NAWI National Alliance for Water Innovation

Bridging thermodynamic data and technoeconomic assessment for solvent extraction

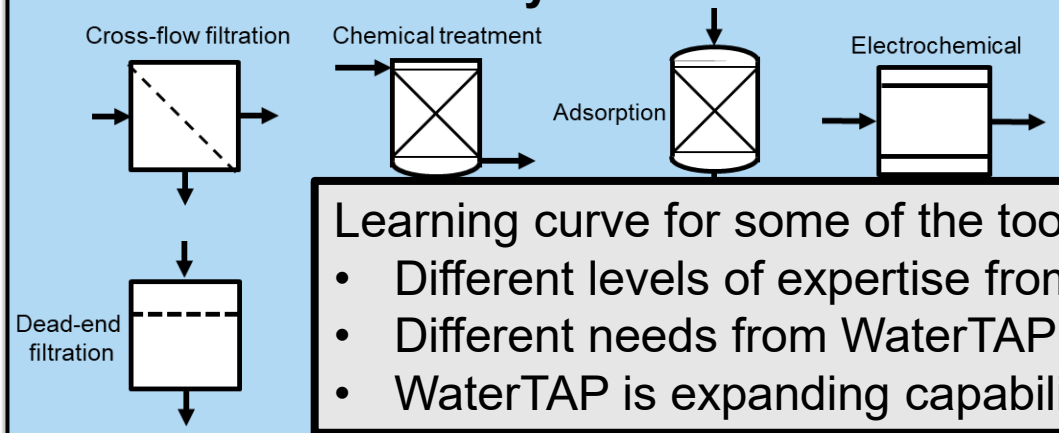
Alejandro Garciadiego, Akshay Deshmukh, Aaron Wilson, Tim Bartholomew, Adam Atia

Thursday, September 19, 2024

WaterTAP models and tools are flexible

Unified

Modular model library:



Core capabilities:

- Simulation to evaluate new device integration
- Optimization to explore complex systems
- …der uncertainty
- …eal-world data
- …lex phenomena

Learning curve for some of the tools can be steep

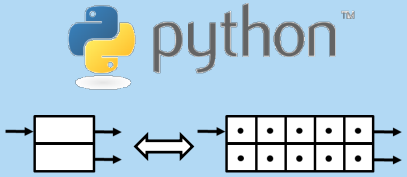
- Different levels of expertise from users
- Different needs from WaterTAP
- WaterTAP is expanding capabilities to increase accessibility!

Flexible

Powerful

Core attributes:

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



$$f(x) = 0$$

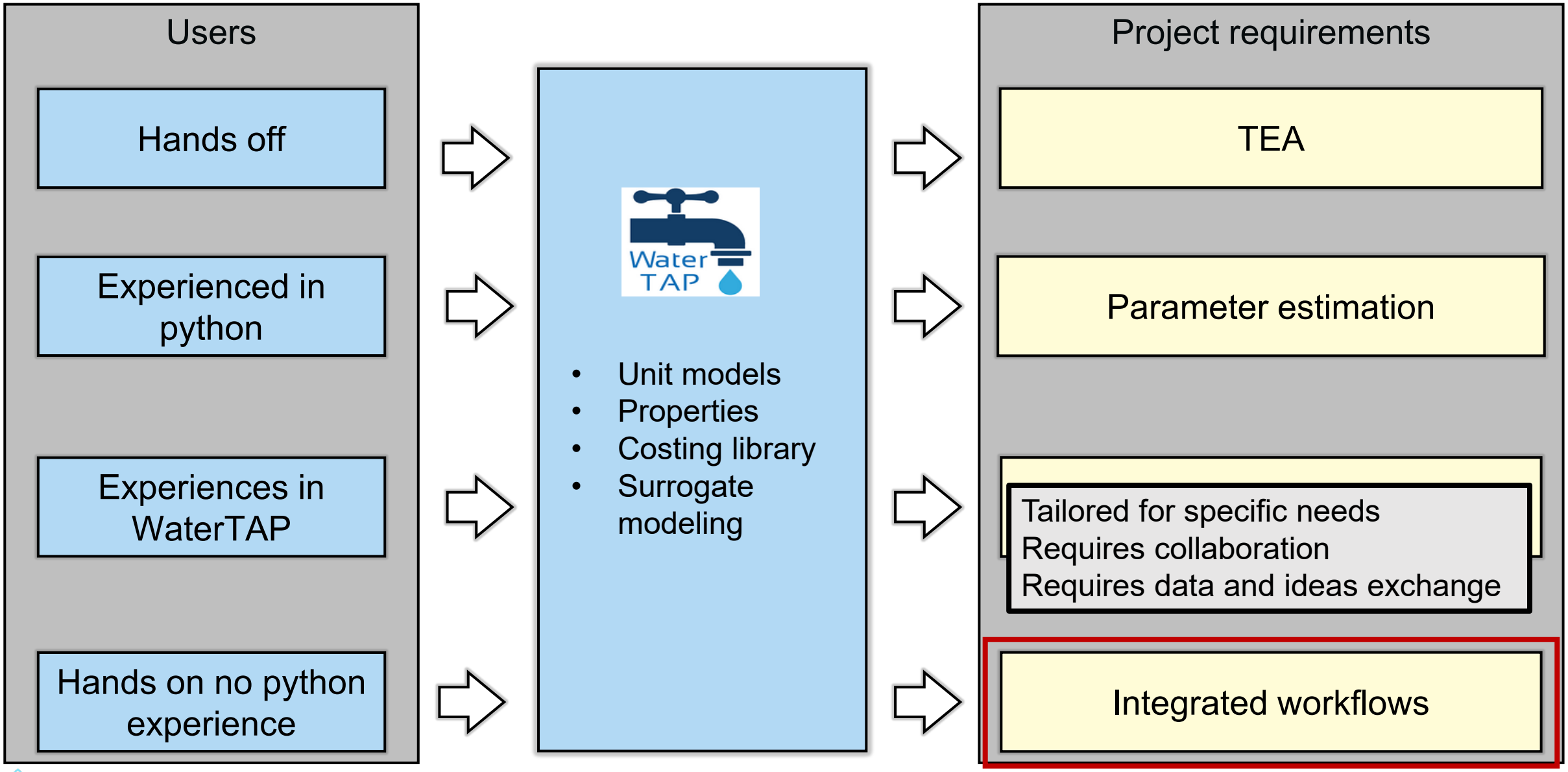
PYOMO

IDAES
Institute for the Design of Advanced Energy Systems

Platform benefits:

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

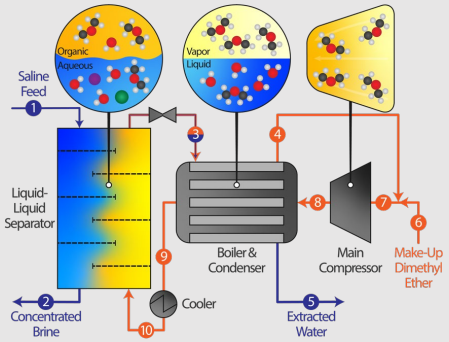
Different needs require different solutions



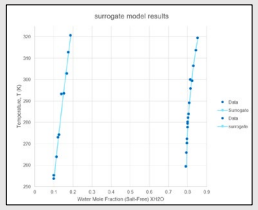
Overview

Solvent extraction

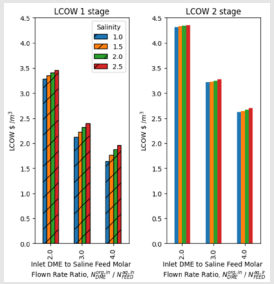
Process



Surrogate modeling

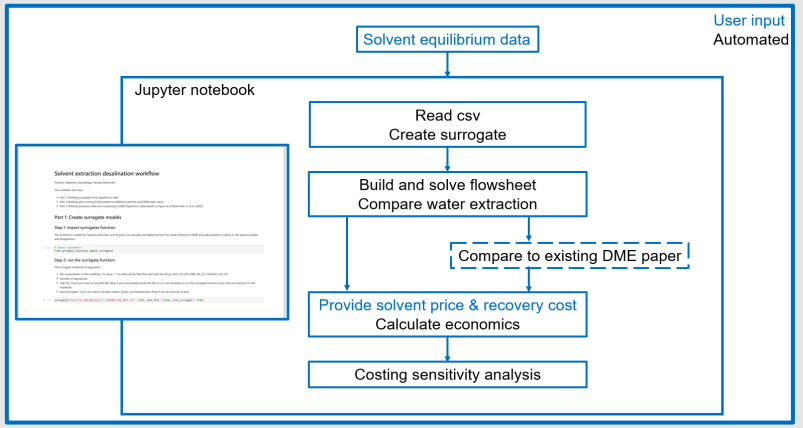


TEA



Workflows

Beginner user



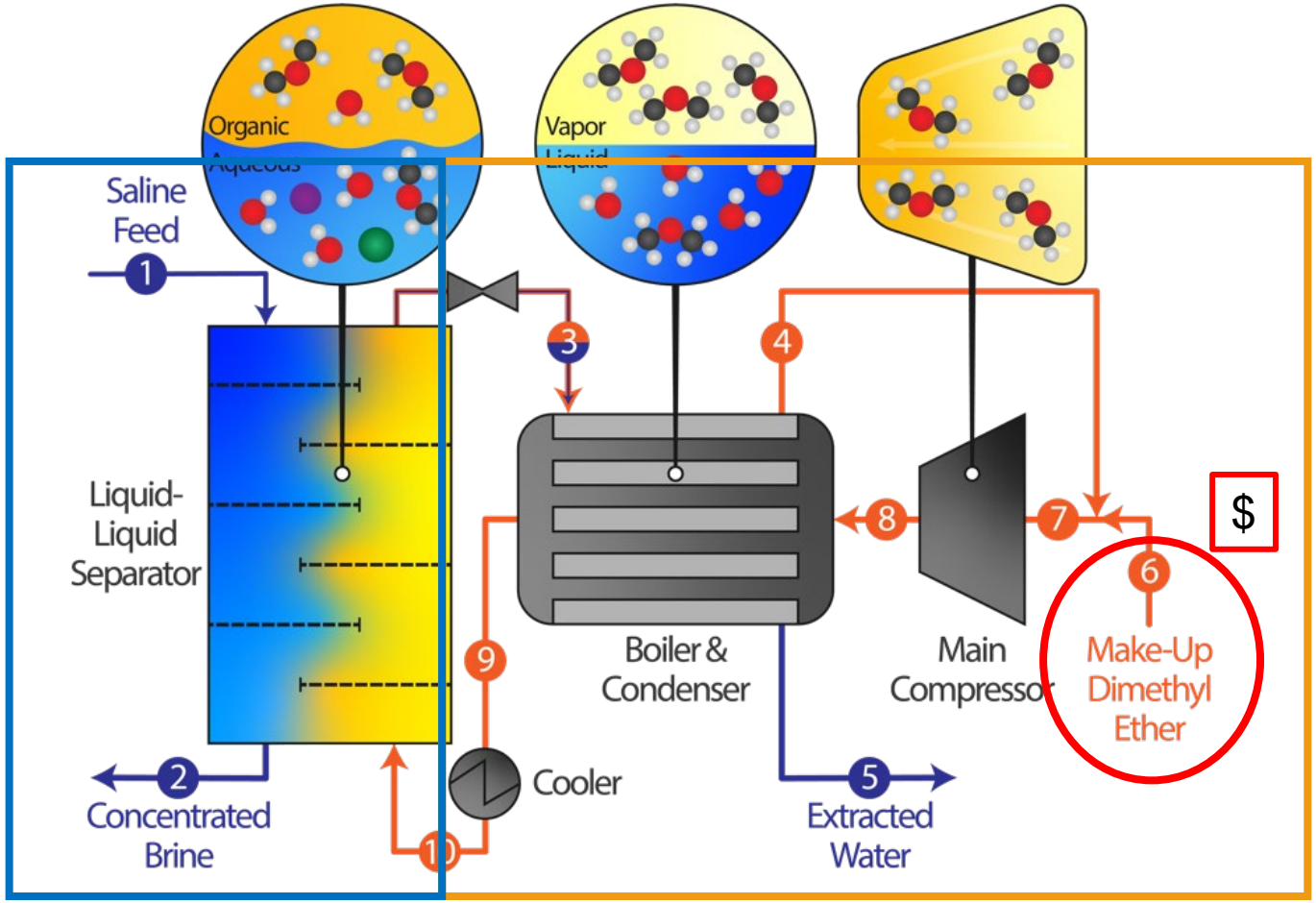
Intermediate user

Property data
Cp parameters
Peng-Robinson parameters
Density
Etc.

Expert user

Build recovery process flowsheet

Solvent extraction process

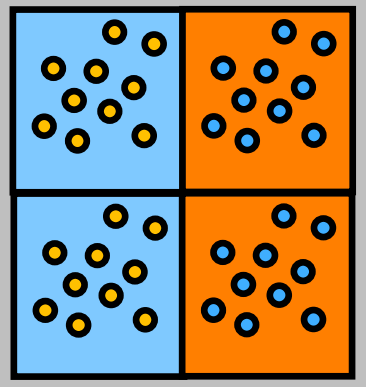


Deshmukh, A., Foo, A. H., Stetson, C., Hyeonseok Lee, H., Orme C. J., Wilson A. D., Lienhard J. H., "Thermodynamics of solvent-driven water extraction from hypersaline brines using dimethyl ether", 2022, Chemical Engineering Journal, Vol. 434, https://www.sciencedirect.com/science/article/pii/S1385894721059611 .

WaterTAP accelerates flowsheet building and TEAs

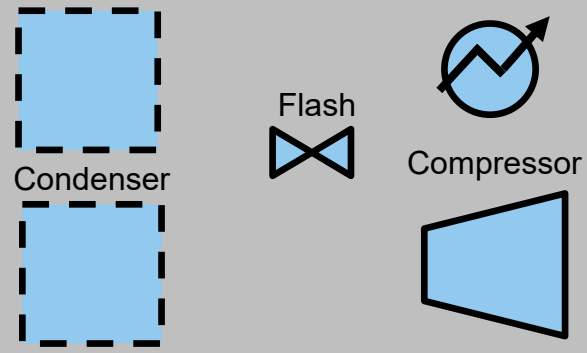
WaterTAP tailored model for the process

PROMMIS

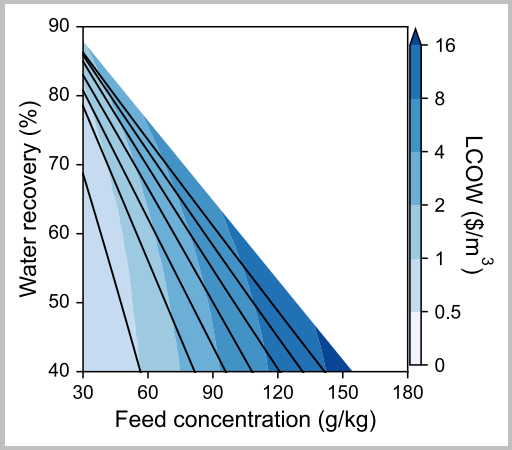


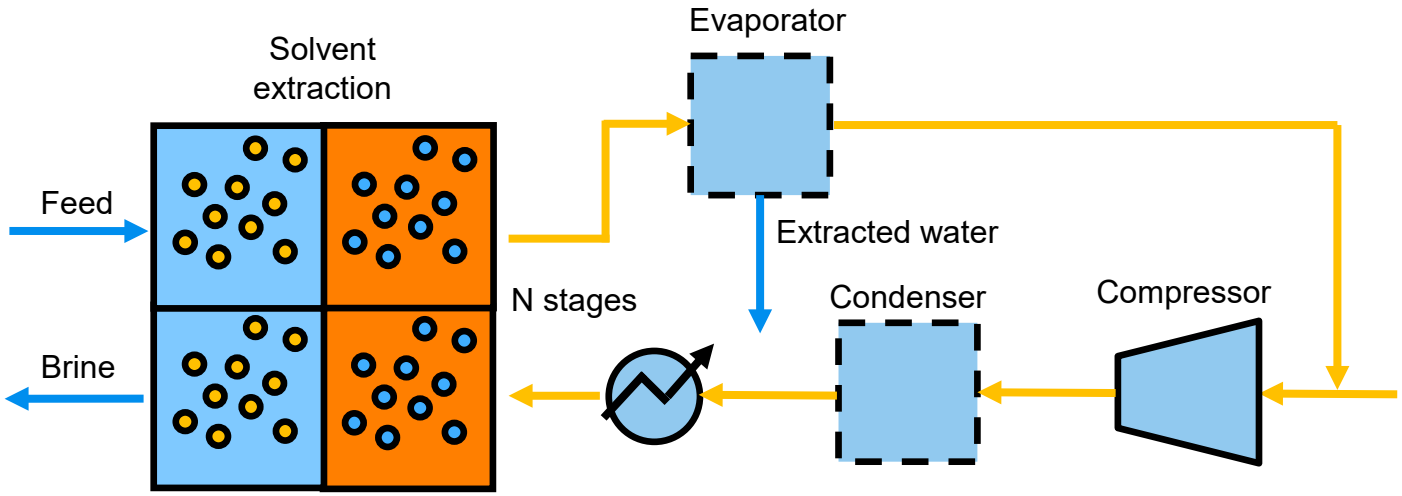
N stages

WaterTAP/IDAES model library

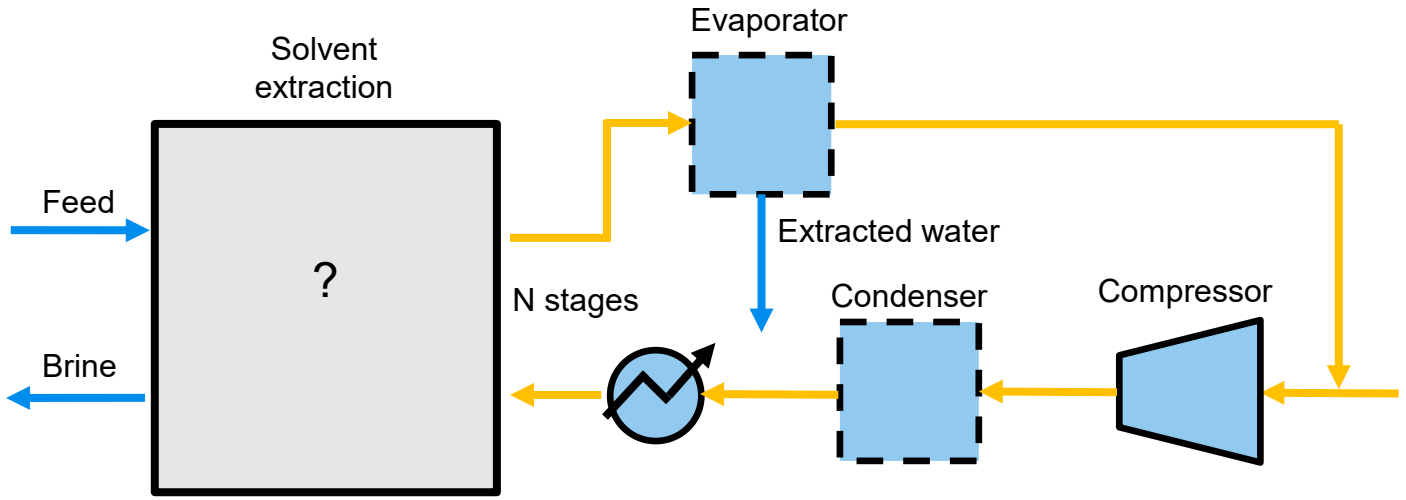


WaterTAP costing library





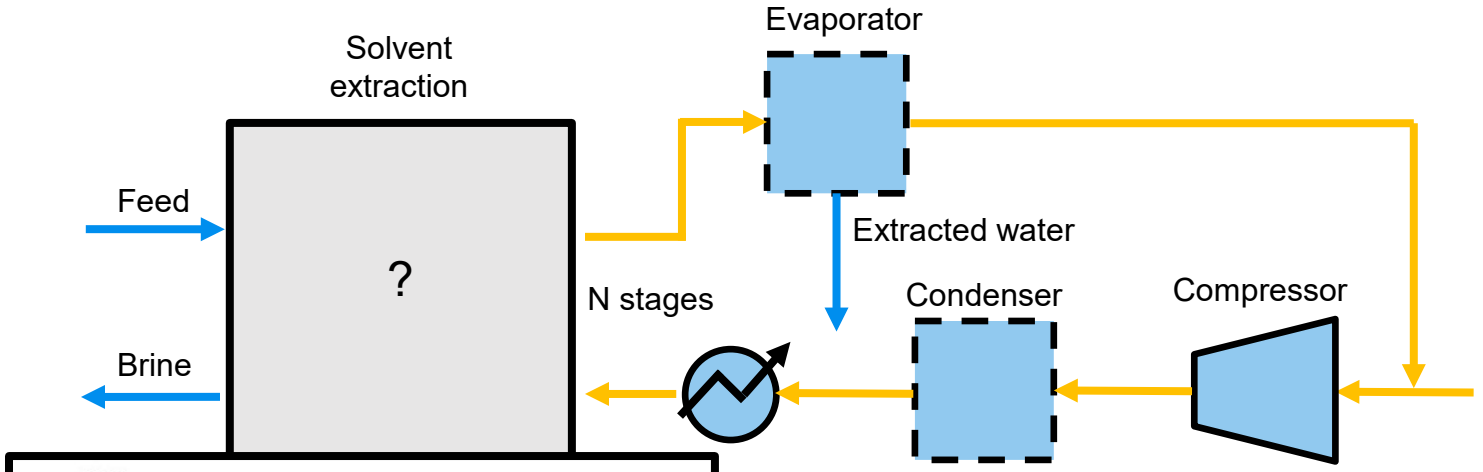
What happens when you do not have a model?



There are many reasons to not have a predictive model:

- Time
- Convergence
- Complexity
- Etc.

Surrogates are a modeling solution



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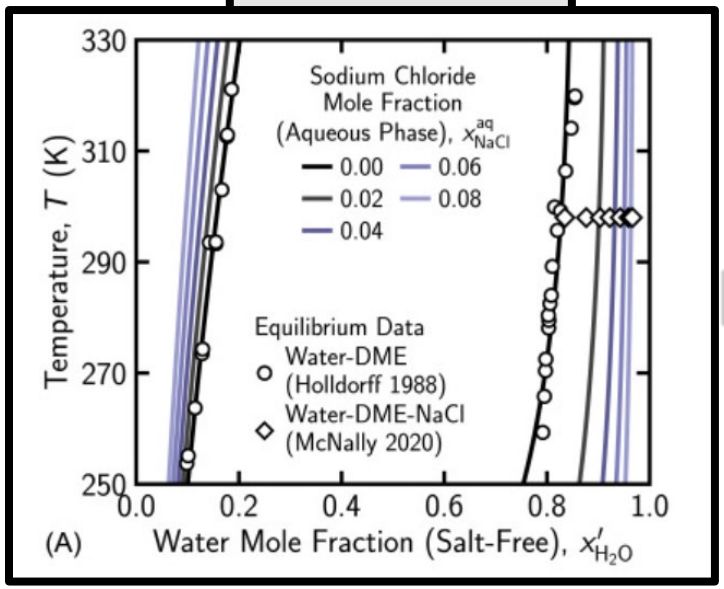

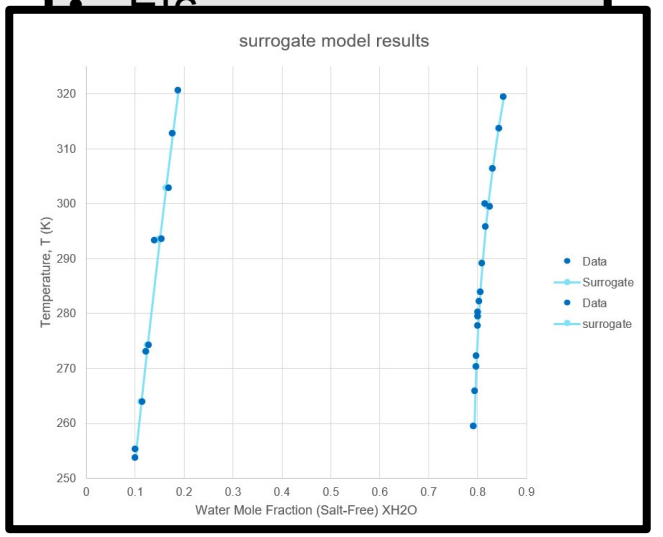

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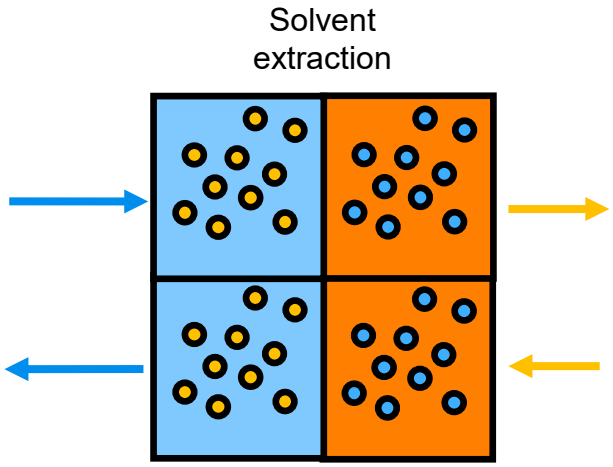
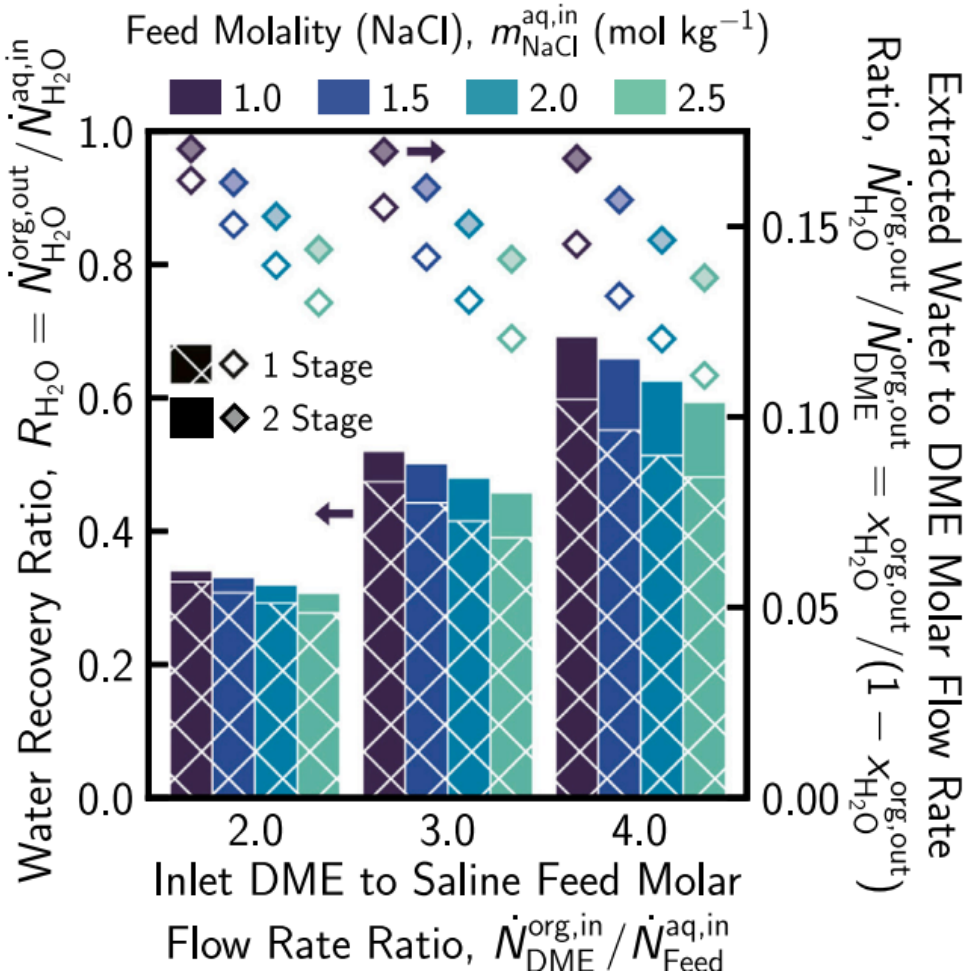
Can surrogate translate to process scale?





Deshmukh, A., Foo, A. H., Stetson, C., Hyeonseok Lee, H., Orme C. J., Wilson A. D., Lienhard J. H., "Thermodynamics of solvent-driven water extraction from hypersaline brines using dimethyl ether", 2022, Chemical Engineering Journal, Vol. 434, https://www.sciencedirect.com/science/article/pii/S1385894721059611 .

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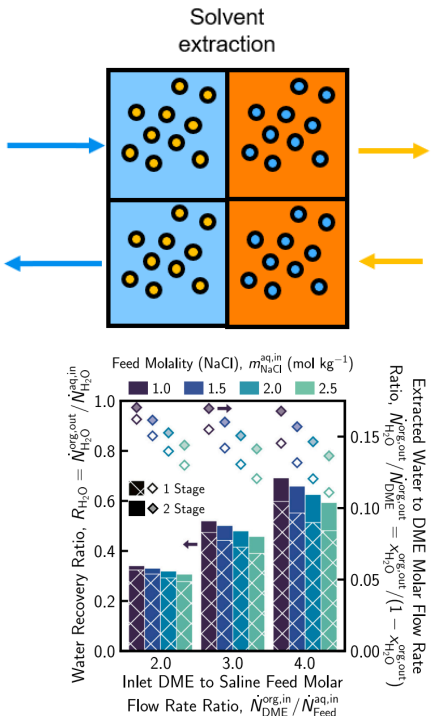
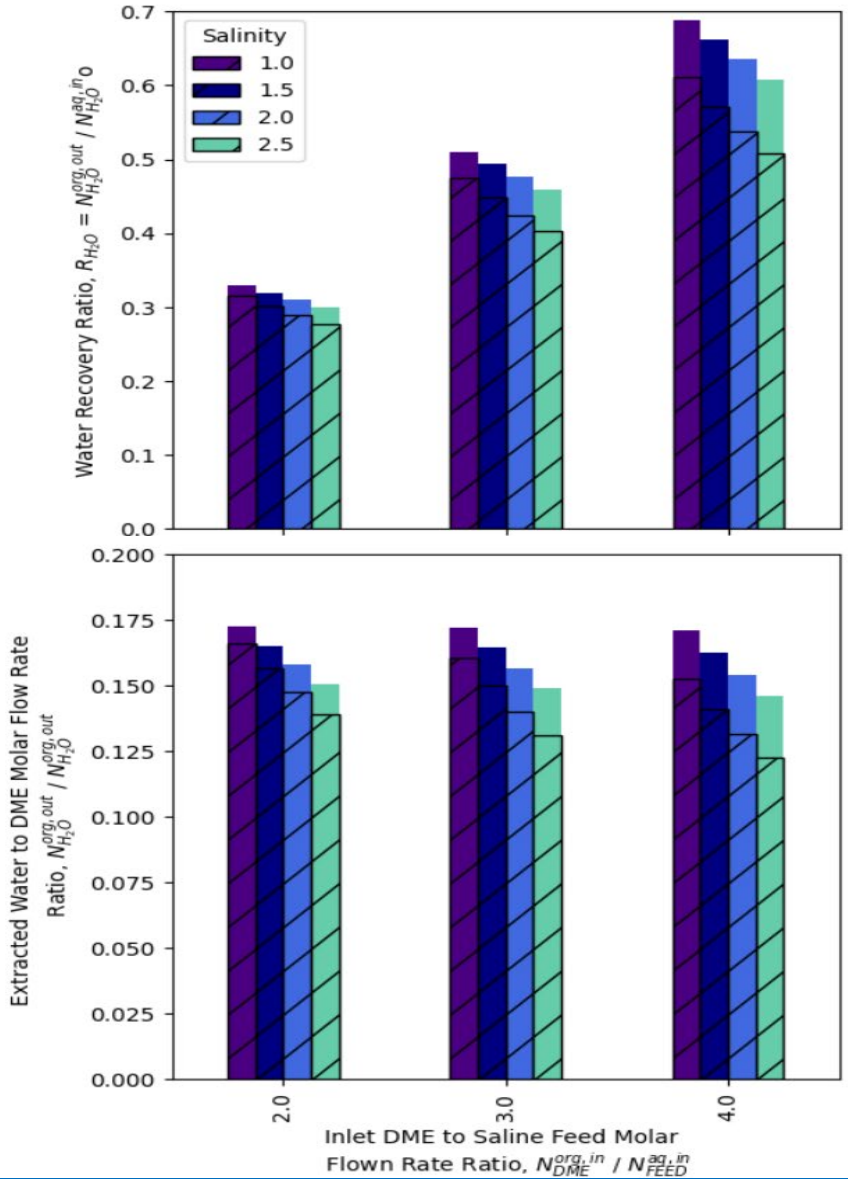
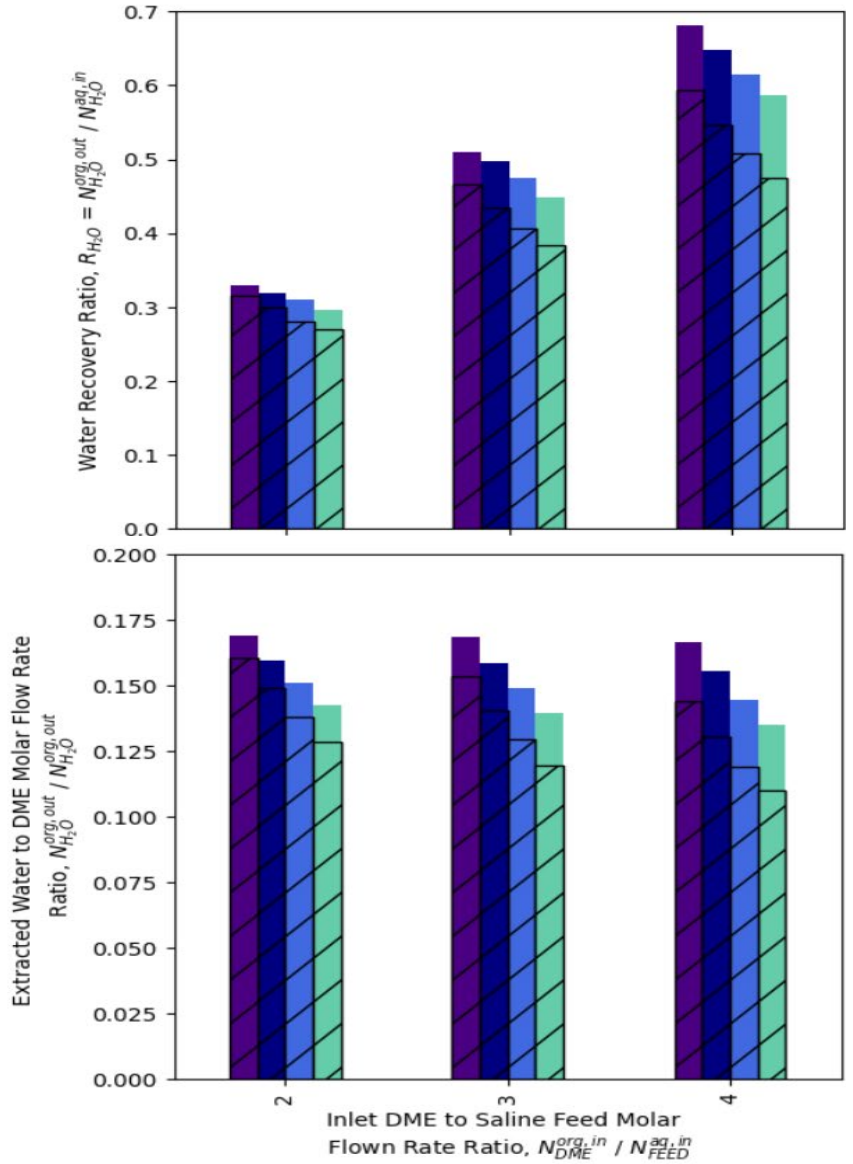
Surrogate are accurate at process scale



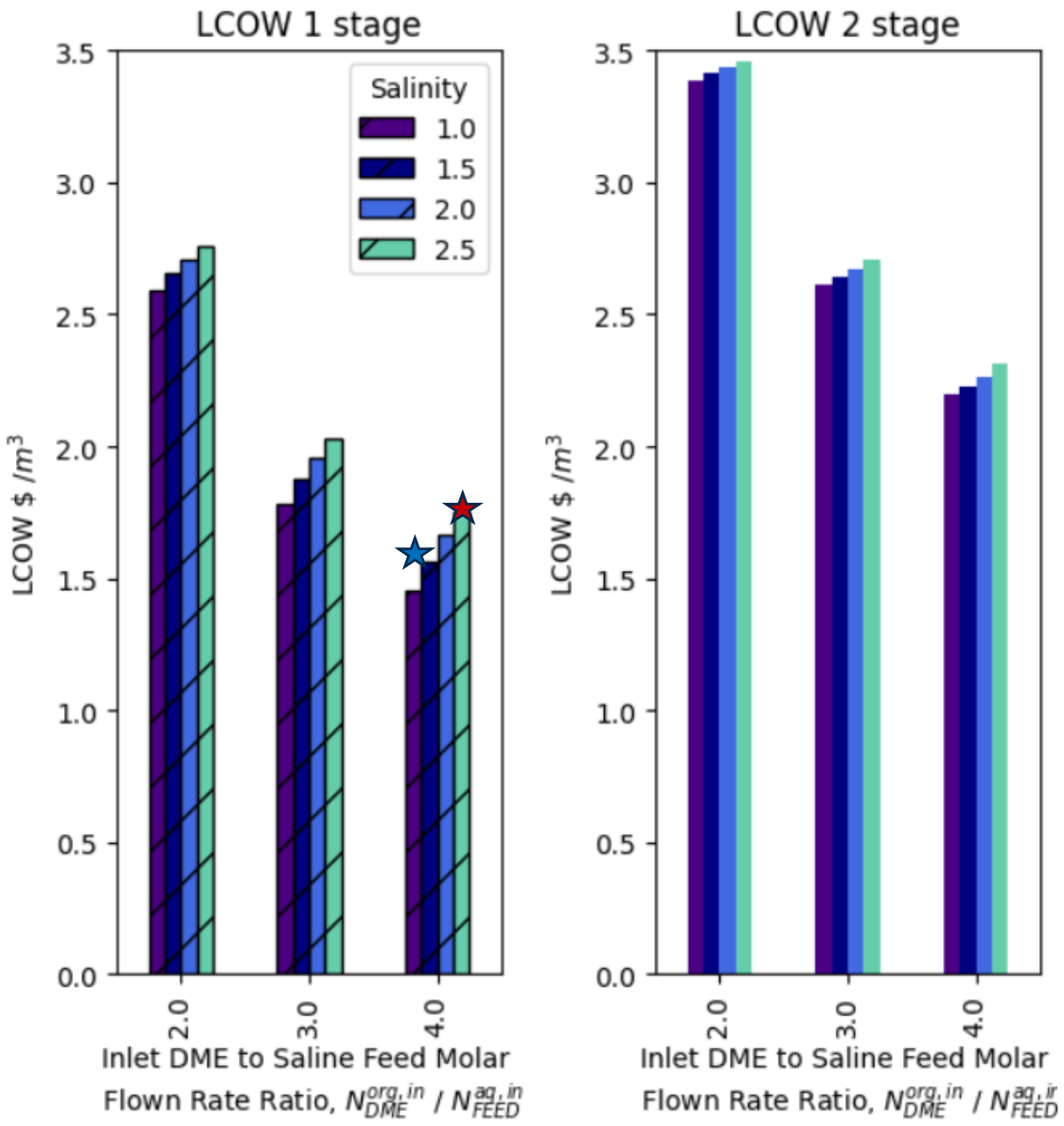
WaterTAP surrogate



Collaborators study



Detailed TEA gives comparable LCOW values



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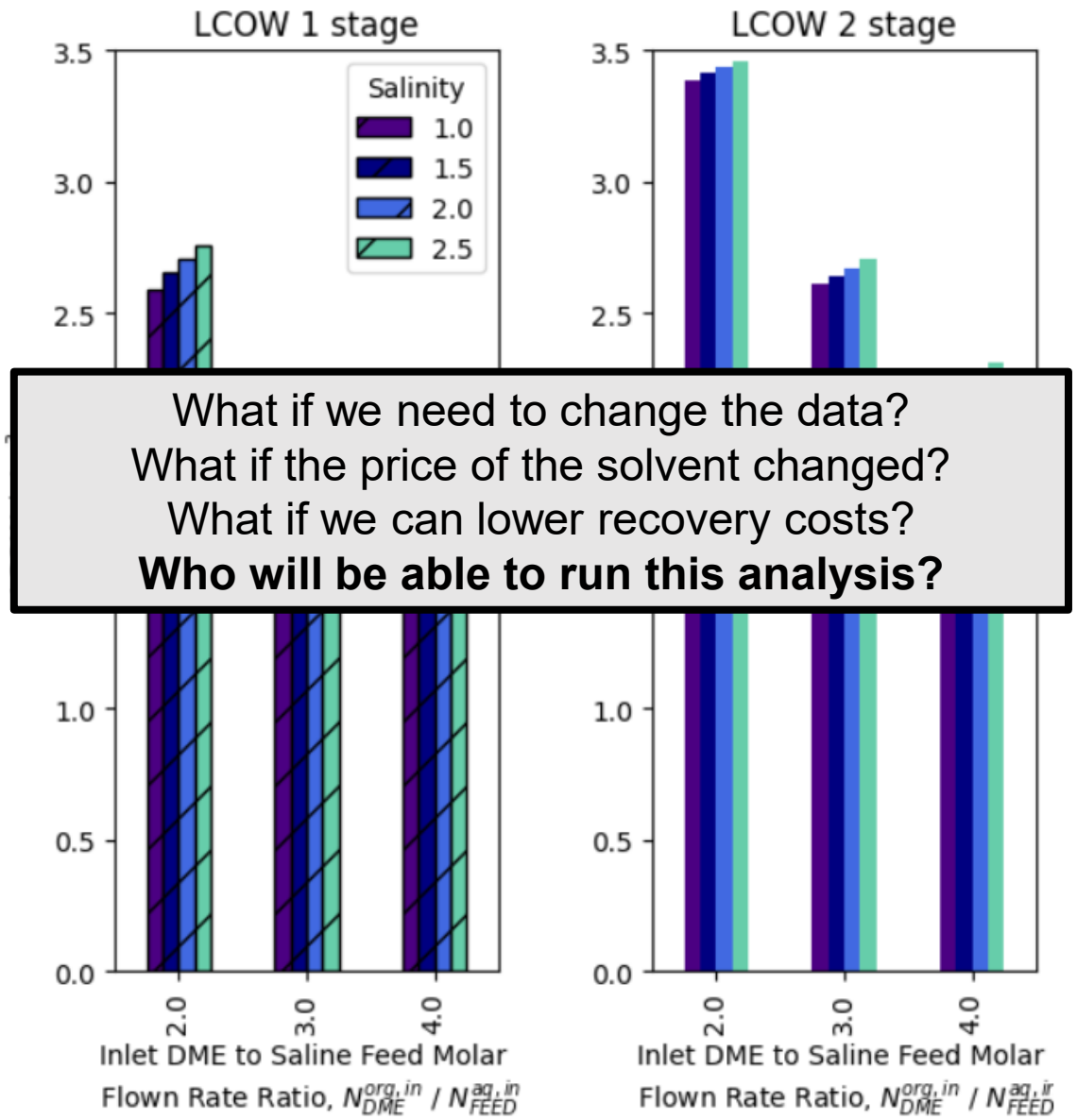
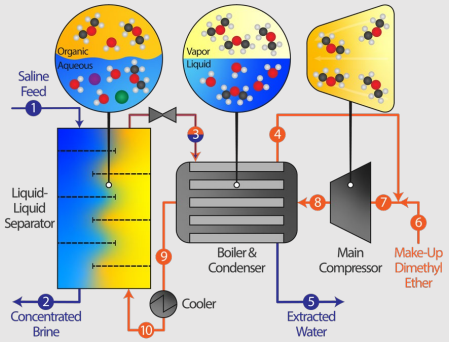


What if we need to change the data?
What if the price of the solvent changed?
What if we can lower recovery costs?
Who will be able to run this analysis?

Overview

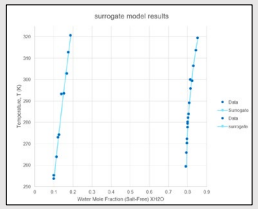
Solvent extraction

Process

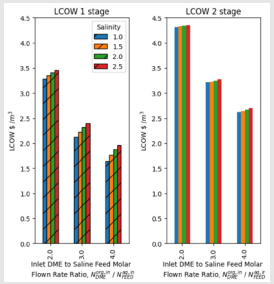


Surrogate modeling

PySMO

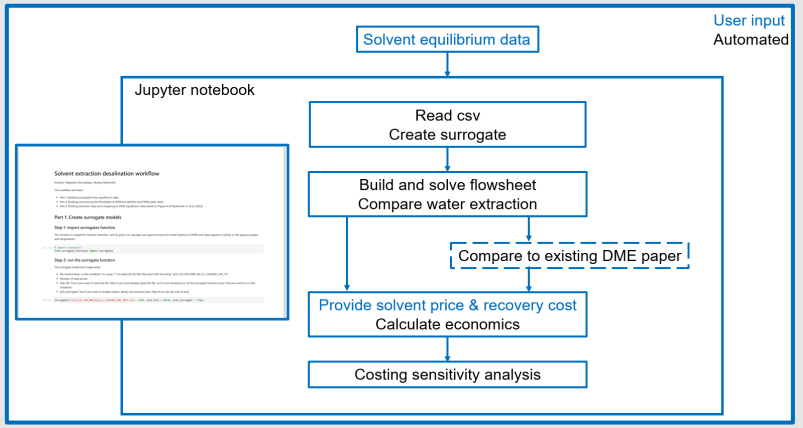


TEA



Workflows

Beginner user



Intermediate user

Property data
Cp parameters
Peng-Robinson parameters
Density
Etc.

Expert user

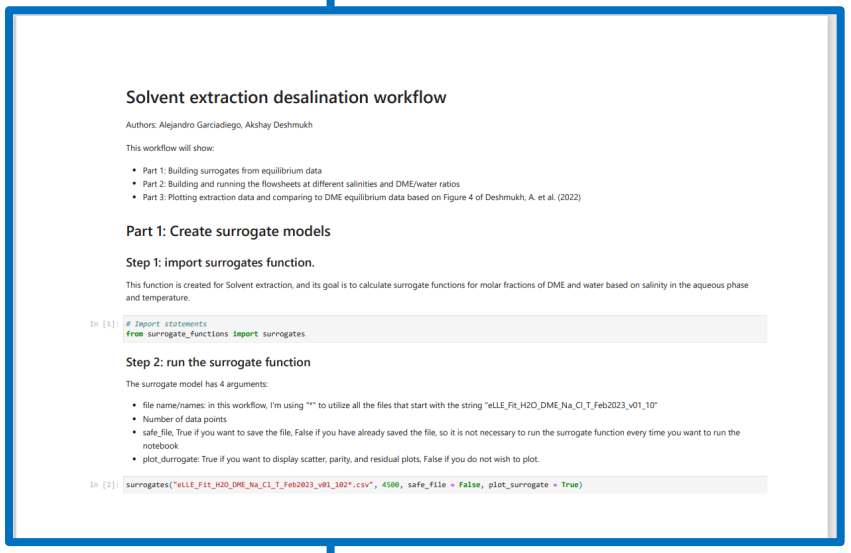
Build recovery process flowsheet

Workflow – Limited expertise (Screen solvents)

User input
Automated

Solvent equilibrium data

Jupyter notebook



Solvent extraction desalination workflow

Authors: Alejandro Garciadiego, Akshay Deshmukh

This workflow will show:

- Part 1: Building surrogates from equilibrium data
- Part 2: Building and running the flowsheets at different salinities and DME/water ratios
- Part 3: Plotting extraction data and comparing to DME equilibrium data based on Figure 4 of Deshmukh, A. et al. (2022)

Part 1: Create surrogate models

Step 1: import surrogates function.

This function is created for Solvent extraction, and its goal is to calculate surrogate functions for molar fractions of DME and water based on salinity in the aqueous phase and temperature.

In [1]:
```
# Import statements
from surrogate_functions import surrogates
```

Step 2: run the surrogate function

The surrogate model has 4 arguments:

- file name/names: in this workflow, I'm using "*" to utilize all the files that start with the string "eLLE_Fit_H2O_DME_Na_Cl_T_Feb2023_v01_10"
- Number of data points
- safe_file, True if you want to save the file, False if you have already saved the file, so it is not necessary to run the surrogate function every time you want to run the notebook
- plot_durrogate: True if you want to display scatter, parity, and residual plots, False if you do not wish to plot.

In [2]:
```
surrogates("eLLE_Fit_H2O_DME_Na_Cl_T_Feb2023_v01_102*.csv", 4500, safe_file = False, plot_surrogate = True)
```

Read csv
Create surrogate

Build and solve flowsheet
Compare water extraction

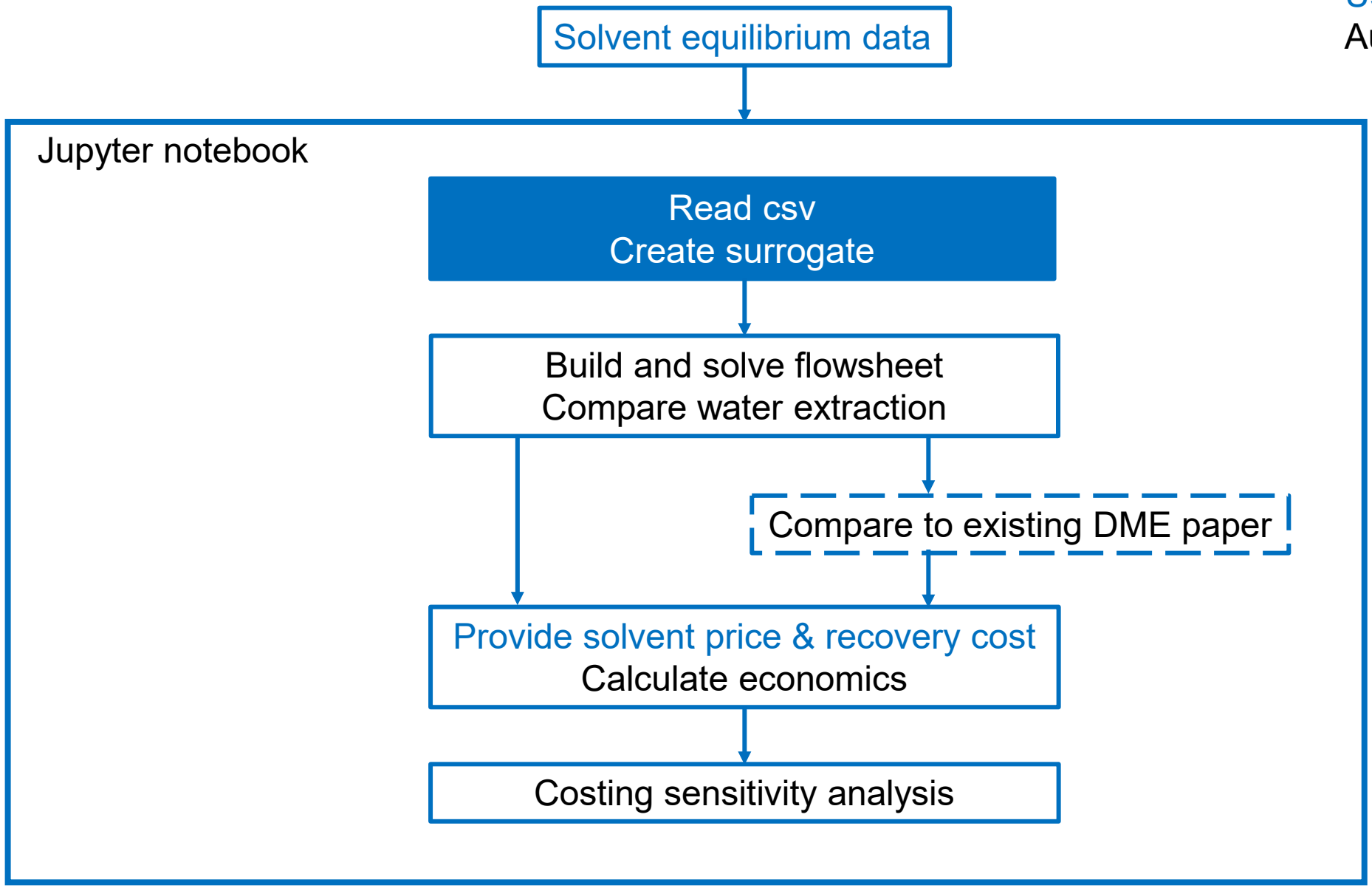
Compare to existing DME paper

Provide solvent price & recovery cost
Calculate economics

Costing sensitivity analysis

Workflow - Data Tailored DME extraction comparison

User input
Automated



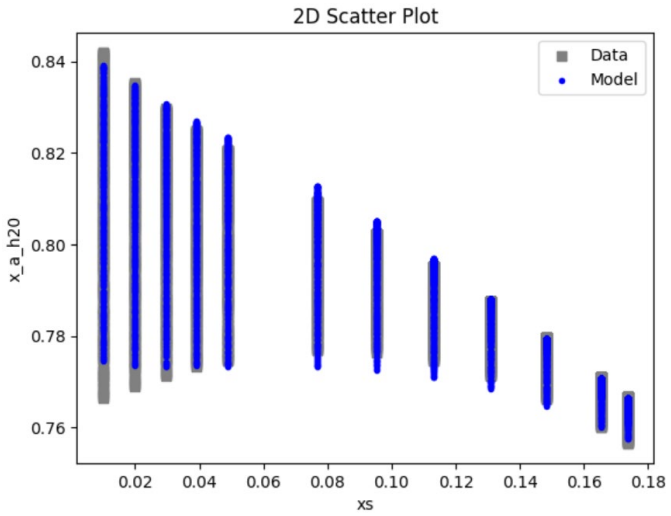
Workflow – surrogate building

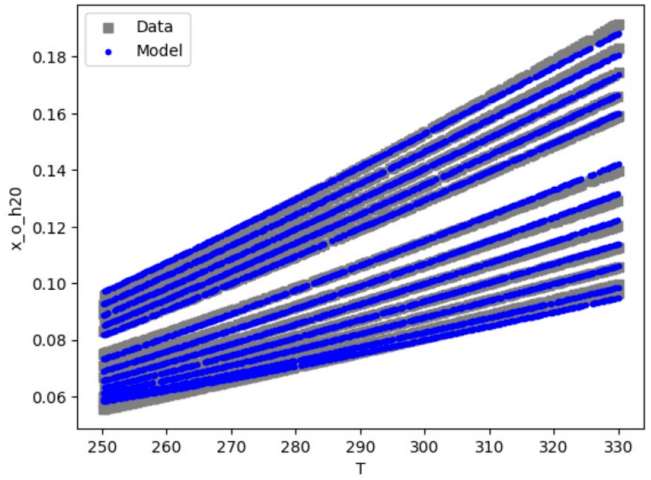
```
surrogates("eLLE_Fit_H2O_DME_Na_Cl_T_Feb2023_v01_102*.csv", 4500, safe_file = False, plot_surrogate = True)
```

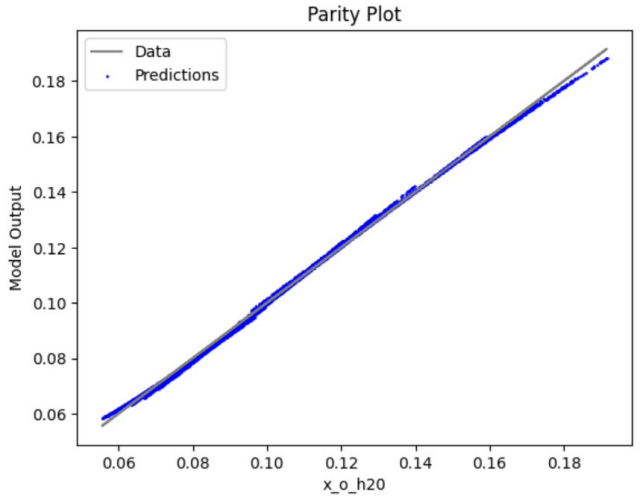
Name of data file and number of experiments

```
-----------------------------------------------------
The final coefficients of the regression terms are:

k                | -0.104655
(x_ 1 )^ 1       | -0.594643
(x_ 2 )^ 1       | 0.015913
(x_ 1 )^ 2       | -0.860408
(x_ 2 )^ 2       | -8.4e-05
(x_ 1 )^ 3       | -6.386718
(x_ 2 )^ 3       | 0.0
(x_ 1 )^ 4       | 25.0484
(x_ 2 )^ 4       | -0.0
x_ 1 .x_ 2       | 0.00421
```

```
Best solution found:
Order:  4  / MAE: 0.000707  / MSE: 0.000001  / R_sq: 0.999060  / Adjusted R^2: 0.999057
```

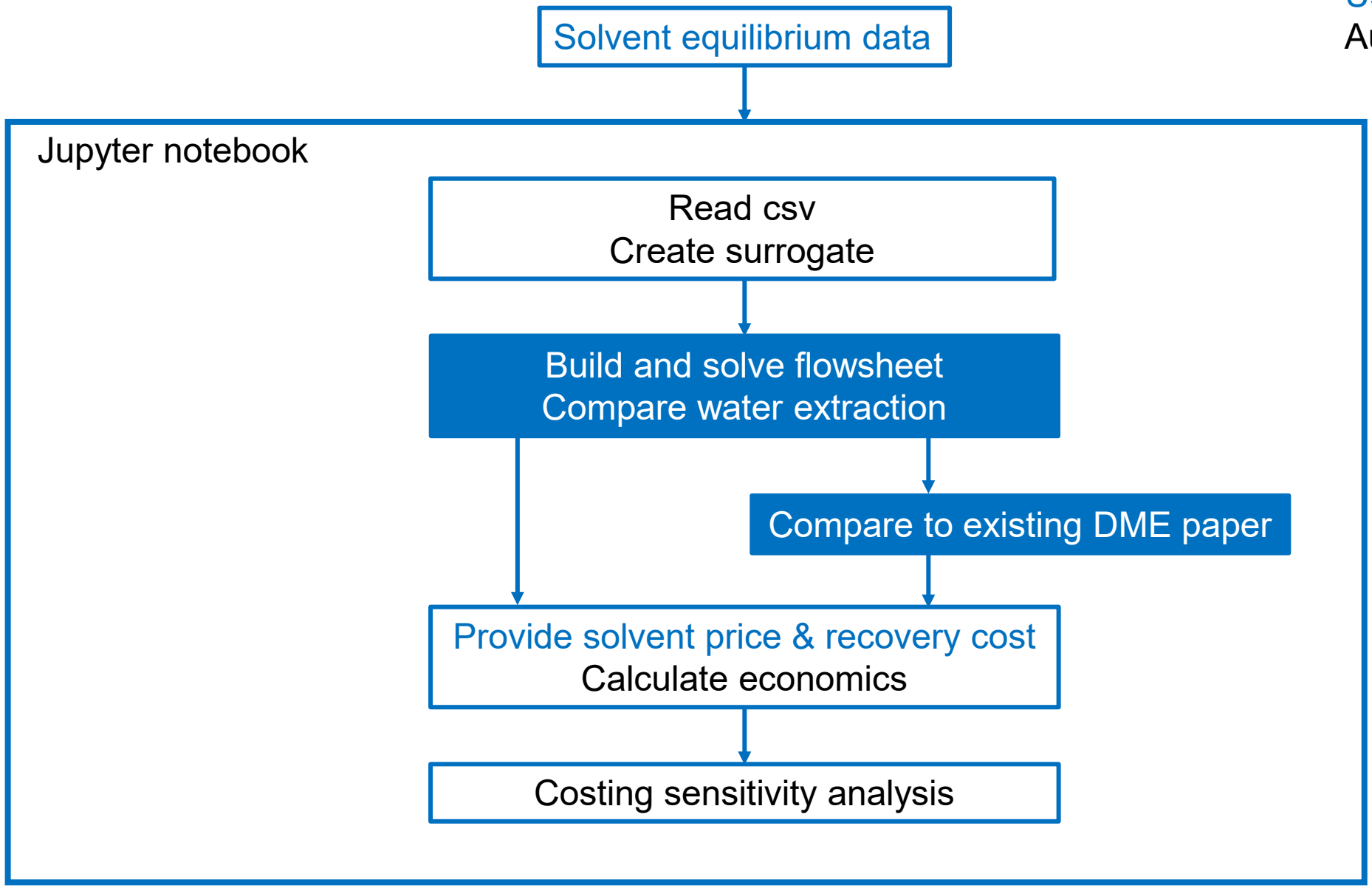






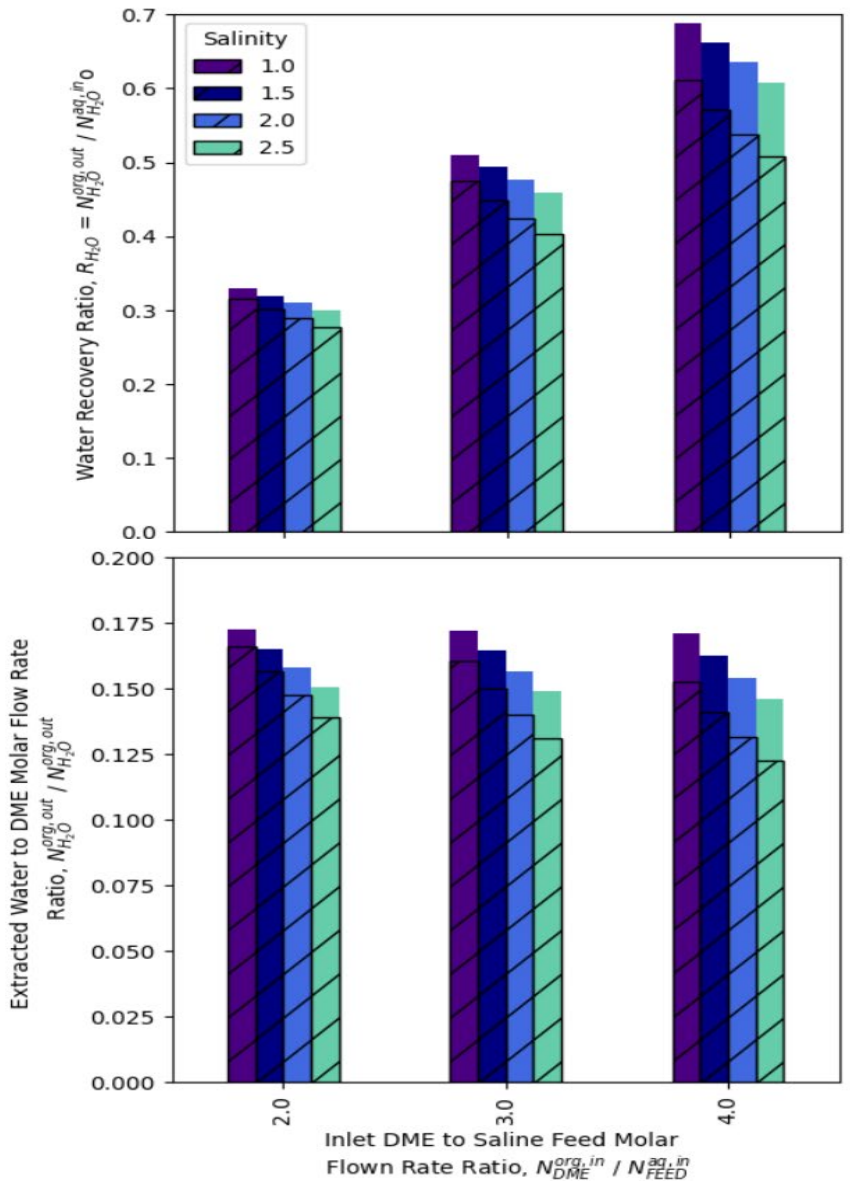
Workflow – Limited expertise (Screen solvents)

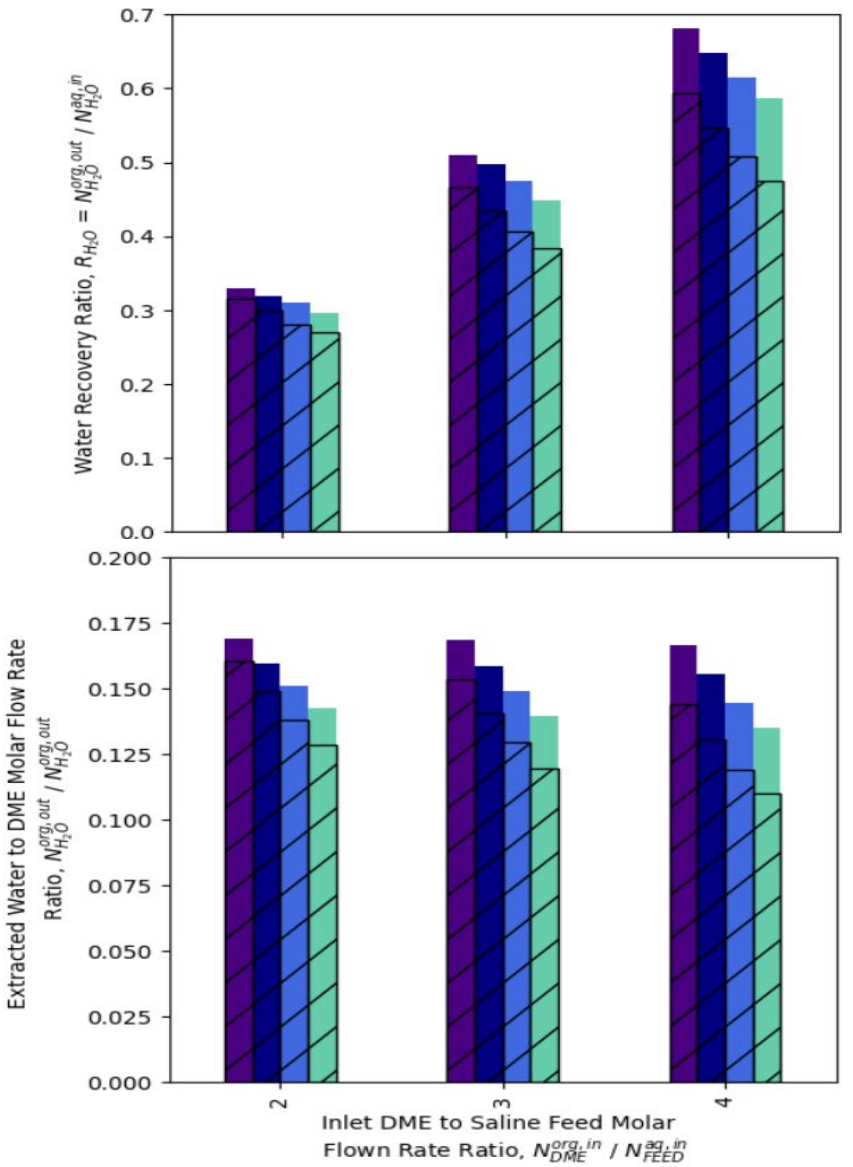
User input
Automated



Workflow – Water extraction

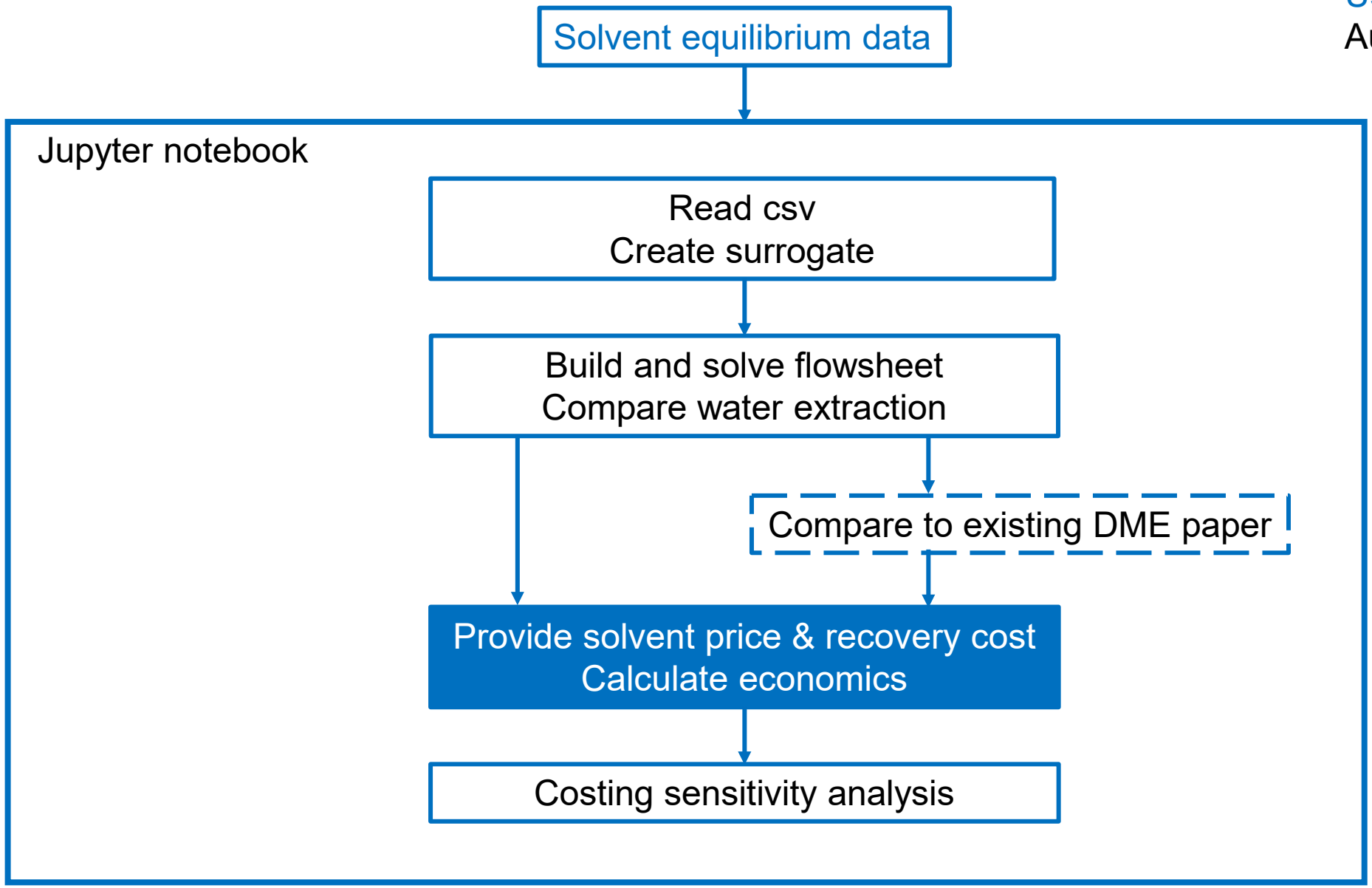
```
DME_f2 = [2, 3, 4]

NaCl_f2 = [0.335449544, 0.519290265, 0.715296575, 0.924717819]
```





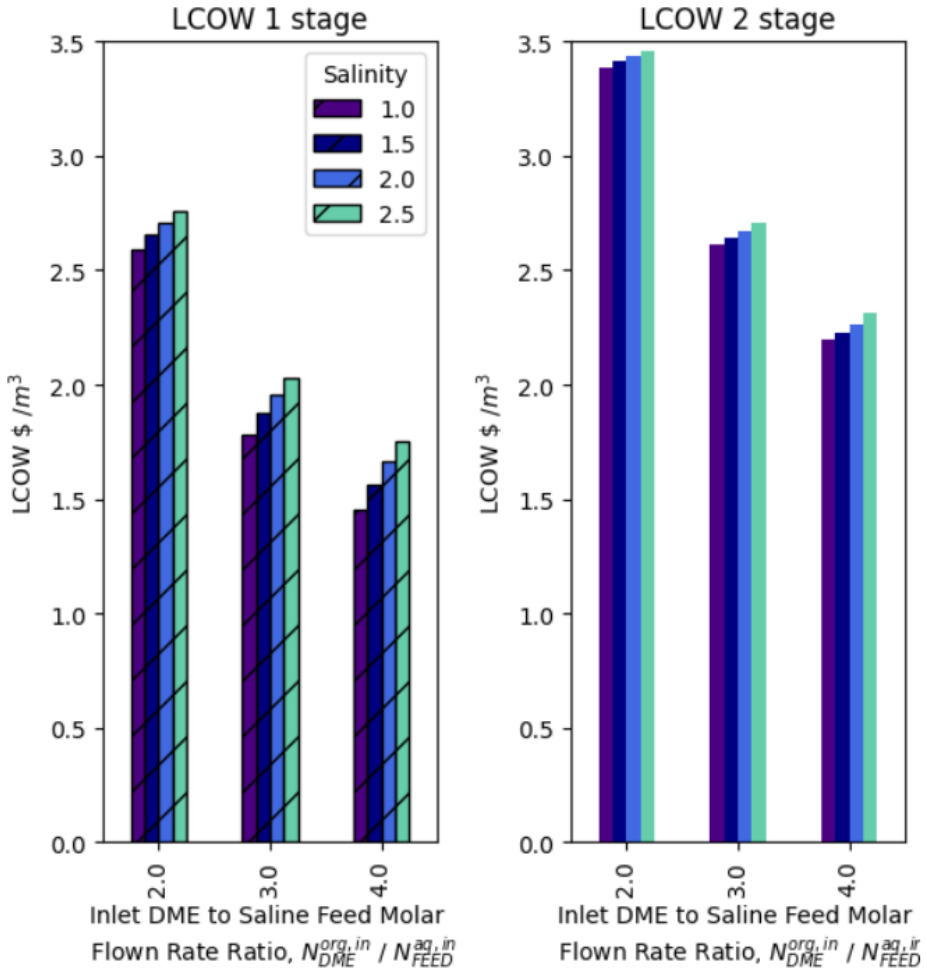
Workflow – Limited expertise (Screen solvents)

User input
Automated

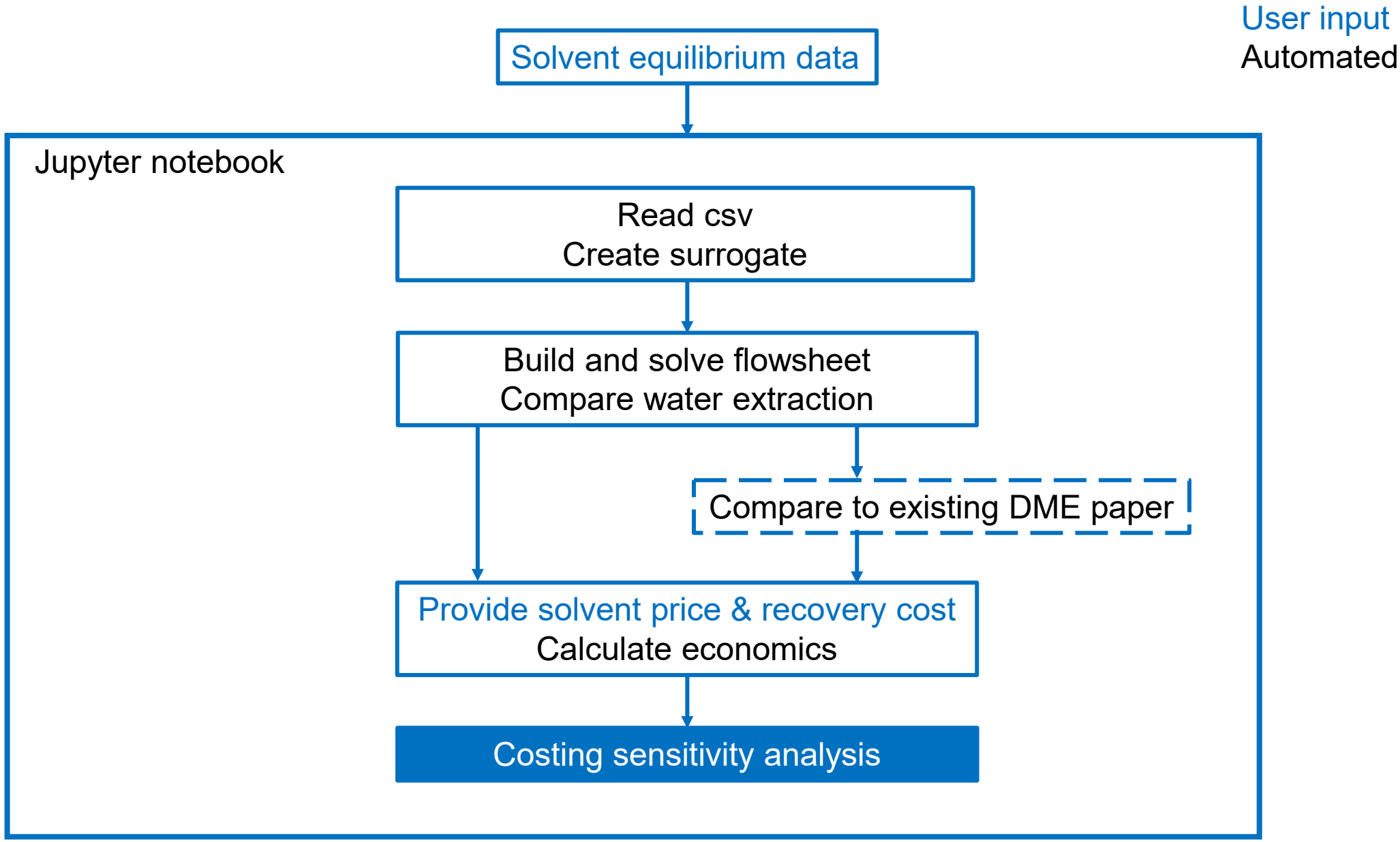


Workflow – LCOW calculation

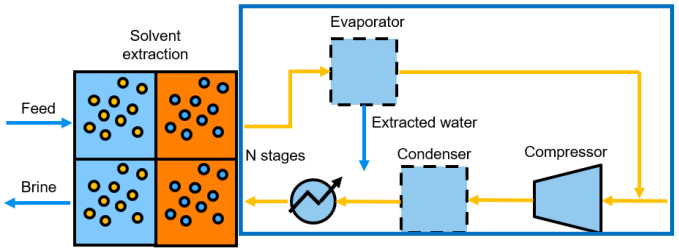
```
m.fs.costing.solvent_cost.fix(0.496) #USD_2020 /kg

recovery_fract = 0.01 # % of inlet solvent

m.fs.costing.solvent_recov.fix(0.0001) # USD_2020 / pyo.units.kg
```



Workflow – Limited expertise (Screen solvents)



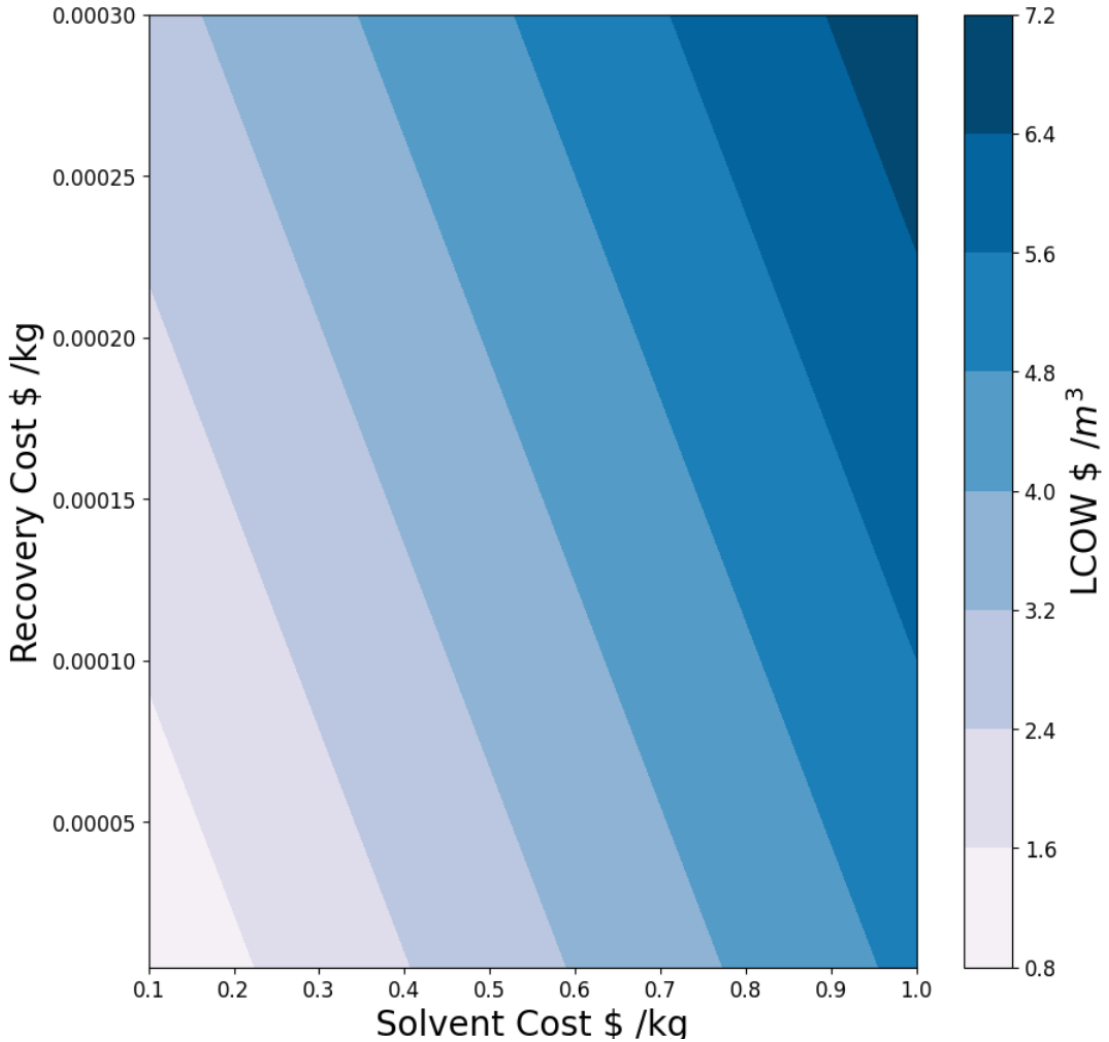
Workflow – Sensitivity analysis



$ Solvent Recovery

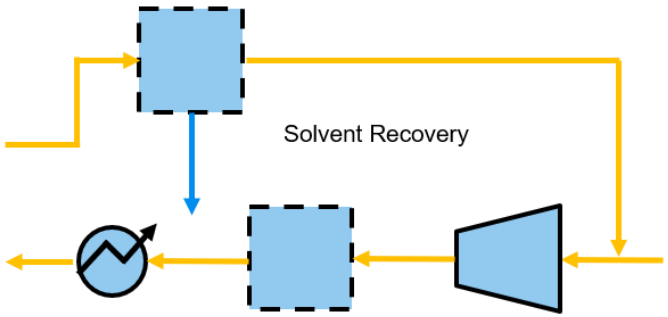
$ Inlet solvent

```
solv_price = np.linspace(0.100, 1.0, num=100)
solv_recov = np.linspace(0.000005, 0.0003, num=100)
```



Workflow – Intermediate expertise (Similar solvents)

User input
Automated



Solvent equilibrium data

Jupyter notebook

Read csv
Create surrogate

Property data json
Cp parameters
Peng-Robinson parameters
Density
Etc.

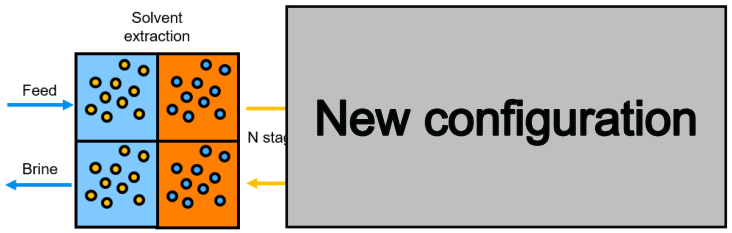
Build flowsheet
Read .and overwrite property packages
Solve flowsheet

Compare water extraction metrics

Provide solvent price & recovery cost
Calculate economics

Costing sensitivity analysis

Workflow – Experienced user (Different recovery process)



Build recovery process flowsheet

Property data json
Cp parameters
Peng-Robinson parameters
Density
Etc.

Solvent equilibrium data

Phyton file

Read csv
Create surrogate

Build flowsheet
Read and overwrite property packages
Solve flowsheet

Compare water extraction metrics

Provide solvent price
Calculate economics

Costing sensitivity analysis

User input
Automated

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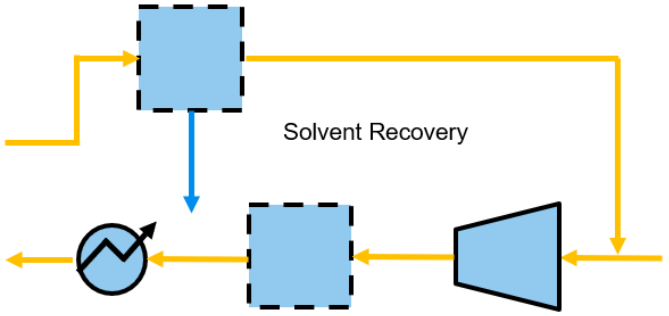
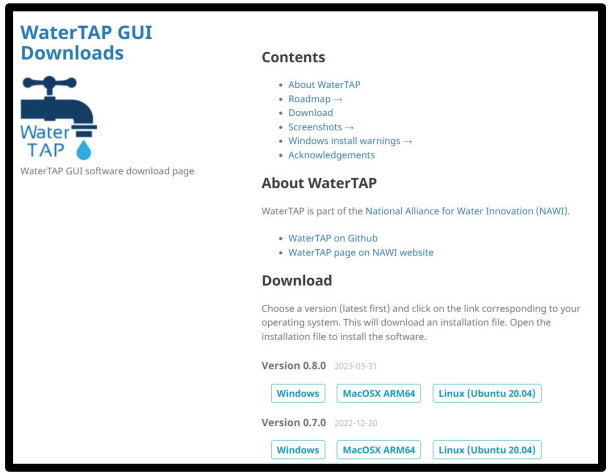
Summary

- WaterTAP tools are flexible
- We can create tailored workflows for users and needs
- We created an easy-to-use solvent screening tool
- WaterTAP is expanding its capabilities and accessibility

Ongoing work

- Release the workflows in the repository
- Add process flowsheet to GUI
- Gap analysis on unit models required for recovery of different types of solvents





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

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