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

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Project Institutions



BERKELEY LAB ABORATORY

Optimization Initiative

Outline

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



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



Flowsheet Visualizer: Stream table



Flowsheet Visualizer: Diagnostics Panel

idaes 🛛 😣	Diagnosti	cs			sample_visualization	€ Refresh	🖬 Save	₽R	eset La	yout	? Help
Diagram								Ð	Q 🖸	0	Ţ
		inlet_1_1		M01	H02 F03 vap_outlet_1						
Stream Table									H	de Fi	elds
Variable	s_inlet_2_1	s_inlet_1_1	s01	s02							
flow_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 pla

- 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 Runner aka WaterTAP UI



Functionality

- <u>API</u> 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://watertaporg.github.io

Flowsheet Runner: Flowsheets List

NAVVI WaterTAP

Flowsheets

— Flowsheet Name 🗸	Last Run	NEW FLOWSHEET +
BSM2 flowsheet	9/4/2024	
BSM2_P_extension flowsheet	7/23/2024	
Dye Desalination flowsheet	9/4/2024	
Electrodialysis with concentrate recirculation flowsheet	9/4/2024	
Generic treatment train flowsheet	9/5/2024	
Granular Activated Carbon (GAC) flowsheet	9/4/2024	
LSRRO flowsheet	9/4/2024	
Mechanical vapor compression flowsheet	9/4/2024	
NF-DSPM-DE flowsheet	9/4/2024	
OARO flowsheet	9/4/2024	
RO with energy recovery flowsheet	9/4/2024	

Flowsheet Runner: Input Page

NAVVI WaterTAP

LSRRO

DEGREES OF FREEDOM: 12



	INPUT OU	ITPUT COMPARE
aved Configurations:		Analysis Type optimization C RESET RU
rimary Pumps	^	Booster Pumps
Pump 1 outlet pressure		Pump 2 efficiency
85 bar	Free 👻	0.75 fraction Fixed -
C Lower		Pump 3 efficiency
0.1 500.0000000		0.75 fraction Fixed -
- Pump 1 efficiency		
0.75 fraction	Fixed 👻	
Pump 2 outlet pressure		Stage 1
65 bar	Free 💌	- Ligo -
C Lower C Upper		 Stage 1 water permeability coefficient
0.1 500.0000000(1.51 LMH/bar Fixed -
		Stage 1 salt permeability coefficient
Pump 2 efficiency		0.13 LMH Fixed -
0.75 fraction	Fixed 👻	C Stage 1 membrane area
- Pump 3 outlet pressure		

Flowsheet Runner: Optimization Output

INPUT

OUTPUT

		DOWNLOAD RESULT	SAVE CONFIGURATION
Category	Variable	Units	Value
Food	Volumetric flow rate	m3/hr	3.6
reed	NaCl concentration	g/L	70
	Pump 1 outlet pressure	bar	85
	Pump 1 efficiency	fraction	0.75
	Pump 2 outlet pressure	bar	65
	Pump 2 efficiency	fraction	0.75
Drim on a Dumon o	Pump 3 outlet pressure	bar	63.6
Primary Pumps	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
Deceter Dumme	Pump 2 efficiency	fraction	0.75
Booster Pumps	Pump 3 efficiency	fraction	0.75
	Stage 1 water permeability coefficient	LMH/bar	1.51
	Stage 1 salt permeability coefficient	LMH	0.13
Otogo 1	Stage 1 width	m	7.42
Stage I	Stage 1 permeate pressure	bar	1
	Stage 1 channel height	mm	1
	Stage 1 space porosity	fraction	0.85
	Stage 1 membrane area	m2	66.46
Membrane area	Stage 2 membrane area	m2	141.22
	Stage 3 membrane area	m2	1.73

Flowsheet Runner: Compare Page

INPUT OUTPUT COMPARE

TABLE VIEW CHART VIEW

	Metric	LSRRO 2 👻	LSRRO 1 -	Value Difference		
Food	Volumetric flow rate	3.6 m3/hr	3.6 m3/hr	0.00		
reed	NaCl concentration	70 g/L	70 g/L	0.00		
	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		
Primary Pumpe	Pump 3 outlet pressure	63.6 bar	63.6 bar	0.06		
Primary Pumps	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		
Poostor Pumps	Pump 2 efficiency	0.5 fraction	0.75 fraction	-0.25		
Booster Pumps	Pump 3 efficiency	0.23 fraction	0.75 fraction	-0.52		
	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	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

NAVVI WaterTAP

LSRRO

DEGREES OF FREEDOM: 12



Model Options v

INPUT OUTPUT

TABLE VIEW CHART VIEW

Net pump work	Energy recovery	Number of stages	Water volumetric recovery	Mass water recovery rate	Salt rejection	Specific en
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)



Flowsheet Runner: Sensitivity (3)

LSRRO

DEGREES OF FREEDOM: 10



Model Options v

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)



Flowsheet Runner plans: Crossproject

Use across IDAES flowsheet projects

 Project branding

 Project flowsheets

			DEGREES OF FREEDOM: 0	
	WaterTAP UI			_
	File Edit View Window Help			
	A PROMMIS			
	Metab		DEG	REES OF FREEDOM: 0
		feed metab_hydrogen	product_methane product_H2O	
Feed			product_hydrogen	10
- Volumetric flow rate 1.18	_	INPUT	PUT COMPARE	
6.76			Analysis Type optimization -	RUN
	Feed	^	Hydrogen reactor	^
	Volumetric flow rate	m3/h Fixed -	Water recovery fraction	Fixed -
	COD concentration		COD conversion	
	6.76	g/L Fixed -	0.22 fraction	Fixed -
			0.05 fraction	Fixed -
			6 h	Fixed -
			Mixer specific power 0.05 kW/m3 of reactor	Fixed -
Hydrogen reactor	stin		Mixer specific power 0.05 kW/m3 of reactor Vacuum specific power 9.19 kW/(kq-H2/h)	Fixed -
Hydrogen reactor	ostir		Mixer specific power 0.05 kW/m3 of reactor Vacuum specific power 9.19 kW/(kg-H2/h) Specific heating 7.88 MJ/m3 of water	Fixed -

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.projectpareto.org/software/

PARETO UI: Pre-built "scenarios"



PARETO UI: Configure scenario

INNII O PARETO	Scenario P2 -		VIEW SCENARIO LIS
Data Input	Optimization Setup Model R	esults	
Input Summary		P2 /	
Network Diagram			
Plots		Input Summary 👻	•
Dynamic Inputs ^	Statiatia	Va	ua Unita
Completions Demand	Total Completions Demand	14464	29 bbl
Disposal Operational	Total Produced Water	2,825,9	53 bbl
Cost	Total Starting Disposal Capacity	2,525,7	14 bbl
Treatment Operational Cost	Total Starting Treatment Capacity		0 bbl
Completions	4		✓
PadOutside System			
Desalination Technologies			
Desalination Sites			
Trucking Time			
Pad Rates			

PARETO UI: Configure scenario inputs (2)

Scenario P2

-

VIEW SCENARIO LIST

		Mad	C								
put Summary		MOde	er Results		F	2 /					
etwork Diagram											
ots										Column & Pow	Filtors
ynamic Inputs 🛛 🔨				С	ompletions	Demand (bb	ol/day)				Thers
Completions Demand	CompletionsPads	T01	T02	T03	T04	T05	T06	T07	T08	Т09	T10
	CP01	0	10,000	50,000	50,000	50,000	50,000	50,000	50,000	50,000	50,0
)isposal Operational	CP02	0	0	0	0	0	0	0	0	0	0
0001	CP03	0	0	0	0	0	0	0	0	0	0
Treatment Operational	•										
Completions PadOutside System											
Desalination Technologies											
Desalination Sites											
Trucking Time											

CONTINUE TO OPTIMIZATION \rightarrow

PARETO UI: Optimize

PARETO	Scenario Baseline -	VIEW SCENA
\rightarrow		
Data Input	Optimization Setup Model Results	
	OPTIMIZATION SETTINGS	
	Objective Selection 🚯	Minimize Cost -
	Solver 🚯	CBC (Free)
	Maximum Runtime 🚯	CBC (Free) Gurobi (Commercial)
	Optimality Gap 🌗	0 %
	Water Quality 👔	False -
	Hydraulics 🚯	False -
	Advanced User Options 🗸	

PARETO UI: Result summary



PARETO UI: Results Sankey diagram



PARETO UI: Override optimizer

PARETO Scenario Baseline $\overline{}$ VIEW SCENARIO LIST \rightarrow 0 Data Input **Optimization Setup** Model Results Dashboard + ADD INFRASTRUCTURE OVERRIDE Sankey Infrastructure Buildout Network Diagram CAPEX Type Destination Technology **Results Tables** ^ To add more options, edit the Pipeline Diameter Values Treatment Facility R02 CB 50,000 bbl/d --table in the data input section. Overview Value PP04 N09 4 \checkmark 6 🔺 Pipeline Construction --in Infrastructure Buildout 0 Pipeline Construction S02 CP01 ---6 in Piped 4 **Pipeline Construction** R02 S02 6 in ---Cost Piped 6 8 Trucked **Pipeline Construction** N09 CP02 4 \square --in 12 Cost Trucked R02 Value **Pipeline Construction** N09 ---6 in Sourced N07 Pipeline Construction N09 ---6 in Value Cost Sourced Rows per page: 50 -1-7 of 7 |< < > >| Pad Storage In Pad Storage Out + ADD INFRASTRUCTURE OVERRIDE Cost Disposal Cost Treatment

PARETO UI: Compare solutions

Scenario Baseline override	ne / Baseline override / Compare S	cenarios		VIEW SCENARIO LIST
Outputs ^ Dashboard	Key KPIs Baseline override vs Baseline	Recycling Rate -49% 14% vs 62%	Disposal -359,584 bbl 686,372 bbl vs 1,045,956 bbl	Sourced +988,395 bbl 1,750,000 bbl vs 761,605 bbl
Static Inputs Manual Overrides	CAPI 20M 15M 10M 5M 0 Baseline override	EX -4%	SM 5M 4M 3M 2M 1M 0 Baseline override	+57%
		Results Co	omparison	

PARETO UI: Show on map (beta)



CONTINUE TO OPTIMIZATION \rightarrow

PARETO UI plans



PARETO UI Q&A



"Superstructure" UI



Functionality

Create and solve superstructures

Initially working with zeroorder 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

PROMMIS Superstructures				9
1 Input Parameters	2 Build Superstructure	3 Results	Ł	EXPORT SOLVE
	Input Parameters			
	Plant Start Year			
	2028		¢	
	Operational Lifetime (years)			
	11		¢	
	Key Components			
	Enter a new component		Đ	
	No items added			

Superstructure: Build



Superstructure: Solve





Superstructure UI plans



- 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



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 [not saved	l yet]		_	• ×	
Session Flowshe	Uncertainty Optimization OUU	Surrogates DRM-Builder	Help (Settings	
Metadata Descr	iption Change Log				
Session Name:	Simple_Flow 2	(required)			
Version:	00.00				
Confidence:	experimental 🔹]			
ID:	3fa49a4516984b1fa9dc2e251f5e772d	(generated)			
Creation Time:		(generated)			
Modification Time:		(generated)			
Working Directory: C:\U	Jsers\jeslick\work\test2				

SFOQUS [not sa 4						
Session - Howsheet Uncertainty Optimization OUU Surrogates DRM-Builder Help S	Settings					
Node Edit						
↓ ↓ Apply ✓ Revert ▶ Run (this node only for testing) ● Stop	Run					
Name: Calc Visible						
Code: -1						
Message: Did not finish Model						
Type: None Model:	• • • • • •					
Dift Ba,c + - Tags						
Name Value Unit Default Min Max Description Tags 1 x1 1.0 8g 0.0 -2.0 2.0 8e []						
7 2 x2 4.0 8h 0.0 -1.0 4.0 8f []						
Output Variables						
Settings Settings						

FOQUS: Run optimization



FOQUS: Connect to Aspen models through "Sinter"



FOQUS: More functions not covered here

😽 FOQUS [not saved	FOQUS [not saved yet]			
Session Flowshee	$ \begin{array}{c} & & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ $	Help Settings		
Metadata Descri	otion Change Log			
Session Name:	Simple_Flow 2 (required)			
Version:	00.00			
Confidence:	experimental 🔹			
ID:	3fa49a4516984b1fa9dc2e251f5e772d (generated)			
Creation Time:	(generated)			
Modification Time:	(generated)			

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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