NAWI

National Alliance
for Water Innovation

WaterTAP – Supporting NAWI

Water treatment Technoeconomic Assessment Platform (WaterTAP)

Kris Villez

September 18th, 2024

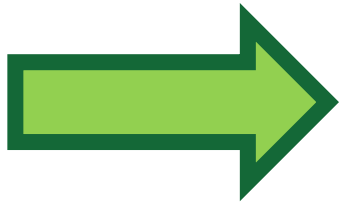
NAWI 1.0 (ends 2026)

- WaterTAP focus
  - Uniform modelling platform for plant-wide modelling
  - Techno-economic analysis software for process selection and design
  - Analysis to guide NAWI R&D efforts

OLI systems, inc.

PROTON®
Membrane Aqueous Chemistry Calculator

BLUE PLAN-IT®
DECISION SUPPORT SYSTEM



NAWI

Up next: Optimized water treatment train design & operation

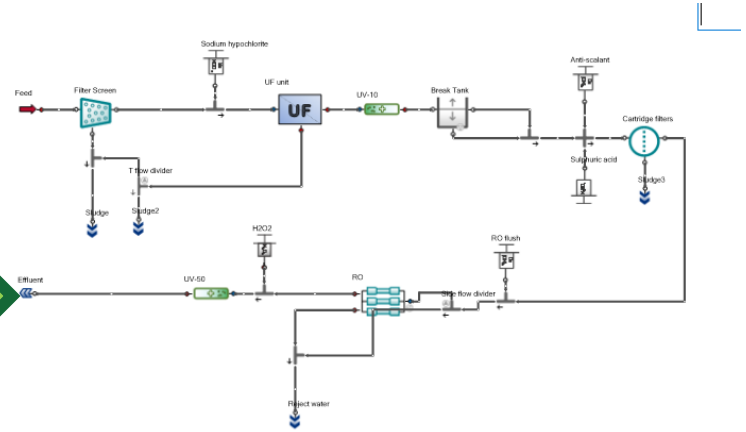
- Industry goals
  - Brackish water: increased water recovery (less brine)
  - Premise-scale water treatment:
    - Autonomy (limited on-site staff)
    - Reliability
  - Industrial cooling/heating:
    - Higher efficacy of treatment to enable alternative water sources
- Using alternative water sources invites new dynamics:
  - Water availability and quality
  - Electricity/resource markets, carbon intensity

Up next: Optimized water treatment train design & operation

Plant

Pilot (physical twin)

Model (digital twin)

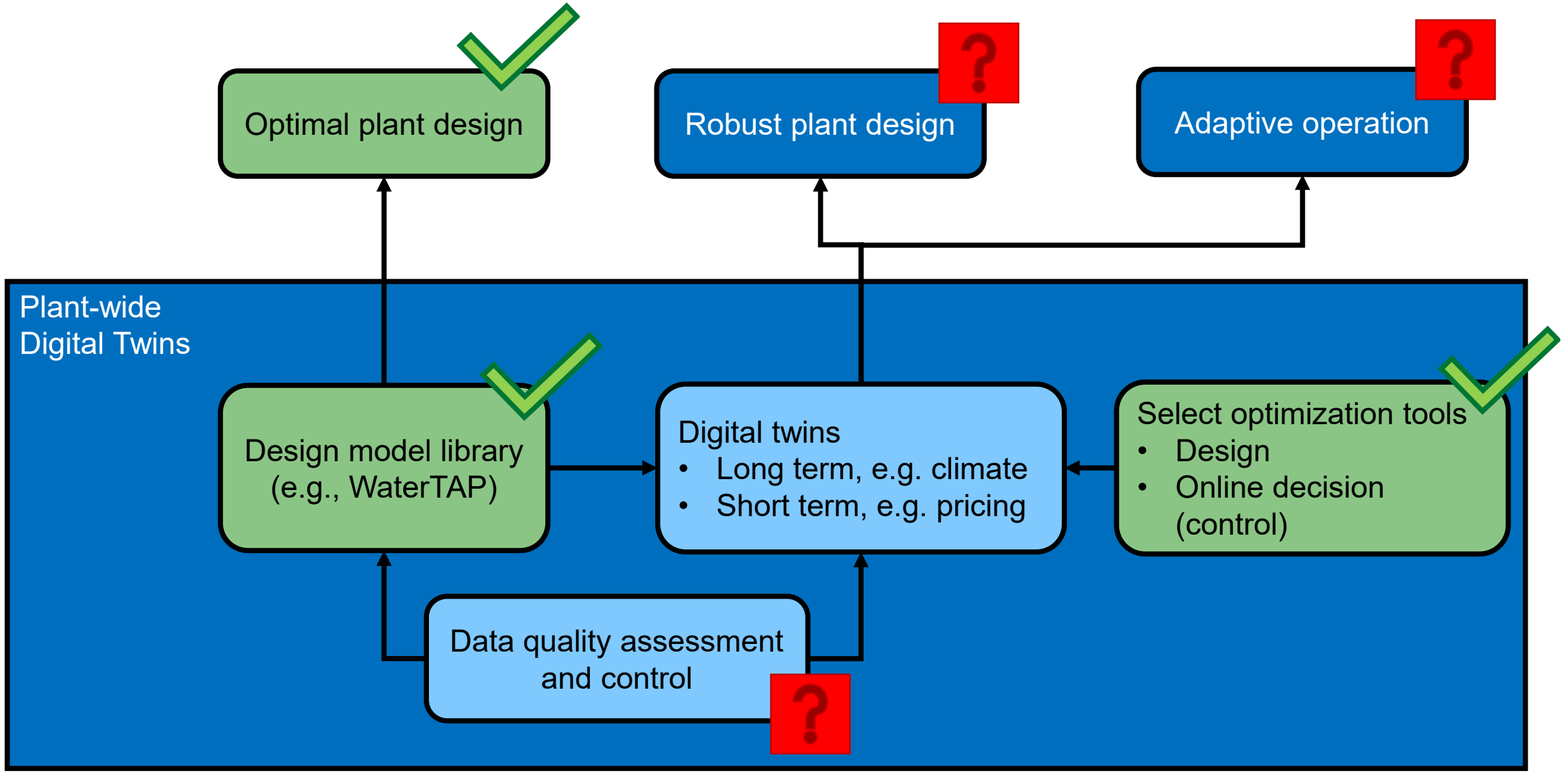


Real-time updating →

← **Optimal operation (MPC)**

← **Experimental design (ED)**

Up next: Optimized water treatment train design & operation



NAWI National Alliance for Water Innovation

WaterTAP Overview

Water treatment Technoeconomic Assessment Platform (WaterTAP)

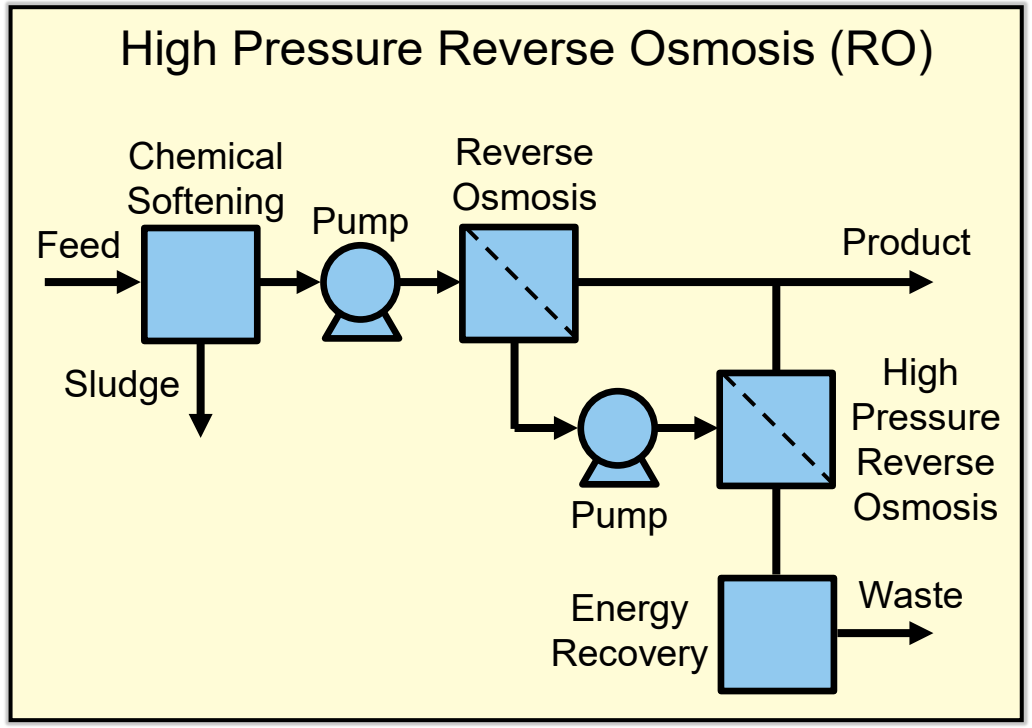
Tim Bartholomew

September 18th, 2024

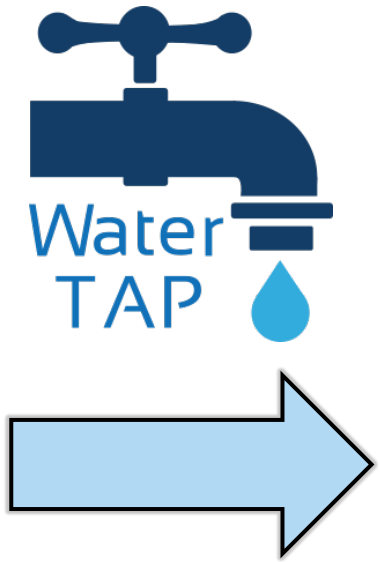
WaterTAP is a software tool for water treatment technoeconomic assessments

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

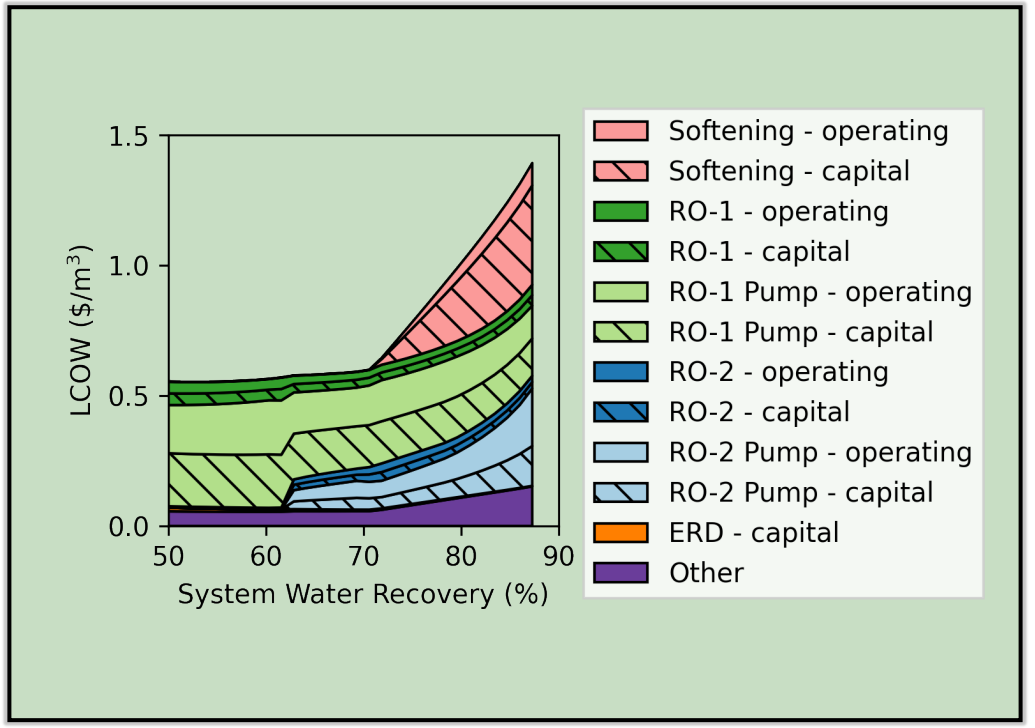
Emerging water treatment technology



Software tool



Technoeconomic assessment



A paradigm shift for water management requires advances in treatment technologies

NAWI

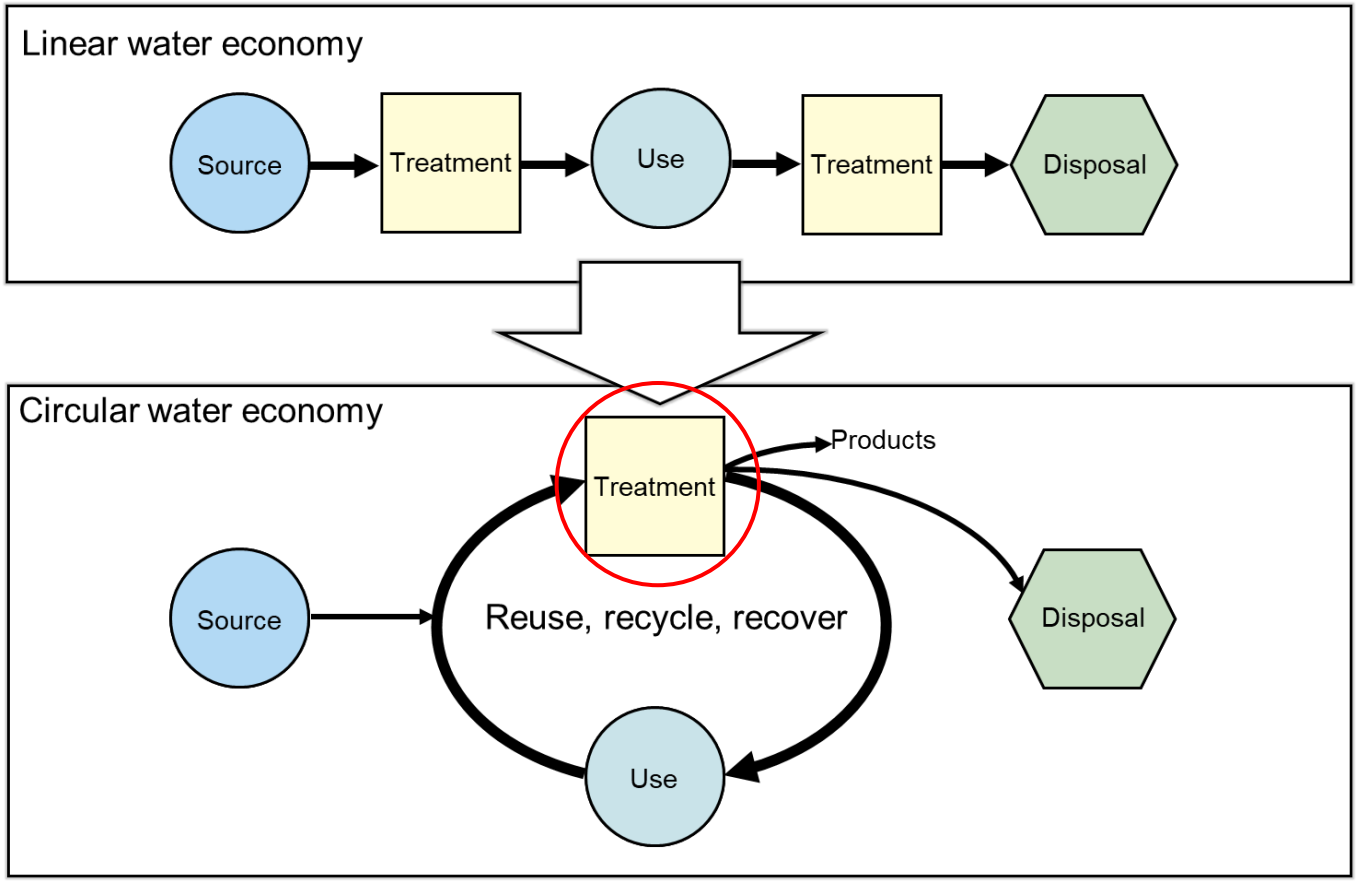
National Alliance for Water Innovation

U.S. DEPARTMENT OF ENERGY

Energy Efficiency & Renewable Energy

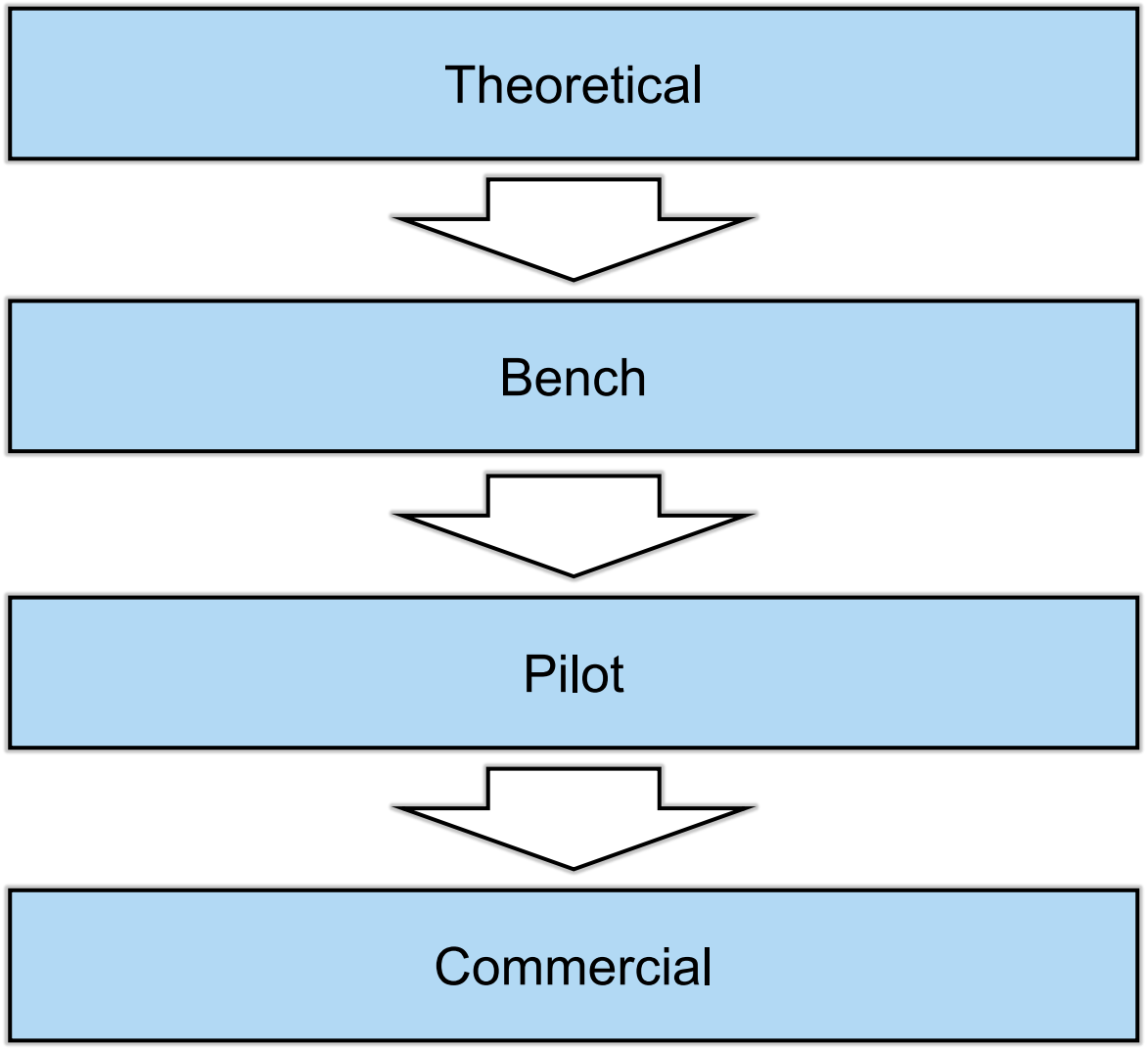
Industrial Efficiency & Decarbonization Office (IEDO)

Solar Energy Technologies Office (SETO)



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

TEA and modeling supports technological innovations throughout the R&D stages



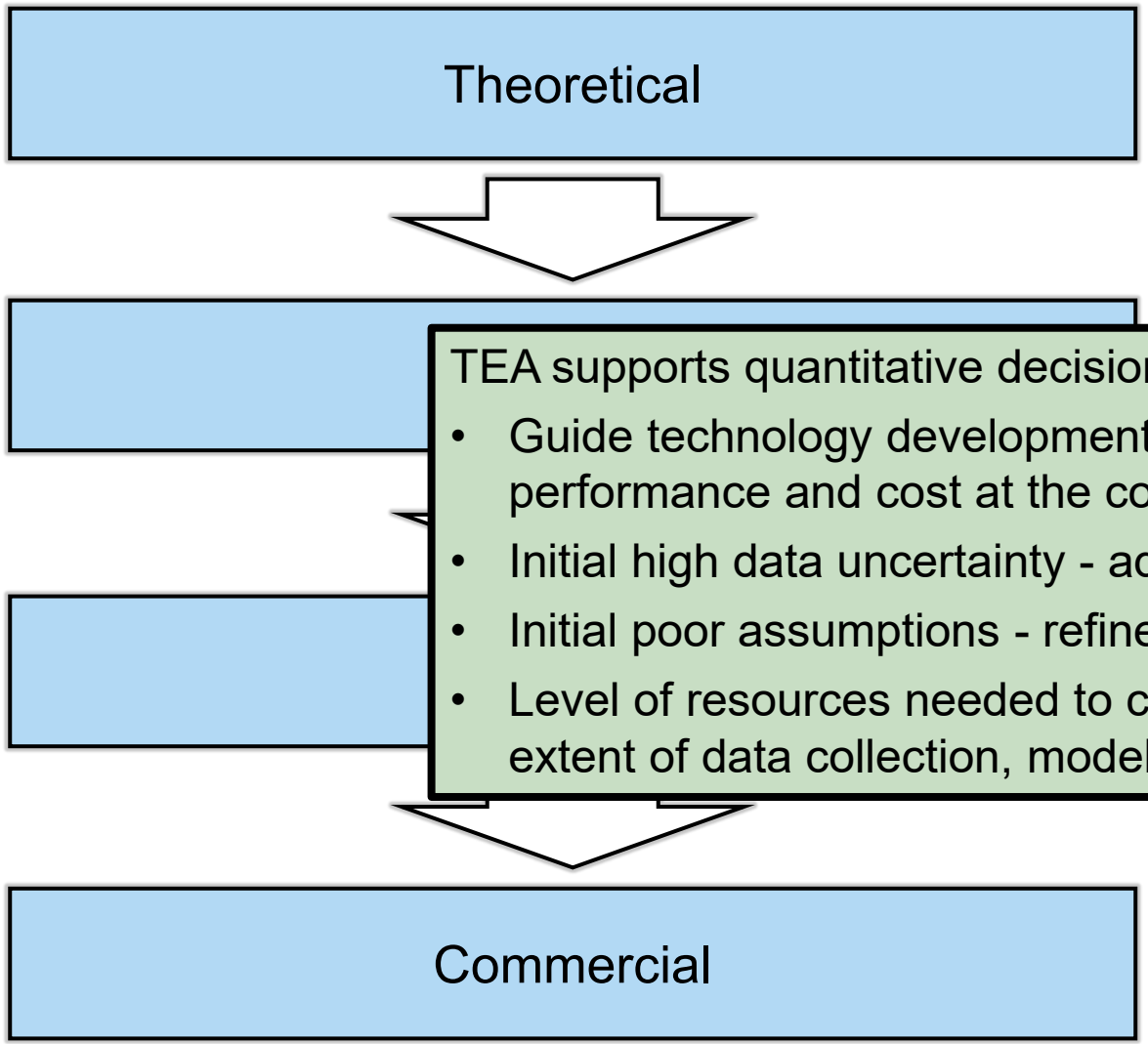
Concrete analyses

- Answers: What is _____?
- Data reconciliation – understanding the system
- Parameter estimation and model validation
- Provide real time insight into operation
- Enable conceptual analysis for recommendations

Conceptual analyses

- Answers: What if _____?
- Estimate performance and cost
- Identify research targets and potential bottlenecks
- Suggest best operation and design
- Compare potential alternatives and set priorities

TEA and modeling supports technological innovations throughout the R&D stages



Concrete analyses

- Answers: What is _____?
- Data reconciliation – understanding the system
- Parameter estimation and model validation
- eration
- ecommendations

TEA supports quantitative decision making throughout R&D lifecycle:

- Guide technology development based on best estimate of performance and cost at the commercial scale
- Initial high data uncertainty - address with sensitivity analyses
- Initial poor assumptions - refine with experimental campaigns
- Level of resources needed to conduct a TEA depends on the extent of data collection, model development, and analysis scope

ses

- Identify research targets and potential bottlenecks
- Suggest best operation and design
- Compare potential alternatives and set priorities

High quality TEA is challenging and time consuming

Existing water treatment software is great for quickly conducting the specific analyses they support

Engineering/consulting firms generally use several tools in a disjointed manner (e.g., Proton for RO, OLI for softening, in house for costing, etc.)

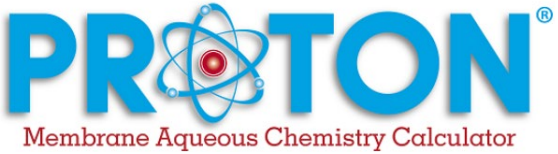
Researchers generally build/implement their own models from scratch (e.g., Excel, Python, MATLAB)

Drawbacks include:

- Inherent limitations due to interfacing between tools
- Time intensive to develop models and capabilities, eventually reducing the quality or scope of analyses
- Not available or extensible by others -> duplicative effort and hard to compare to previous work

Water Application Value Engine (WAVE)

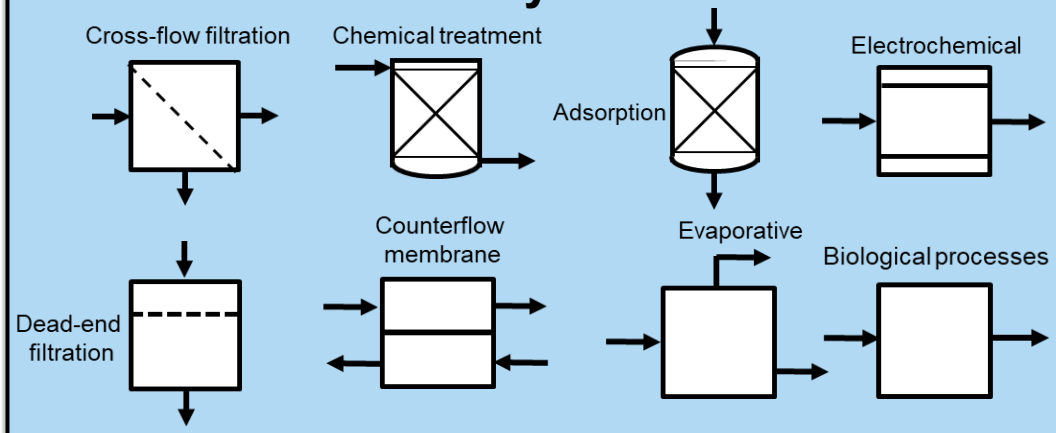
The SUper MOdel (Sumo)



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

Unified

Modular model library:



Software release:

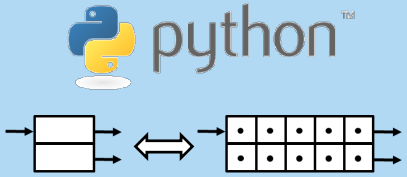
- Publicly accessible on GitHub
- Released every quarter
- https://github.com/watertap-org/watertap
- https://watertap.readthedocs.io/en/latest/
- `pip install watertap`

Flexible

Powerful

Core attributes:

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



$$f(x) = 0$$

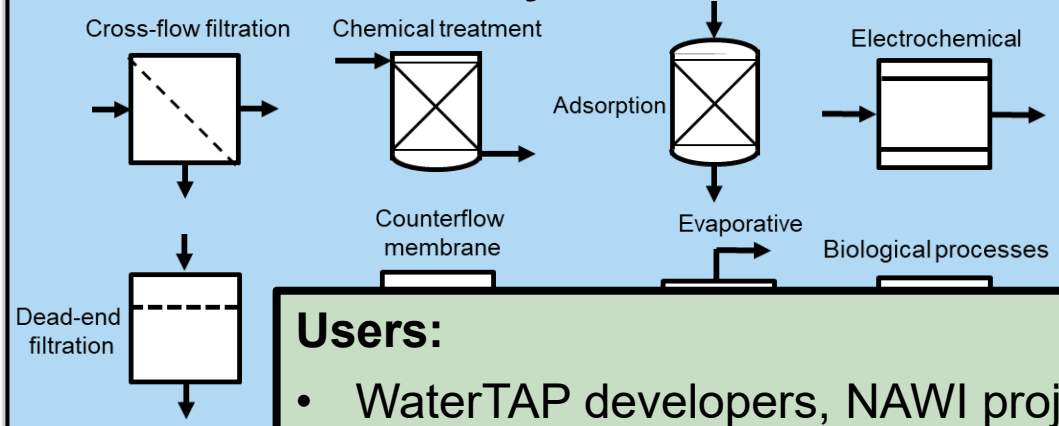
Core capabilities:

- 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

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

Unified

Modular model library:



Software release:

- Publicly accessible on GitHub
- Released every quarter
- https://github.com/watertap-org/watertap

...pcs.io/en/latest/

...p

Users:

- WaterTAP developers, NAWI project collaborators
- Other programs (e.g., PrOMMiS, CoWERC)

Use:

- Code based interface (primary)
- Graphical user interface (secondary)

Flexible

Core attrib...

- Open-s...
- Multi-hi...
- Custom...

Powerful

- Equation oriented
- IDAES compatible

PYOMO

IDAES Institute for the Design of Advanced Energy Systems

...device integration

...mplex systems

...sider uncertainty

- Parameter estimation to fit real-world data
- Data-driven models for complex phenomena

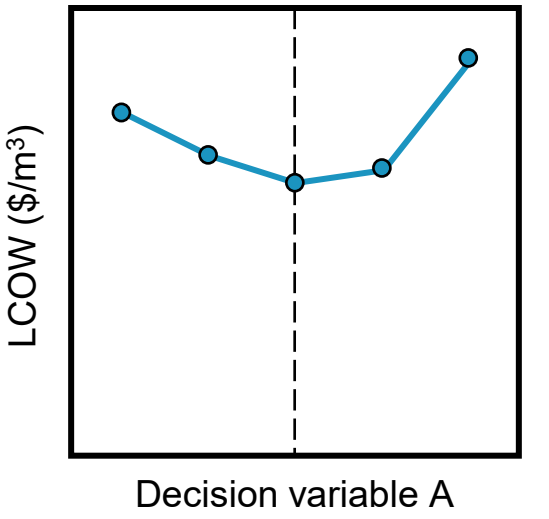
Dan Gunter: 1:30 today (Panel 1), 11:30am tomorrow (main room)

Mathematical optimization greatly expands TEAs

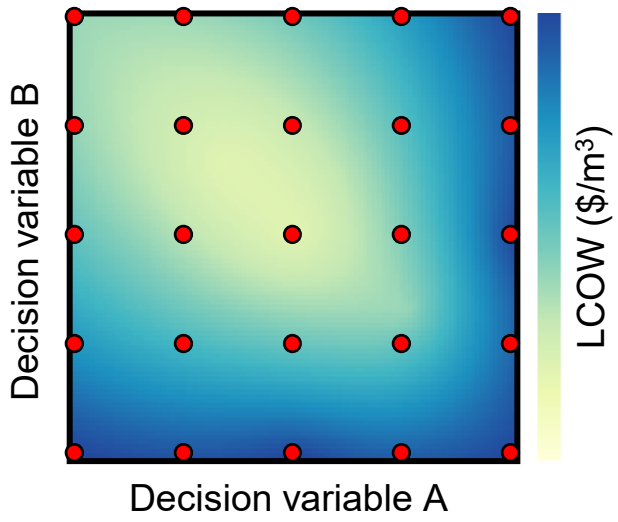
Simulation based modeling focuses on **decision variables**

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

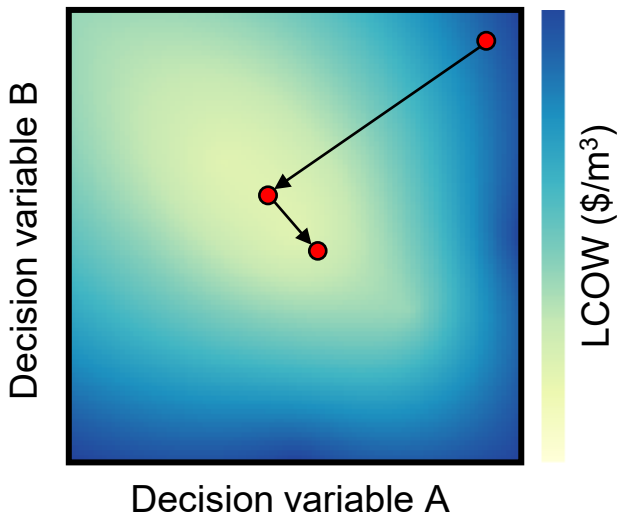
Simulation based sensitivity



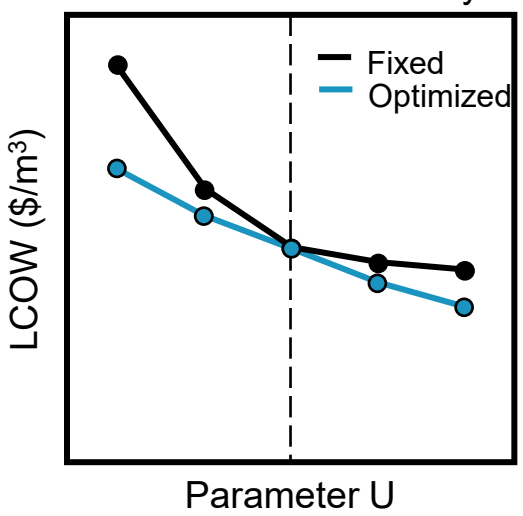
Simulation based optimization



Mathematical optimization



Parameter sensitivity

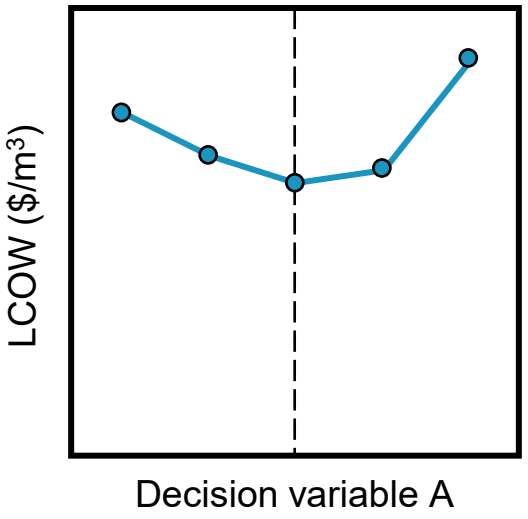


Mathematical optimization greatly expands TEAs

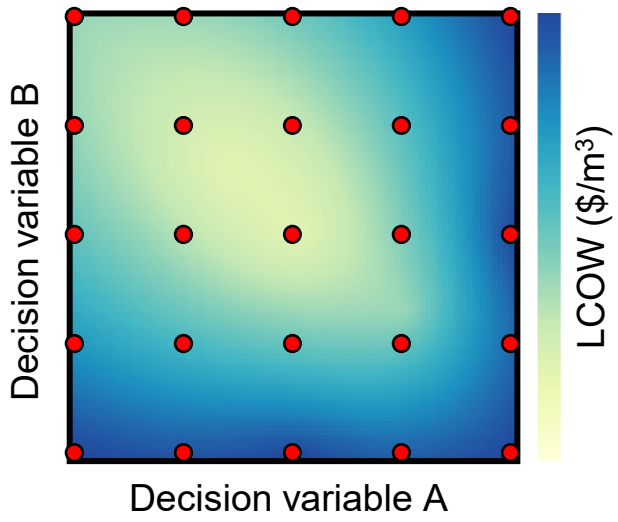
Simulation based modeling focuses on **decision variables**

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

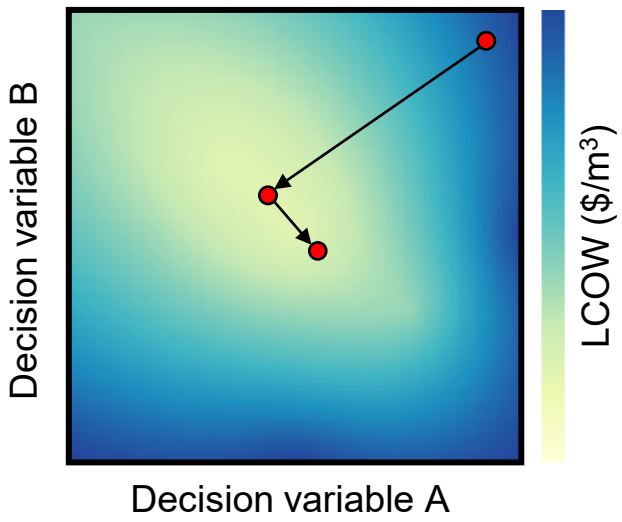
Simulation based sensitivity



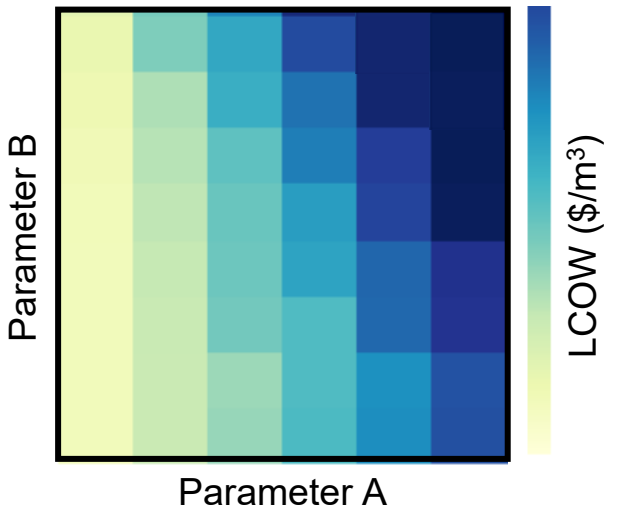
Simulation based optimization



Mathematical optimization



Dual parameter analysis



Equation oriented methods provide this optimization capability, but it requires all models to support it (Pyomo and IDAES)

NAWI

Detailed water chemistry is supported on WaterTAP

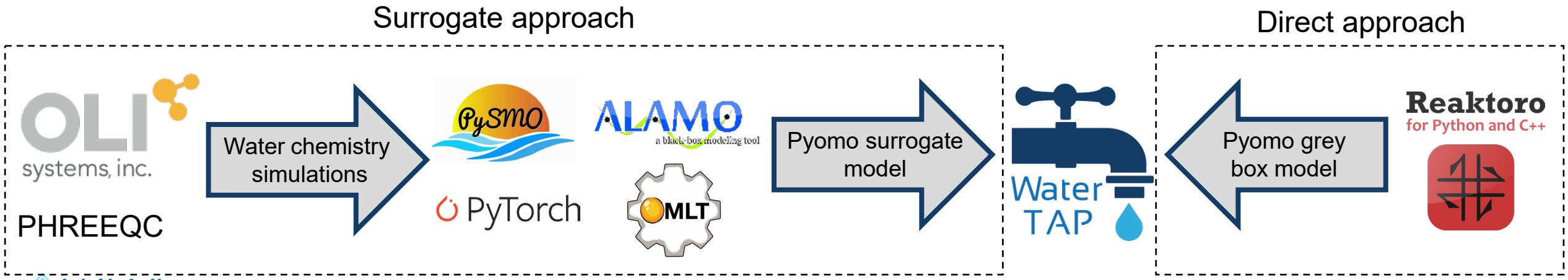
Modeling complex water chemistry is challenging and data intensive

- 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)

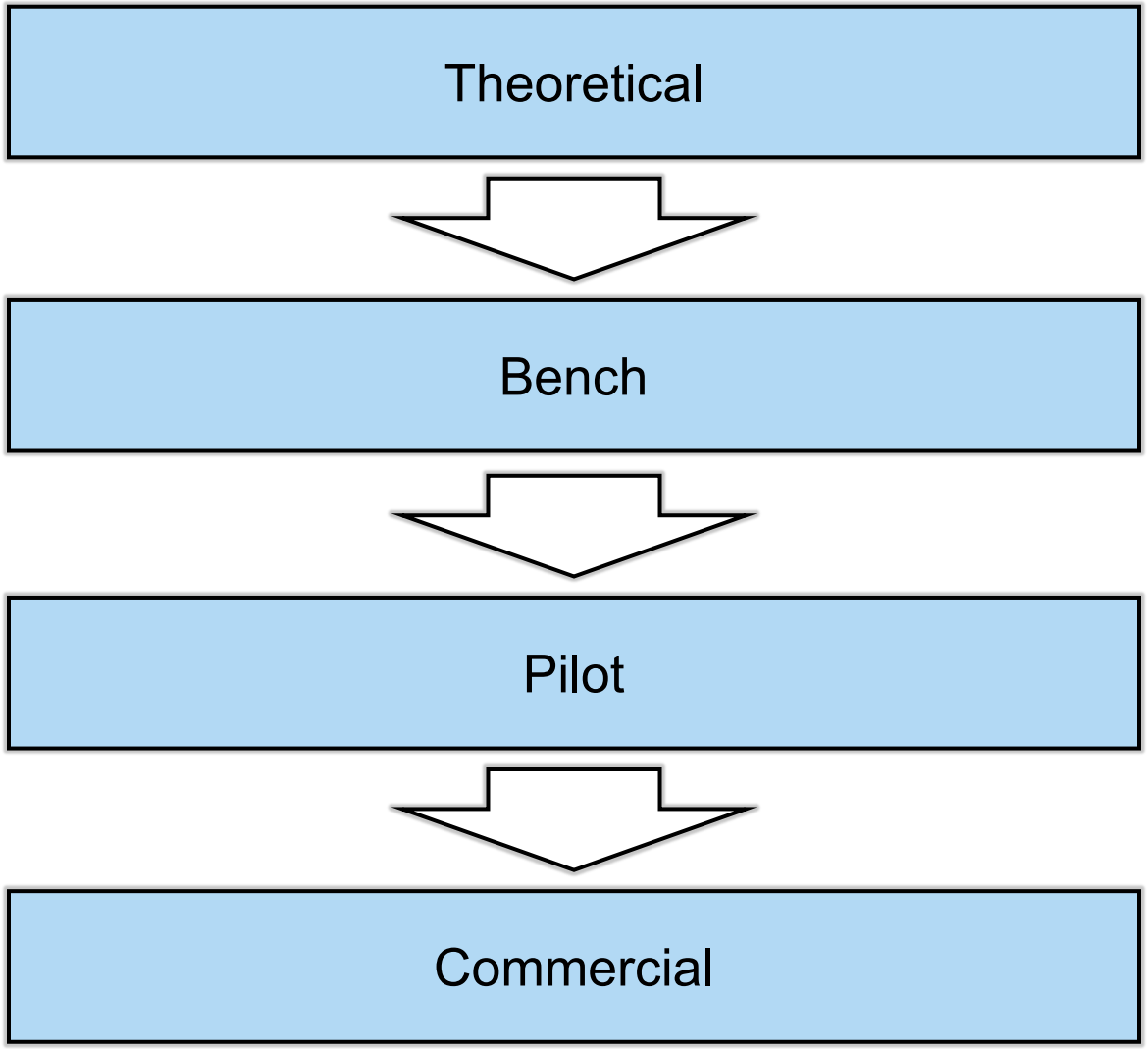
- Data availability limits the species than can be considered
- Large models pose challenges for mathematical optimization

WaterTAP leverages external water chemistry software



Alex Dudchenko: 4:30pm today, 5pm tomorrow (main room)

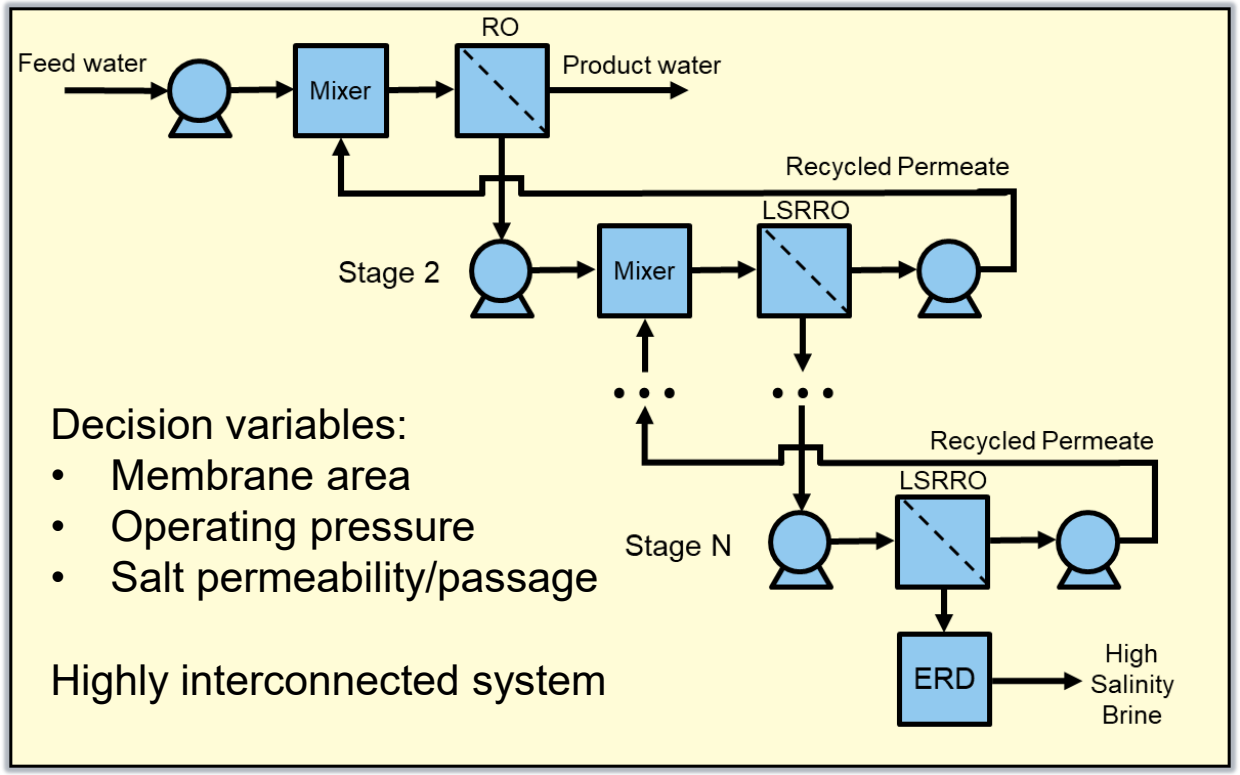
WaterTAP has multiple examples supporting technologies throughout all the development stages



Exploring the potential of a novel membrane process

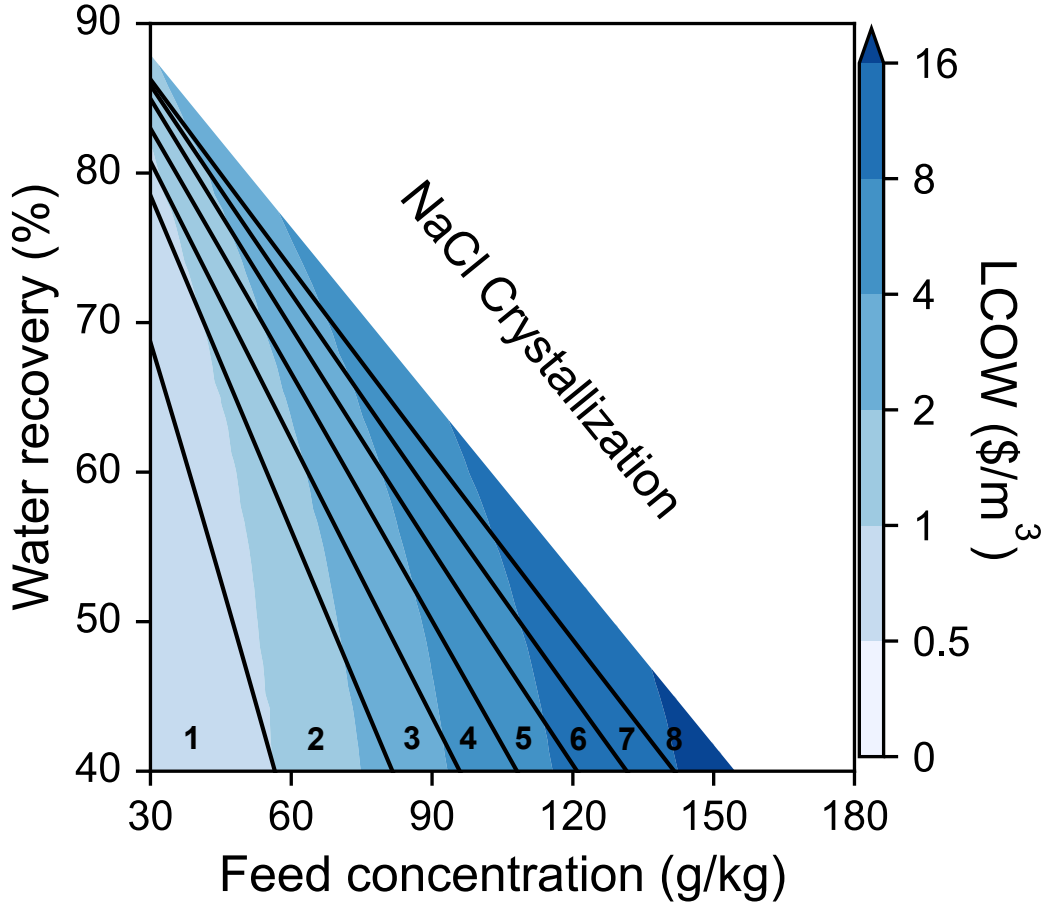
Theoretical

Low salt rejection reverse osmosis (LSRRO)



Decision variables:
- Membrane area
- Operating pressure
- Salt permeability/passage

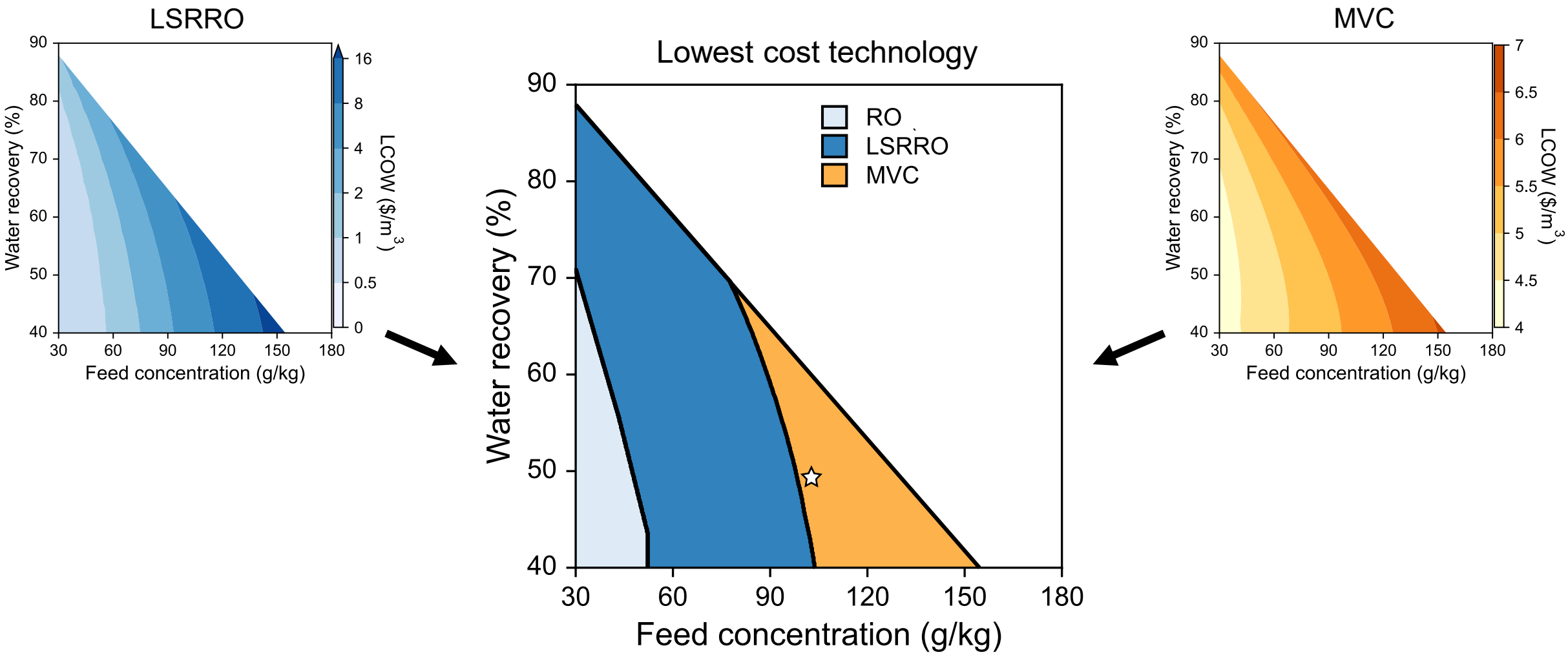
Highly interconnected system



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

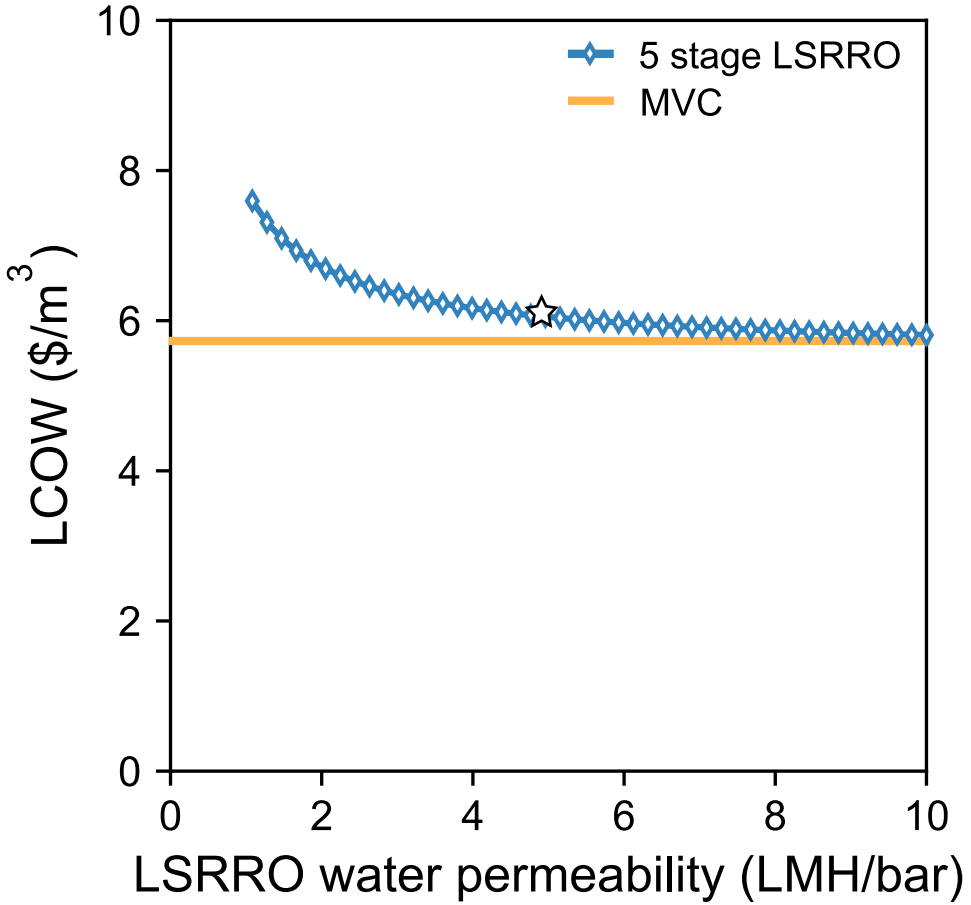
Quantifying technoeconomic viability through comparison

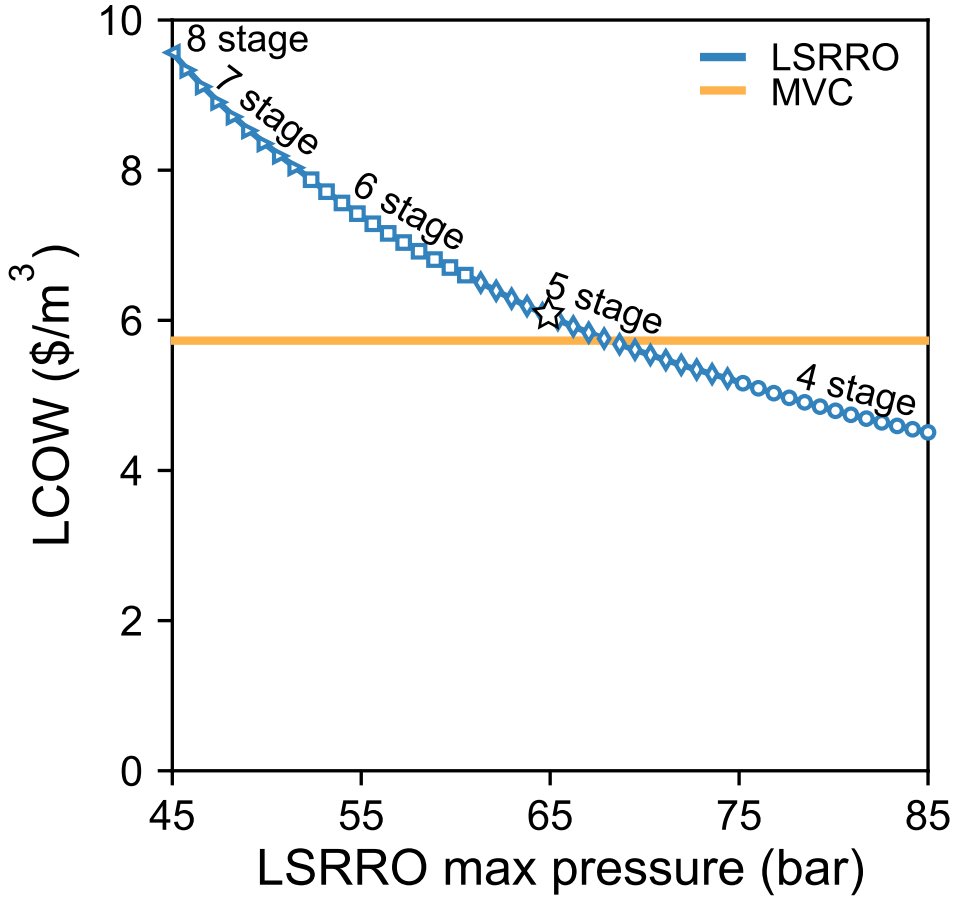
Case: 100 g/kg and 50% water recovery



Using sensitivity analysis to prioritize development

Case: 100 g/kg and 50% water recovery



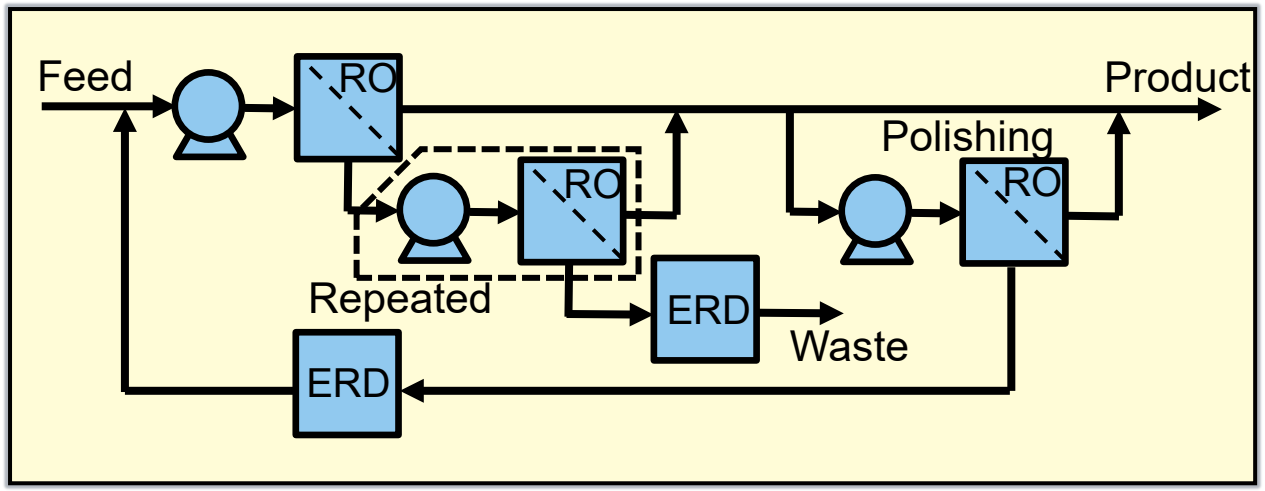


Atia et al. *Desalination.* 2023, 551, 116407

Projecting the implications of bench-scale data

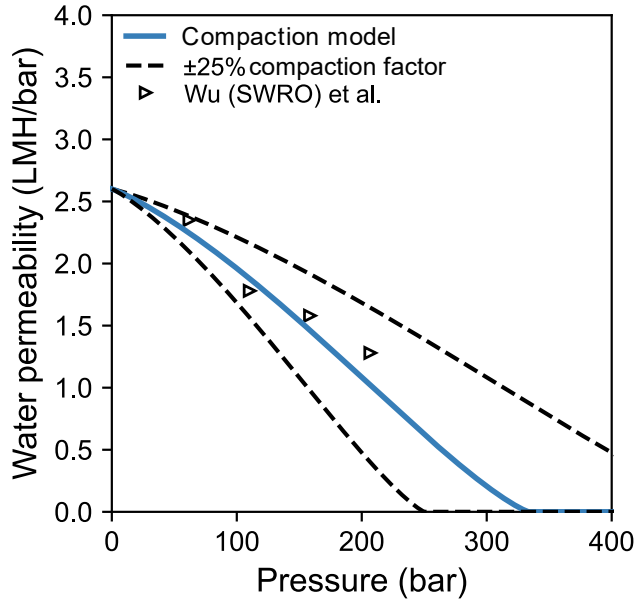
Bench

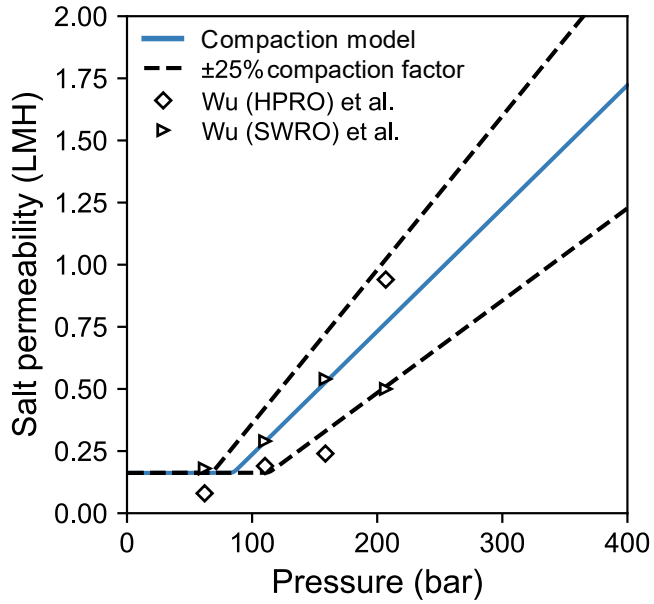
High pressure reverse osmosis (HPRO)



Two known challenges:

- Membrane compaction at high pressures decreases water permeability and increases salt permeability



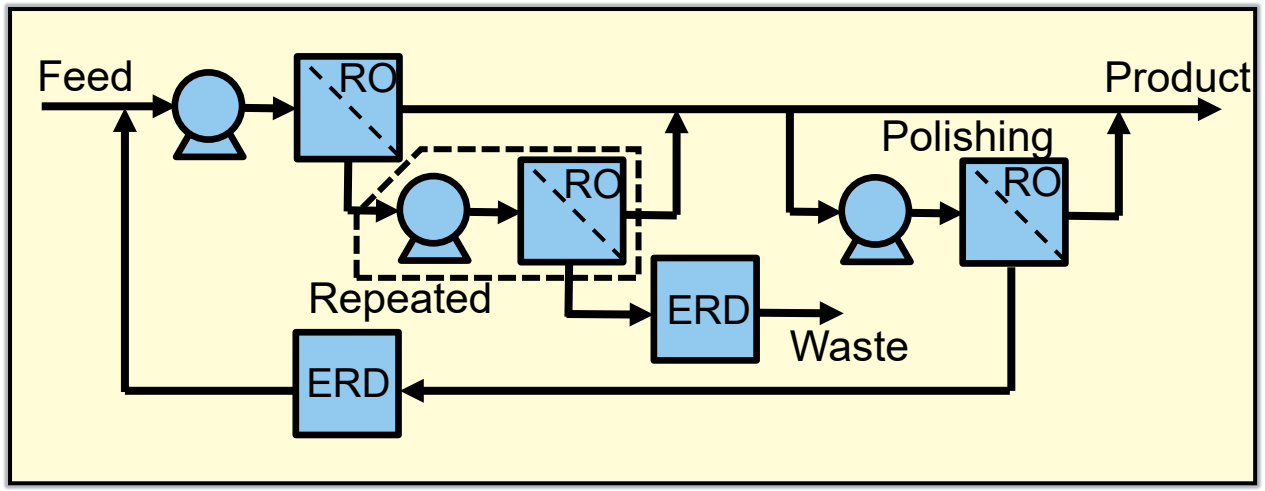


NAWI

Projecting the implications of bench-scale data

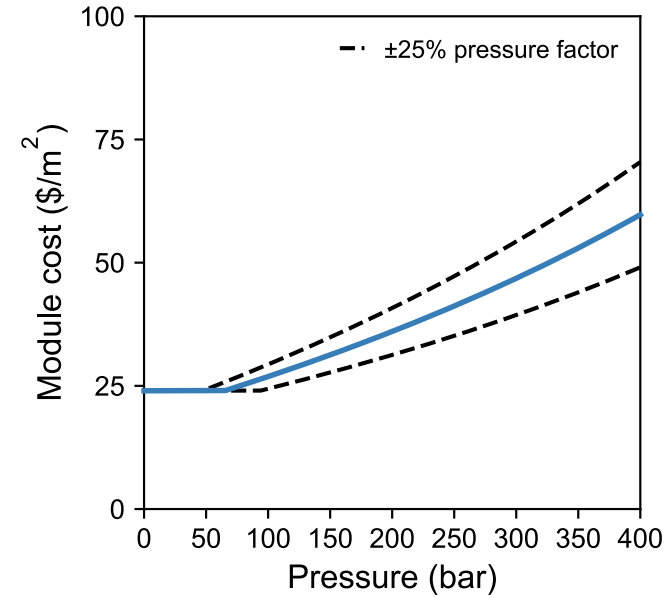
Bench

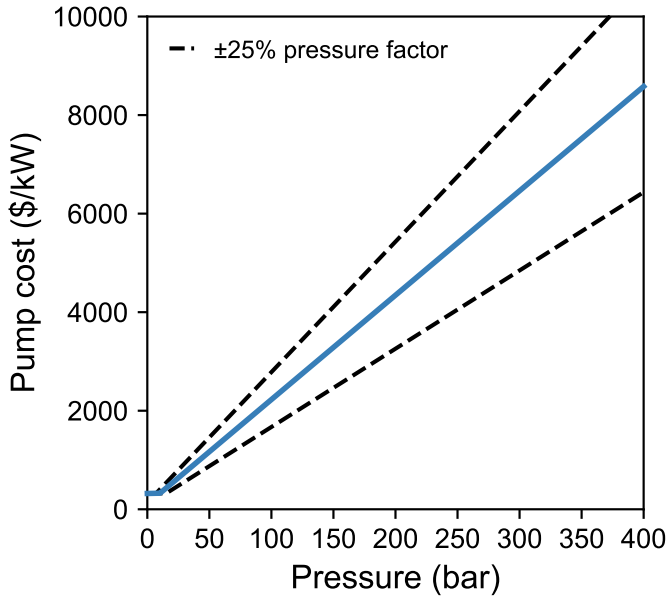
High pressure reverse osmosis (HPRO)



Two known challenges:

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



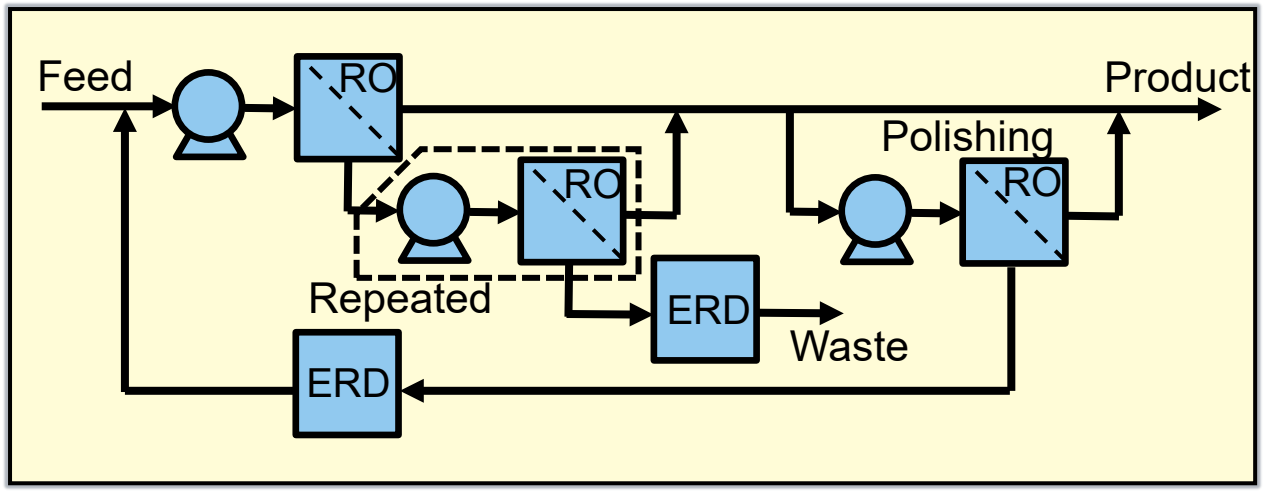


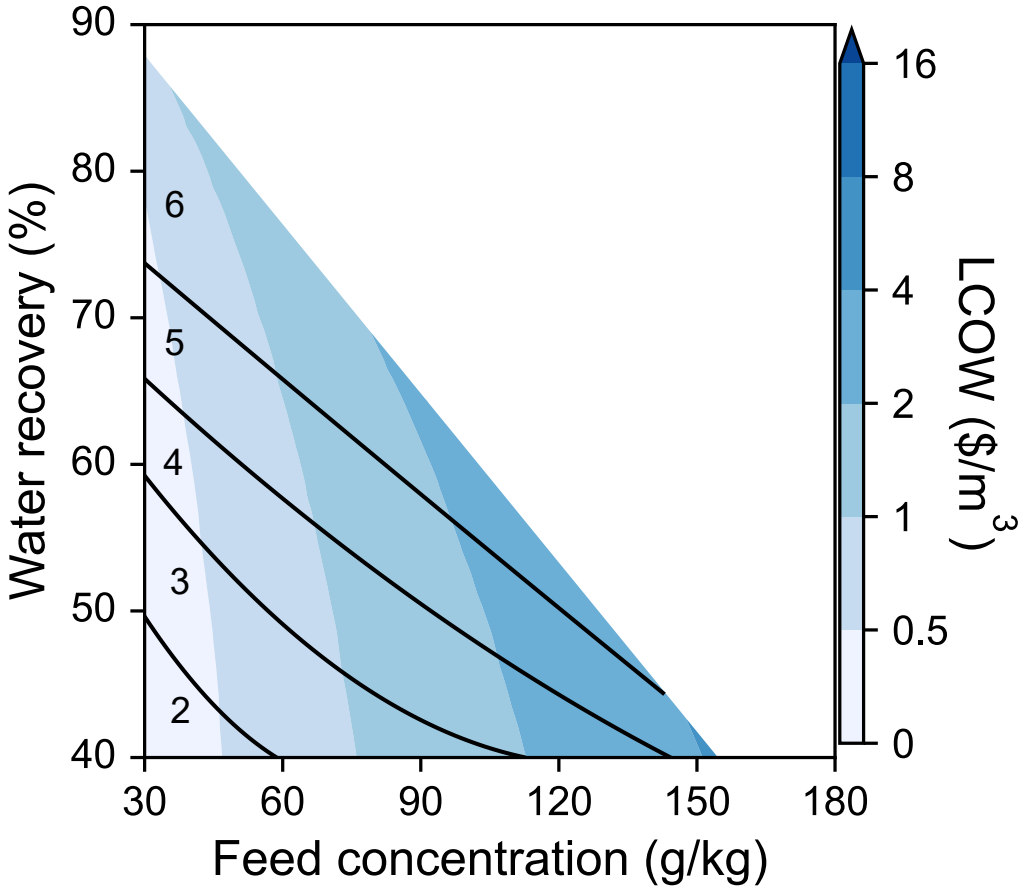
NAWI

Projecting the implications of bench-scale data

Bench

High pressure reverse osmosis (HPRO)





Two known challenges:

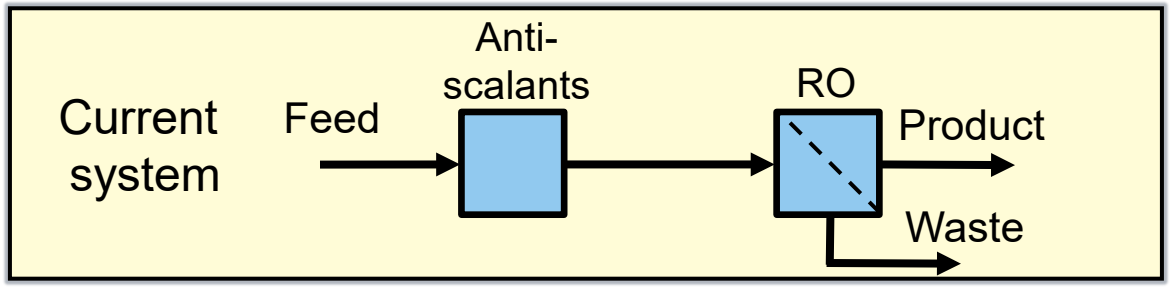
- Membrane compaction at high pressures decreases water permeability and increases salt permeability
- Equipment that operates at higher pressures are more expensive

NAWI

Assisting pilot design and operation

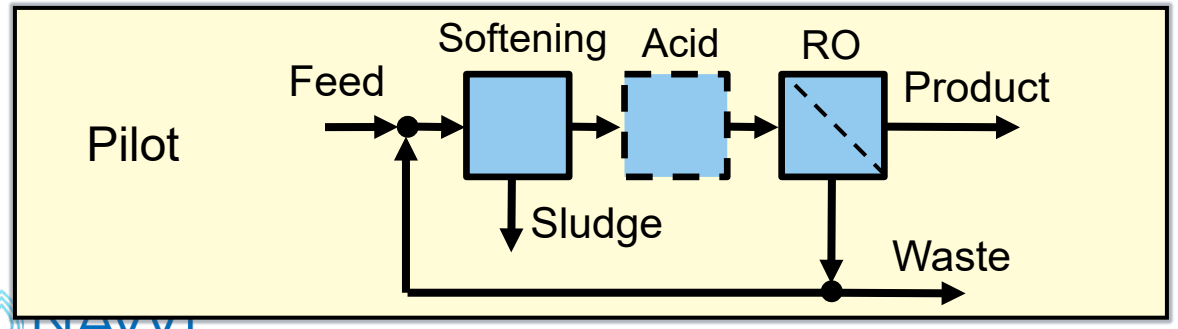
Pilot

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



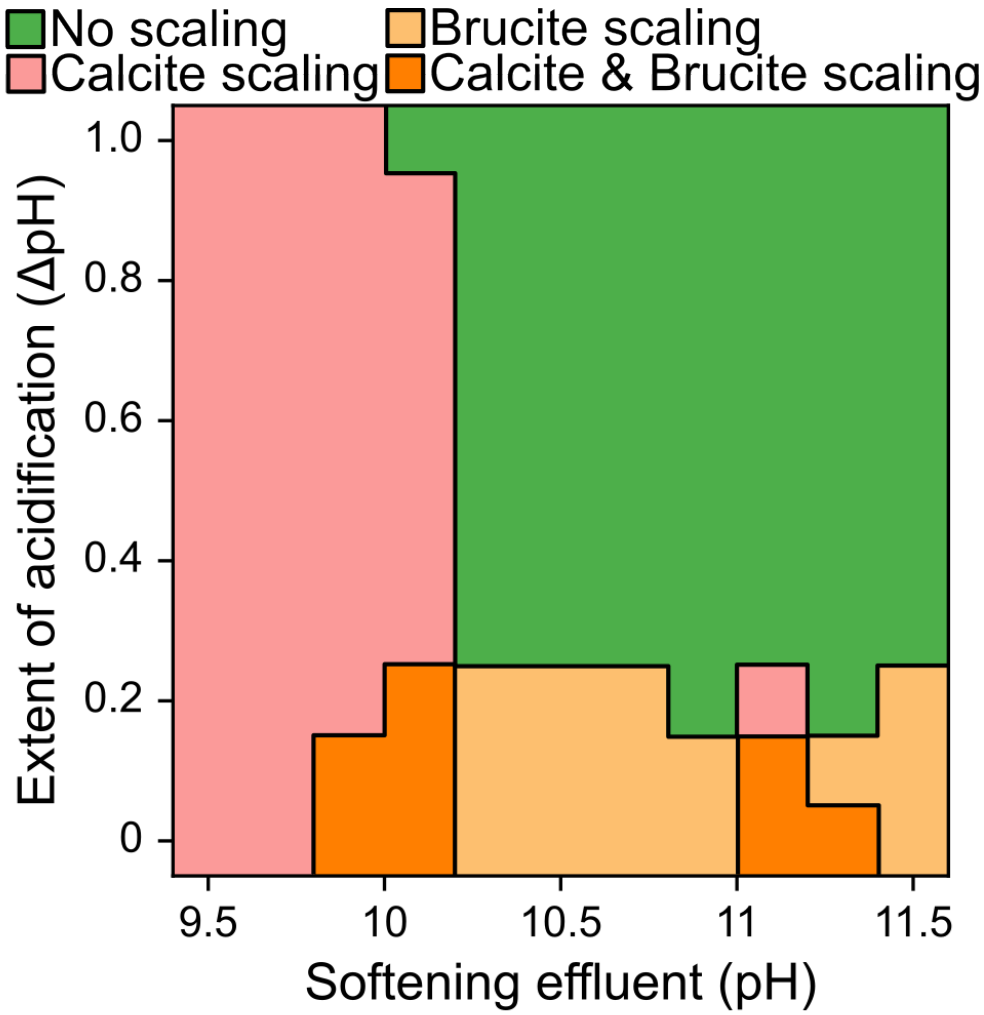
Pilot seeks to address two issues:

- 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

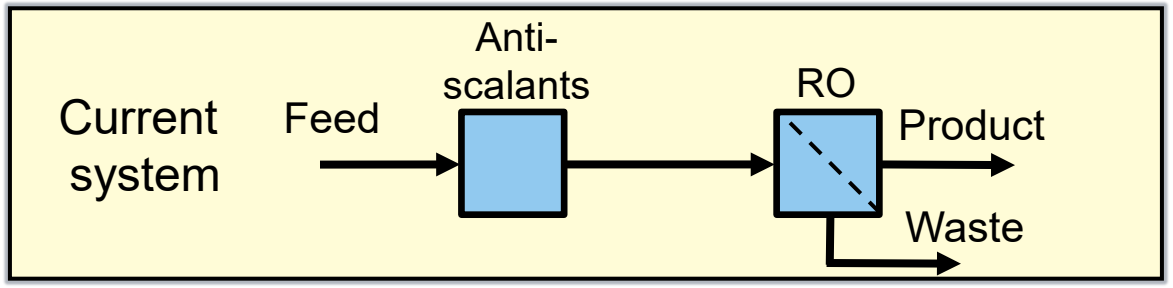
Prof. Manish Kumar



Assisting pilot design and operation

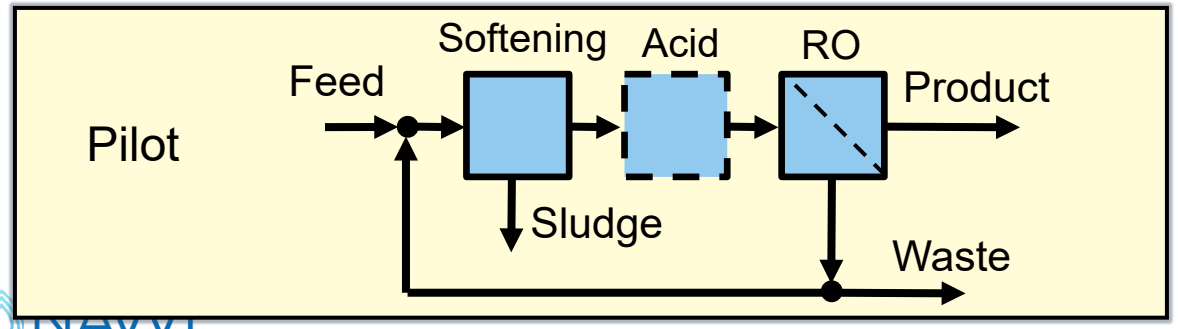
Pilot

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

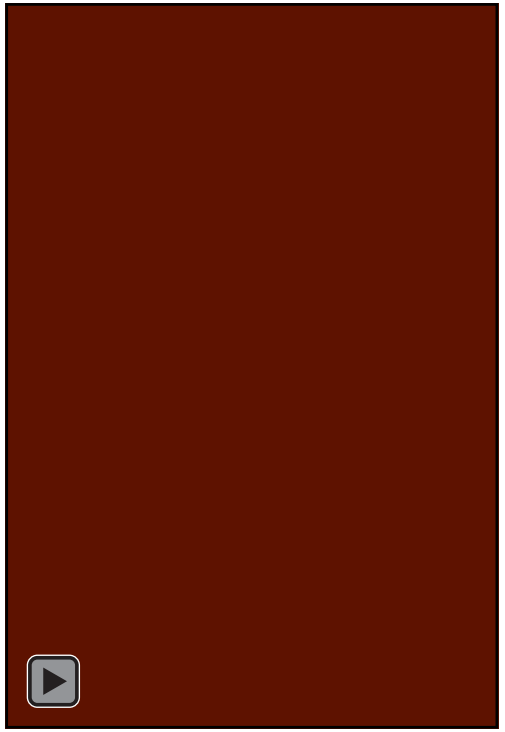


Pilot seeks to address two issues:

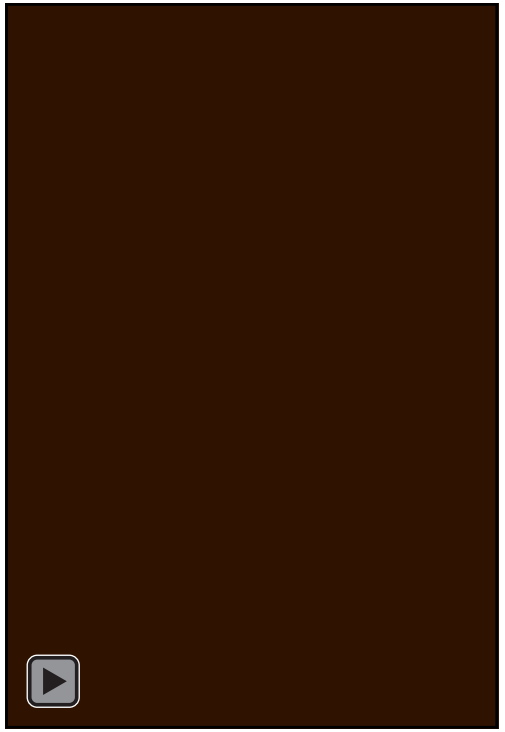
- Mineral scaling even with significant antiscalant dosing (at a high cost)
- High disposal volumes with only 50% water recovery



Before



After



Benefits:

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

Cons:

- Lime softening and waste sludge generation

Supporting commercial-scale retrofit

Commercial

CalPolyPomona

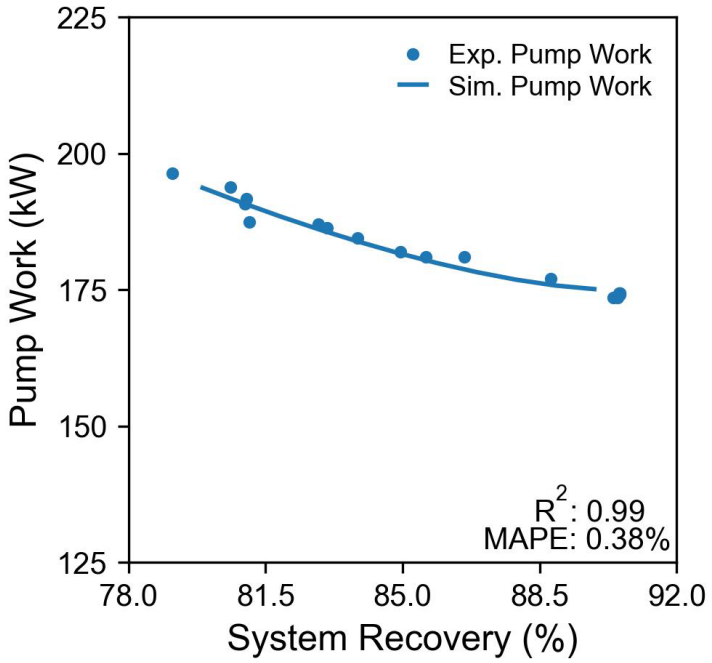
Chino Basin Desalter

Prof. Mingheng Li

Commercial brine concentration

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



NAWI

Zach Binger: 8:30am tomorrow (WaterTAP breakout)

Supporting commercial-scale retrofit

Commercial

CalPolyPomona

Chino Basin Desalter

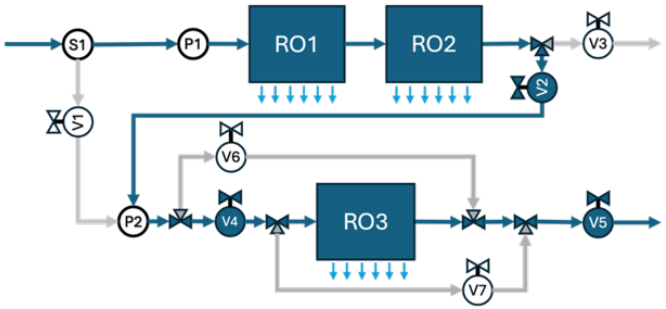
Prof. Mingheng Li

Commercial brine concentration

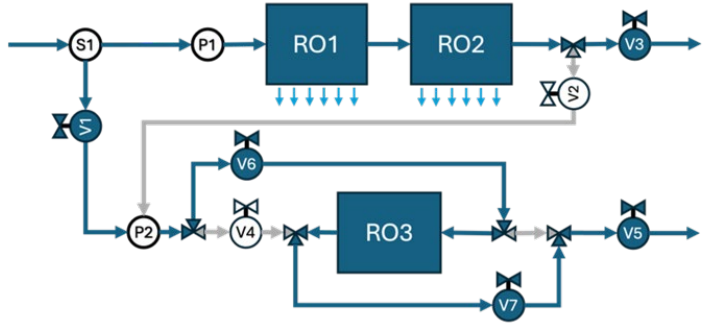
Analysis seeks to evaluate a potential retrofit:

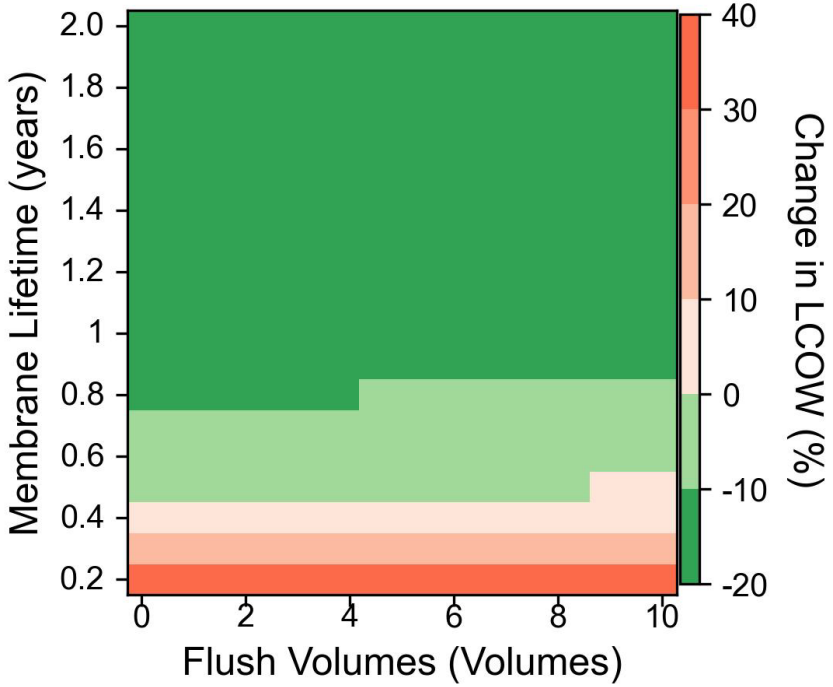
- Reduce disposal costs by increasing recovery
- Potentially add third stage RO with feed flow reversal to mitigate mineral scaling

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?

NAWI

Zach Binger: 8:30am tomorrow (WaterTAP breakout)

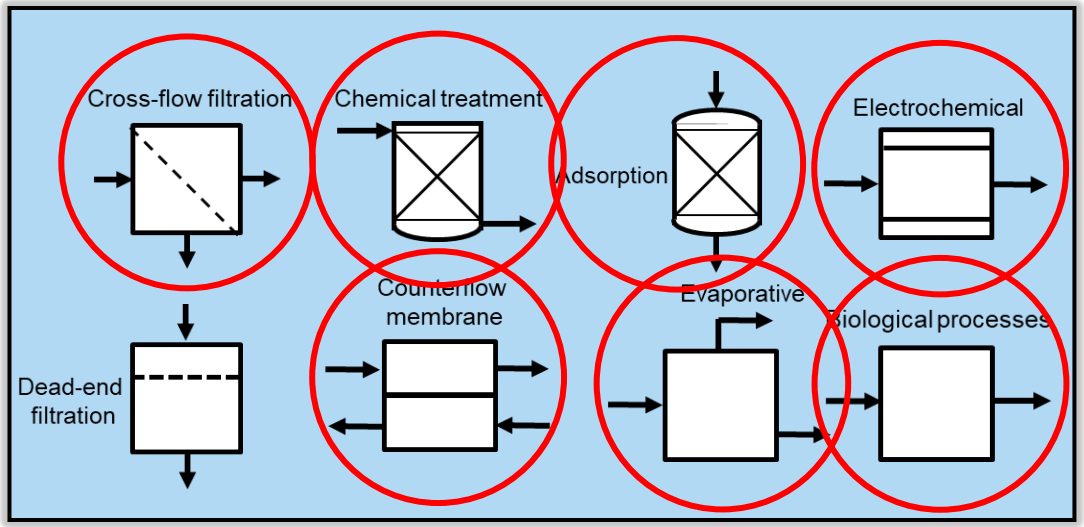
WaterTAP has a broad water treatment library

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 kinetic reactors



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

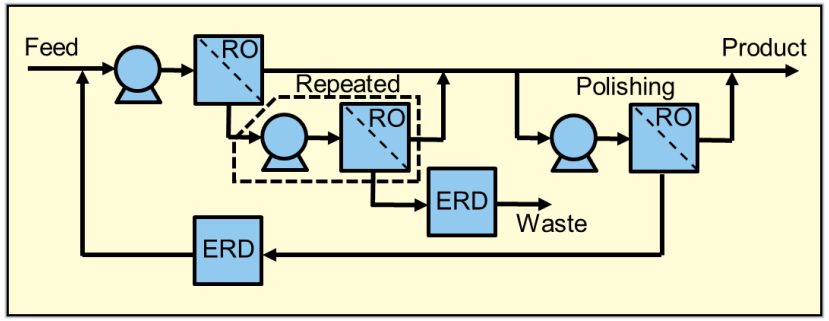
Biological:
- Activated sludge
- Anaerobic digestor

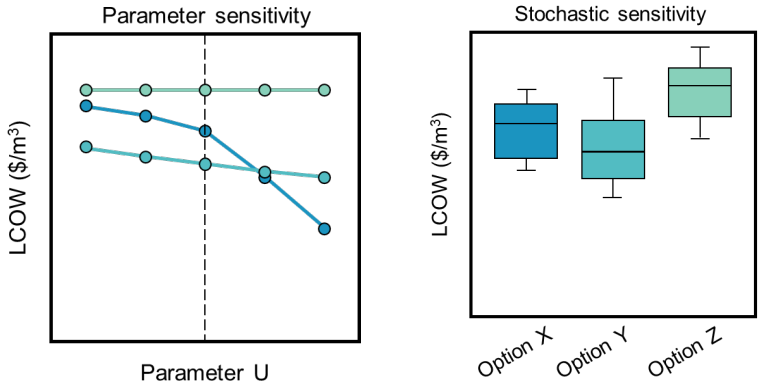
Auxiliary equipment:
- pumps, heat exchangers, mixers, splitters

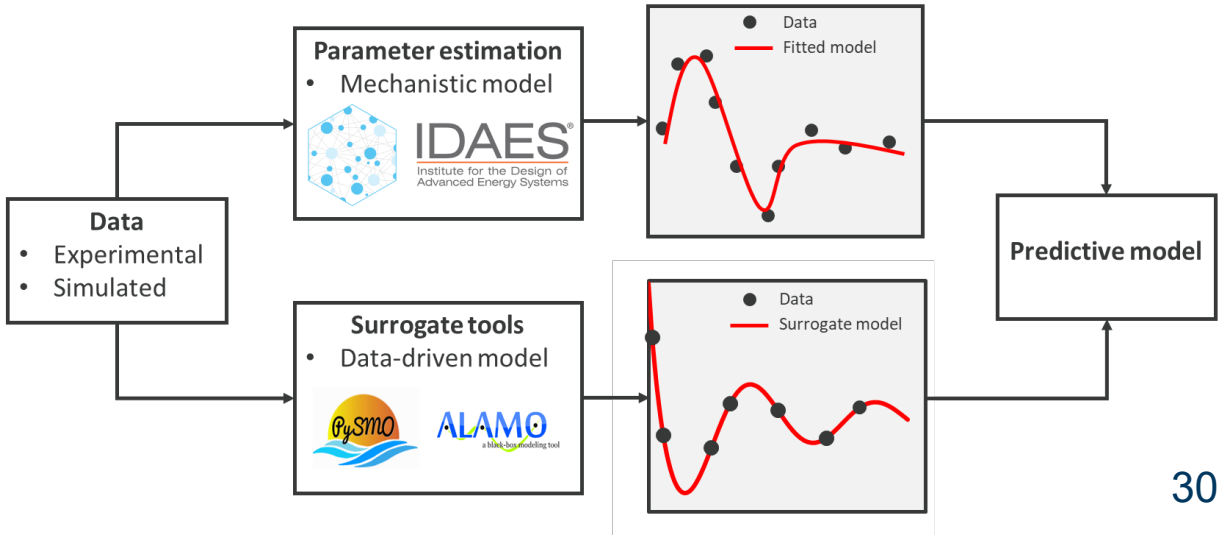
Hunter Barber: 8:55am tomorrow (WaterTAP breakout)

WaterTAP has several valuable core capabilities

- Simulation and optimization of treatment trains assembled from modular model library
- Parametric sensitivity analyses
- Stochastic sensitivity analyses
- Parameter estimation
- Surrogate modeling







WaterTAP has several valuable core capabilities

- Simulation and
  trains assemble
- Parametric sens
- Stochastic sens
- Parameter estin
- Surrogate mode

Water TAP

"An equation-oriented, optimization-based integrated process modeling platform"

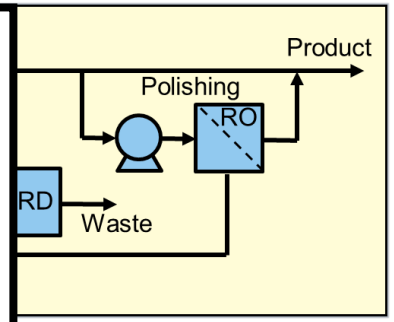
IDAES
Institute for the Design of Advanced Energy Systems

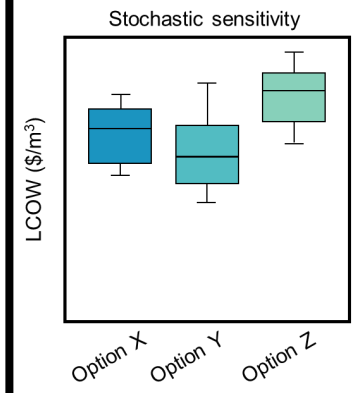
2020 R&D 100 WINNER

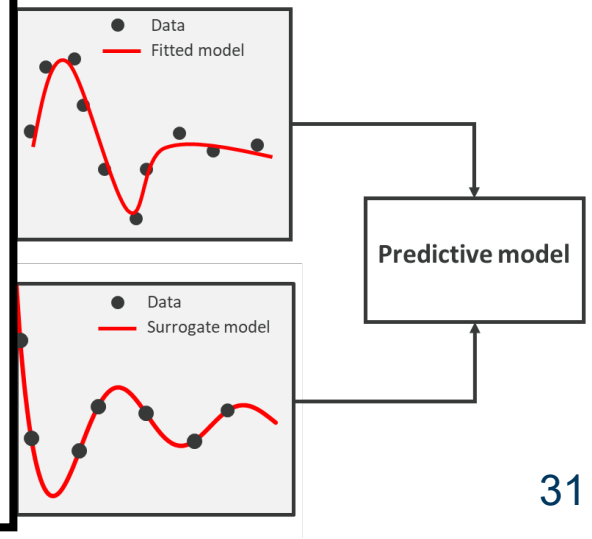
"Rich software environment for formulating and analyzing optimization applications"

PYOMO

2016 R&D 100 WINNER







NAWI

WaterTAP has several valuable core capabilities

- Simu
  train
- Para
- Stoc
- Para
- Surr

Akshay Rao: 9:25am tomorrow (WaterTAP breakout)

Alejandro Garciadiego: 9:50am tomorrow (WaterTAP breakout)

DISPATCHES → Water TAP ↔ PROMMIS

Process Optimization and Modeling for Minerals Sustainability

"An equation-oriented, optimization-based integrated process modeling platform"

IDAES

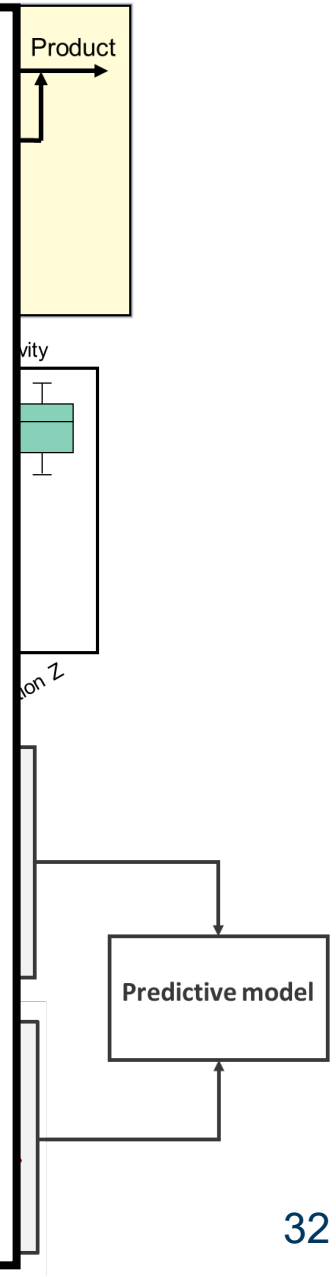
Institute for the Design of Advanced Energy Systems

2020 R&D 100 WINNER

"Rich software environment for formulating and analyzing optimization applications"

PYOMO

2016 R&D 100 WINNER



NAWI

WaterTAP is pivoting for NAWI 2.0 (2025-2029)

Previous focus:

- Technoeconomic assessments (TEA) for researchers

Future development:

- Provide technical assistance for pilot projects
  - Dynamic modeling and controls
  - Model based design of experiments
  - Robust optimization
- Analysis tool for consultants/engineers
  - Demonstrate value with industry case studies
  - Specifically support high demand analyses

IDAES
Institute for the Design of Advanced Energy Systems

PyROS

Alex Dowling and Chrysanthos Gounaris:
1pm tomorrow (Main room)

WaterTAP is pivoting for NAWI 2.0 (2025-2029)

Previous focus:

- Technoeconomic assessments (TEA) for researchers

Future

- Provide
  - Dy
  - M
  - R
- Analysi
  - Demonstrate value with industry case studies
  - Specifically support high demand analyses

WaterTAP provides a platform that is:

- Unified – broad treatment technologies and applications
- Flexible – customizable, modular, hierarchical
- Powerful – advanced simulation and optimization capabilities

A centralized platform enables TEAs to be more:

- Reproducible – can run codes that are publicly accessible
- Comparable – can updated previous analyses with new parameters
- Extendable – can modify and build upon previous models

ES
Design of
gy Systems

os

Thank you

- **National Energy Technology Laboratory:** David Miller, Tim Bartholomew, Andrew Lee, Markus Drouven, 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, Johnson Dhanasekaran, Fahim Abdullah

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