

NAWI WaterTAP User Interface for Model Analysis and Comparison

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Motivation and Goals

WaterTAP models are written in Python code using the IDAES framework (IDAES-IP).

WaterTAP library

IDAES Integrated Platform

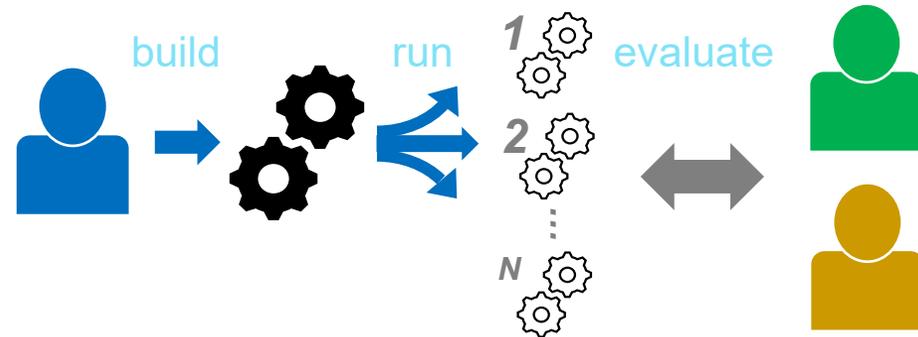
Pyomo + Optimization Solvers

They are highly configurable, and powerful, but also quite complex to configure and run

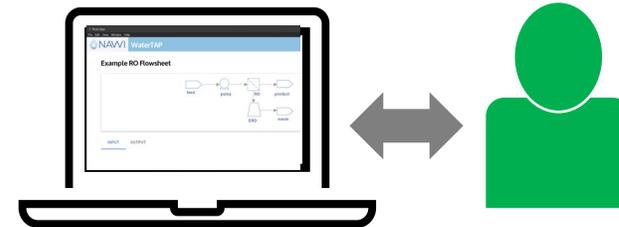
```
= ConcreteModel()
fs = FlowsheetBlock(default={"dynamic": False})
fs.properties = props.SeawaterParameterBlock()
fs.costing = WaterTAPCosting()

unit models
fs.feed = Feed(default={"property_package": m.fs.properties})
fs.pump = Pump(default={"property_package": m.fs.properties})
fs.RO = ReverseOsmosis0D(default={
    "property_package": m.fs.properties,
    "has_pressure_change": True,
    "pressure_change_type": PressureChangeType.calculated,
    "mass_transfer_coefficient": MassTransferCoefficient.calculated,
    "concentration_polarization_type": ConcentrationPolarizationType.calculated})
fs.erd = EnergyRecoveryDevice(default={"property_package": m.fs.properties})
fs.product = Product(default={"property_package": m.fs.properties})
```

Models, once created, are often run many times with different parameters -- perhaps by others



The WaterTAP UI interactively runs, analyzes, and compares existing models



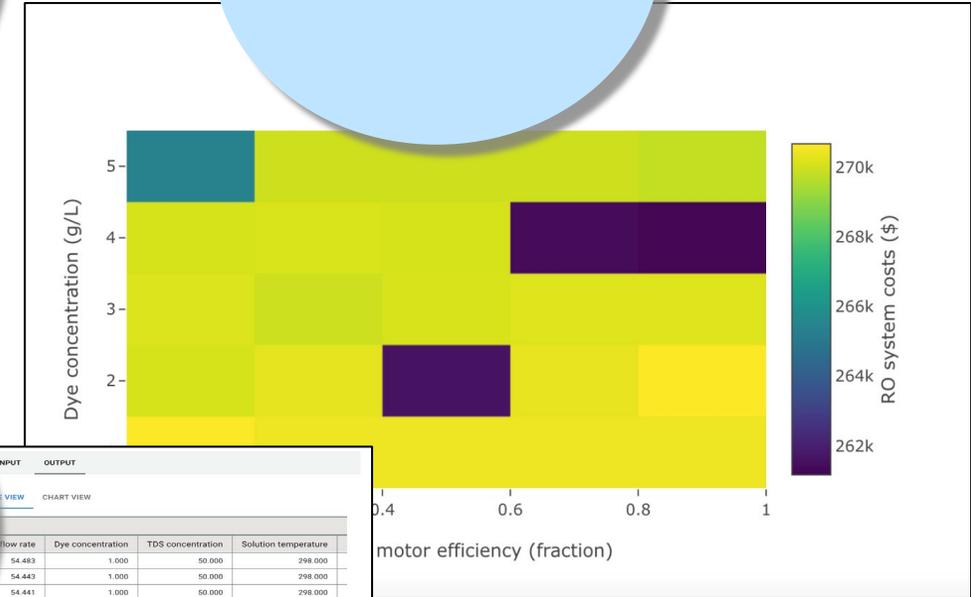
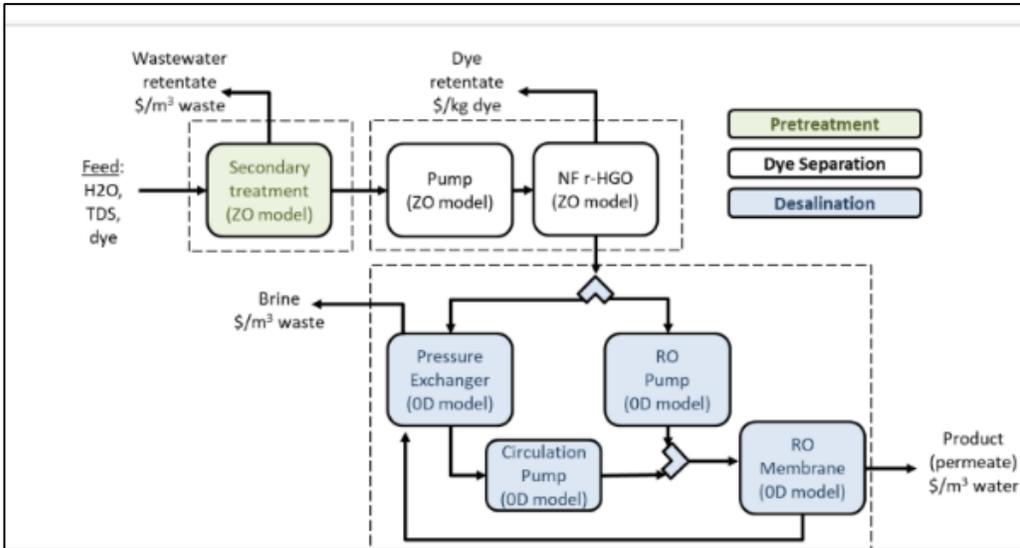
Capabilities Overview

MODEL

**EDIT MODEL
PARAMETERS**
—
SOLVE

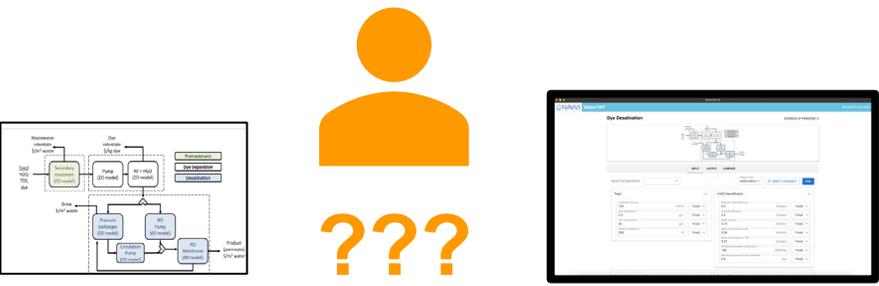
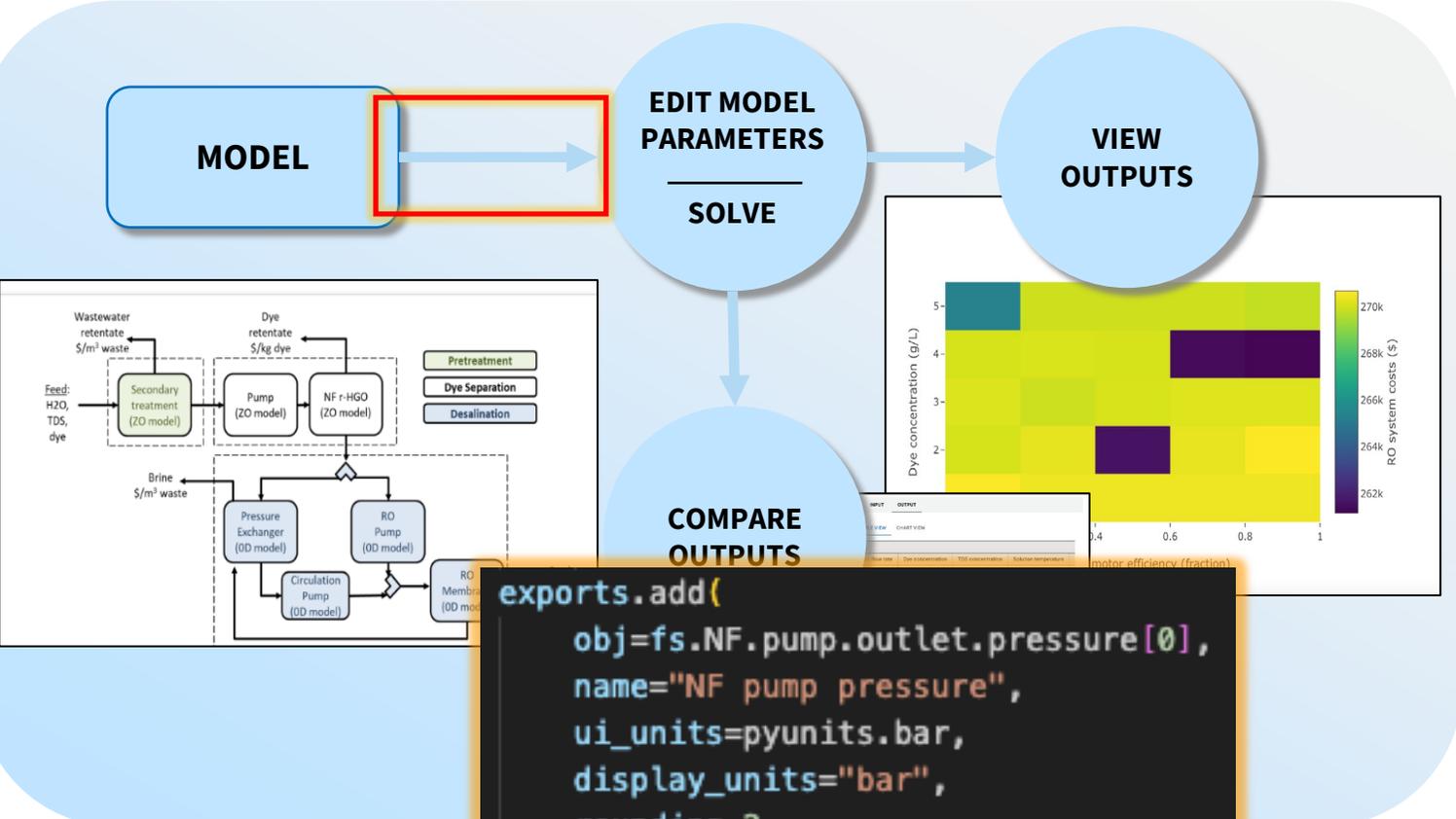
**VIEW
OUTPUTS**

**COMPARE
OUTPUTS**



Flow rate	Dye concentration	TDS concentration	Solution temperature
54.483	1.000	50.000	298.000
54.443	1.000	50.000	298.000
54.441	1.000	50.000	298.000
54.443	1.000	50.000	298.000
54.442	1.000	50.000	298.000
54.394	2.000	50.000	298.000
54.439	2.000	50.000	298.000
52.683	2.000	50.000	298.000
54.443	2.000	50.000	298.000
54.514	2.000	50.000	298.000
54.440	3.000	50.000	298.000
54.389	3.000	50.000	298.000
54.420	3.000	50.000	298.000
54.441	3.000	50.000	298.000
54.441	3.000	50.000	298.000
54.439	4.000	50.000	298.000
54.449	4.000	50.000	298.000
54.439	4.000	50.000	298.000
52.684	4.000	50.000	298.000
52.642	4.000	50.000	298.000

Capability: Export Existing Model to UI



Developer chooses

- Variables, constraints, or combinations, to show
- Variables that can be edited and made fixed/free
- Variable ranges
- Units for variables (can be different from internal model units)

```

exports.add(
  obj=fs.NF.pump.outlet.pressure[0],
  name="NF pump pressure",
  ui_units=pyunits.bar,
  display_units="bar",
  rounding=2,
  description="NF pump pressure",
  is_input=True,
  input_category="NF design",
  is_output=True,
  output_category="NF design",
)
    
```



Example export Python code for pump outlet pressure

Capability: Edit model parameters (variables)

MODEL

EDIT MODEL
PARAMETERS

SOLVE

VIEW
OUTPUTS

INPUT OUTPUT COMPARE

Analysis Type
optimization

RESET FLOWSHEET

RUN

Feed

Volumetric flow rate
3600

L/h

Fixed

Ca₂₊ concentration

NF design

NF pump pressure
3

bar

Free

Lower
1

Upper

NF area
50

m²

Free

Lower
0

Upper
1000

NF water recovery
0.046

fraction

Free

Lower
0

Upper
0.95

NF CAPEX

Membrane cost
15

\$/m²

Fixed

Membrane replacement rate
0.2

fraction/year

Fixed

Feed

Volumetric flow rate

3600

L/h

Fixed

Ca₂₊ concentration

257.99

mg/L

Fixed

SO_{4_2-} concentration

1010.98

mg/L

Fixed

HCO₃₋ concentration

384.99

mg/L

Fixed

Na₊ concentration

738.98

mg/L

Fixed

Cl₋ concentration

890.93

mg/L

Fixed

K₊ concentration

9

mg/L

Fixed

Mg₂₊ concentration

90

mg/L

Fixed

NF design

NF pump pressure

3

bar

Free

Lower
1

Upper

NF area

50

m²

Free

Lower
0

Upper
1000

NF water recovery

0.046

fraction

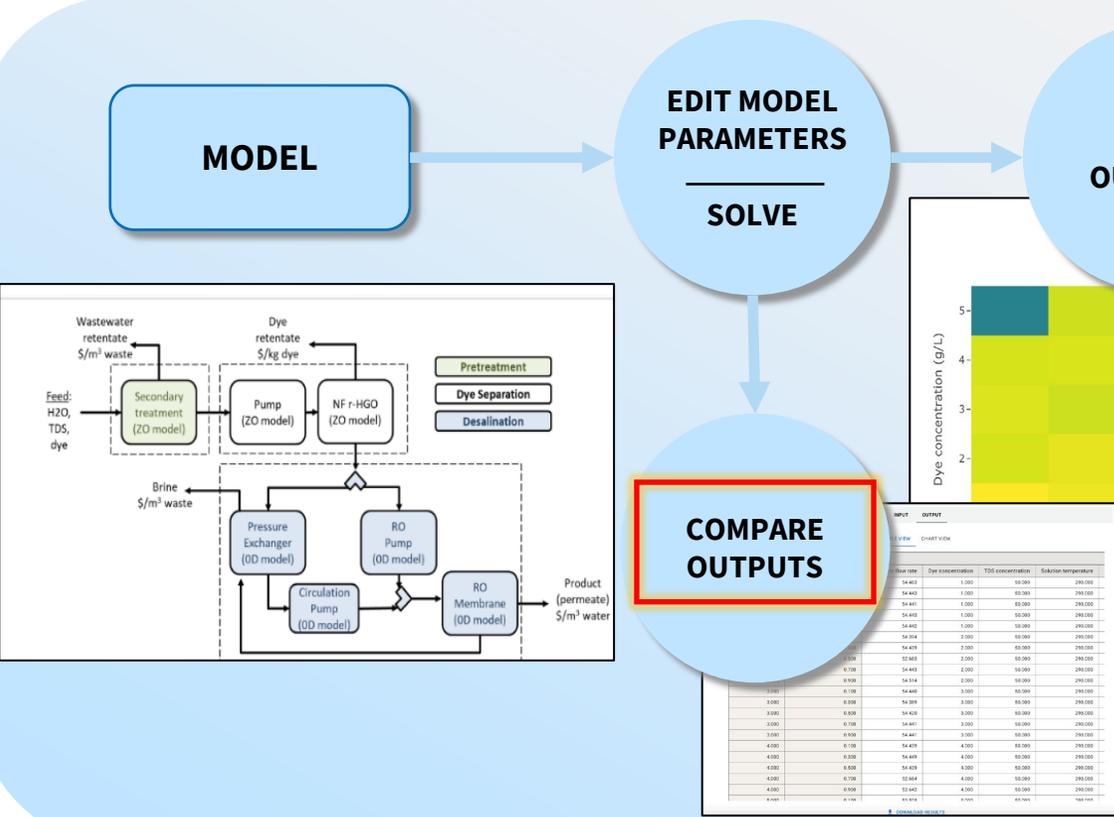
Free

Lower
0

Upper
0.95

HTC

Capability: View and compare outputs



	Metric	Dye Desalination 2 ▾	Dye Desalination 1 ▾	Value Difference
Feed	Volumetric flow rate	53 m3/h	120 m3/h	-67.31
	Dye concentration	1 g/L	2.5 g/L	-1.50
	TDS concentration	50 g/L	50 g/L	0.00
	Solution temperature	298 K	298 K	0.00
rHGO Nanofiltration	NF pump- motor efficiency	0.5 fraction	0.9 fraction	-0.40
	NF pump efficiency	0.4 fraction	0.9 fraction	-0.50
	Water recovery	0.9 fraction	0.75 fraction	0.15
	Mass removal fraction, dye	0.5 fraction	0.98 fraction	-0.48
	Mass removal fraction, TDS	0.27 fraction	0.27 fraction	0.00
	NF Water permeability Coefficient, A	0.58 LMH/bar	100 LMH/bar	-99.42
	Net driving pressure across membrane	6.9 bar	6.9 bar	0.00
	Solute Rejection- dye	0.44 fraction	0.98 fraction	-0.54
	Solute Rejection- tds	0.18 fraction	0.02 fraction	0.16
	Membrane area	11728.39 m**2	128.89 m**2	11599.50
Secondary Wastewater Treatment	Specific energy consumption per inlet flow rate	1897.81 kWh/m3	0.14 kWh/m3	1897.67
Reverse Osmosis	RO Water permeability coefficient, A	4e-12 m**2*s/kg	4e-12 m**2*s/kg	0.00
	RO Salt permeability coefficient, B	4e-8 m/s	4e-8 m/s	0.00
	RO high-pressure pump efficiency	0.8 fraction	0.8 fraction	0.00
	RO booster pump efficiency	0.8 fraction	0.8 fraction	0.00
	Isobaric pressure exchanger efficiency	0.95 fraction	0.95 fraction	0.00
Pump cost	94 \$(/m*3/hr)	94 \$(/m*3/hr)	0.00	

- Save inputs and outputs for later
- Compare side-by-side
- Export results to a table

Capability: Sensitivity analysis (parameter sweeps)

MODEL → **EDIT MODEL PARAMETERS** → **VIEW OUTPUTS**

SOLVE

Feed

- Volumetric flow rate: 280 m3/h Fixed
- Dye concentration: 0.2 kg/m3 Fixed
- TDS concentration: 2 kg/m3 Fixed
- Solution temperature: 298 K Free
- Lower: 273.15 Upper: 1000

rHGO Nanofiltration

- NF pump- motor efficiency: 0.9 fraction Fixed
- NF pump efficiency: 0.75 fraction Fixed
- Water recovery: 0.83 fraction Free
- Lower: 0 Upper: 1.0000001
- Mass removal fraction, dye: 0.99 fraction Sweep**
- Lower: 0 Upper: 0.99 Num. samples: 10
- Mass removal fraction, TDS: 0.21 fraction Fixed
- NF Water permeability Coefficient, A: 105 LMH/bar Fixed
- Net driving pressure across membrane: 7 bar Fixed

Run "sweep" over one (or more!) variables

Output Metric: RO brine disposal

RO brine disposal (\$/year)

Mass removal fraction, dye (fraction)

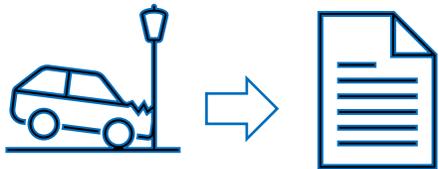
Dye concentration (g/L)

NF pump- motor efficiency (fraction)

Parameter	Value	Unit	Fixed
Volumetric flow rate	280	m3/h	Fixed
Dye concentration	0.2	kg/m3	Fixed
TDS concentration	2	kg/m3	Fixed
Solution temperature	298	K	Free
NF pump- motor efficiency	0.9	fraction	Fixed
NF pump efficiency	0.75	fraction	Fixed
Water recovery	0.83	fraction	Free
Mass removal fraction, dye	0.99	fraction	Sweep
Mass removal fraction, TDS	0.21	fraction	Fixed
NF Water permeability Coefficient, A	105	LMH/bar	Fixed
Net driving pressure across membrane	7	bar	Fixed

Potential Future Work

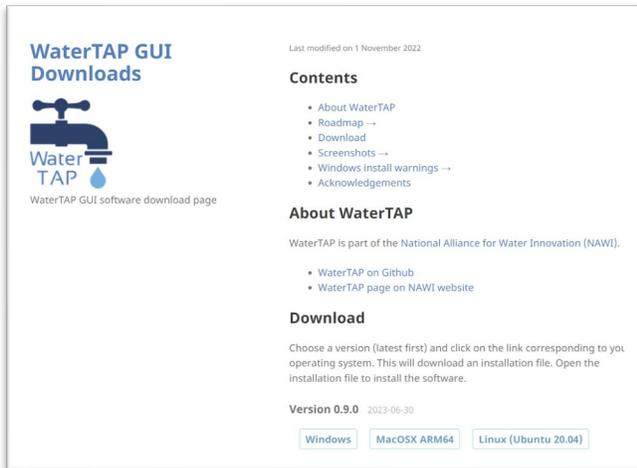
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  name="NF pump pressure",  
  ui_units=pyunits.bar,  
  display_units="bar",  
  rounding=2,  
  description="NF pump pressure",  
  is_input=True,  
  input_category="NF design",  
  is_output=True,  
  output_category="NF design",  
)
```



- Improve adding new flowsheet
 - Graphical “flowsheet export” tool
 - Select variables etc.
 - Output code that can be easily edited for advanced features not covered by the GUI (e.g. custom calculations for objects to export, specialized build & solve logic)
 - (Beginnings of common structure that could be used for graphical flowsheet builder)
- Improve error & non-convergence reporting
 - Help non-developer user communicate details of what went wrong
 - Include inputs, outputs, logs, diagnostics report
 - Provide instructions for how to send, etc.

Summary

- WaterTAP UI provides a no-code ability to:
 - View WaterTAP model parameters, change them, and solve the model
 - Compare outputs from different parameter choices
 - Perform “parameter sweeps” for sensitivity analyses
 - Export results from all of the above as tables for other analyses/tools



The WaterTAP UI can be **easily** installed for Windows, Mac OSX, and UNIX using a native (graphical) installer



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Thank you