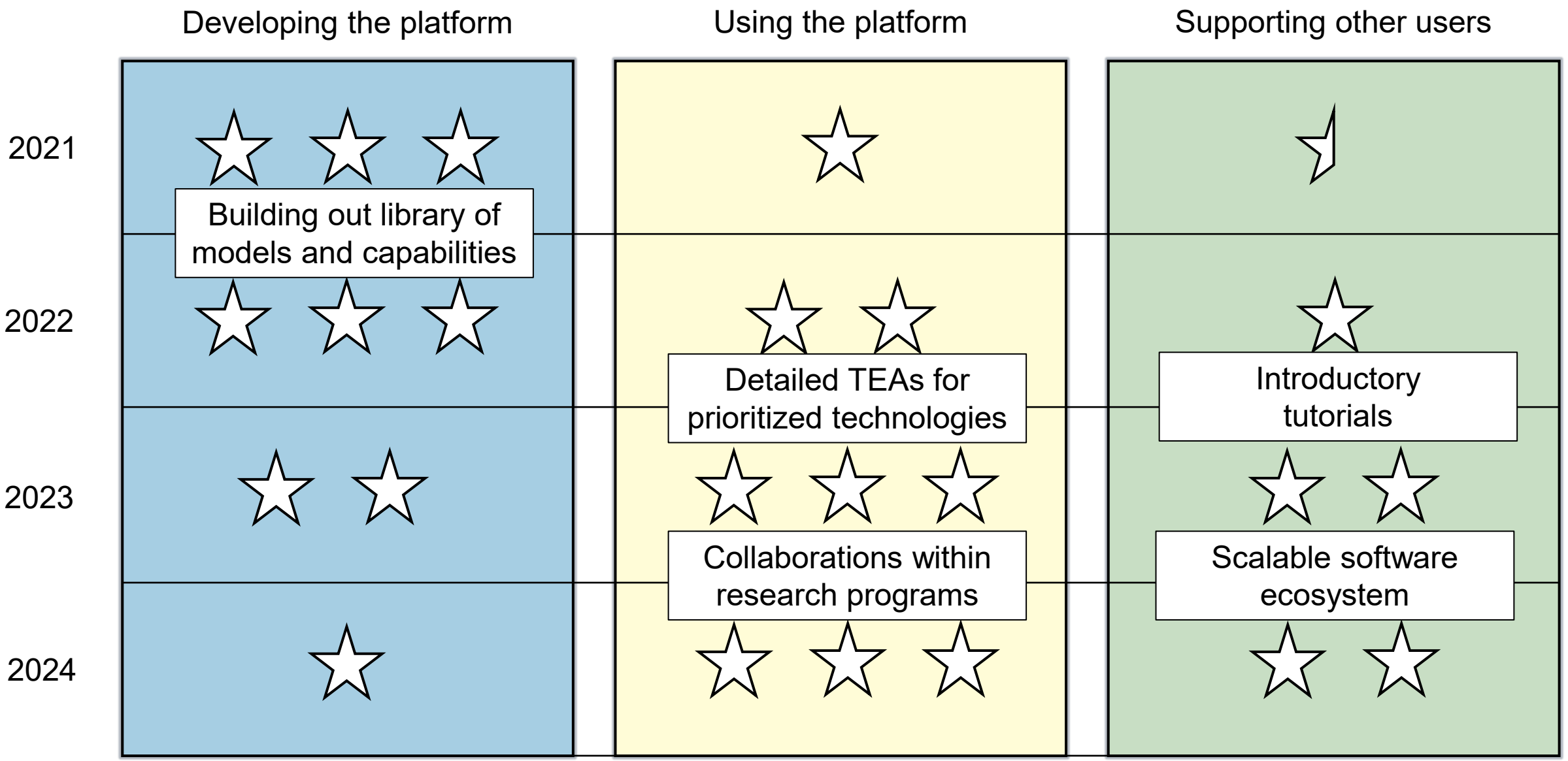
**System streams**
- Product hardness 200 mg/L
- Product volume flow 3443.3 L/h
- Feed hardness 1016.29 mg/L
- Disposal hardness 18953.43 mg/L
- Disposal volume flow 156.7 L/h

**Process cost and opertaing metrics**
- System cost 0.6 $/m^3
- System energy consumption 0.1632 kWhr/m^3

**NF intrinsic rejection**
- Ca_2+ intrinsic rejection 0.976946 fraction
- SO4_2- intrinsic rejection 0.998638 fraction
- HCO3_- intrinsic rejection 0.876292 fraction
- Na_+ intrinsic rejection 0.857046 fraction
- Cl_- intrinsic rejection 0.805398 fraction
- K_+ intrinsic rejection 0.856489 fraction
- Mg_2+ intrinsic rejection 0.977174 fraction

**NF observed rejection**

# Future work focusing on analyses and supporting users



# Thank you


- **National Energy Technology Laboratory:** David Miller, Tim Bartholomew, Markus Drouven, Andrew Lee, Andres Calderon-Vergara, Adam Atia, Chenyu Wang, Marcus Holly, Travis Arnold, Hunter Barber, Alejandro Garciadiego, Elmira Shamlou, Zhuoran Zhang, Savannah Sakhai

- **Lawrence Berkeley National Laboratory:** Deb Agarwal, Dan Gunter, Keith Beattie, Oluwamayowa Amusat, Jangho Park, Ludovico Bianchi, Jennifer Stokes-Draught, Xiangyu Bi, Michael Pesce

- **National Renewable Energy Laboratory:** Ben Knueven, Ethan Young, Jared Allen, Jordan Macknick, Kurby Sitterley, Kinshuk Panda, Zach Binger, Mukta Hardikar, Paul Vecchiarelli

- **Oak Ridge National Laboratory:** Srikanth Allu, Austin Ladshaw, Gavin Wiggins

- **SLAC National Accelerator Laboratory**: Alex Dudchenko