User Interfaces for *IDAES, NAWI WaterTAP, PrOMMiS, PARETO, and CCSI²* Status, Plans, and Discussion

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2024 PSE Summit

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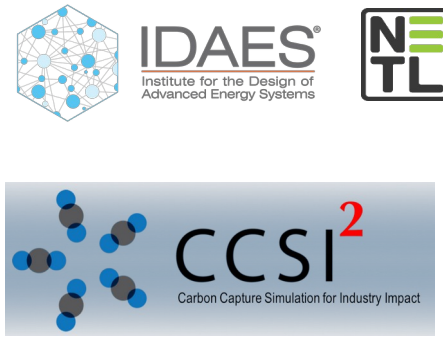
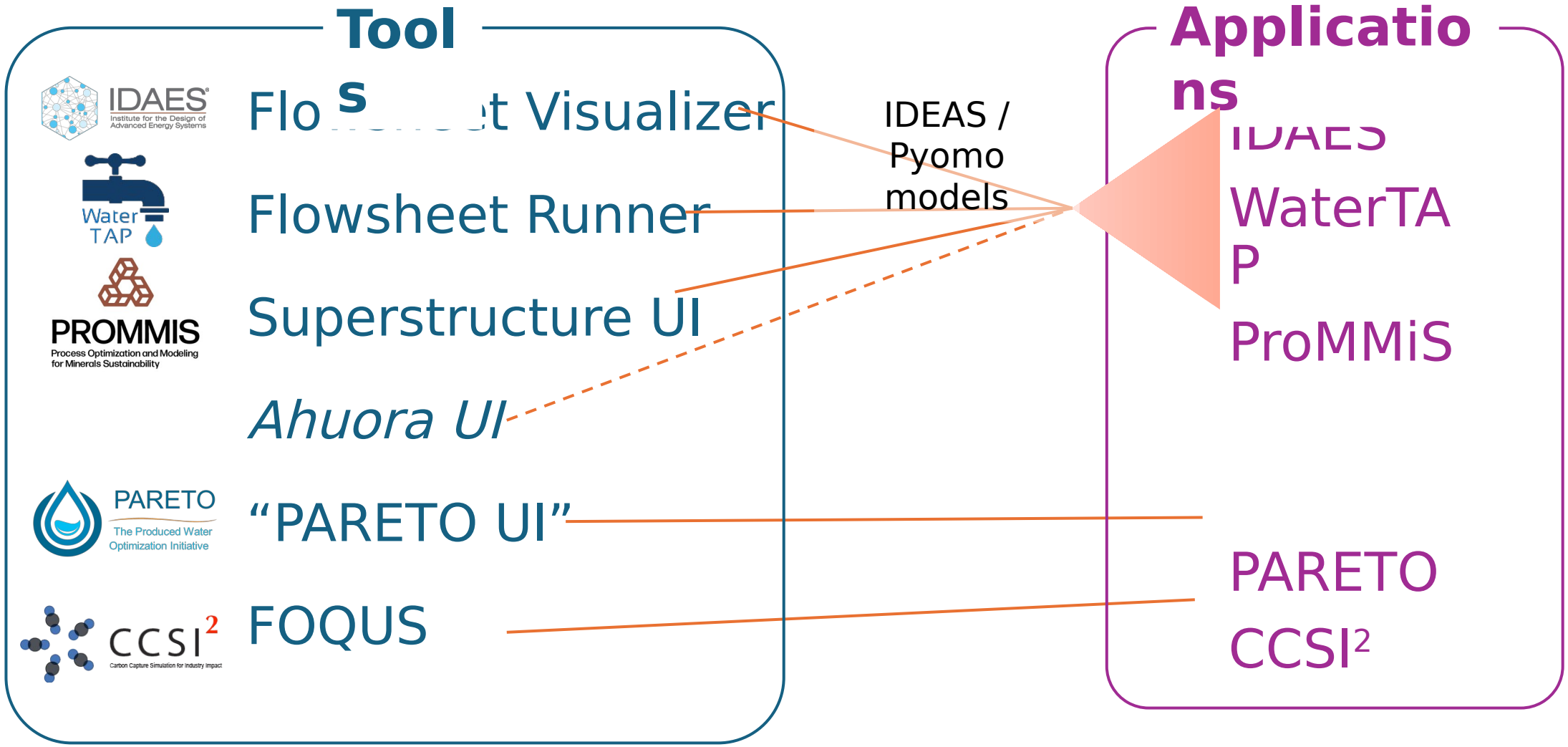
Project Institutions



Outline

- Overview
- Walk-through of current UIs
  - Status
  - Plans
  - Q&A
- Summary
- Q&A

Overview


Tools
IDAES
Institute for the Design of Advanced Energy Systems
Flowsheet Visualizer
Water TAP
Flowsheet Runner
PROMMIS
Process Optimization and Modeling for Minerals Sustainability
Superstructure UI
Ahuora UI
PARETO
The Produced Water Optimization Initiative
"PARETO UI"
CCSI²
Carbon Capture Simulation for Industry Impact
FOQUS
IDEAS / Pyomo models
Applications
IDAES
WaterTAP
ProMMiS
PARETO
CCSI²

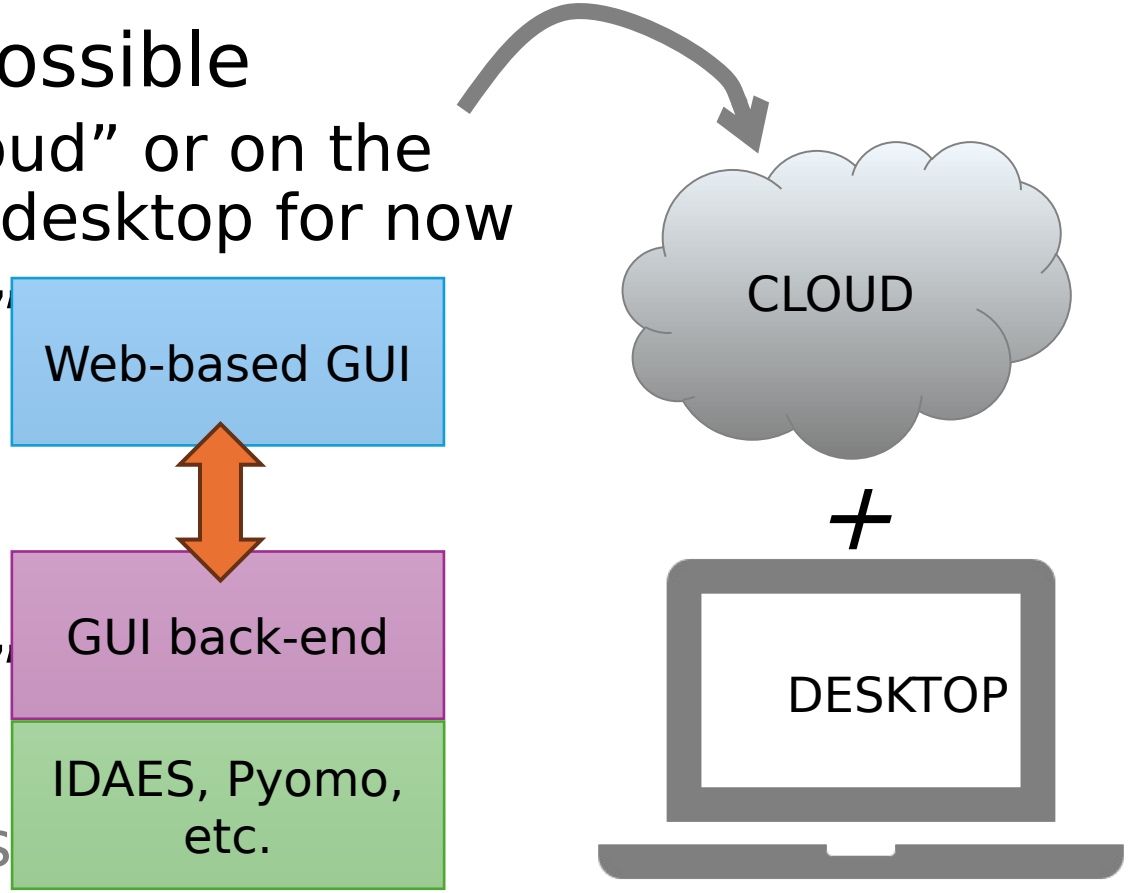
General strategy

- Limited funding – don’t try to be all things to all people
- Engage with users & communities -> understand needs
- Target two communities
  - Developers, including Uni partners et al.
  - Advanced users

    Do *not* target naïve users, except as viewers of results pages

General development principles

- Use Web technologies where possible
  - Allows for deployment in “the cloud” or on the desktop (e.g., Electron) – mostly desktop for now
- Use the same front-end “stack”
  - ReactJS - Interactivity
  - Material UI – Look and feel
  - Plotly – Plots and graphing
- Use the same back-end “stack”
  - Python
  - FastAPI – library to handle reques



Tool walk-through

- Current status
  - Basics
    - Functionality
    - Types of models
    - Installation
  - Examples/screenshots
- Plans
  - New features
  - Improvements, refactorings
- Q&A

Flowsheet Visualizer

Functionality

Automatic layout of flowsheets in Python code

Save as image

View stream table

Start from script, console, or Jupyter Notebook

View and run diagnostics

In Notebook, updates to flowsheet reflected in diagram

Types of models

IDAES/Pyomo

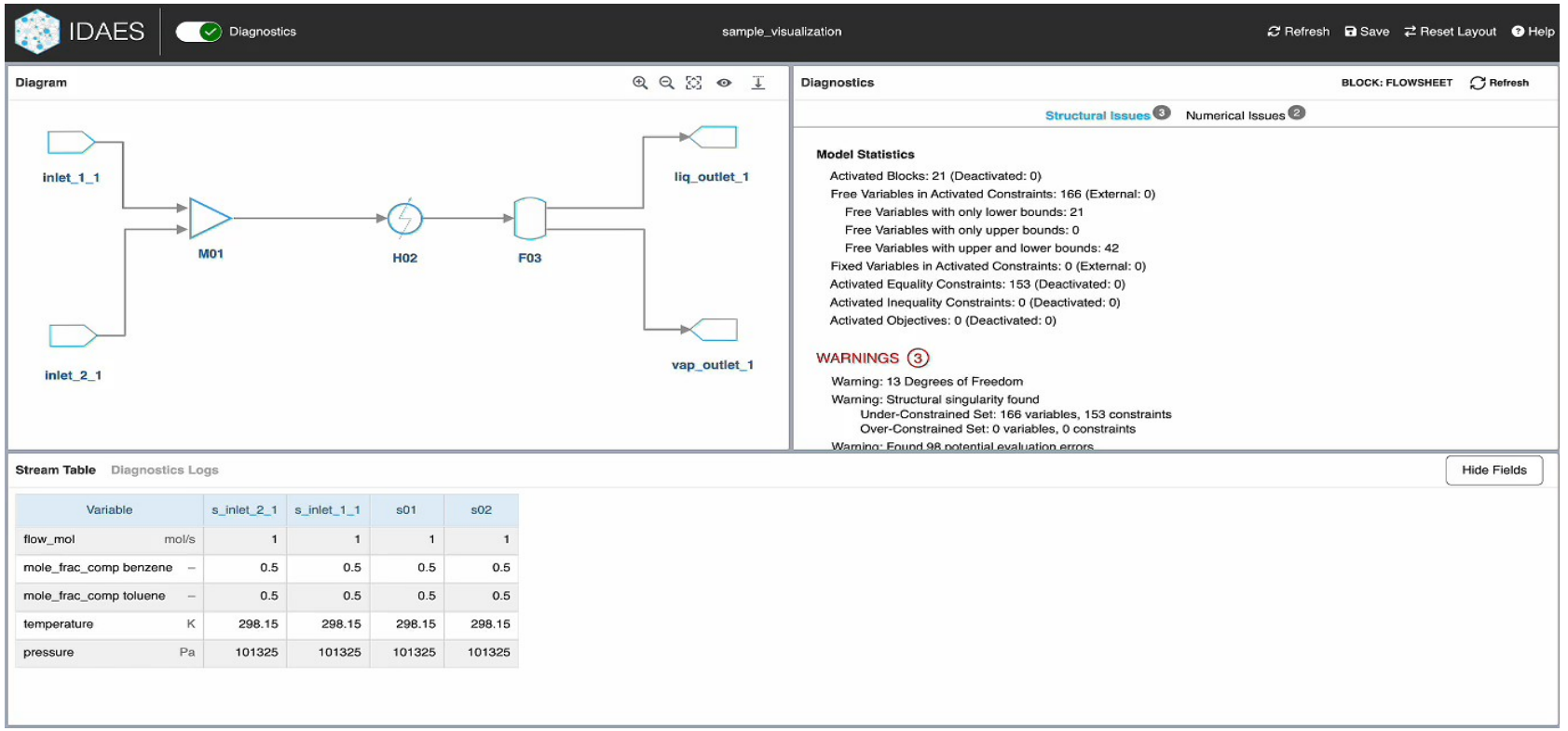
Installation

Install IDAES Toolkit with '[ui]' :

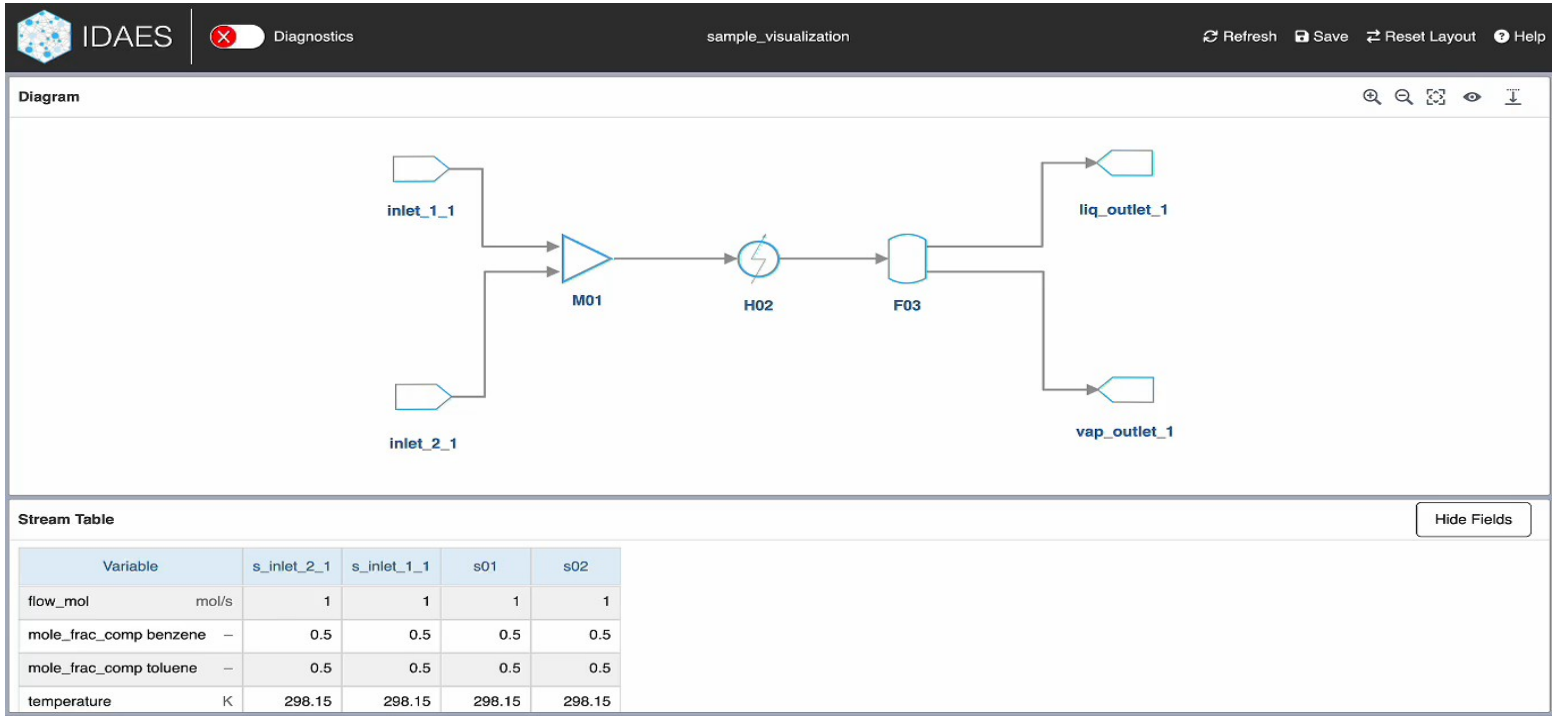
```
pip install ideas-pse[ui]
```

Docs: https://idaes-ui.readthedocs.io

Flowsheet Visualizer: Layout

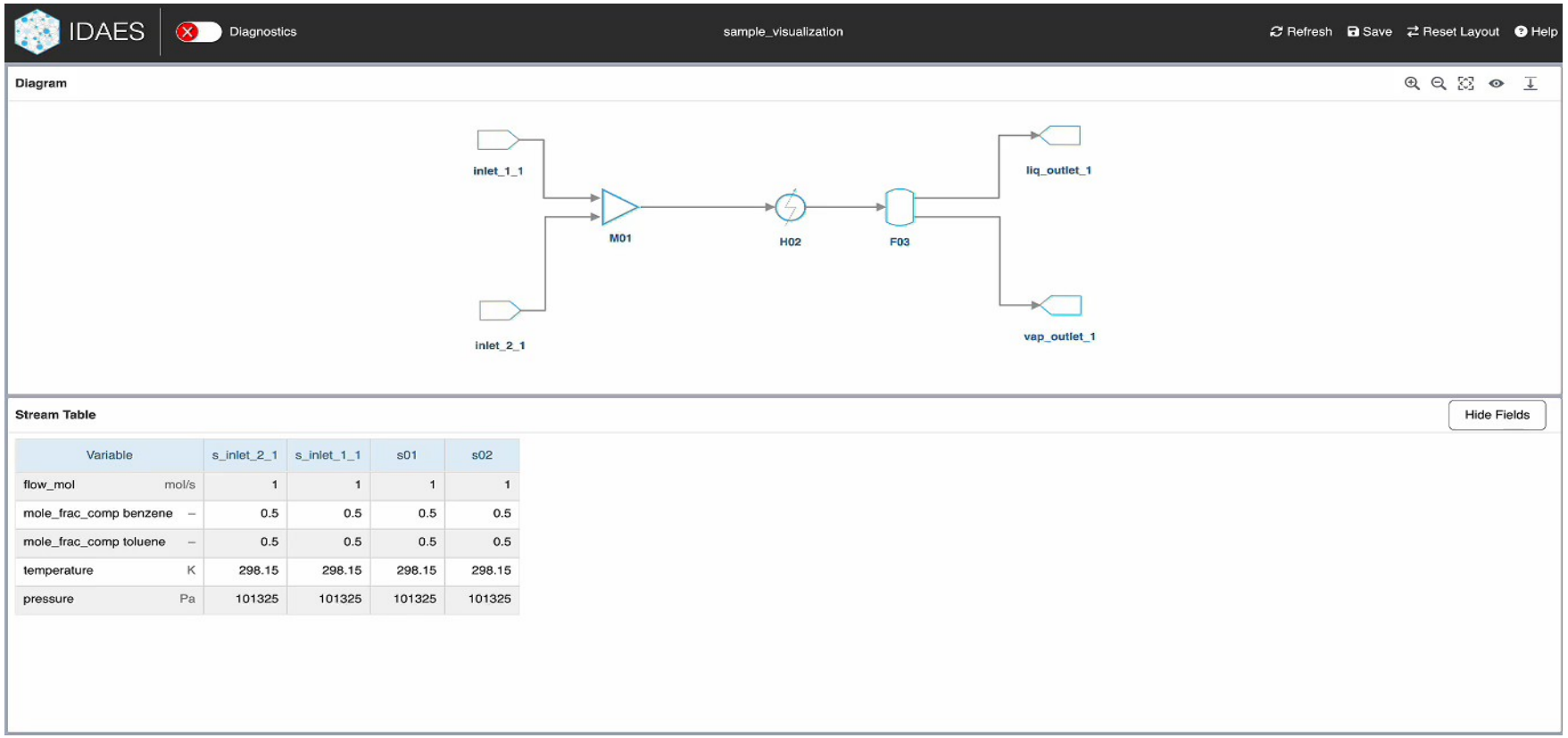


Flowsheet Visualizer: Rearrange diagram

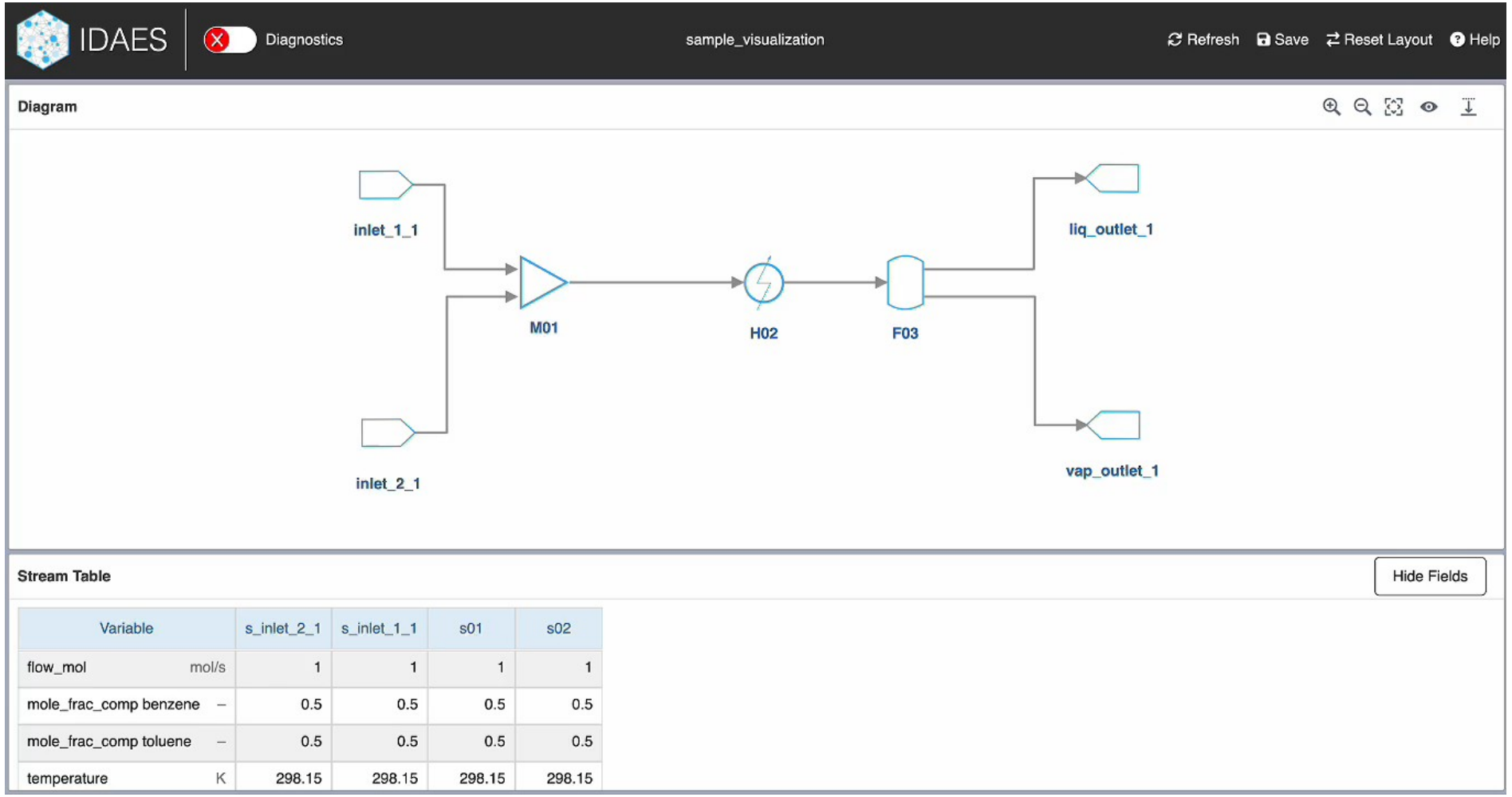


Variable		s_inlet_2_1	s_inlet_1_1	s01	s02
flow_mol	mol/s	1	1	1	1
mole_frac_comp benzene	–	0.5	0.5	0.5	0.5
mole_frac_comp toluene	–	0.5	0.5	0.5	0.5
temperature	K	298.15	298.15	298.15	298.15

Flowsheet Visualizer: Stream table

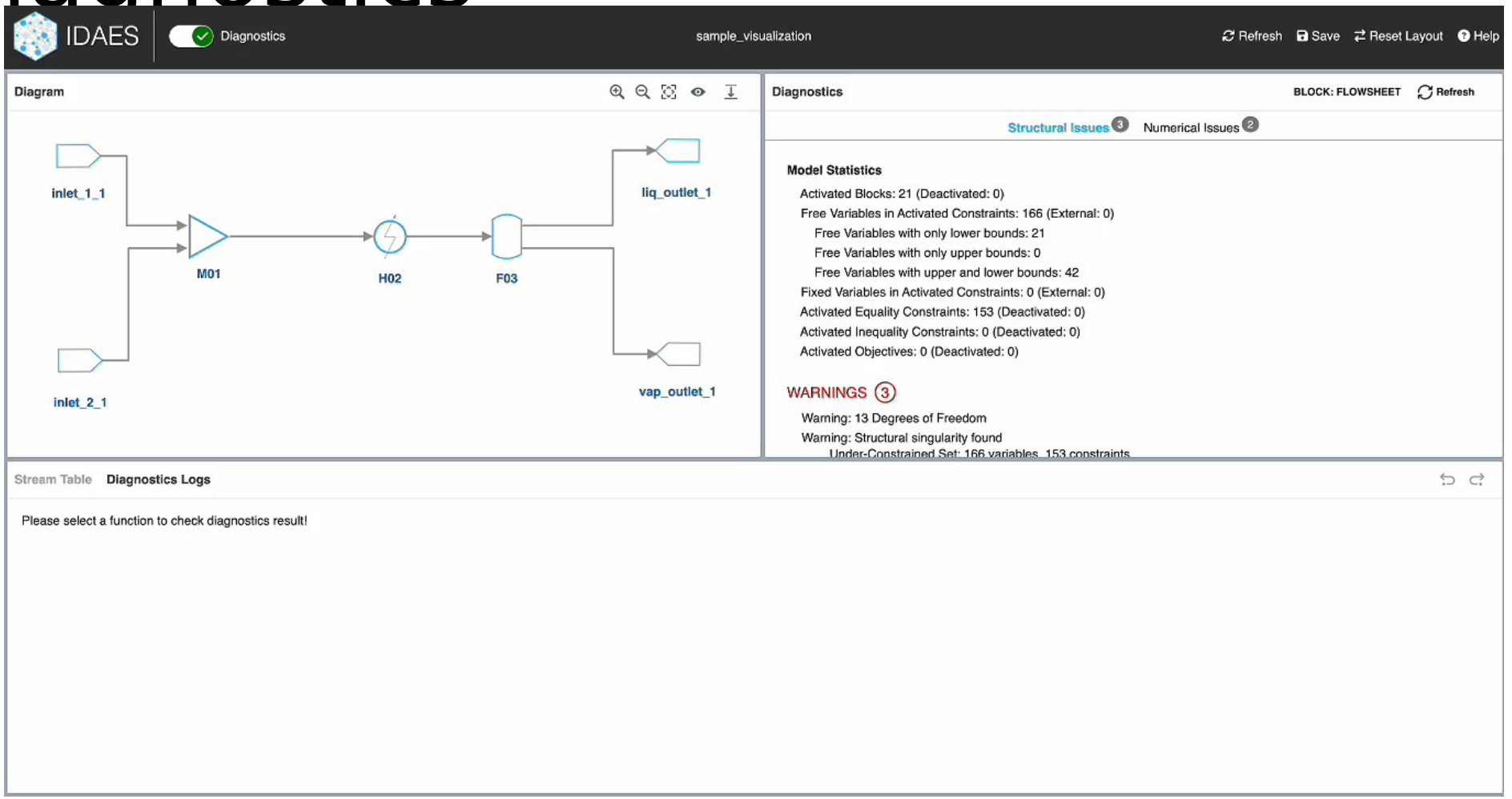


Flowsheet Visualizer: Diagnostics Panel



Variable		s_inlet_2_1	s_inlet_1_1	s01	s02
flow_mol	mol/s	1	1	1	1
mole_frac_comp benzene	–	0.5	0.5	0.5	0.5
mole_frac_comp toluene	–	0.5	0.5	0.5	0.5
temperature	K	298.15	298.15	298.15	298.15

Flowsheet Visualizer: Run diagnostics



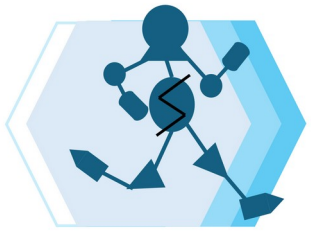
Flowsheet visualizer plans

IDAES®
Institute for the Design of Advanced Energy Systems

- Bugfixes, possible minor enhancements
- No major features planned in this cycle
- Possible future enhancements include:
  - View details of any unit / stream
  - Improved diagnostics workflow and visualization
  - Editing of model variables
  - Integration with Flowsheet Runner

Flowsheet visualizer Q&A

IDAES®
Institute for the Design of Advanced Energy Systems



Flowsheet Runner aka WaterTAP UI

Functionality

- API for devs to export IDAES model output, input variables
- Select model from list
- Set inputs
  - Free/fixed
  - Sweep over range
- Solve (ipopt, etc.)
- Compare different runs
- Sensitivity analysis results

Types of models

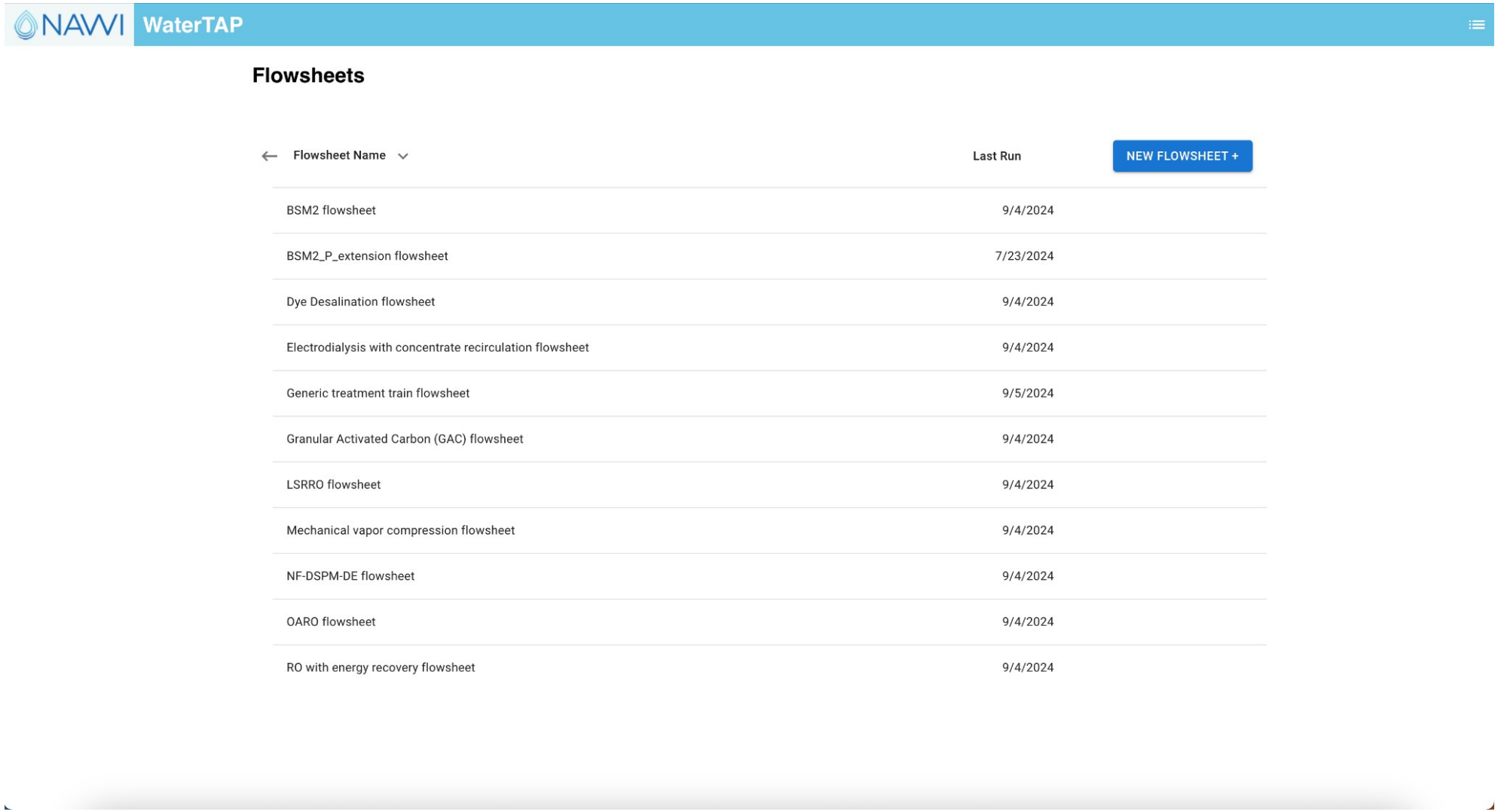
IDAES / Pyomo

Installation

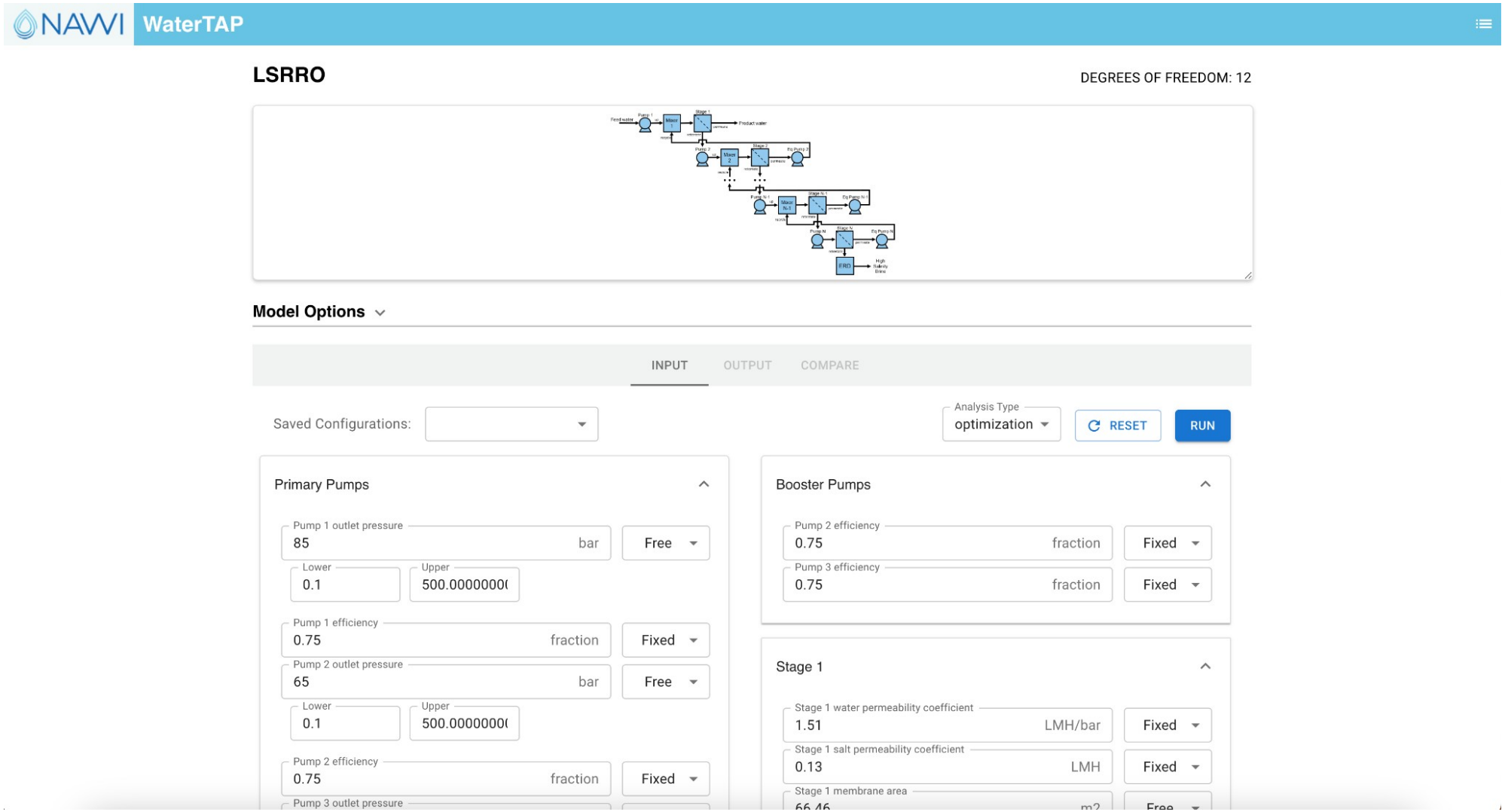
Local install, 1-click

https://watertap-org.github.io

Flowsheet Runner: Flowsheets List



Flowsheet Runner: Input Page



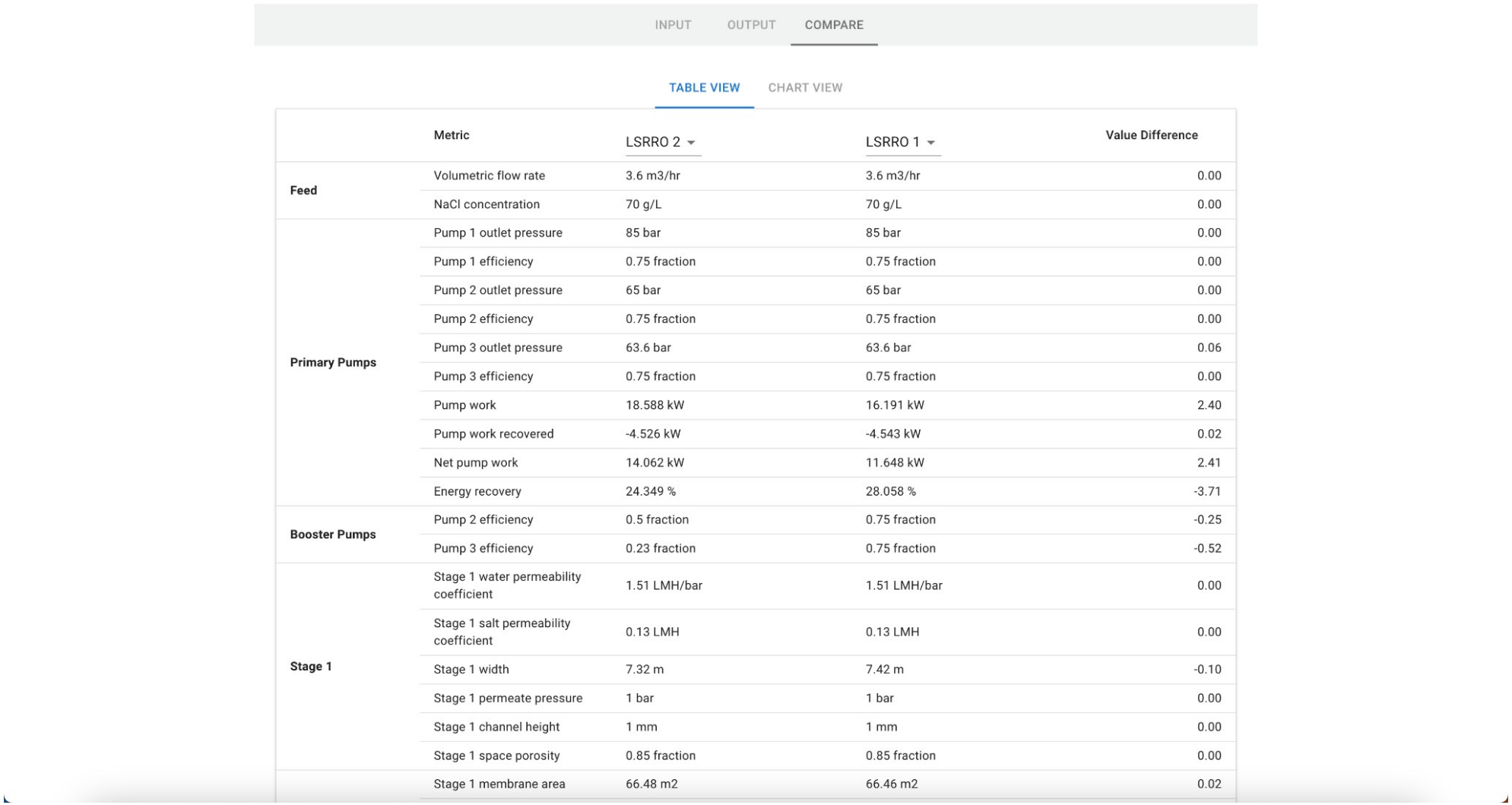
Flowsheet Runner: Optimization Output

INPUT | OUTPUT | COMPARE

DOWNLOAD RESULT | SAVE CONFIGURATION

Category	Variable	Units	Value
Feed	Volumetric flow rate	m3/hr	3.6
	NaCl concentration	g/L	70
Primary Pumps	Pump 1 outlet pressure	bar	85
	Pump 1 efficiency	fraction	0.75
	Pump 2 outlet pressure	bar	65
	Pump 2 efficiency	fraction	0.75
	Pump 3 outlet pressure	bar	63.6
	Pump 3 efficiency	fraction	0.75
	Pump work	kW	16.191
	Pump work recovered	kW	-4.543
	Net pump work	kW	11.648
	Energy recovery	%	28.058
Booster Pumps	Pump 2 efficiency	fraction	0.75
	Pump 3 efficiency	fraction	0.75
Stage 1	Stage 1 water permeability coefficient	LMH/bar	1.51
	Stage 1 salt permeability coefficient	LMH	0.13
	Stage 1 width	m	7.42
	Stage 1 permeate pressure	bar	1
	Stage 1 channel height	mm	1
	Stage 1 space porosity	fraction	0.85
Membrane area	Stage 1 membrane area	m2	66.46
	Stage 2 membrane area	m2	141.22
	Stage 3 membrane area	m2	1.73

Flowsheet Runner: Compare Page



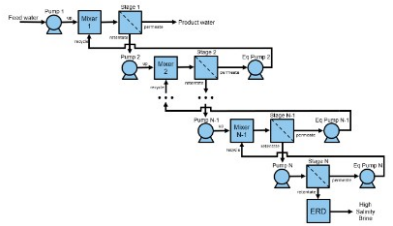
	Metric	LSRRO 2	LSRRO 1	Value Difference
Feed	Volumetric flow rate	3.6 m3/hr	3.6 m3/hr	0.00
	NaCl concentration	70 g/L	70 g/L	0.00
Primary Pumps	Pump 1 outlet pressure	85 bar	85 bar	0.00
	Pump 1 efficiency	0.75 fraction	0.75 fraction	0.00
	Pump 2 outlet pressure	65 bar	65 bar	0.00
	Pump 2 efficiency	0.75 fraction	0.75 fraction	0.00
	Pump 3 outlet pressure	63.6 bar	63.6 bar	0.06
	Pump 3 efficiency	0.75 fraction	0.75 fraction	0.00
	Pump work	18.588 kW	16.191 kW	2.40
	Pump work recovered	-4.526 kW	-4.543 kW	0.02
	Net pump work	14.062 kW	11.648 kW	2.41
	Energy recovery	24.349 %	28.058 %	-3.71
Booster Pumps	Pump 2 efficiency	0.5 fraction	0.75 fraction	-0.25
	Pump 3 efficiency	0.23 fraction	0.75 fraction	-0.52
Stage 1	Stage 1 water permeability coefficient	1.51 LMH/bar	1.51 LMH/bar	0.00
	Stage 1 salt permeability coefficient	0.13 LMH	0.13 LMH	0.00
	Stage 1 width	7.32 m	7.42 m	-0.10
	Stage 1 permeate pressure	1 bar	1 bar	0.00
	Stage 1 channel height	1 mm	1 mm	0.00
	Stage 1 space porosity	0.85 fraction	0.85 fraction	0.00
	Stage 1 membrane area	66.48 m2	66.46 m2	0.02

Flowsheet Runner: Sensitivity

NAWI WaterTAP

LSRRO

DEGREES OF FREEDOM: 12



Model Options

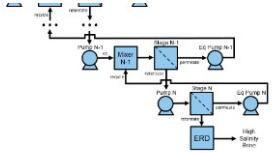
INPUT OUTPUT

TABLE VIEW CHART VIEW

Net pump work	Energy recovery	Number of stages	Water volumetric recovery	Mass water recovery rate	Salt rejection	Specific ene
19.675	19.448	3.000	31.296	31.914	99.289	
15.933	22.435	3.000	35.611	36.314	99.289	
13.847	24.802	3.000	37.412	38.150	99.289	
12.543	26.621	3.000	38.425	39.184	99.289	
11.648	28.058	3.000	39.081	39.853	99.289	

DOWNLOAD RESULTS

Flowsheet Runner: Sensitivity (2)

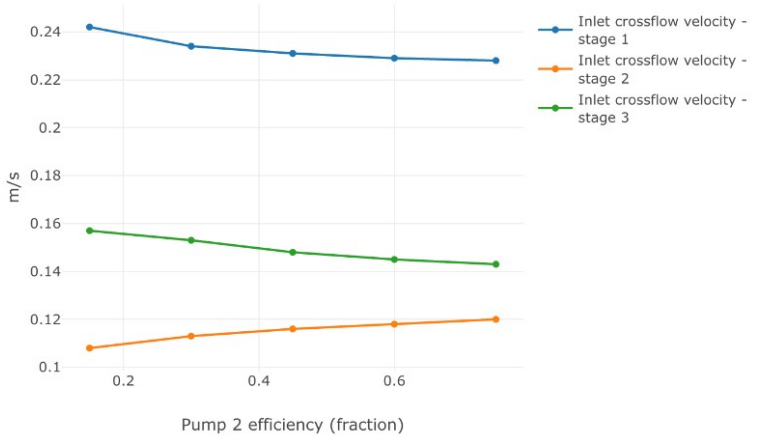


Model Options

INPUT OUTPUT

TABLE VIEW CHART VIEW

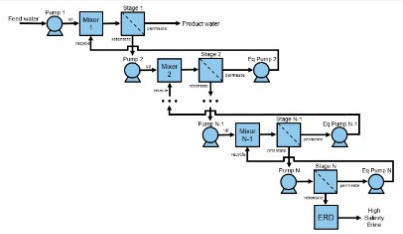
3
Average water flux - stage 1
Average water flux - stage 2
Average water flux - stage 3
Average NaCl flux - stage 1
Average NaCl flux - stage 2
Average NaCl flux - stage 3
Inlet Reynolds number - stage 1
Inlet Reynolds number - stage 2
Inlet Reynolds number - stage 3
Inlet crossflow velocity - stage 1
Inlet crossflow velocity - stage 2
Inlet crossflow velocity - stage 3



Flowsheet Runner: Sensitivity (3)

LSRRO

DEGREES OF FREEDOM: 10



Model Options

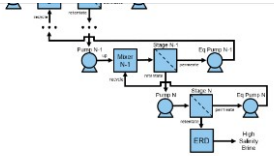
INPUT OUTPUT

TABLE VIEW CHART VIEW

Salt permeability coefficient - stage 3	Average water flux - stage 1	Average water flux - stage 2	Average water flux - stage 3	Average NaCl
11.375	21.042	8.500	11.534	
12.016	21.043	8.704	12.216	
12.600	21.044	8.917	12.893	
12.600	21.054	10.209	12.349	
12.600	21.054	10.209	12.349	
12.600	21.054	10.209	12.348	
12.600	21.061	11.071	12.317	
12.600	21.061	11.071	12.317	
12.600	21.061	11.071	12.316	

DOWNLOAD RESULTS

Flowsheet Runner: Sensitivity (4)

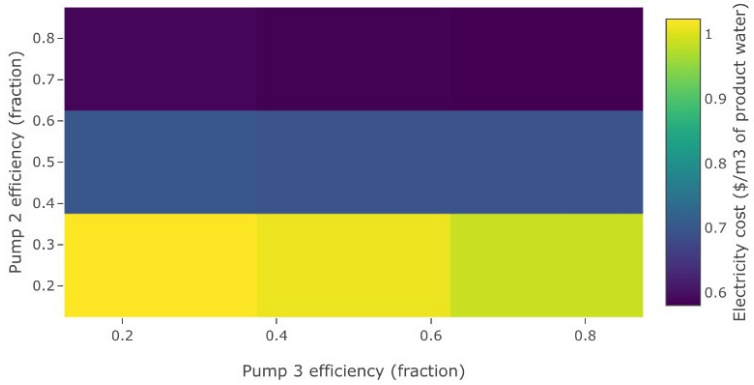


Model Options

INPUT OUTPUT

TABLE VIEW CHART VIEW

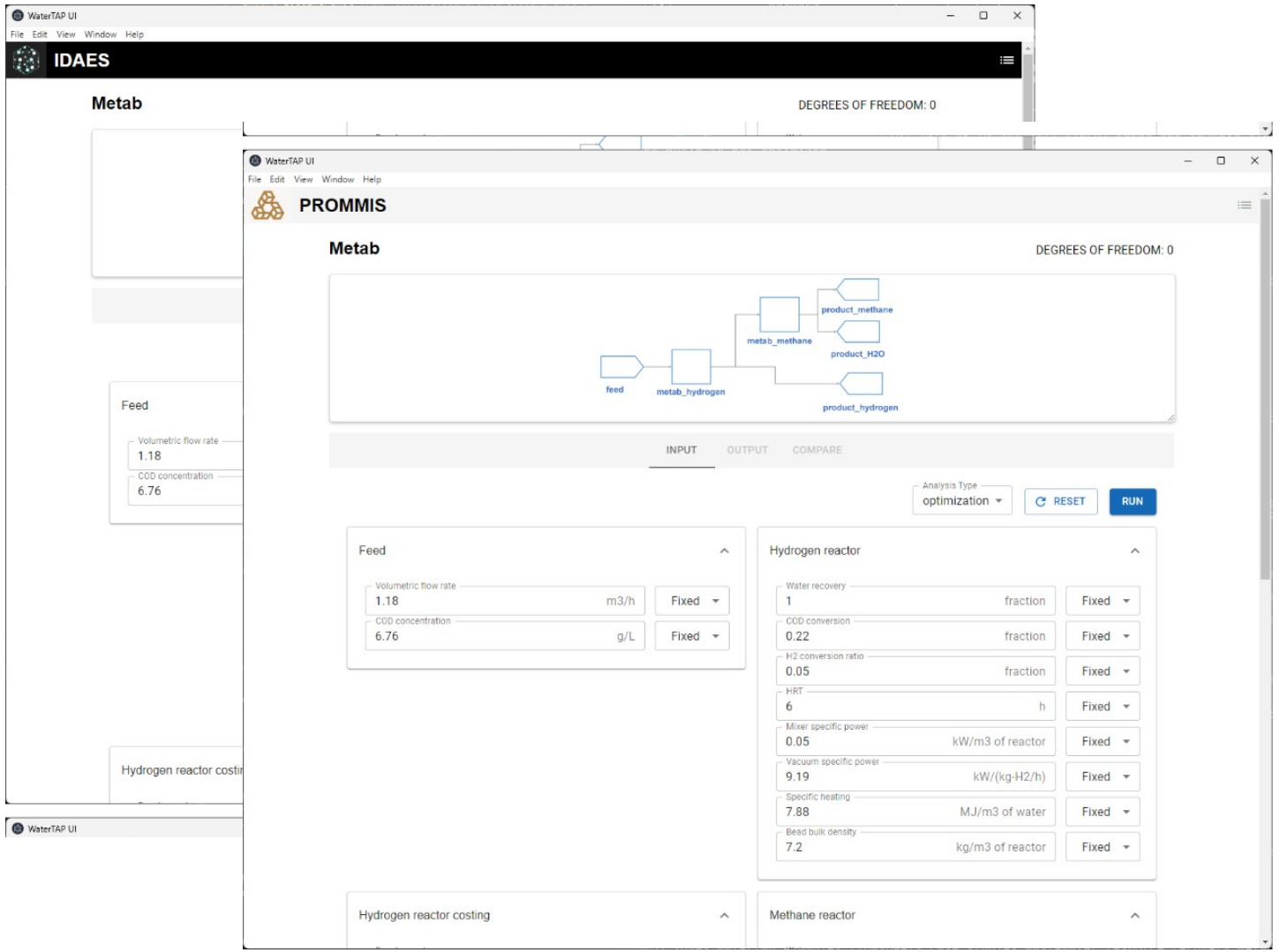
- Mass water recovery rate
- Salt rejection
- Specific energy consumption
- Electricity cost
- Total membrane area
- Annual feed flow
- Annual water production
- Levelized cost of water
- Total CAPEX LCOW
- Primary pump CAPEX LCOW
- Booster pump CAPEX LCOW
- Energy recovery device CAPEX LCOW
- Membrane CAPEX LCOW



Flowsheet Runner plans: Cross-project

Use across IDAES flowsheet projects

- Project branding
- Project flowsheets



Flowsheet Runner plans

- Software repository alignment with cross-project goals
  - Better dependency management and maintenance
- Add support for IDAES “decision support” applications
- Streamline API/tools to add existing flowsheets
- *Possible integration with Ahuora GUI*

Flowsheet runner Q&A

PARETO UI

Functionality

Decision-support tool for produced water management

Given a network of sources, sinks, etc., optimize infrastructure buildout alternatives

User can edit any input, or override optimization choices

Compare solutions with tables and charts

Types of models

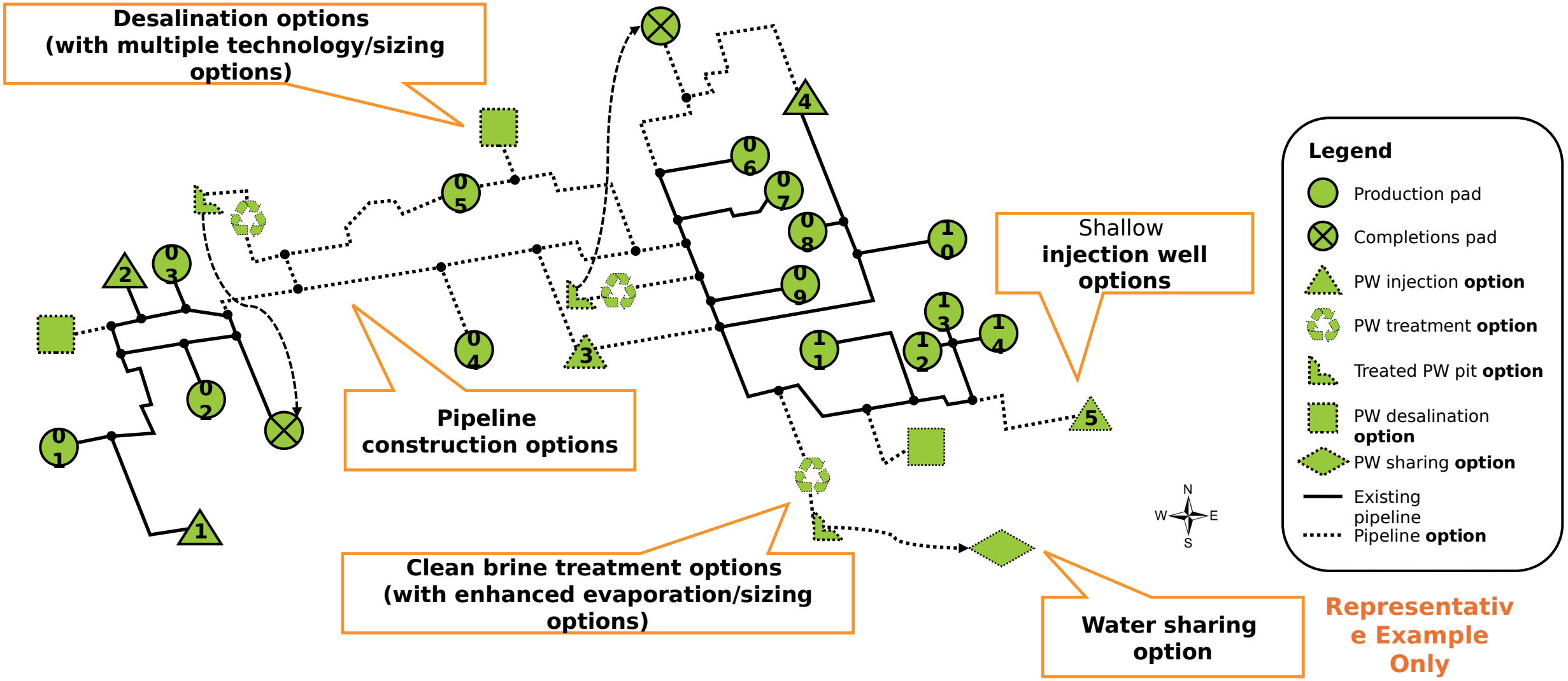
Pyomo PW networks created from Excel spreadsheets

Installation

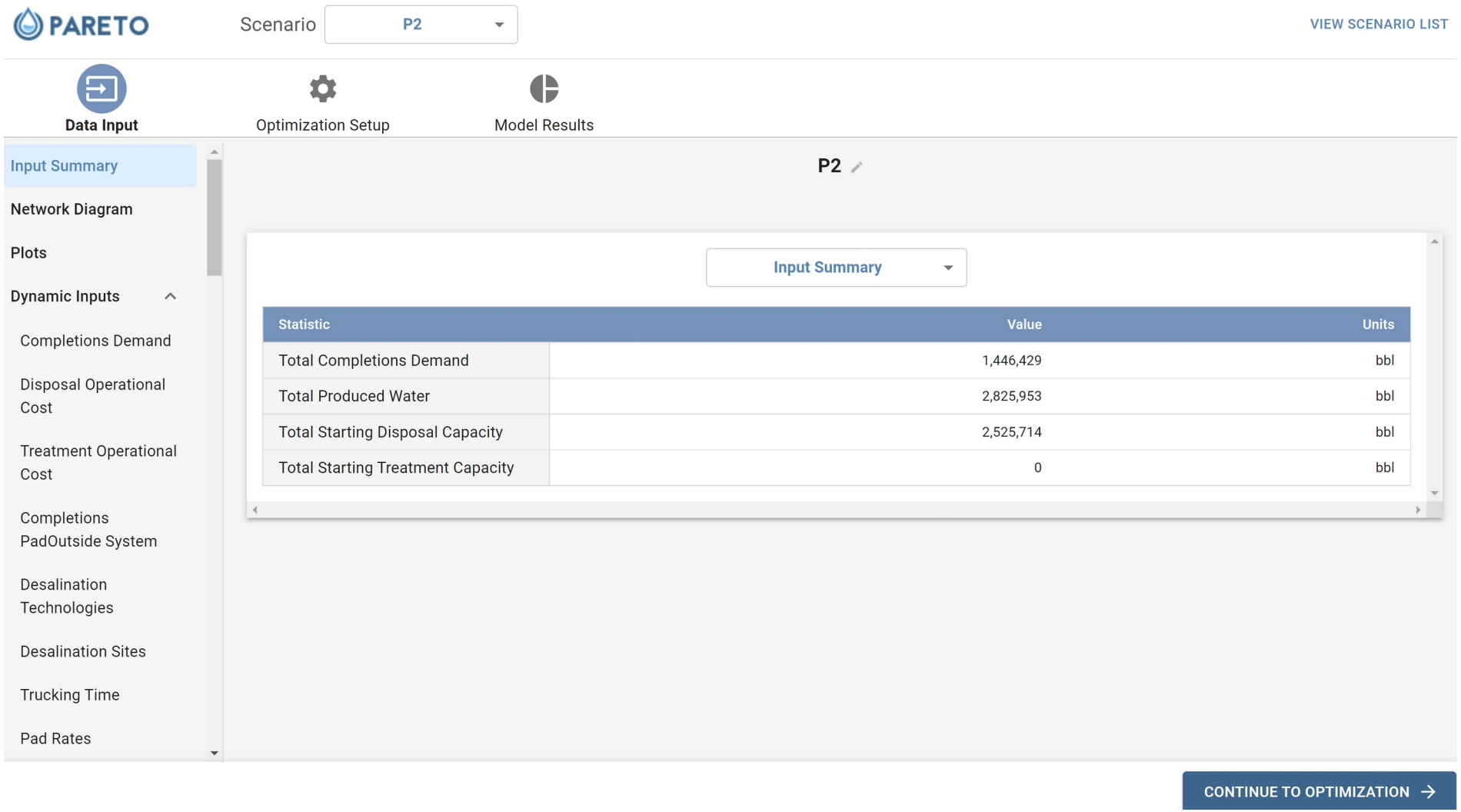
One-click native installer

Docs: https://www.project-pareto.org/software/

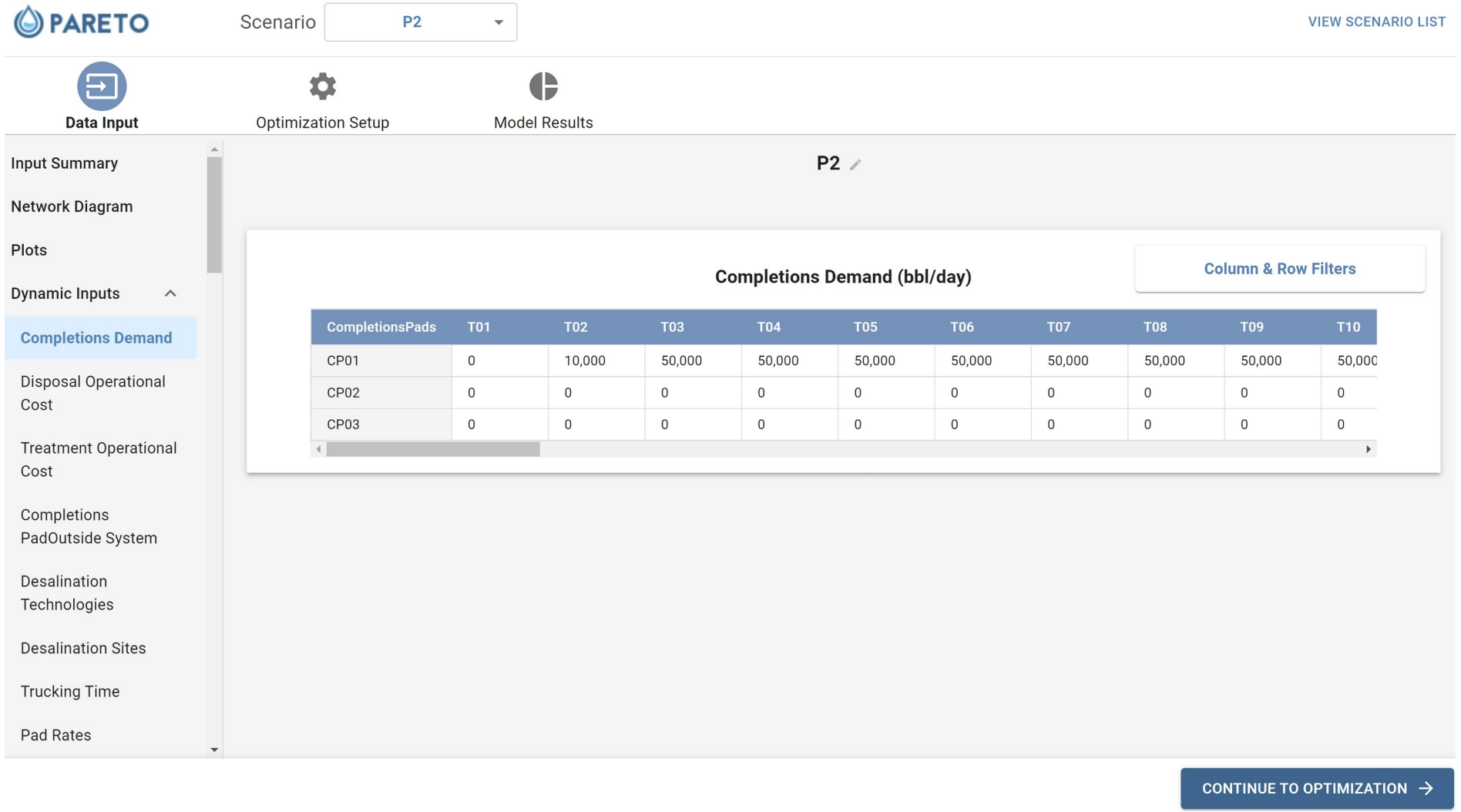
PARETO UI: Pre-built “scenarios”



PARETO UI: Configure scenario inputs

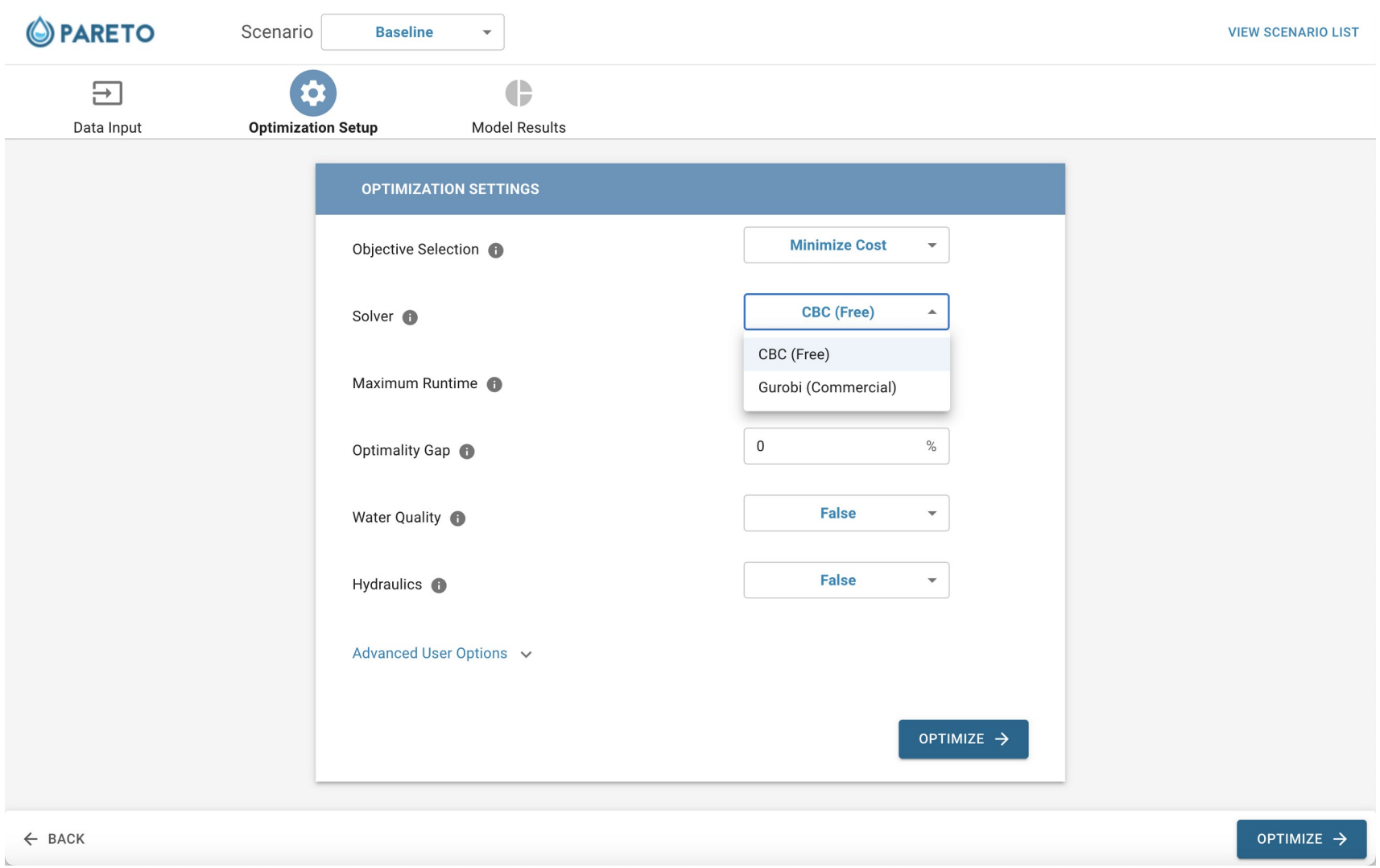


PARETO UI: Configure scenario inputs (2)

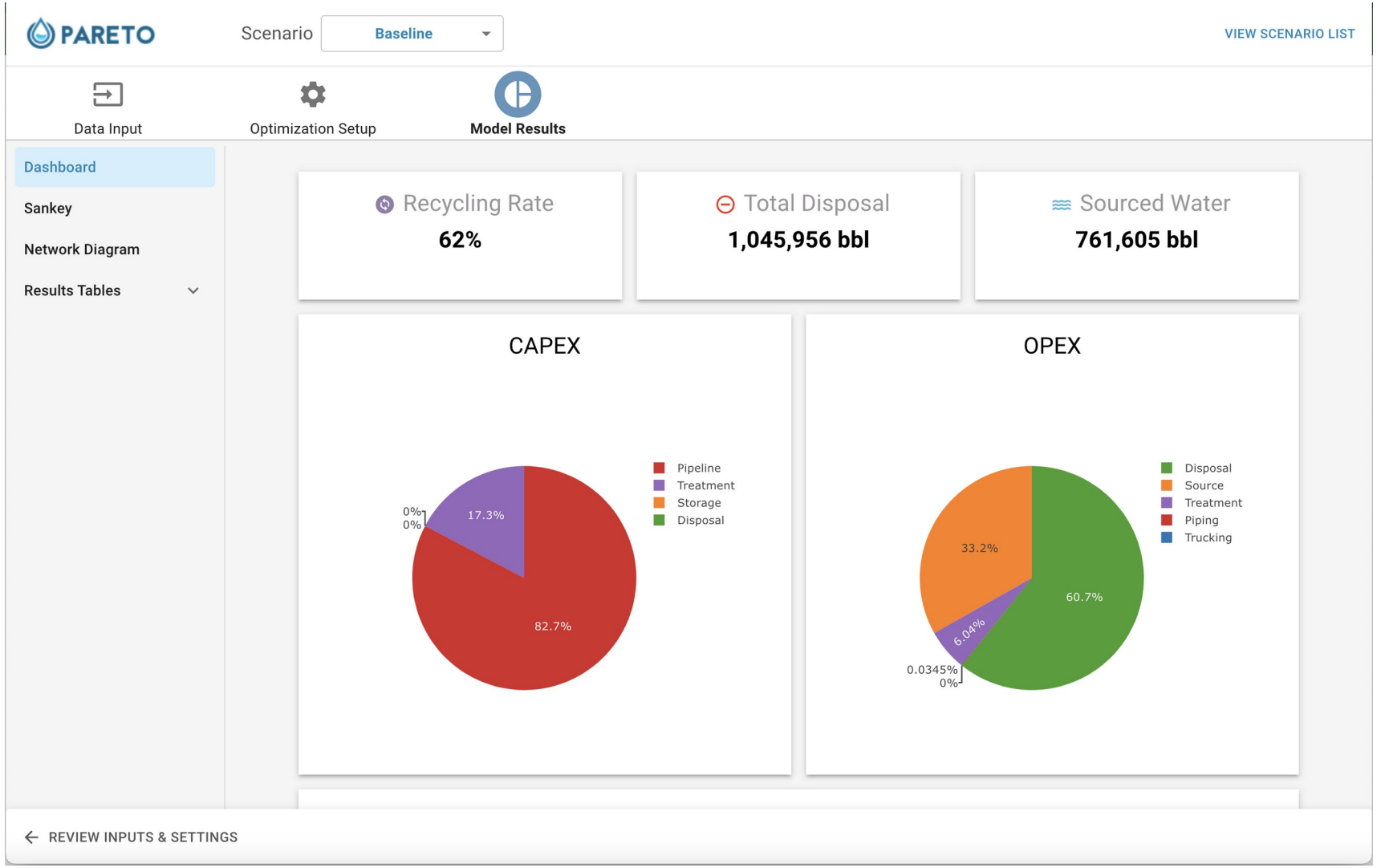


CompletionsPads	T01	T02	T03	T04	T05	T06	T07	T08	T09	T10
CP01	0	10,000	50,000	50,000	50,000	50,000	50,000	50,000	50,000	50,000
CP02	0	0	0	0	0	0	0	0	0	0
CP03	0	0	0	0	0	0	0	0	0	0

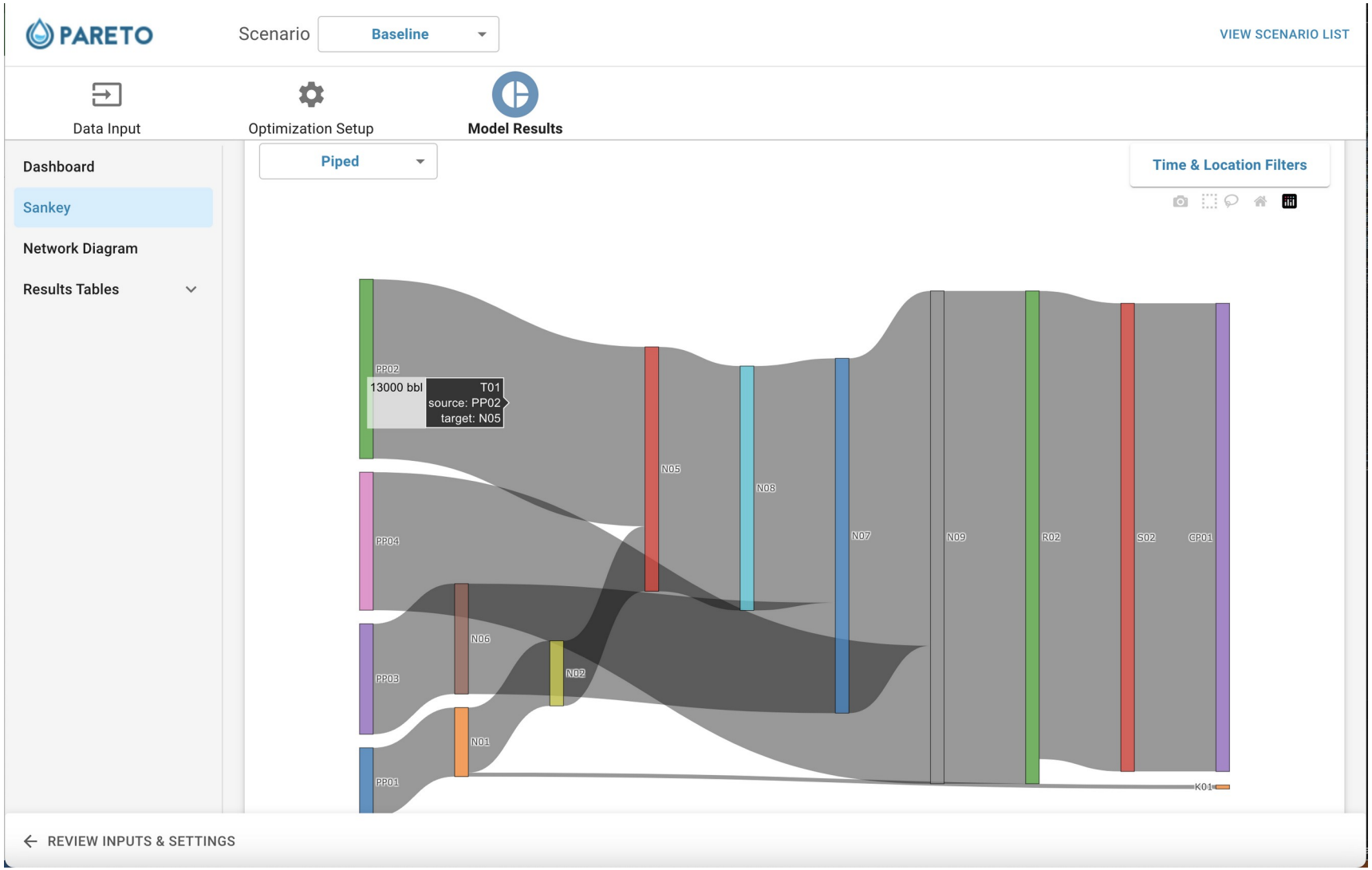
PARETO UI: Optimize



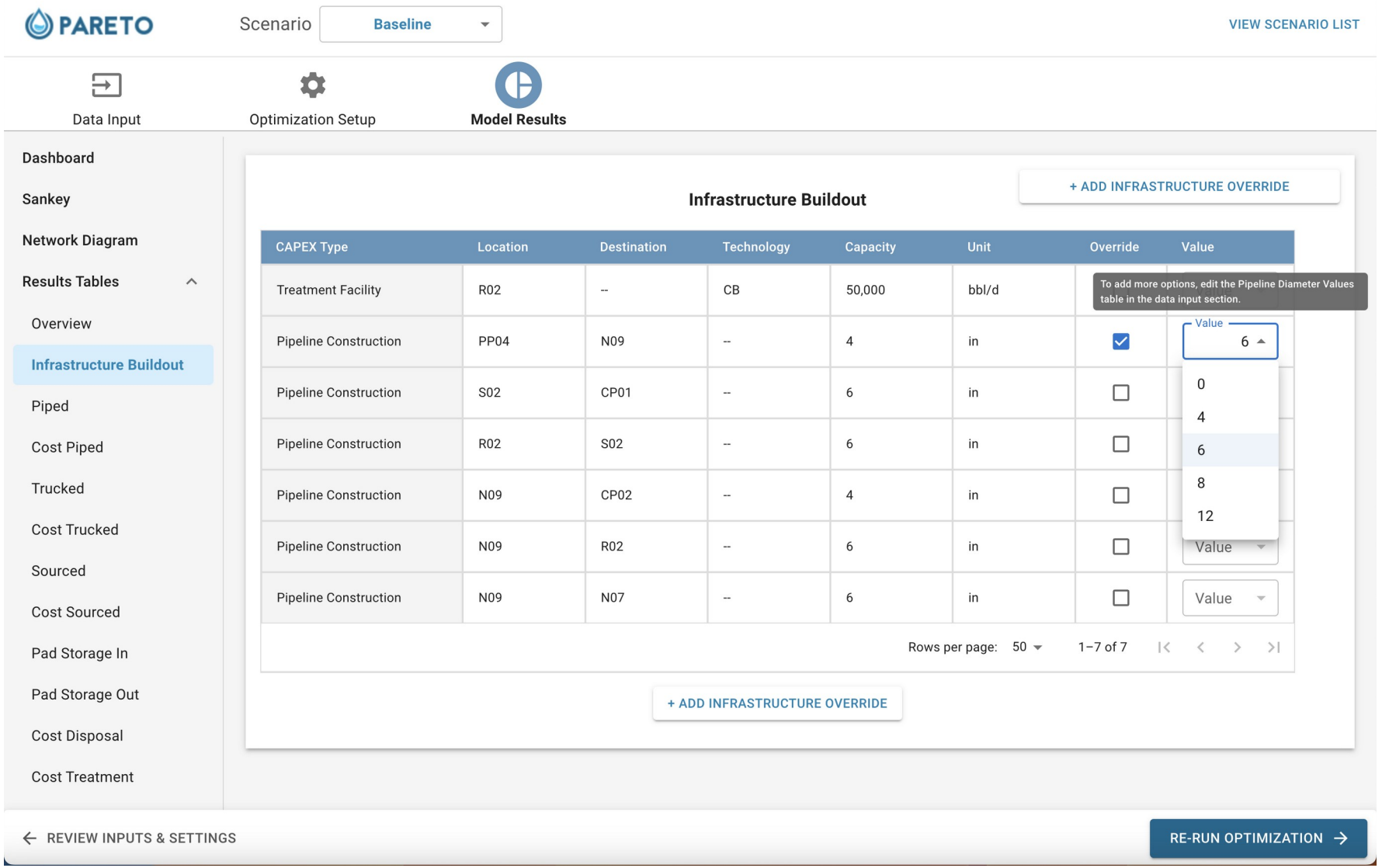
PARETO UI: Result summary



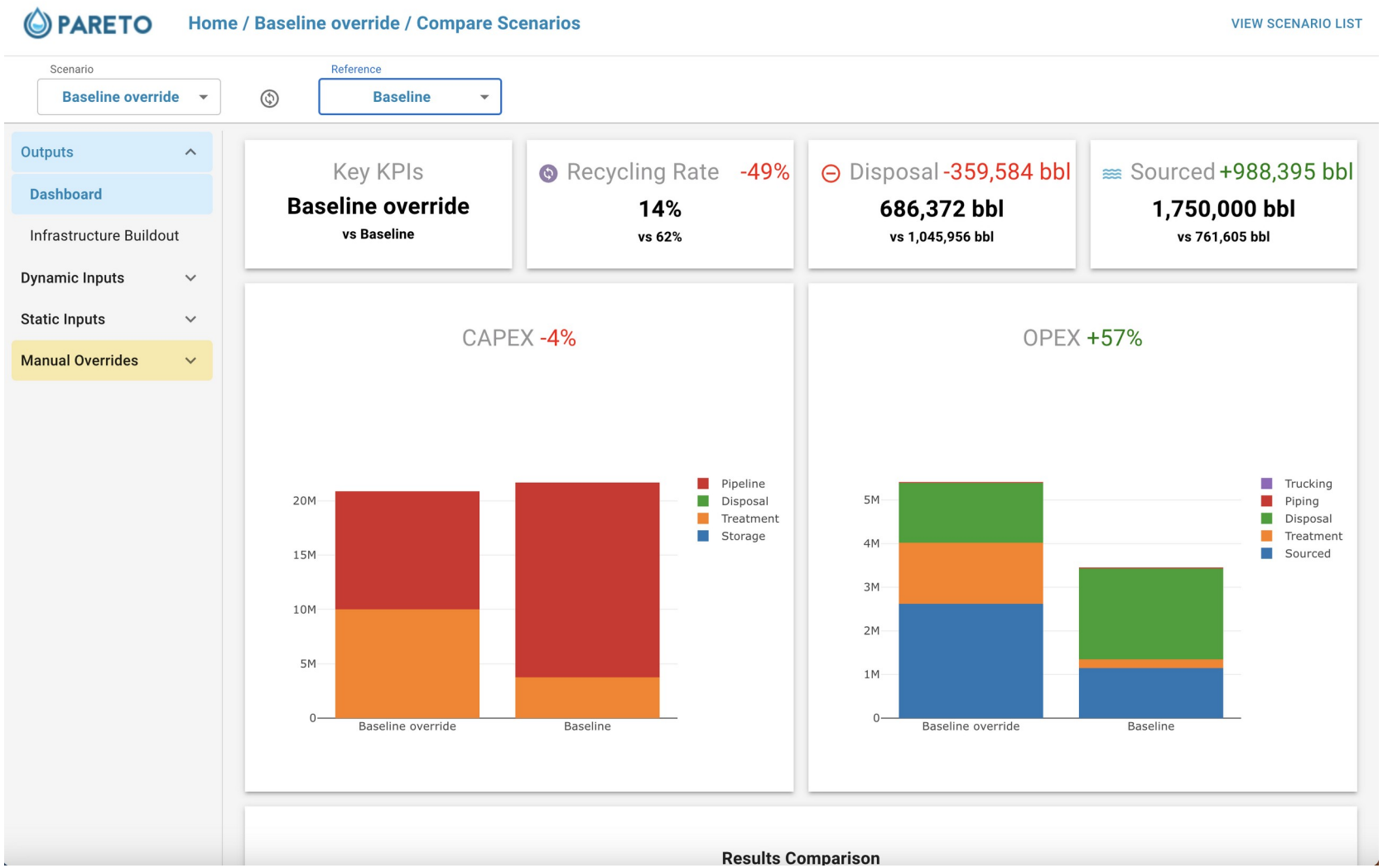
PARETO UI: Results Sankey diagram



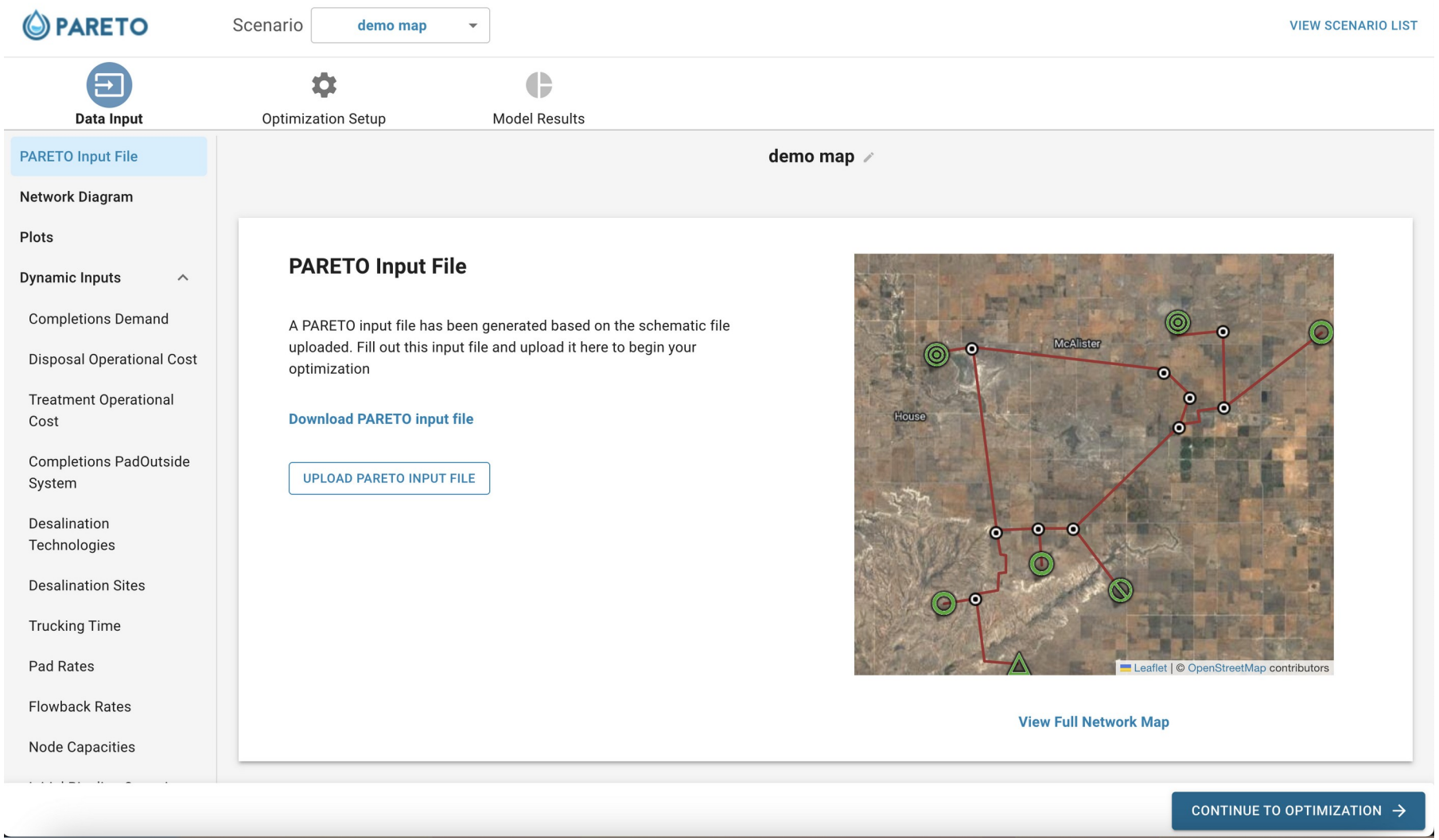
PARETO UI: Override optimizer decisions



PARETO UI: Compare solutions



PARETO UI: Show on map (beta)



PARETO UI plans

PARETO
The Produced Water Optimization Initiative

PARETO UI Q&A

PARETO
The Produced Water Optimization Initiative

“Superstructure” UI

PROMMIS
Process Optimization and Modeling for Minerals Sustainability

Functionality

Create and solve superstructures

Initially working with zero-order known performance

Goal: Build Pyomo models to incorporate more complex technology options

Types of models

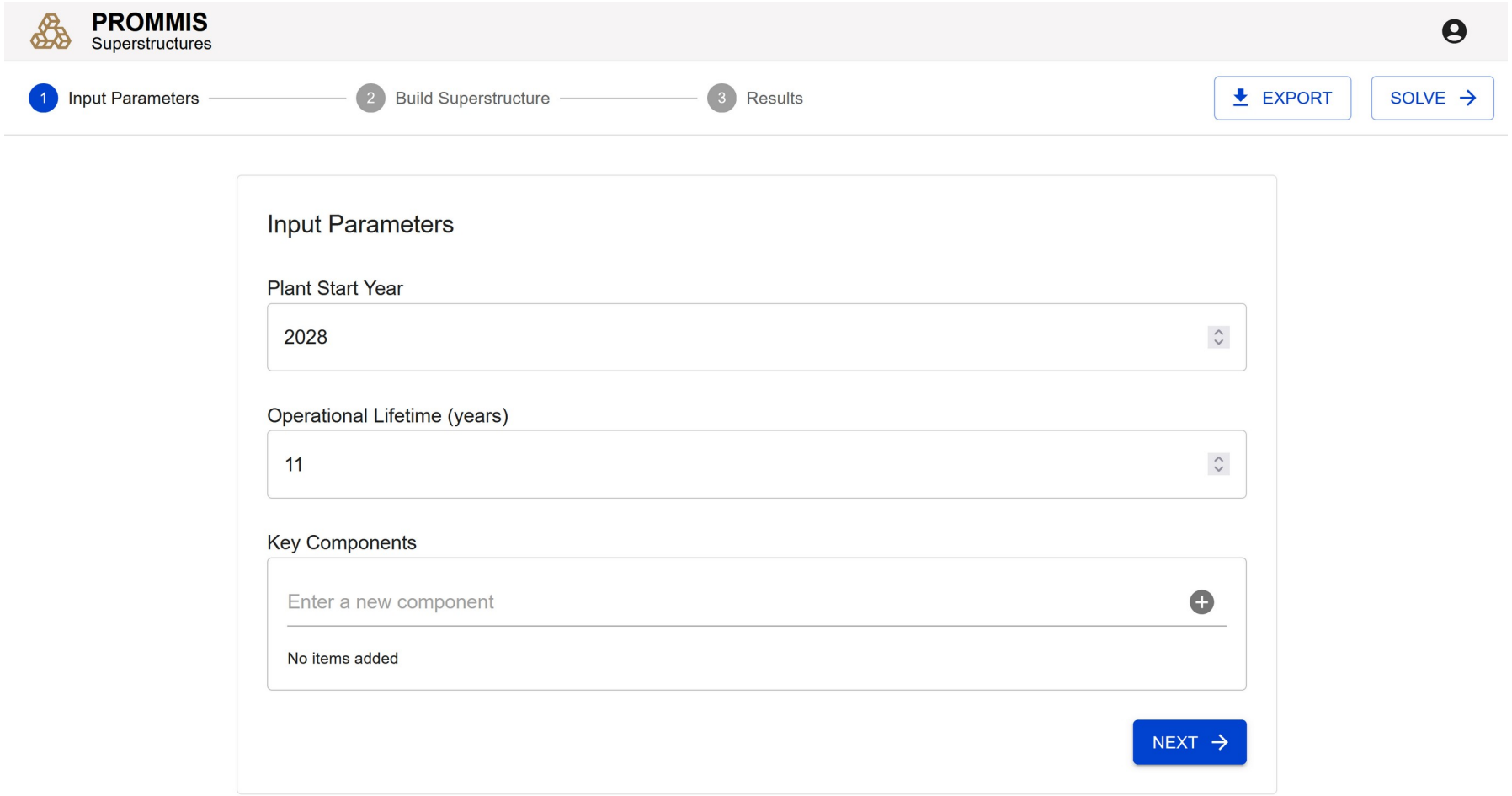
IDAES / Pyomo

Installation

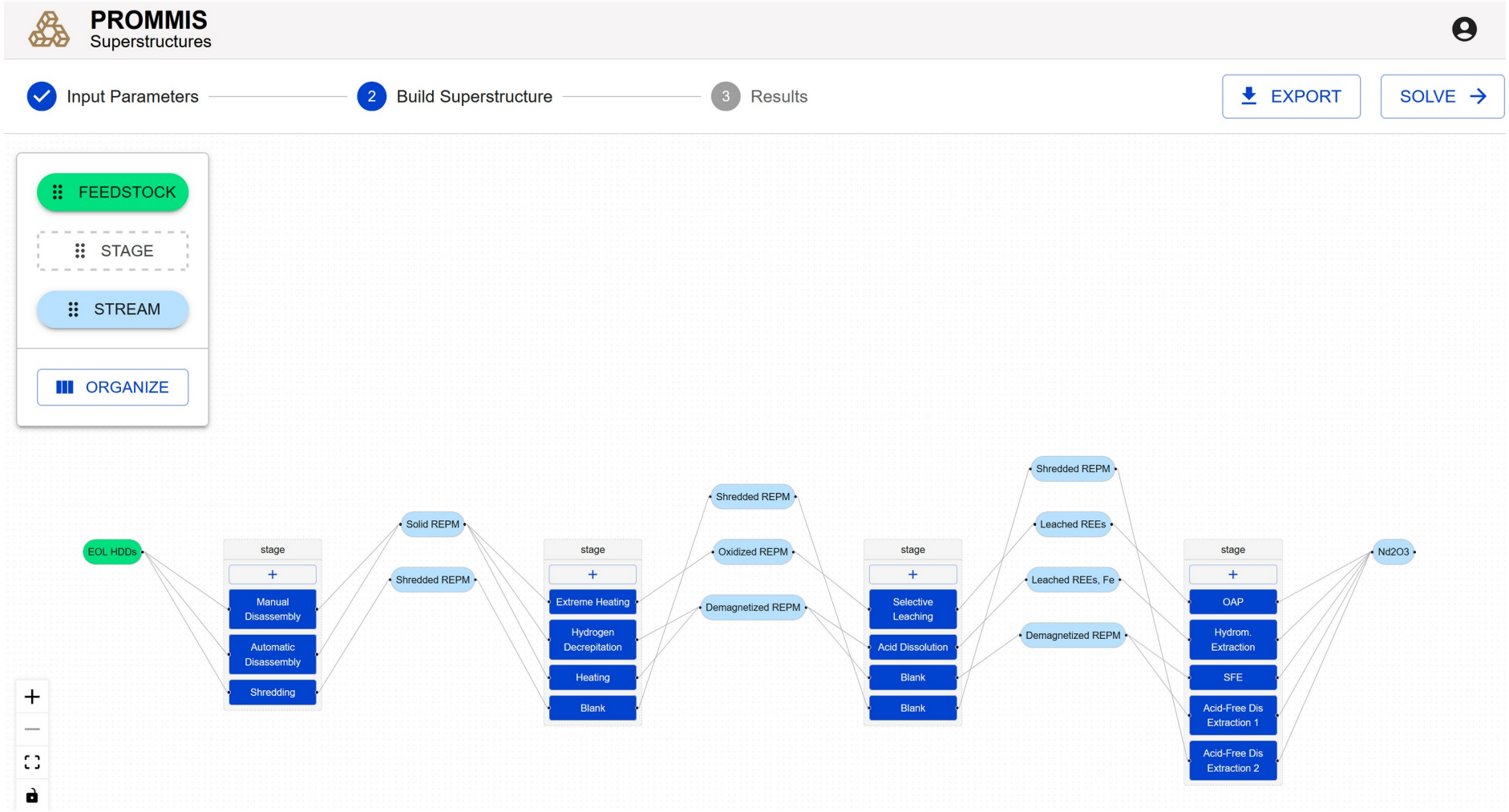
WIP, currently only from source

https://github.com/prommis/prommis-ui

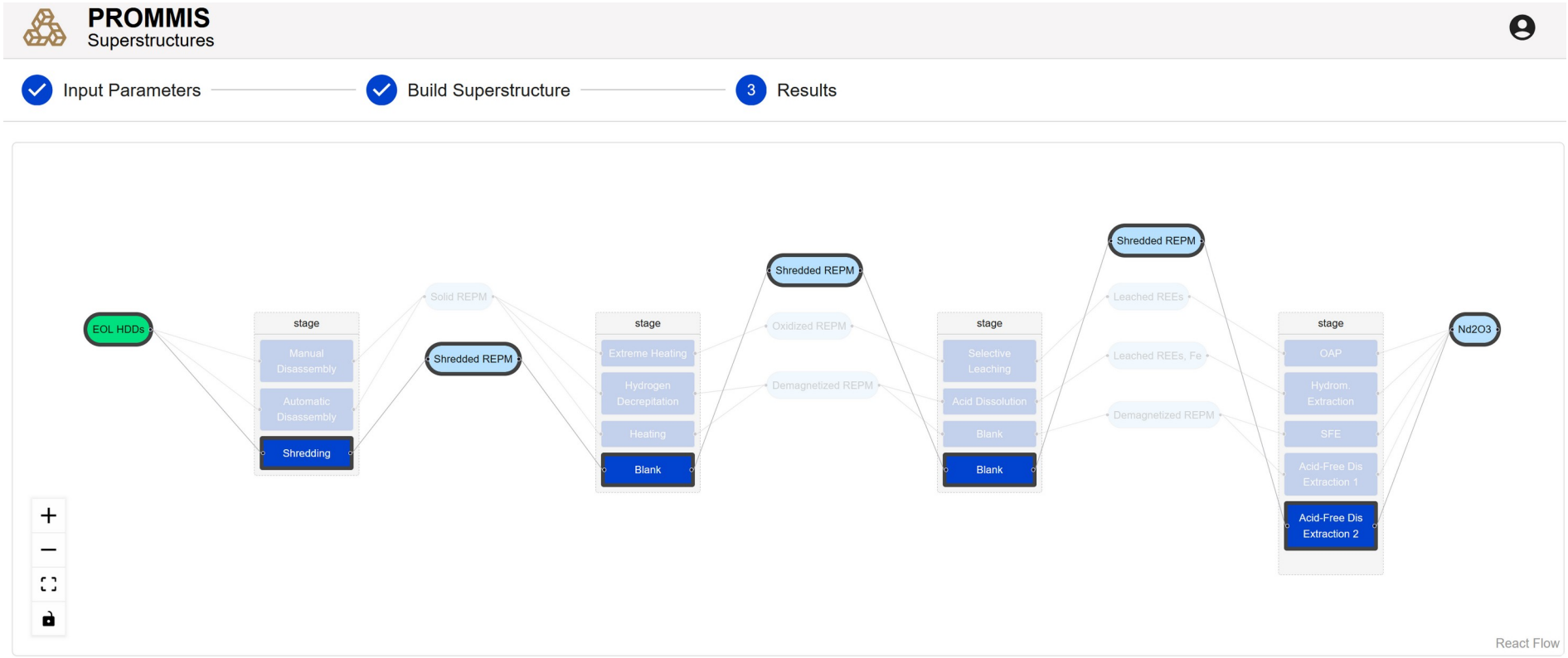
Superstructure: Create



Superstructure: Build



Superstructure: Solve



Stream Table

Component	Units	Shredding Inlet	Blank Inlet	Blank Inlet	Acid-Free Dis. Extraction 2 Inlet	Outlet

Superstructure UI plans

PROMMIS
Process Optimization and Modeling for Minerals Sustainability

- Finish prototype
  - Build zero-order models with known performance for technologies
- UX testing/feedback with real users
- Additional applications
  - PrOMMiS
  - Other PSE projects

Superstructure UI Q&A

PROMMIS
Process Optimization and Modeling for Minerals Sustainability

FOQUS

Framework for Optimization, Quantification of Uncertainty, and Surrogates

Functionality

Run Aspen, gPROMS models

Also run IDAES or Pyomo models

Optimization, UQ, sDOE, surrogate modeling

Run on desktop (Python GUI)

Types of models

Aspen, gPROMS (with license)

IDAES/Pyomo

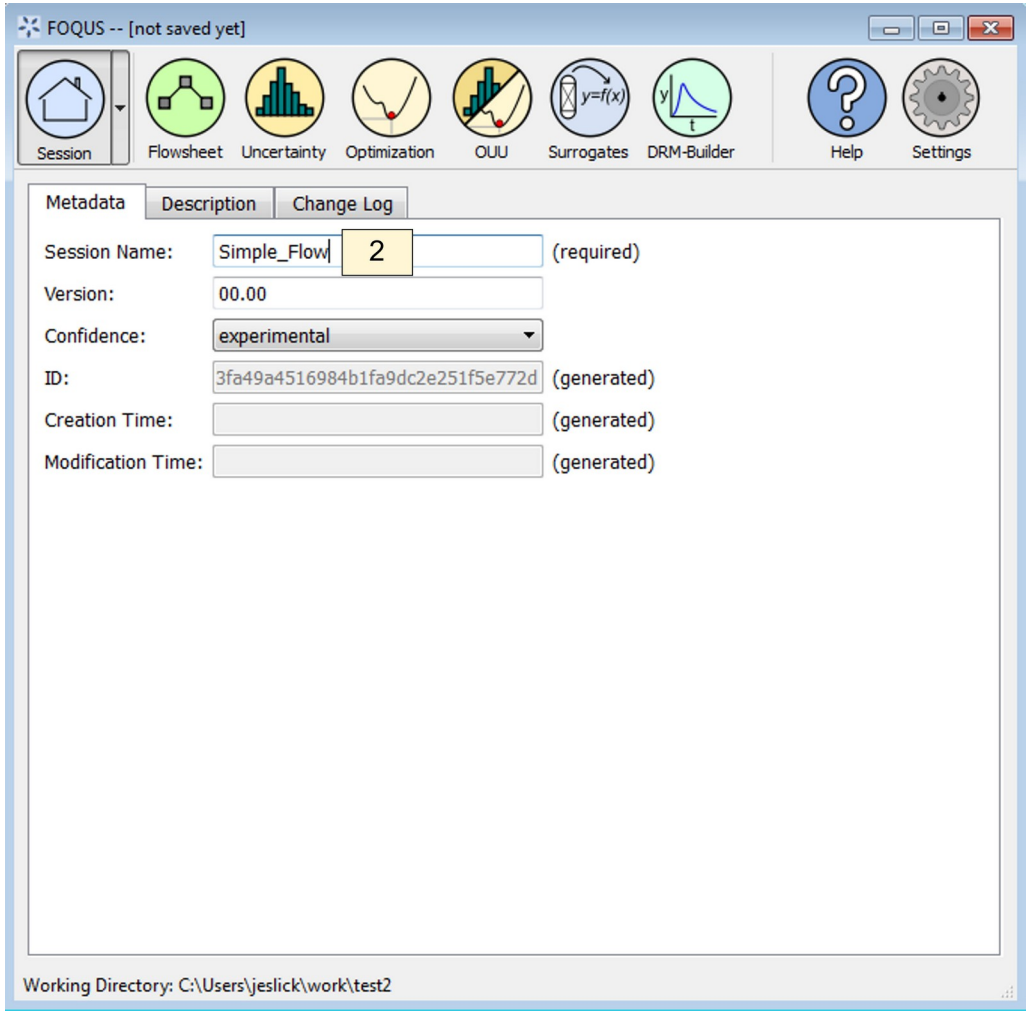
Installation

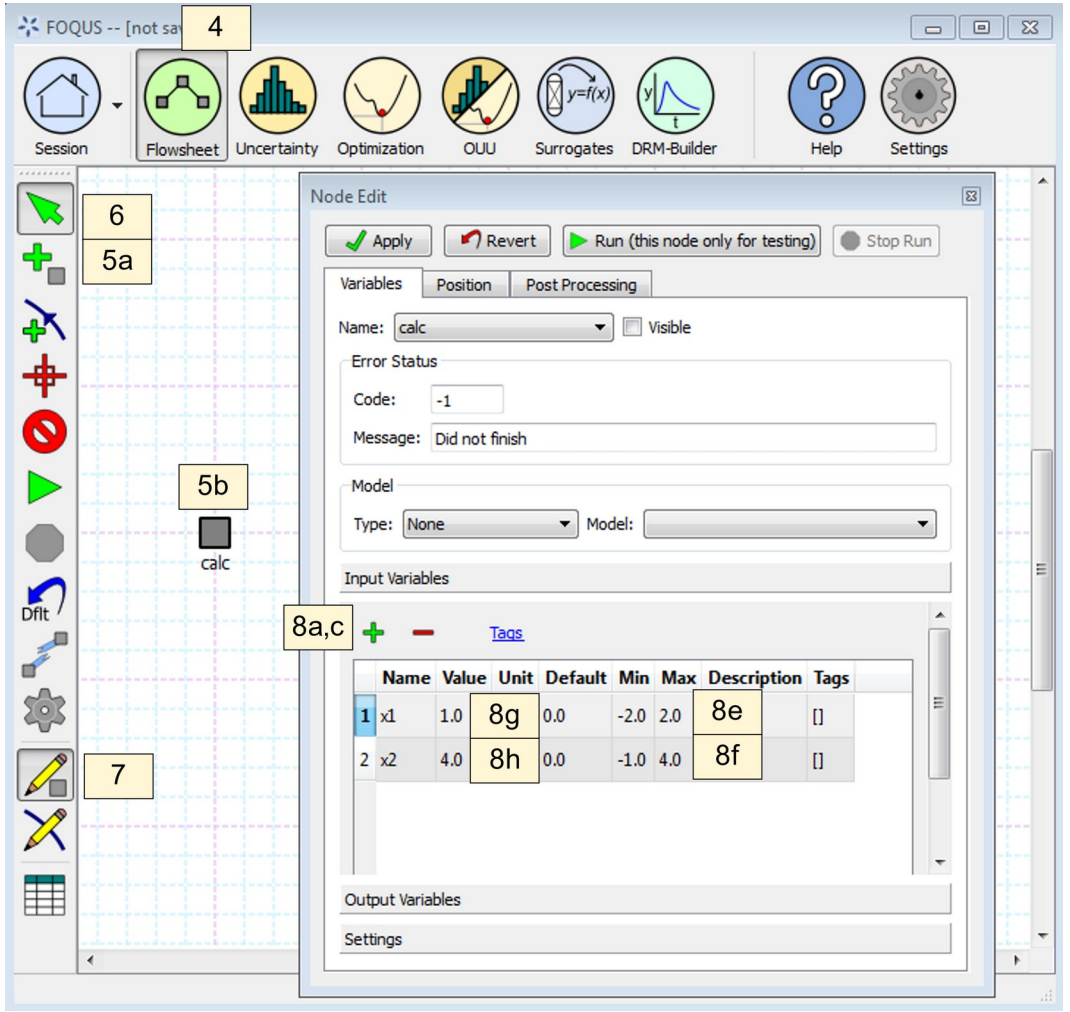
Python local install:

```
pip install ccsi-foqus
```

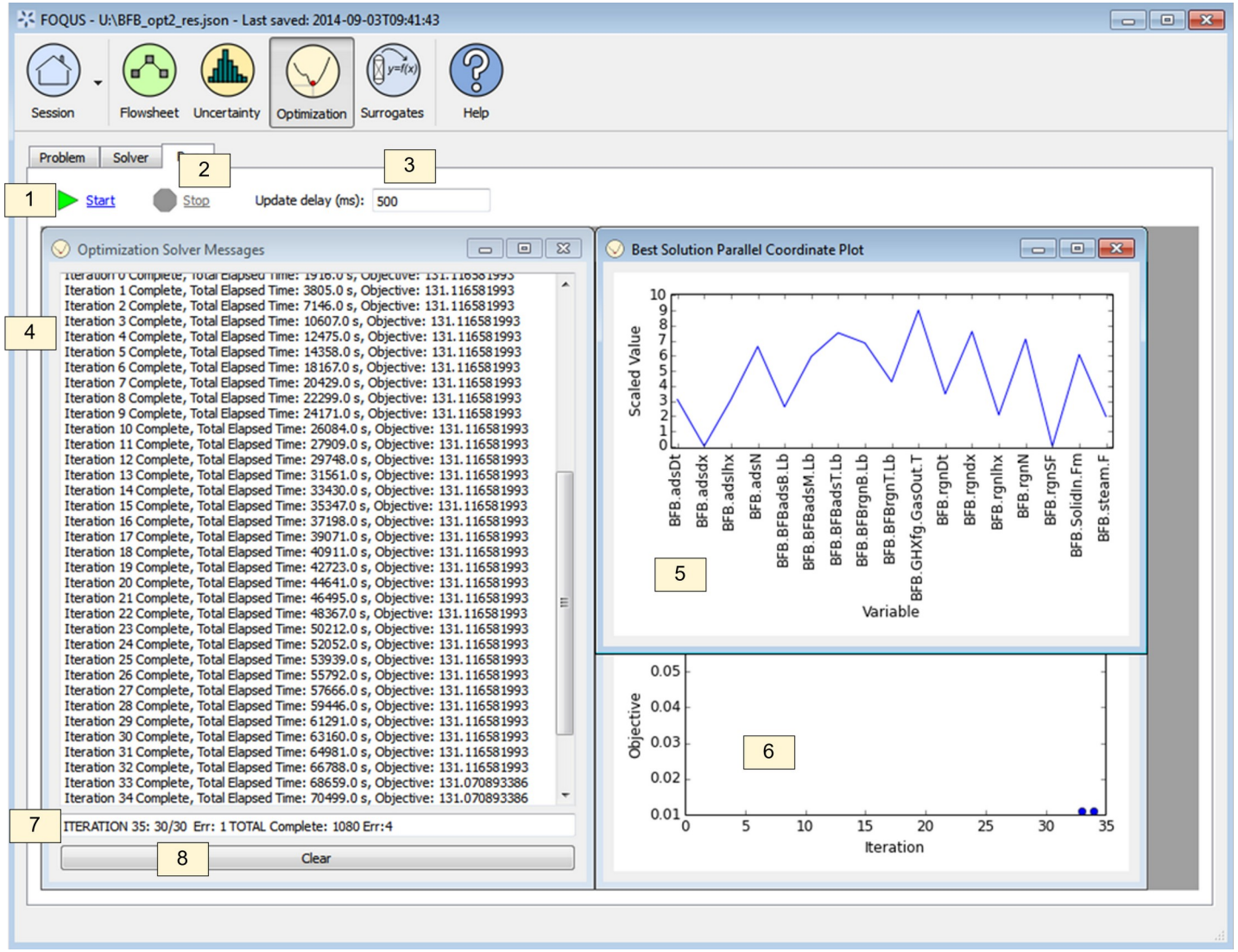
Docs: https://foqus.readthedocs.io

FOQUS: Create a flowsheet

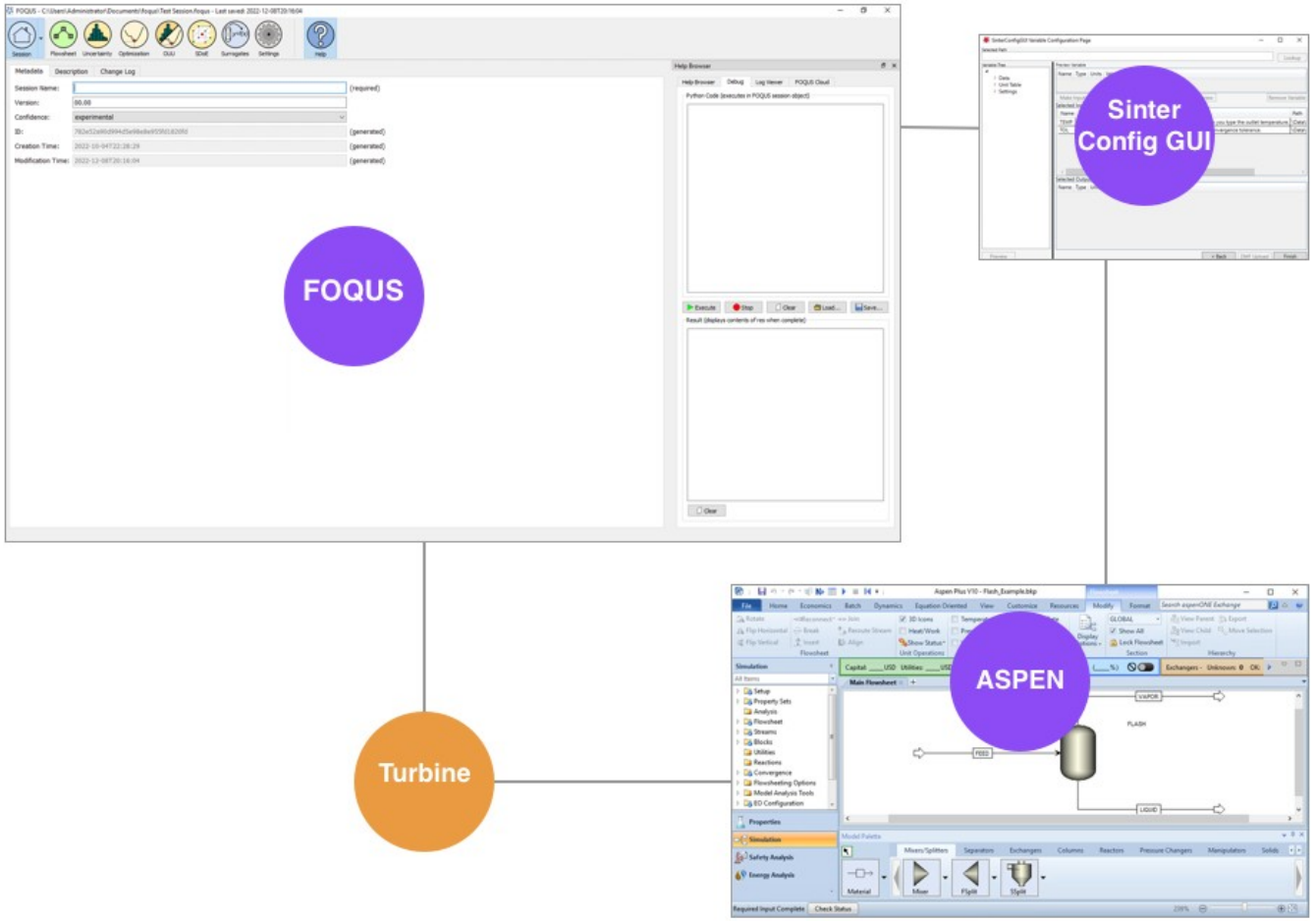




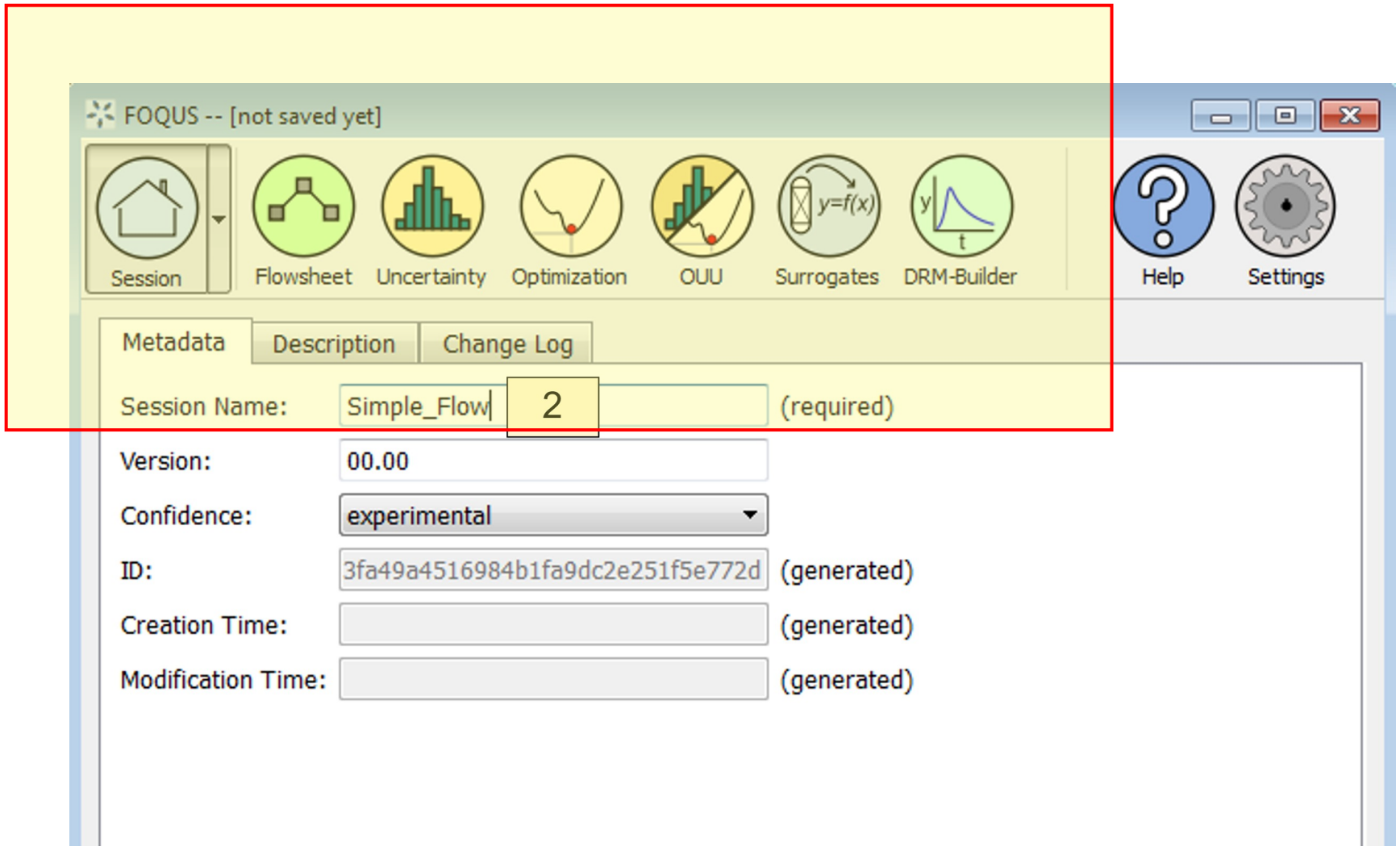
FOQUS: Run optimization



FOQUS: Connect to Aspen models through “Sinter”



FOQUS: More functions not covered here



FOQUS plans

- Refer to CCSI2 leadership for details
- UI is currently in maintenance mode
  - Integration with other tools could require refactor into Web stack

Summary

- Flowsheet Visualizer
  - Developer-focused, view and run diagnostics on flowsheets
- Flowsheet Runner
  - User-focused, parameterize and run flowsheets and sensitivity analyses
- PARETO UI
  - User-focused, parameterize and run produced water models
- Superstructure UI
  - User-focused, create and run (constrained) superstructure models
- FOQUS
  - Developer-focused, create and run Aspen or Pyomo flowsheets, many additional analysis features

Final Q&A

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Acknowledgement and Disclaimer

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