NAWI National Alliance for Water Innovation

Incorporating Detailed Water Chemistry with Process-Scale Cost Optimization

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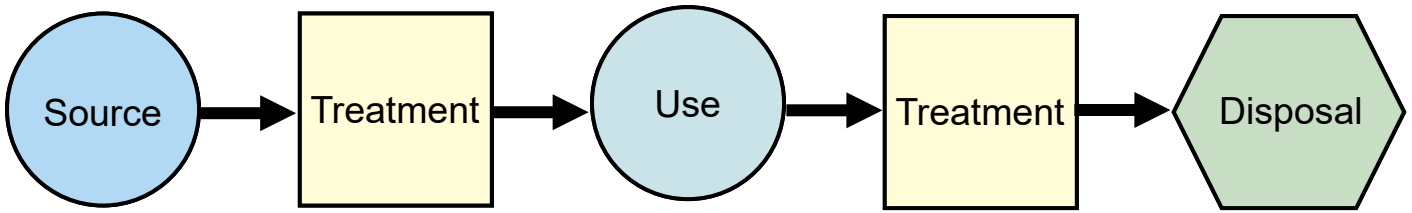
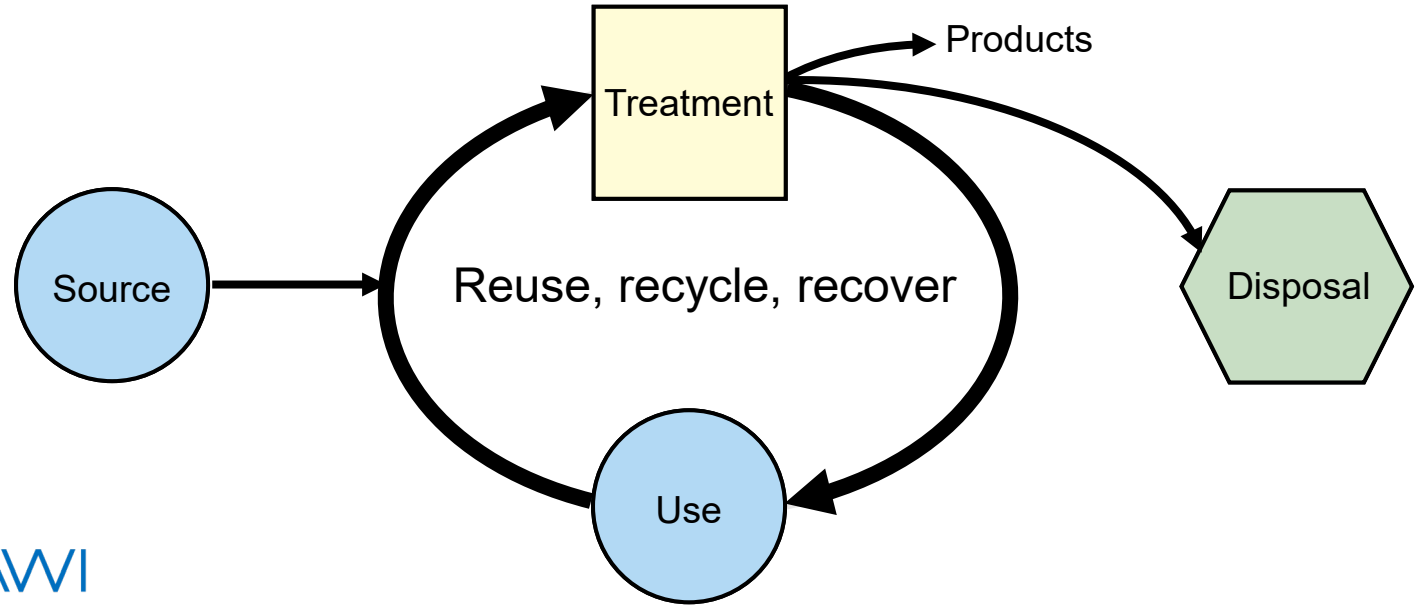
There is a growing demand for high water recovery desalination

Current 20th century paradigm - linear water economy



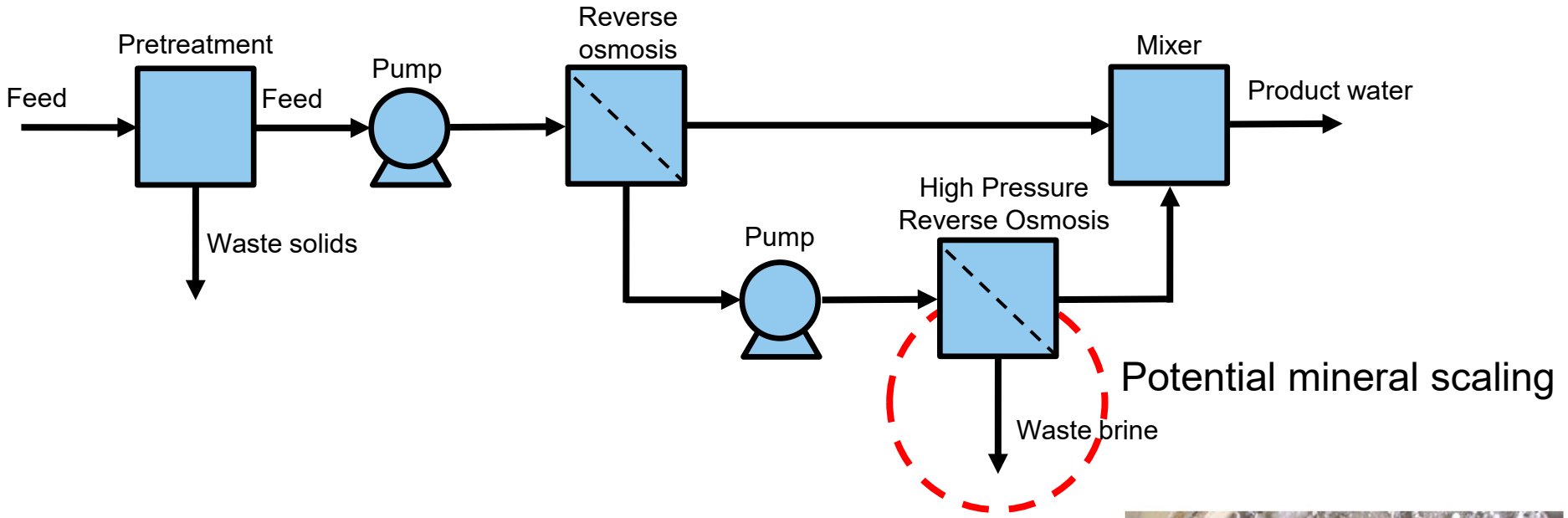
- Centralized treatment
- Large distribution systems
- Discharge to the environment
- Traditional water sources

Potential 21st century paradigm – circular water economy



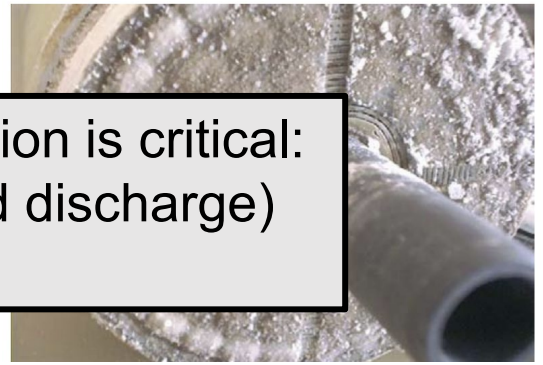
- Distributed fit for purpose treatment
- Limited transport
- Nutrient and mineral recovery
- Limited disposal
- Nontraditional water sources

Considering mineral precipitation and scaling is essential for evaluating high recovery systems



Accurately modeling mineral scaling and precipitation is critical:

- Defines key extent of treatment (minimum liquid discharge)
- Establishes the need for pretreatment



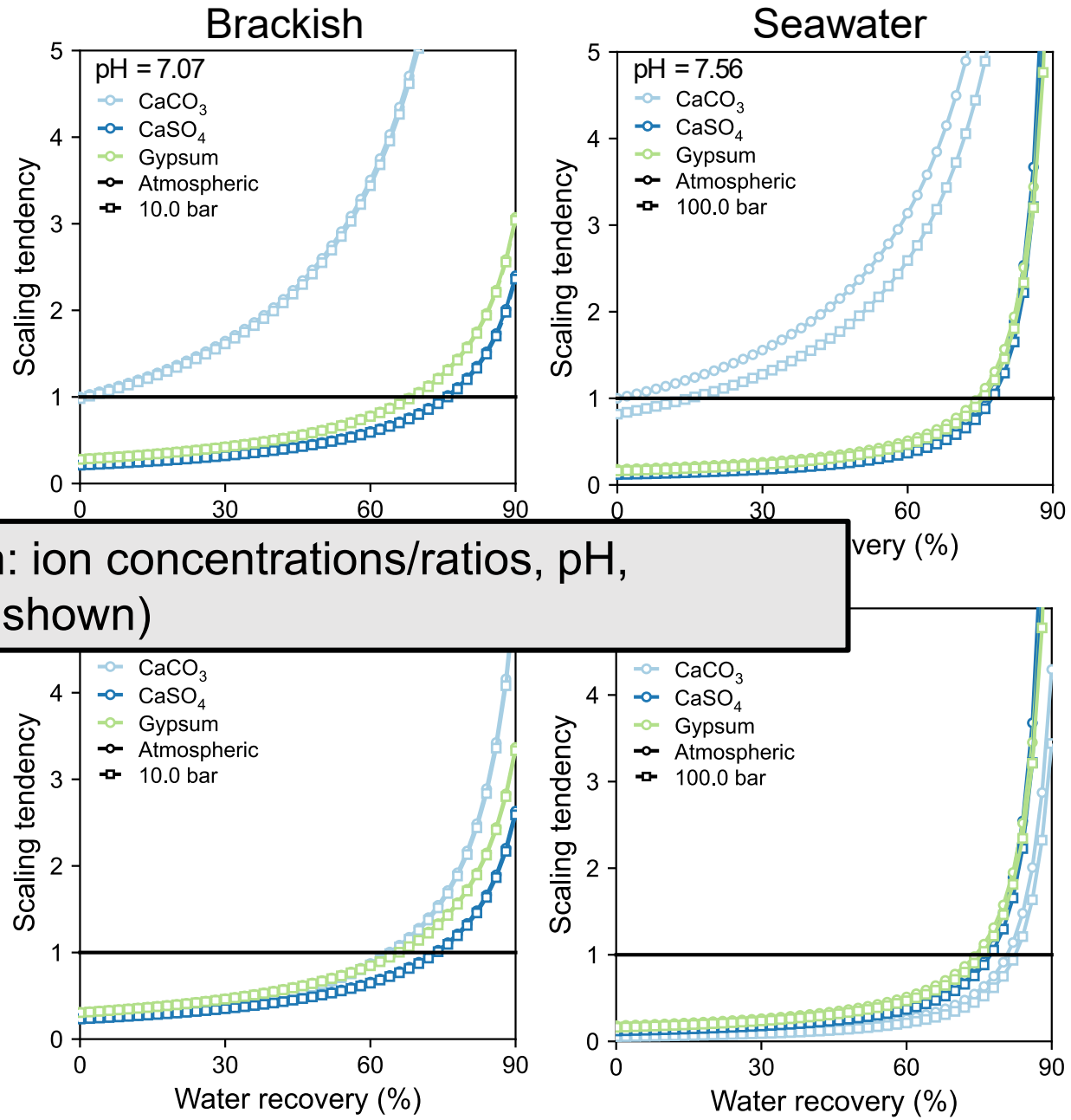
Calcium sulfate scaling on RO element

Chesters and Armstrong. 2013. *IDA World Congress on Desalination and Water Reuse*

Mineral scaling is dependent on many dimensions

	Concentration (mg/L)	
Components	Brackish	Seawater
Na	739	10,556
K	9	380
Ca	258	400
Mg		
Cl		
SO4		
HCO3	385	140
Total TDS	3,388	34,360

Mineral scaling depends on: ion concentrations/ratios, pH, pressure, temperature (not shown)



Modeling complex water chemistry is challenging and data intensive

Components
Na
K
Ca
Mg
Cl
SO4
HCO3

Mineral scaling and precipitation is dependent on speciation

- Numerous reactions and interractions across aqueous, vapor, and solid species
- Activities, solubility/scaling tendencies, diffusivity
- Dependen
- pH, tempe

Carbonation Process

$H_2O \leftrightarrow H^+ + OH^-$

$CaOH^+ \leftrightarrow Ca^{2+} + OH^-$

$CaHCO_3^+ \leftrightarrow Ca^{2+} + HCO_3^-$

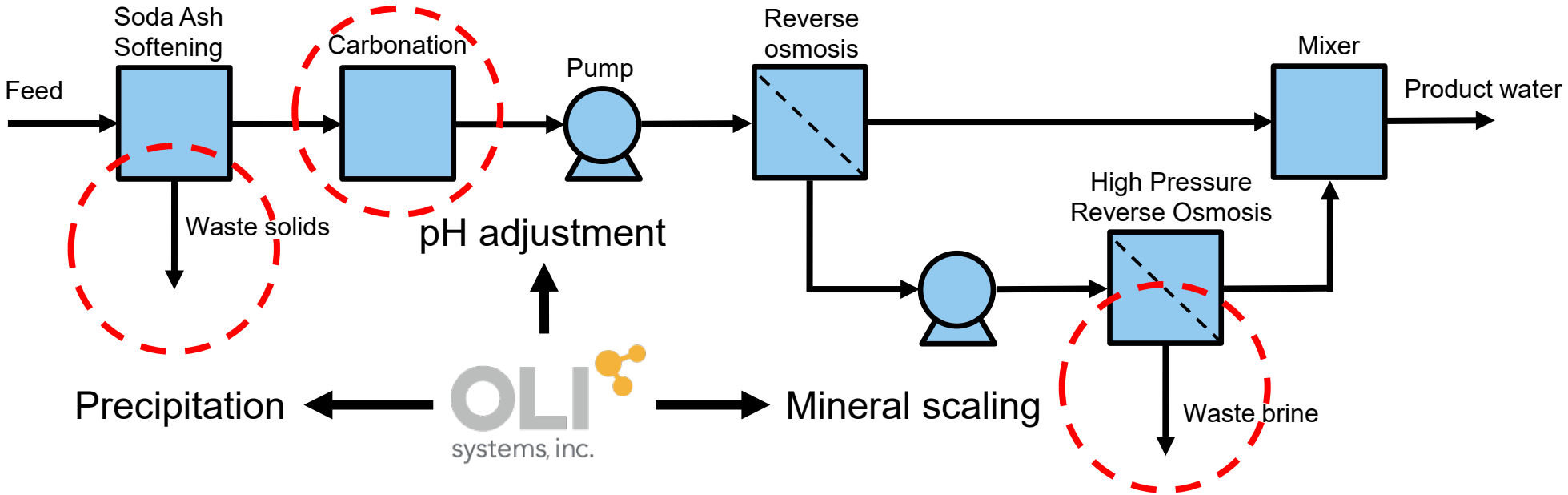
$H_2CO_3 \leftrightarrow CO_{2\,(aq)} + H_2O$

$H_2CO_3 \leftrightarrow H^+ + HCO_3^-$

$HCO_3^- \leftrightarrow H^+ + CO_3^{2-}$

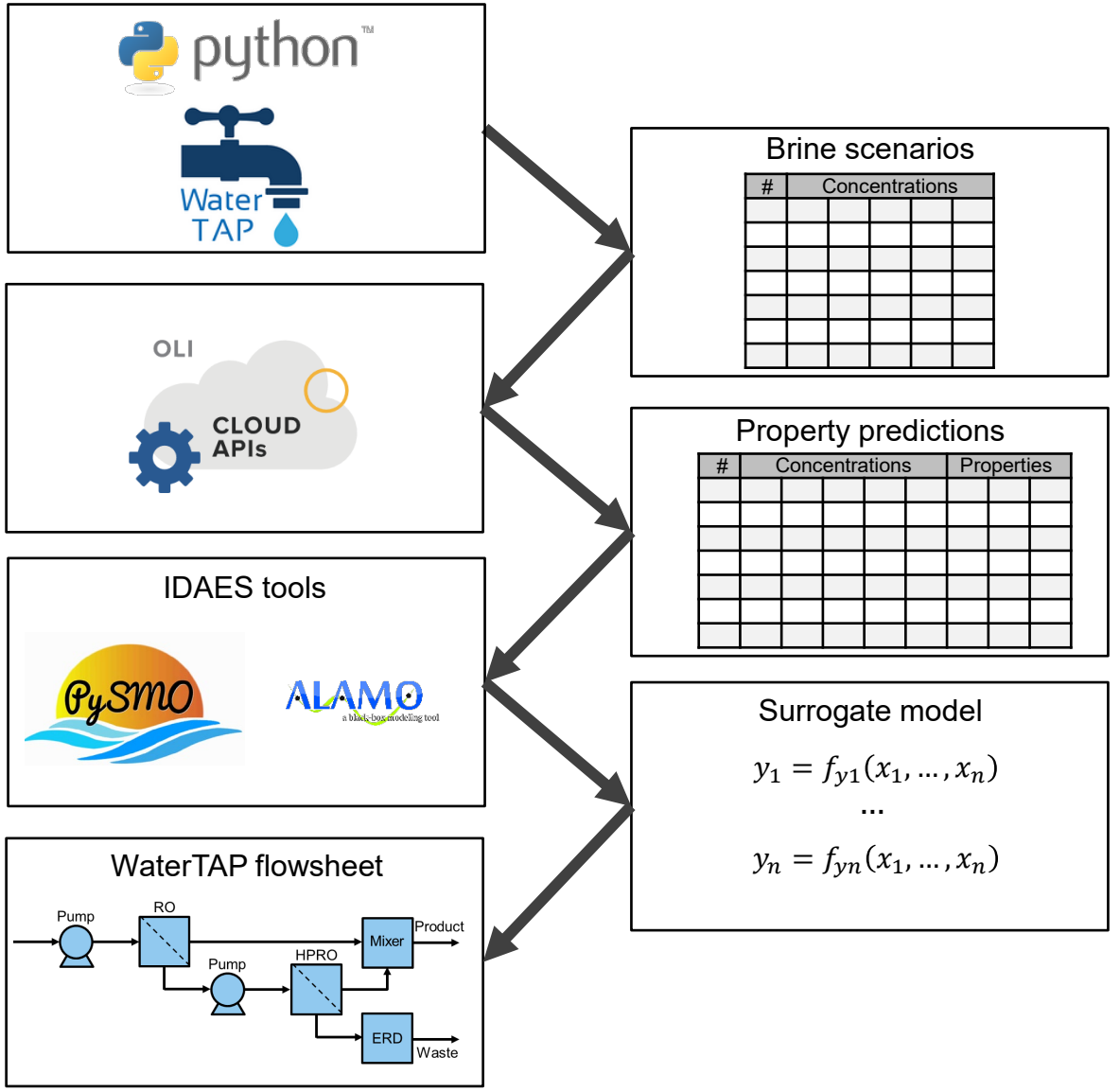
- Electrolyte theoretical models have numerous terms and parameters to represent all of the interactions (e.g., MSE, Pitzer, eNRTL)
- Data availability limits the species that can be considered
- Large models pose challenges for optimization

Integrating OLI and WaterTAP enables detailed water chemistry with process-scale cost optimization



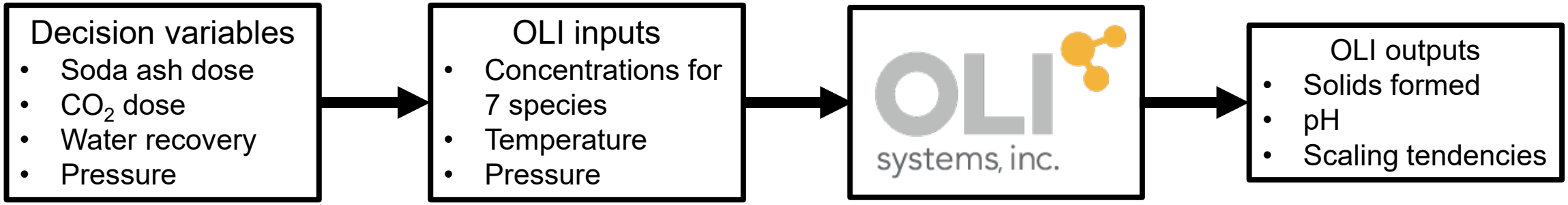
Integrating OLI as a surrogate in WaterTAP

1. Generate relevant brine scenarios
2. Use OLI Cloud API to calculate properties for brine scenarios
3. Use IDAES tools to fit a surrogate model to OLI properties
4. Use WaterTAP flowsheet with the OLI surrogate model



Lessons learned from developing surrogates

1. It is critical to limit the number of independent variables for the simulated space
   - Number of simulations grows dramatically with the variables: $N_{sim} = (N_{steps})^{N_{vars}}$
     - 50k simulations with 4 variables and 15 steps
   - Best approach is to determine the critical decision variables for the optimization



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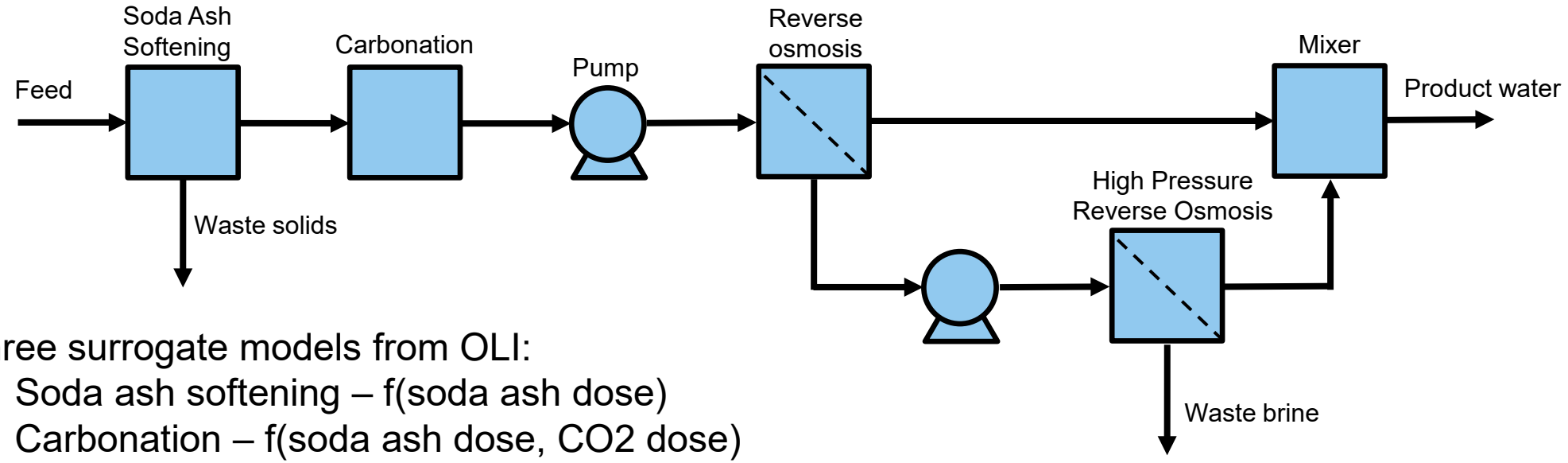
2. Radial basis function (RBF) surrogate models with adaptative sampling performed best
    - Regression model equivalents did not fit as well and were plagued by local solutions
    - RBFs were the most accurate, useful, and flexible
        - Low mean and maximum absolute error for large spaces
        - Even RBFs with 100s of terms solved quickly
        - Sampling techniques provide an easy way to hone the model

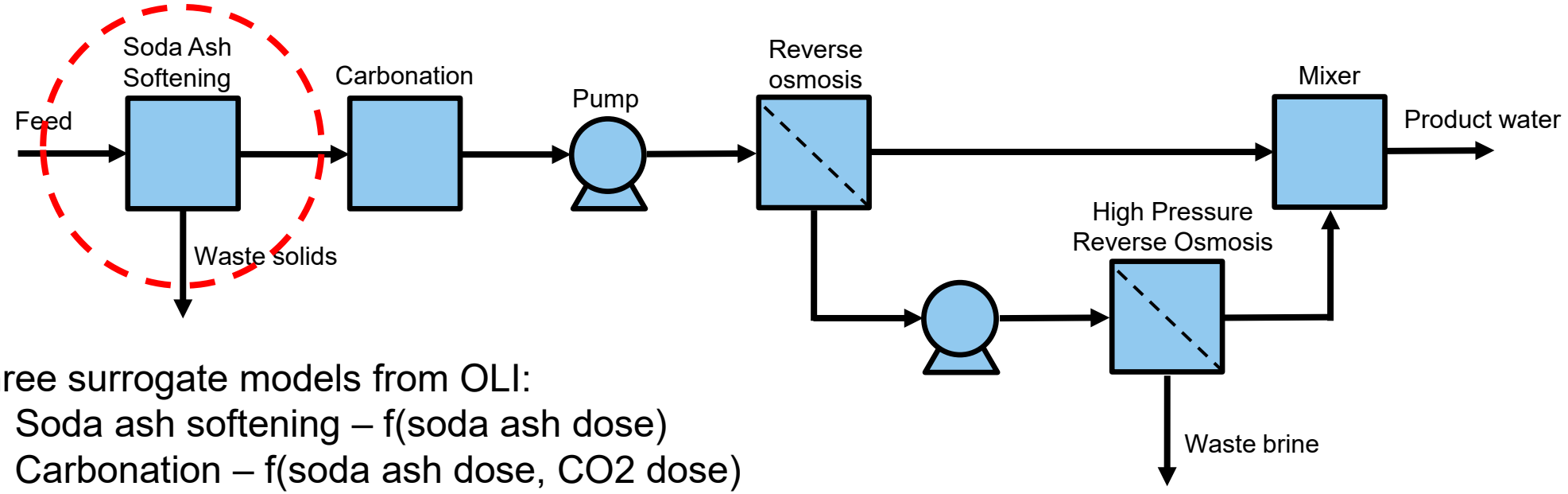
Developing accurate surrogate models



Three surrogate models from OLI:

1. Soda ash softening – f(soda ash dose)
2. Carbonation – f(soda ash dose, CO2 dose)
3. Mineral scale prediction at the end of RO – f(soda ash dose, CO2 dose, system recovery, pressure)

Developing accurate surrogate models



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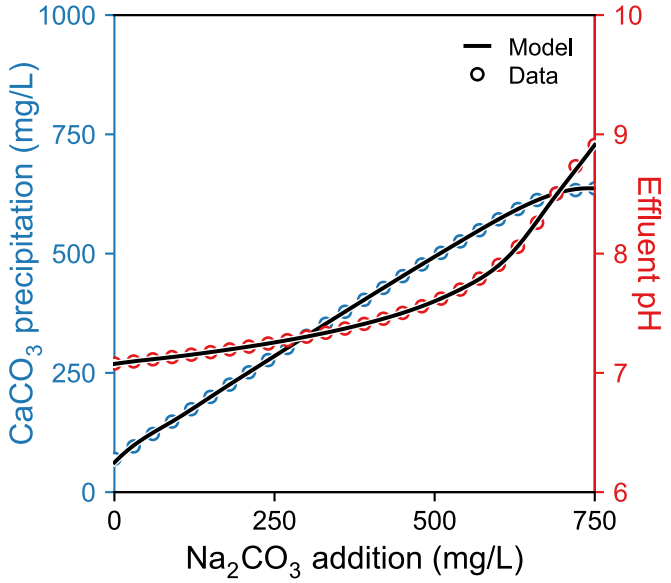
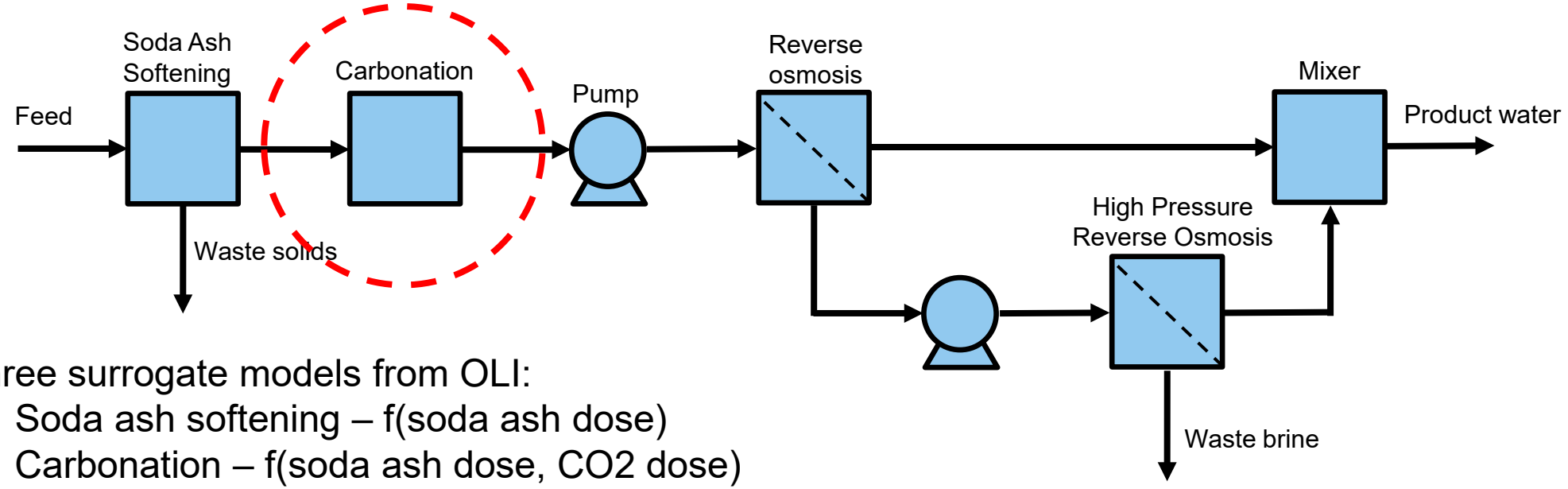


0-750 soda ash dose, steps of 10, 76 total simulated points

Surrogate model	CaCO3 (s) concentration	pH
Model size (No. terms)	13	13
Model training time (s)	0.07	0.08
R^2	0.9999	0.9998
Mean Absolute Error	0.510	0.0031
Maximum Absolute Error	7.59 mg/L	0.0315

Developing accurate surrogate models



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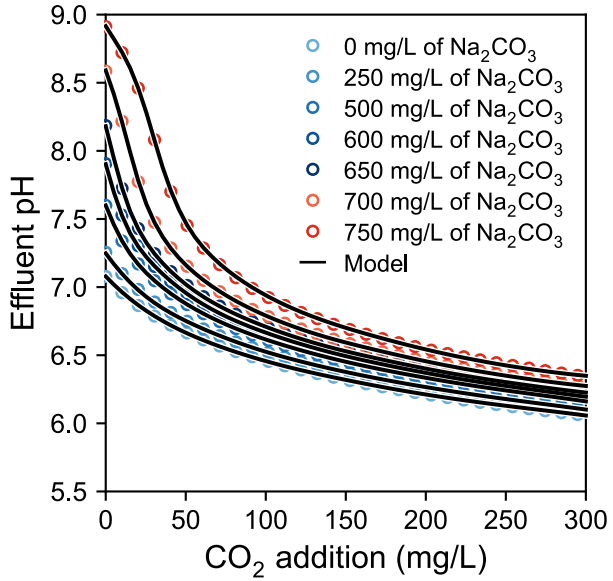


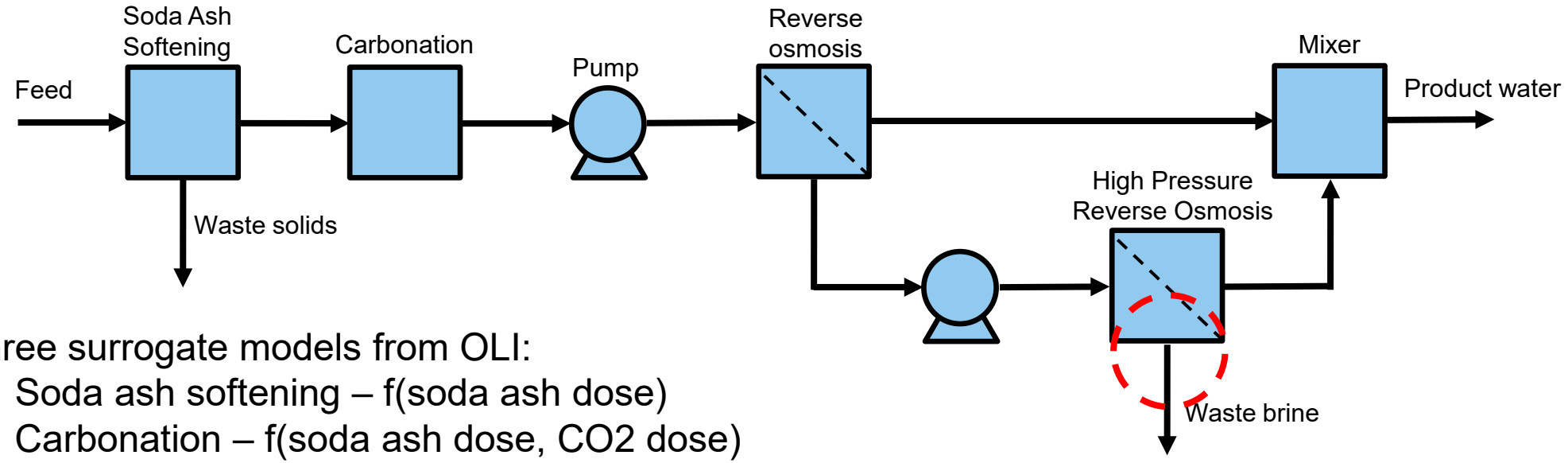
0-750 soda ash dose (76 steps), 0-300 CO2 dose (60 steps), 4560 total simulations

Surrogate model	pH
Model size (No. terms)	101
Model training time (s)	445
R^2	0.9999
Mean Absolute Error	0.0011
Maximum Absolute Error	0.0086

← adaptive sampling

- Uniform grid 51-point sample
- Adaptive 50-point for highest absolute error (AE)

Developing accurate surrogate models



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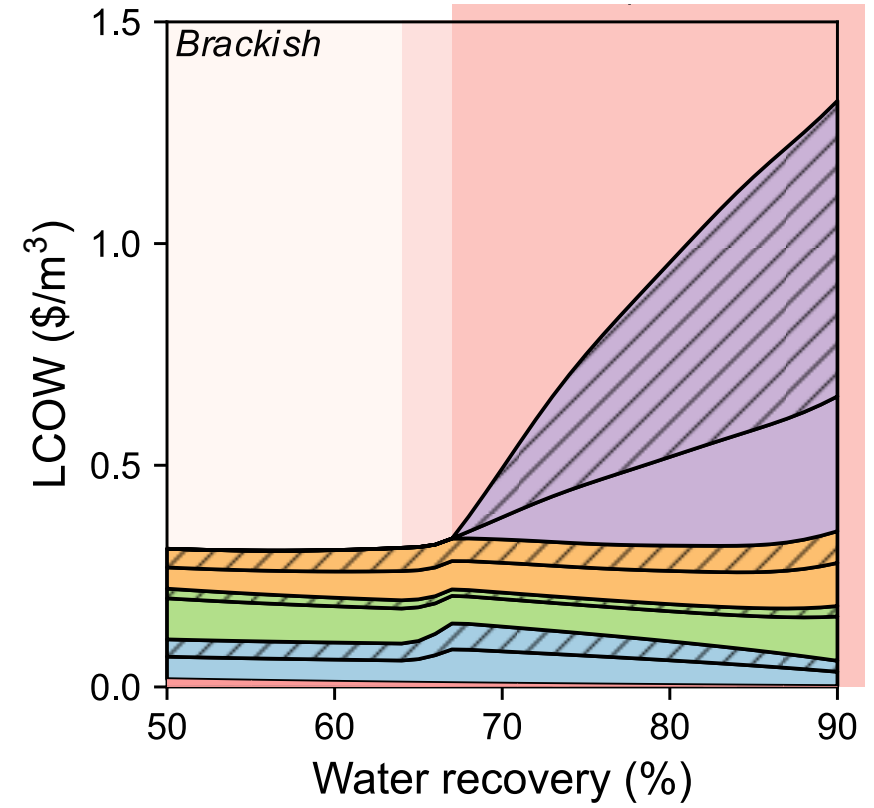
OLI simulation	min - max (no. steps)
Soda ash dose (mg/L)	0 – 750 (16)
CO_2 dose (mg/L)	0 – 300 (16)
Water recovery (%)	48 – 94 (24)
Hydraulic pressure (bar)	10 – 110 (11)

36,864 total simulated points

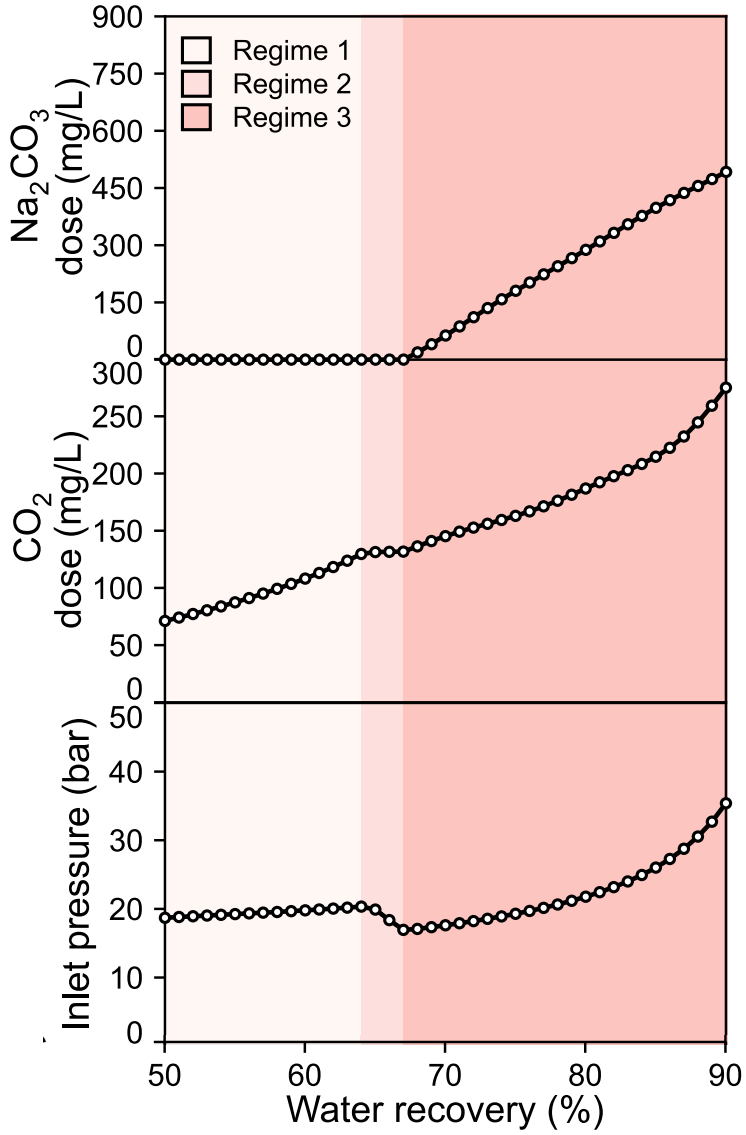
SI surrogate model	CaCO3	Gypsum
Model size (No. terms)	150	150
Model training time (s)	8,370	10,300
R^2 (0.75 < ST < 1.25)	0.96	0.99
Mean Absolute Error (0.75 < ST < 1.25)	0.0233	0.0183
Classification accuracy (%)	99.5	99.8

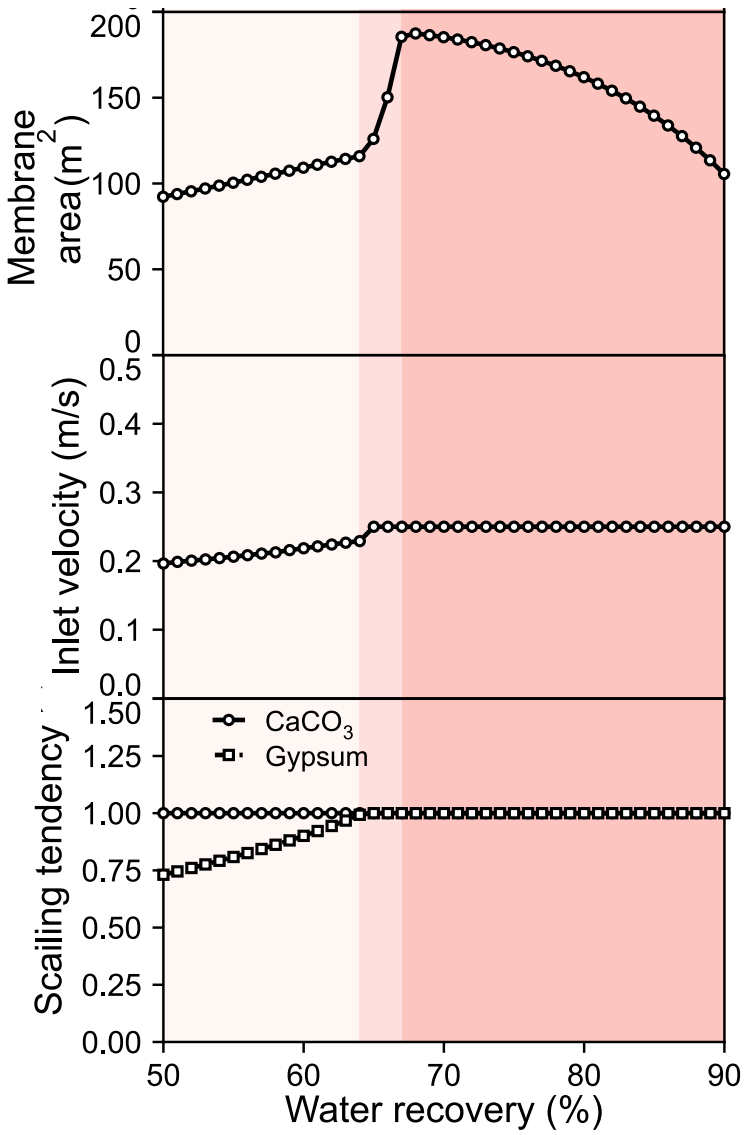
- Uniform 50-point sample
- Adaptive 50-point for highest AE and misclassified
- Adaptive 50-point for highest AE in region of interest

Can optimize full treatment train across water recovery

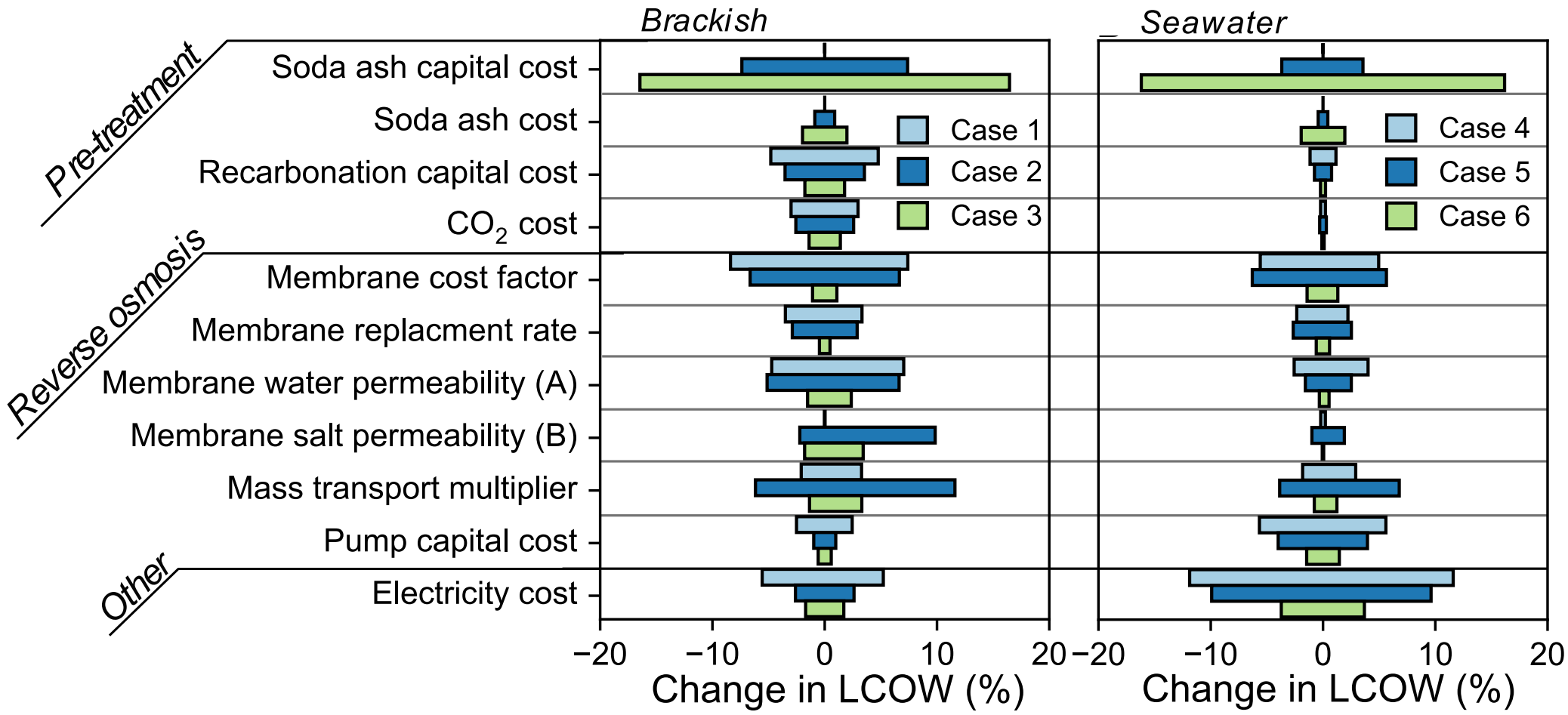


Determining optimal pretreatment and desalination





Expanding the analysis through sensitivities



WaterTAP and OLI demonstrated integrated capabilities

- Directly incorporated detailed water chemistry predictions with rigorous mathematical cost optimization at the process-scale
- This work was enabled by the surrogate modeling tools in IDAES
- Surrogates based on flowsheet level decision variables and that used RBFs with adaptive sampling performed best
- WaterTAP and OLI believe this work shows significant promise and are expanding it for other analyses – crystallization, antiscalants, corrosion

Acknowledgements and disclaimer

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OLI Systems: Leslie Miller, Adi Bannady, AJ Gerbino, John Pagan

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Questions

Regressions fit data, RBFs interpolate data

Regression models

- Most common type of surrogate

Linear: $y = b + m\,x$

Polynomial: $y = \beta_0 + \sum_p \sum_{i=1}^{n} \beta_{ii} x_i^p$

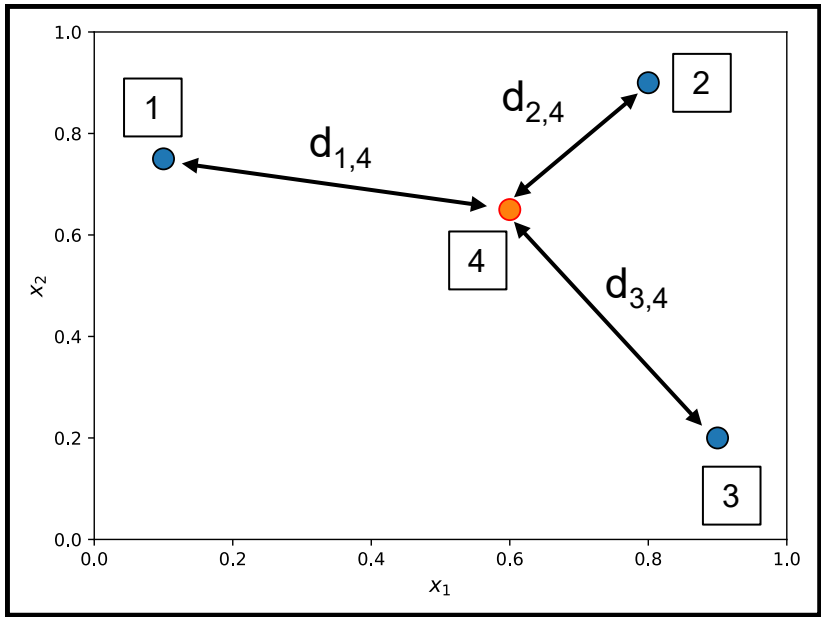
General: $y = \beta_0 + \sum_p \sum_{i=1}^{n} \beta_{ii} x_i^p + \sum_{i=1}^{n} \sum_{i<j}^{n} \beta_{ij} x_i x_j$

Can add other terms: $x_i/x_j,\ x_i^2 x_j, \sin x_i, \log x_j$

- Objective: $\min_{\beta} \sum \left(y_{true} - y_{predicted}\right)^2$
- Evaluate fit based on key metrics:
  - Root mean squared error (RMSE)
  - Coefficient of determination (R^2)
  - Mean absolute error (MAE)
  - Maximum absolute error

Radial basis functions (RBFs)

- General idea: value of any unknown point in domain is a function of its distance from the all known points around it



$y = \sum_{i=1}^{n} \omega_i \cdot \aleph(x - x_i)$ Transformation functions

$y_4 = \omega_{1,4} \cdot \aleph(d_{1,4}) + \omega_{2,4} \cdot \aleph(d_{2,4}) + \omega_{3,4} \cdot \aleph(d_{3,4})$

- Objective: $\min_{\omega} \sum \left(y_{true} - y_{predicted}\right)^2$