PrOMMiS overview

Advances in Modeling Capabilities for Critical Mineral Separation Technologies

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NETL

CMU ESI Seminar
April 2026

Disclaimer

This presentation and comments are based on my personal experiences

Please note that they are not the official statement by Department of Energy/NETL

A little bit about myself…

PROMMIS
Process Optimization and Modeling for Minerals Sustainability

- **Ph.D. in Chemical Engineering – CMU**
    - **Process optimization**
- **ExxonMobil Upstream Research Company (Houston, TX)**
    - **Supply chain optimization**
- **ExxonMobil Research & Engineering (Fairfax, VA)**
    - **Refinery scheduling optimization**
- **BASF (Florham Park, NJ)**
    - **Operations research manager**
- **NETL – Systems Analysis / Research & Innovation Center (Pittsburgh, PA)**
    - **Process Systems Engineering**

Acknowledgements

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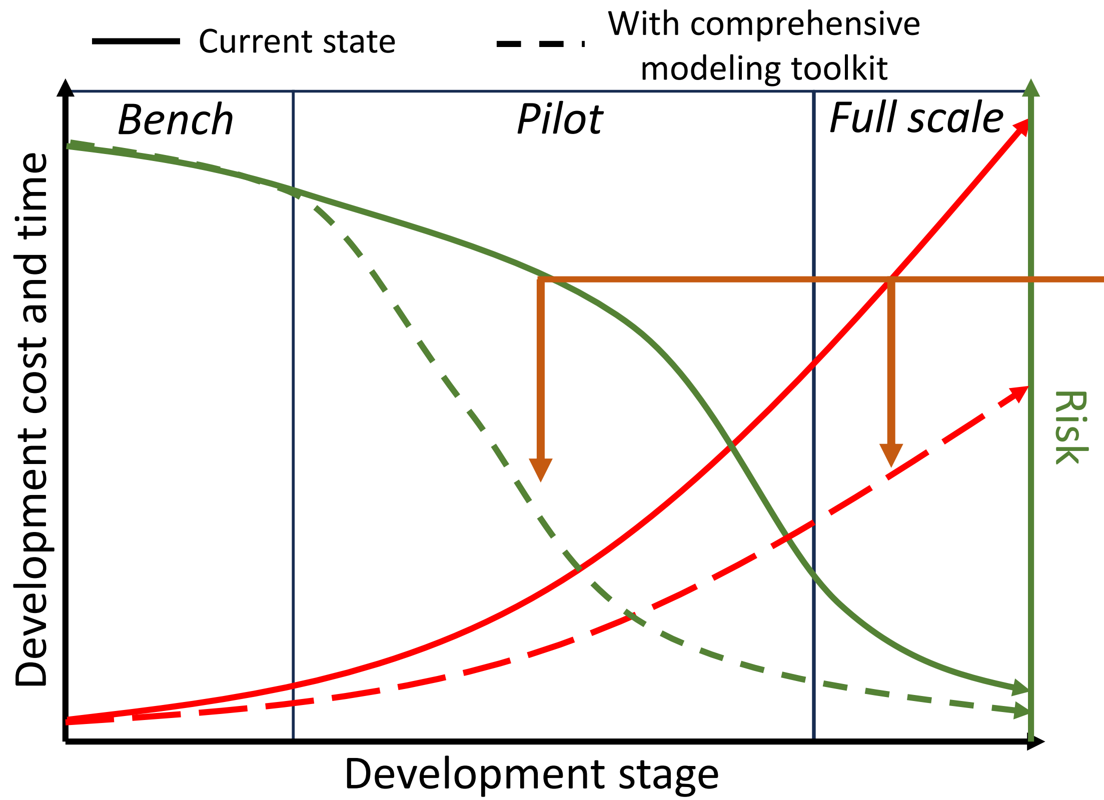
PrOMMiS: Process Optimization and Modeling for Minerals Sustainability

PROMMIS
Process Optimization and Modeling for Minerals Sustainability

Objective: **Accelerate scale-up** and **deployment** of innovative CM & REE processes and establish the toolkit to compress future RD timelines by **leveraging IDAES** and a **decade** of **DOE CM & REE investment**.

Typical R&D roadmap and blocks



Prior DOE investments

CM & REE process experience

CMI Critical Materials Innovation Hub

REECM Rare Earth Elements and Critical Minerals from Coal and Coal-Based Resources

Process modeling capabilities

PYOMO

IDAES Institute for the Design of Advanced Energy Systems

PROMMIS **A long-lasting tool set for accelerating development of CM & REE technologies**

- Open-source
- Equation-oriented
- Multi-hierarchical
- Unified modeling structure

PrOMMiS: Process Optimization and Modeling for Minerals Sustainability

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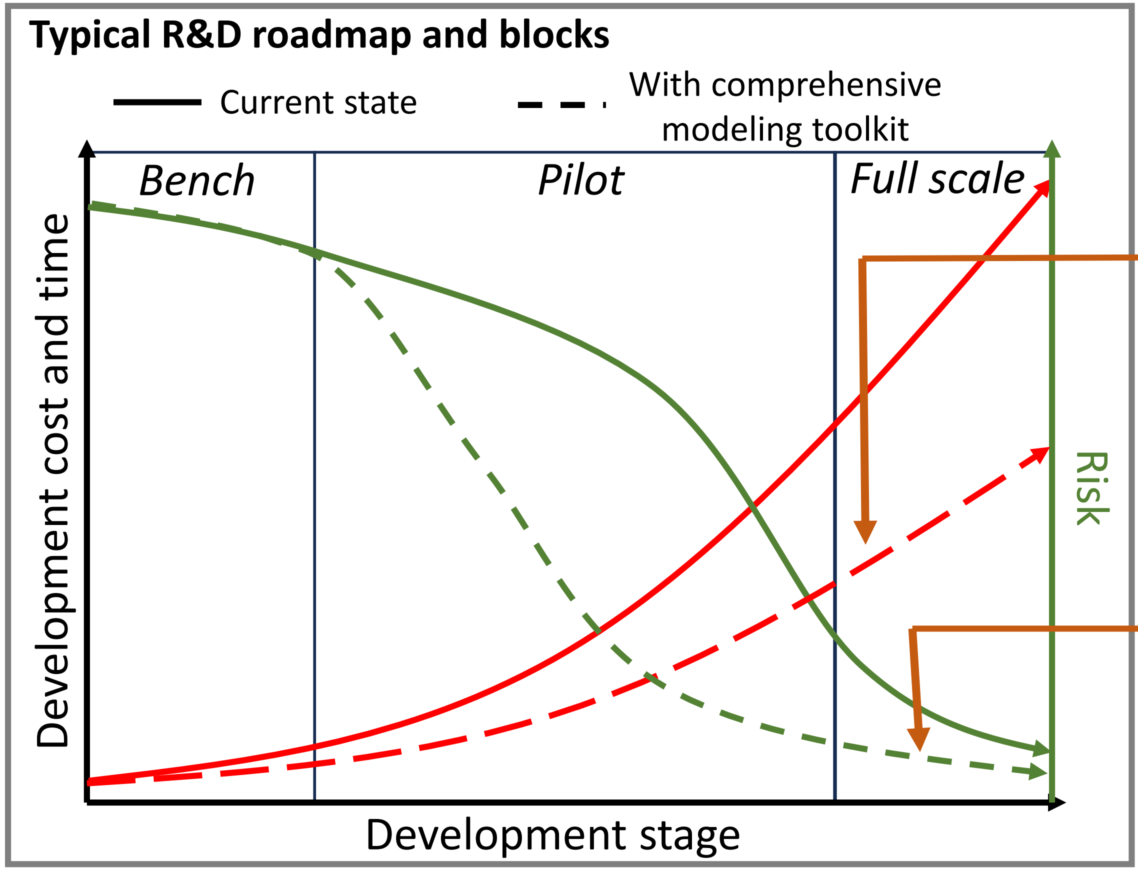
Objective: **Accelerate scale-up** and **deployment** of innovative CM & REE processes and establish the toolkit to compress future RD timelines by **leveraging IDEAS** and a **decade** of **DOE CM & REE investment**.



PROMMIS

1. Simulating and optimizing process design and operation
2. Reduce risk from uncertainties in process design, feedstock, etc.
3. Enable workforce development for future CM & REE facilities
4. Enable long-term planning for process integration and supply chain planning

1. Optimize separation processes trains
2. Quantify parameter and process uncertainty
3. Reduce manufacturing inconsistency risk

Reduce modeling timeline

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Framework

IDAES Institute for the Design of Advanced Energy Systems

Properties:
- Implemented as modular blocks
- Flexibility to choose state variables, use different property packages in the same flowsheet
- Flexible formulation of equations

Ports:
- Can connect to any other Port with the same members automatically
- Translator blocks to connect Ports with different state variables

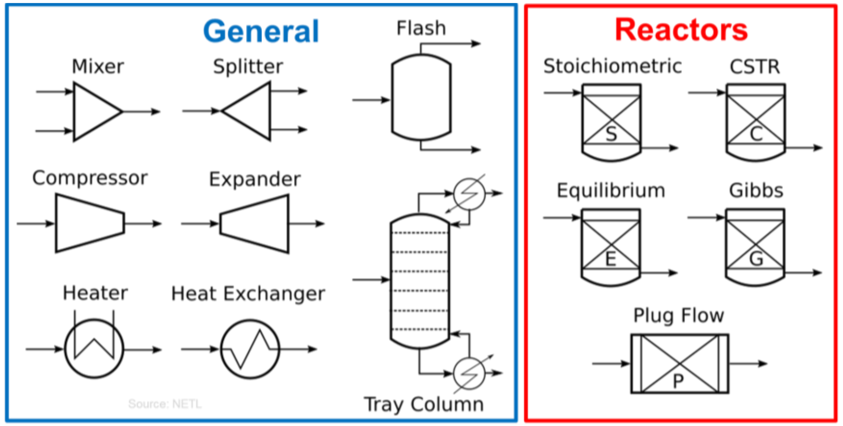
Control Volumes:
- Control Volumes can be connected together to develop complex multi-scale models
- Prebuilt **methods** for common forms of **balance equations**

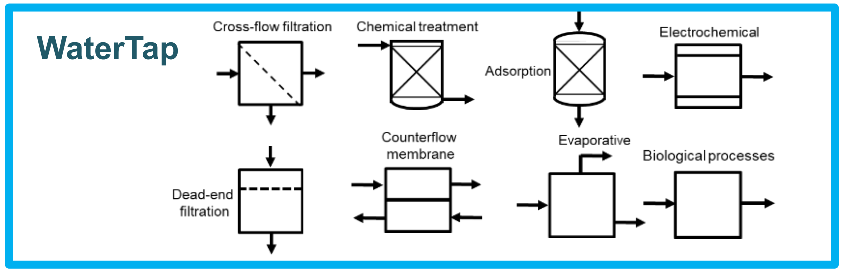
Initialization:
- Custom initialization routines
  - Reliability and convergence tools
- IDAES diagnostics toolset (structural analysis, …)

Extensive model and property library

IDAES Institute for the Design of Advanced Energy Systems

Water TAP





Standardize costing utilizing NETL's QGESS

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Data Management

- NETL QGESS Reports[1]
- FEED Studies
- Legacy Models
- Public References

Costing Correlations – Equipment

Excel

Step 1: Identify/select reference source to obtain RP, RC, EXP values
Step 2: Fit data for a given expression (Guthrie's method)
Step 3: Validation/Verification to system

$$\mathrm{SC} = \mathrm{RC}\left(\frac{\mathrm{SP}}{\mathrm{RP}}\right)^{\mathrm{EXP}} \qquad \mathrm{EXP} = \frac{\ln\left(\frac{\mathrm{RC1}}{\mathrm{RC2}}\right)}{\ln\left(\frac{\mathrm{RP1}}{\mathrm{RP2}}\right)}$$

SC: Scaled Bare Erected Cost
RC: Reference Bare Erected Cost
SP: Scaled Parameter
RP: Reference Parameter
EXP: Cost scaling exponent

Obtained from reference source

Obtained from multiple data points of reference source, or typical values

Implementation

Excel → Python Dictionary → IDAES Costing Framework → Total Plant Costing & Optimization

[1] NETL's QGESS: Capital Cost Scaling Methodology Revision 4

https://github.com/IDAES/idaes-pse/

Data driven model parametrization and development

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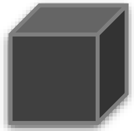
Data Source

Experimental Data

Black-Box Models (e.g., ASPEN, Prescient, CFD)



IDAES Models or Properties

Sampling

Common Sampling Tools

idaes.
surrogate.sampling

PySMO

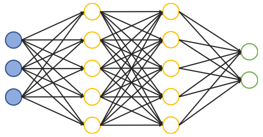
ALAMO
a black-box modeling tool

Model Selection and Training

parmest

ALAMO
a black-box modeling tool

PySMO



IDAES ML Surrogates

RIPE

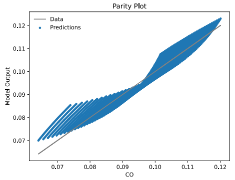
HELMET

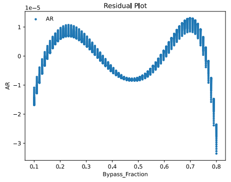
Visualization and Validation

Standard Metrics

RMSE = 0.291E-1
R2 = 0.988

Plotting and Visualization Tools





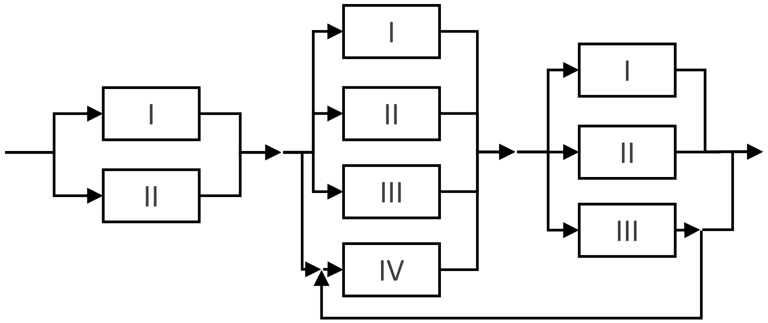
Integrated IDAES Model

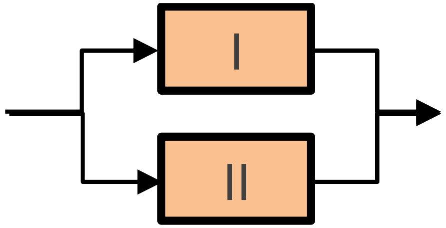
EO Model: Correlation, Property Package, Unit Model

Direct Evaluation

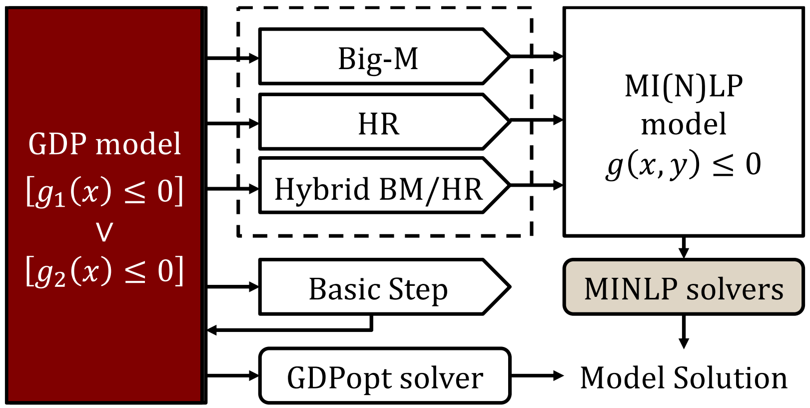
z[0.75, 1.0] = 3.02965425e-01

Automated design of optimal separation trains





$$\begin{bmatrix} Y_1 \\ g_1(x) \le 0 \end{bmatrix} \vee \begin{bmatrix} Y_2 \\ g_2(x) \le 0 \end{bmatrix}$$



PrOMMiS Modeling Framework	Pyomo.GDP Disjunctive Modeling	General GDP Solution Approaches

- Models built using IDAES framework and process model library
- High-level representation of superstructure with disjunctions
- Automatic conversion to MINLP with Pyomo.GDP
- Gives access to rigorous, competitive MINLP solvers

Design of processes under uncertainty

Industrial processes must be able to perform satisfactorily in light of model uncertainties.

Two types of variables in robust process design:

- Design Variables (set during construction):
  - Membrane stage length
- Control Variables (adjustable during operation):
  - Flows (feed, diafiltrate, recycle, products)

Potential Sources of Uncertainty

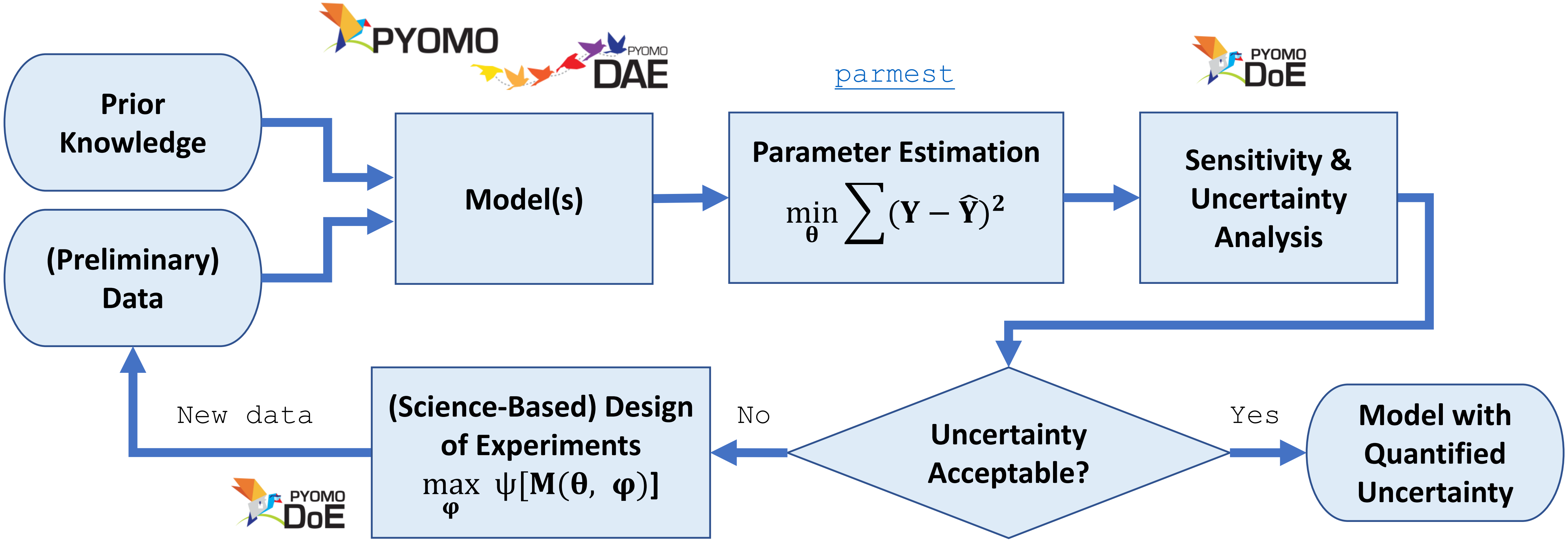
- Location and rate of **fouling**
- **Feedstock** flow rate and solute concentrations
- **Manufacturing variation**
  - Seek to ensure optimal performance for up to *N* units underperforming

Pyomo Robust Optimization Solver (**PyROS**) can obtain robust optimal solutions that are feasible for all realizations of uncertainty[3,4]

$$
\begin{aligned}
\min_{x\in\mathcal{X}} \quad \max_{q\in\mathcal{Q}} \quad \min_{\substack{z\in\mathbb{R}^{n_z},\\ y\in\mathbb{R}^{n_y}}} \quad & f_1(x) + f_2(x,z,y,q) & \\
\text{s.t.} \quad & g_i(x,z,y,q) \le 0 & \forall i \in \mathcal{I} \\
& h_j(x,z,y,q) = 0 & \forall j \in \mathcal{J}
\end{aligned}
$$

[3] Isenberg, NM, Sherman, JA, Siirola, JD, & Gounaris, CE. PyROS: The Pyomo Robust Optimization Solver. *Forthcoming.* 2024.

Accelerated experimental efforts



$\boldsymbol{\theta}$ = unknown parameters (sieving coefficients), $\hat{\mathbf{Y}}$ = model prediction of measured variables, $\mathbf{Y}$ = observed values of measured variables, $\mathbf{M}$ = Fischer information matrix, $\boldsymbol{\varphi}$ = design vector containing control variables, ψ = scalar measure (determinant/trace/minimum eigenvalue)

Wang, J., & Dowling, A. W. (2022). *AIChE Journal*

Integration with advanced chemistry models

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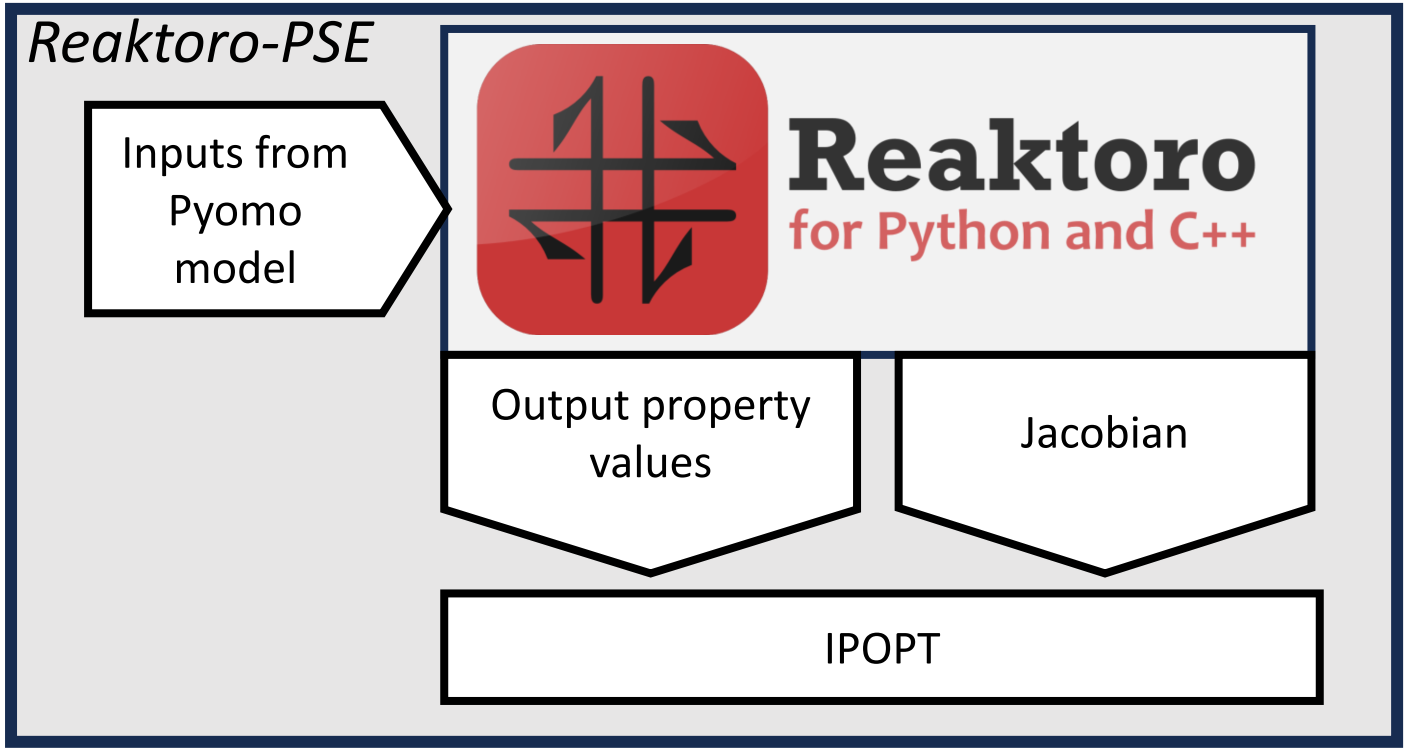
Reaktoro is a platform for simulation of chemical reactions:

- Access to large number of databases
- Access to a number of activity models
- Estimates a large number of chemical, thermodynamic, and aqueous properties

Provides access to direct derivatives as a function of user inputs:

- Enables integration into Pyomo via Graybox modeling approach



OLI cloud API integration

- Available on WaterTAP-org GitHub: https://github.com/watertap-org/reaktoro-pse

Leveraging existing PSE+ tools for PrOMMiS

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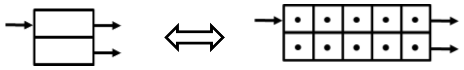
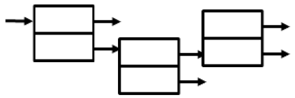
DOE developed modeling toolkit

PYOMO IDAES Institute for the Design of Advanced Energy Systems

- Open-source GitHub python
- Equation oriented $f(x) = 0$
- Multi-hierarchical 
- Unified modeling structure 

Rich model libraries

IDAES Institute for the Design of Advanced Energy Systems : Common unit operations

WaterTAP : Water treatment unit operations

PrOMMiS : CM & REE unit models

Advanced capabilities

Model fitting tools
Surrogate model tools
Superstructure optimization
Robust Optimization
Science based design of experiments
External chemistry software integration

PySMO MLT PySTAR PYOMO GDP PyROS PYOMO DoE OLI Reaktoro for Python and C++

Open source and accessible

Publicly accessible on GitHub

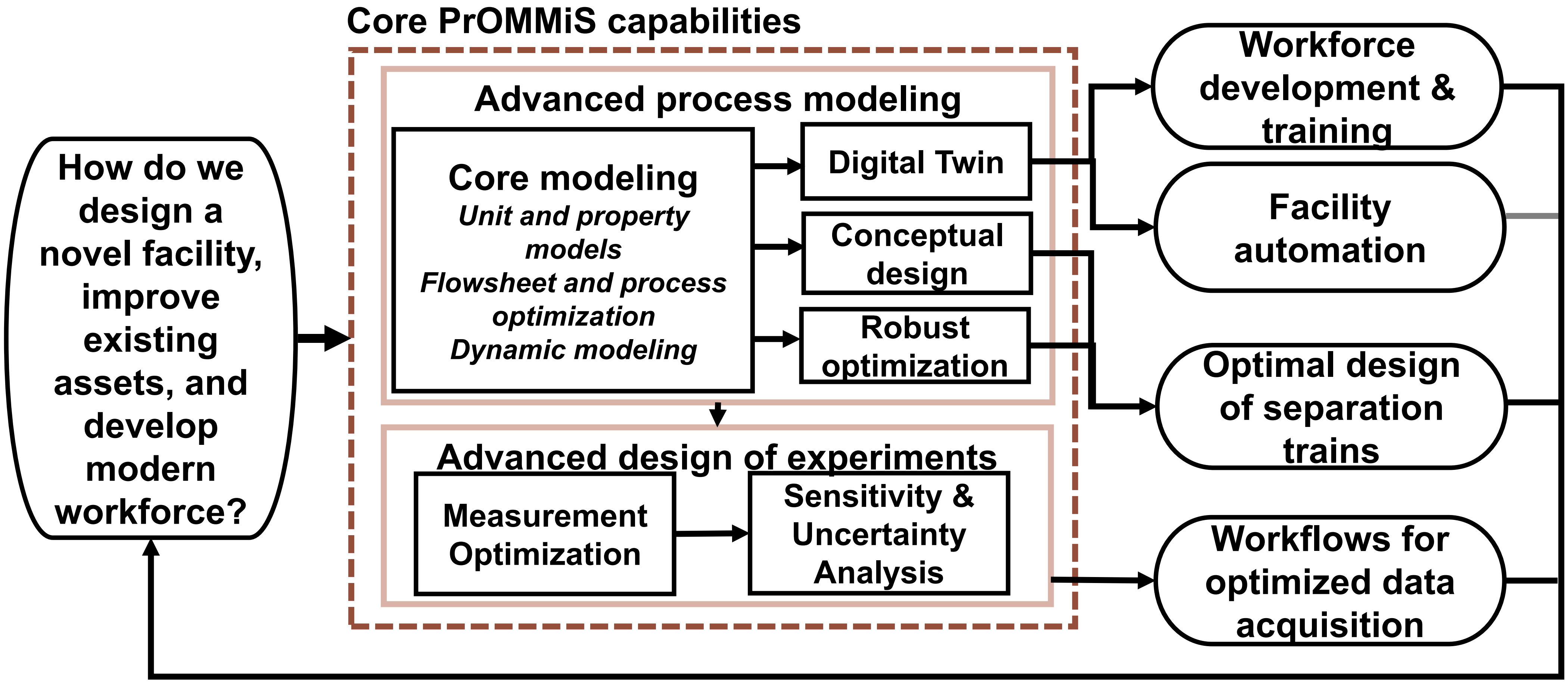
- https://github.com/Pyomo
- https://github.com/IDAES
- https://github.com/watertap-org
- https://github.com/prommis

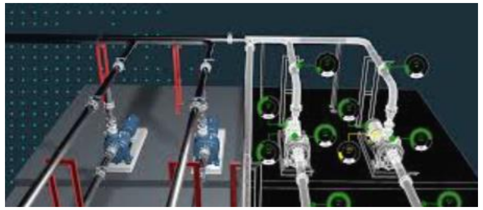
GitHub

User interfaces

- Code based interface (primary)
- Limited graphical user interface (secondary)

PrOMMiS core capabilities





PrOMMiS case studies

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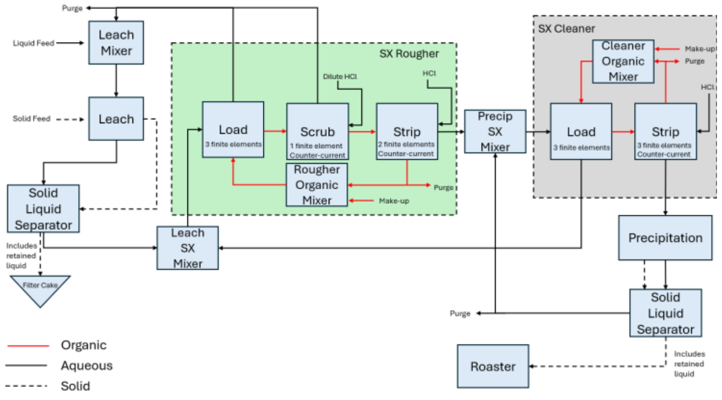
University of Kentucky pilot



- Model library
- Costing library
- Model fitting tools
- Superstructure optimization
- Surrogate model tools

IDAES
Institute for the Design of Advanced Energy Systems

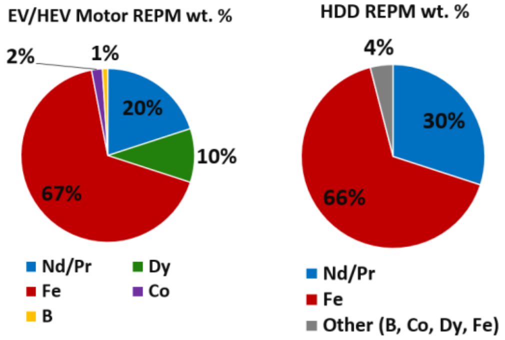
WaterTAP

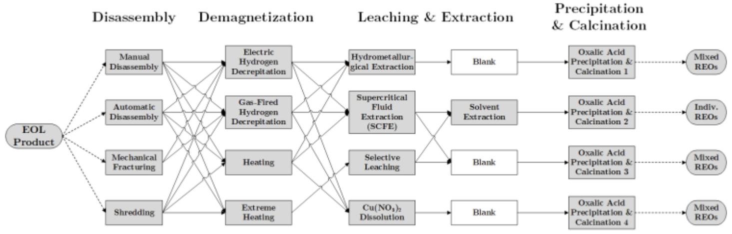
PySMO

PySTAR

PYOMO GDP

End Of Life CM recovery

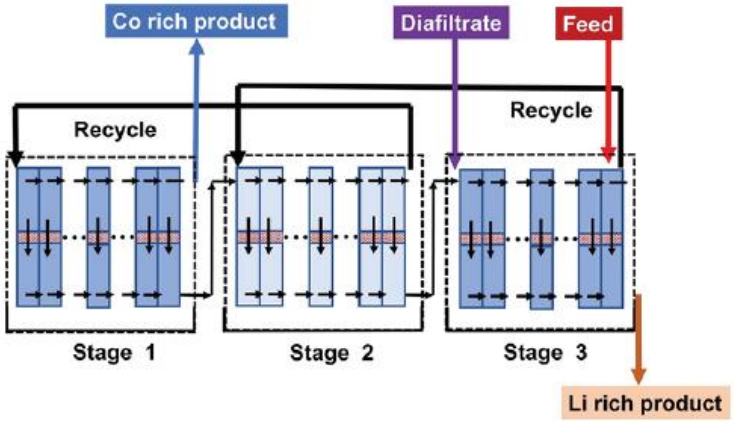




Superstructure optimization

PYOMO

Separation of Lithium and cobalt through diafiltration



- Robust Optimization
- Science based design of experiments

PYOMO GDP

PyROS

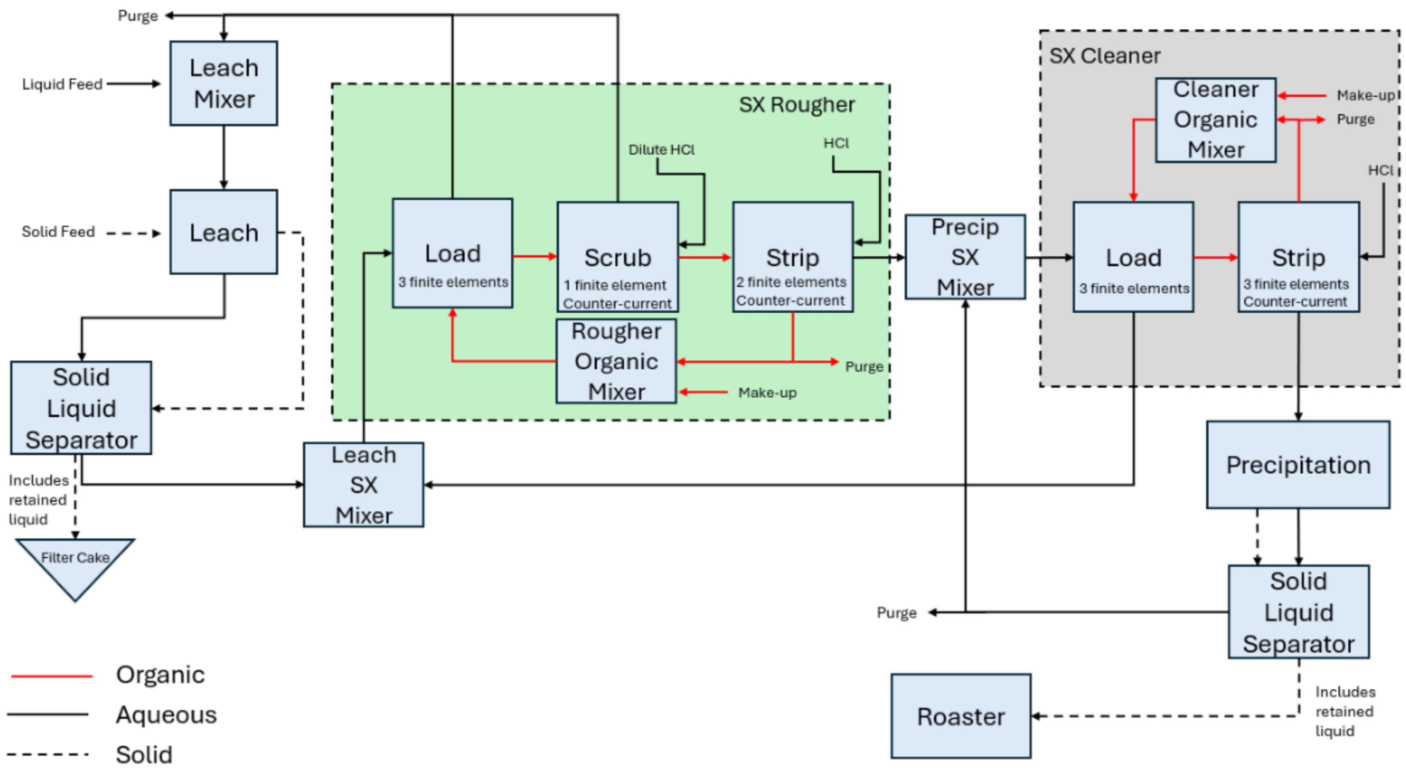
PYOMO DoE

Code base tutorial

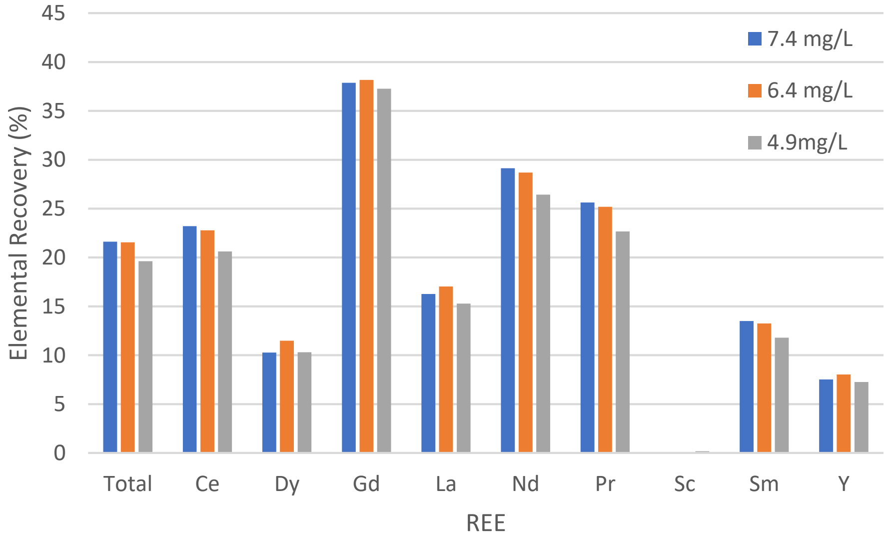
UKy Flowsheet Tutorial

This tutorial will show how to build, initialize, and simulate the West Kentucky No.13 Coal Refuse flowsheet. The inputs into this flowsheet are case study-specific, so users should not expect the flowsheet to solve if the values are significantly altered.

- Useful Links:
  - Public Github Repository: https://github.com/prommis/prommis/tree/main
  - UKy Flowsheet Code: https://github.com/prommis/prommis/blob/main/src/prommis/uky/uky_flowsheet.py



Precipitator recovery vs. Oxalic Acid Dosage



https://github.com/prommis/prommis/blob/main/docs/tutorials/uky_flowsheet-solution.ipynb

Conceptual Design of Solvent Extraction

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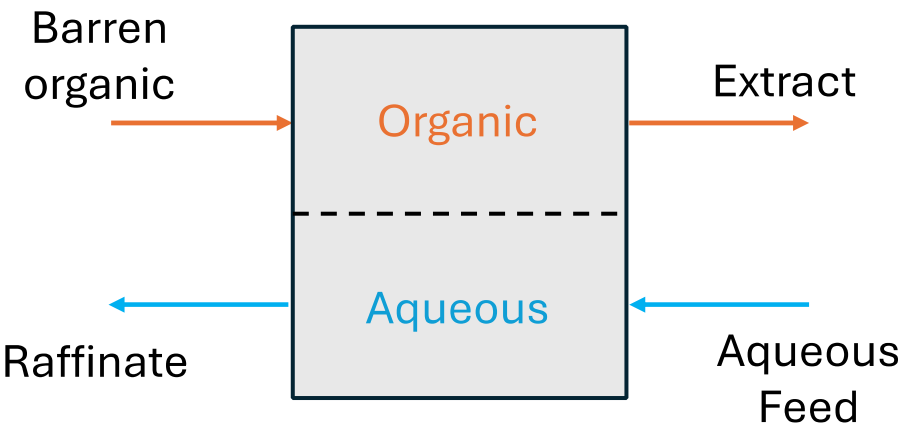
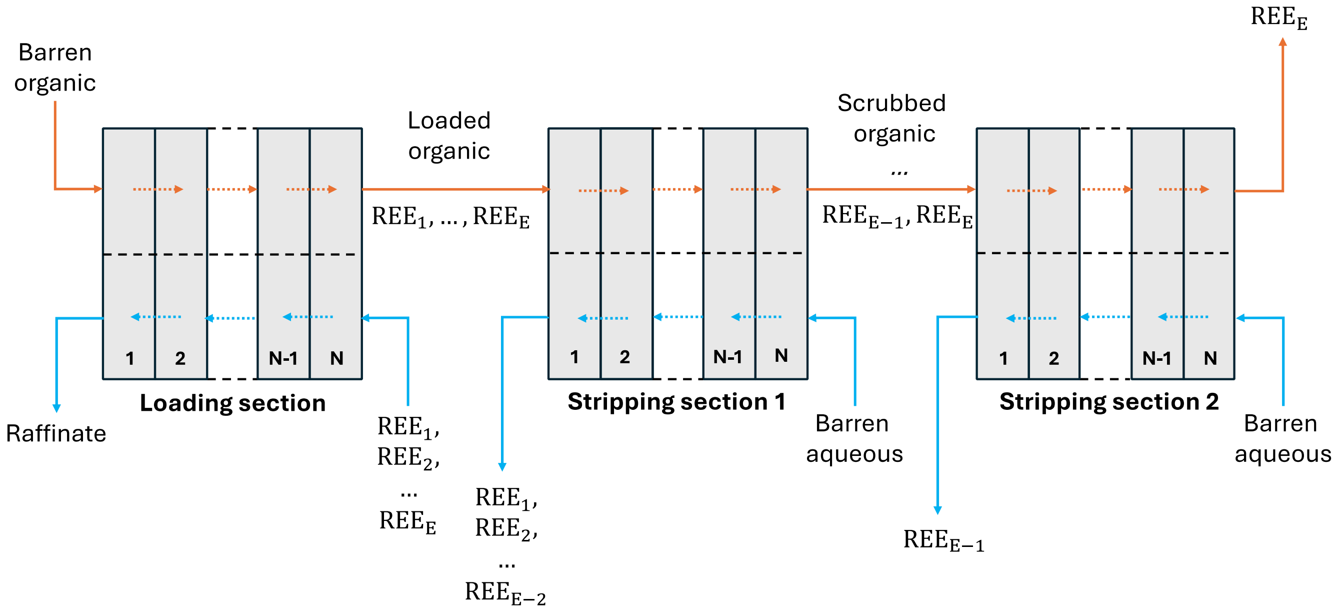
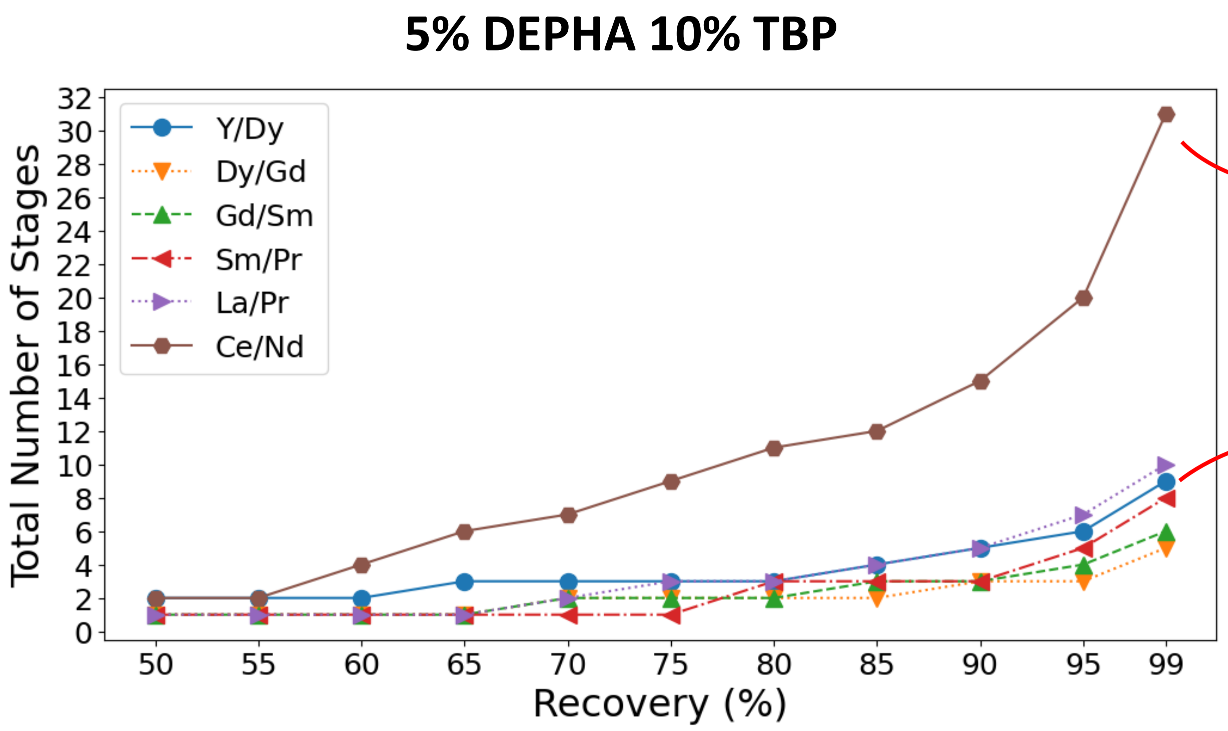
- Solvent extraction refers to the distribution of solute between two <u>*immiscible phases*</u>
    - The system does not form a single phase after mixing



Single stage

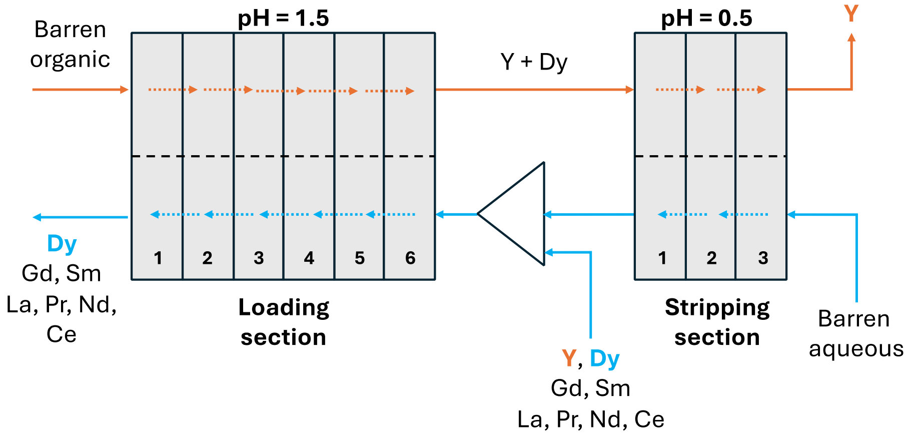


Conceptual Design of Solvent Extraction



Cerium (Ce) – Neodymium (Nd) Separation	
85%	7 L.Stages at pH 5.0, 5 S.Stage at pH 2.5
90%	10 L.Stages at pH 5.0, 5 S.Stage at pH 2.0
95%	16 L.Stages at pH 5.0, 4 S.Stage at pH 0.5
99%	14 L.Stages at pH 5.0, 17 S.Stages at pH 3.0

Solved to global optimality with average runtime of 20s per node



Enhancement of costing libraries

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Front End Loader (2 yd^3)	Front End Loader (10 yd^3)	Bucket Elevator	Jaw Crusher	VSI Crusher	Roll Crusher
Vibrating Screen	Storage Bins	Dry Ball Mill	PE Tanks	Steel Tanks	Tank Mixer
Elevator Motor	Process/Slurry Pump	Thickener	Filter Press	Conveyor	Roaster
Gas Scrubber	Spray Chamber Quencher (77k-60k cfm)	Spray Chamber Quencher (60k-230k cfm)	Chiller	Solution Heater	Belt Filter
BioLeach Tanks	Blower	Mixer Settler	HDD Recycling Shredder (2700 drives/hour)	HDD Recycling Furnace (Hydrogen Decrepitation)	Membranes*
	Nanofiltration*	Reverse Osmosis*	Ion Exchange*		

* WaterTap library

References:

[2] Keim, Steven Anthony, and Naumann, Hans. Production of Salable Rare Earths Products from Coal and Coal Byproducts in the U.S. Using Advanced Separation Processes (Final Technical Report). United States: N. p., 2019. Web. doi:10.2172/1569277.

[3] Honaker, Rick, Werner, Joshua, Yang, Xinbo, Zhang, Wencai, Noble, Aaron, Yoon, Roe-Hoan, Luttrell, Gerald, and Huang, Qingqing. **Pilot-Scale Testing of an Integrated Circuit for the Extraction of Rare Earth Minerals and Elements from Coal and Coal Byproducts Using Advanced Separation Technologies.** United States: N. p., 2021. Web.

[4] Honaker, Rick Q., Werner, Joshua, Nawab, Ahmad, Zhang, Wencai, Noble, Aaron, Free, Michael, and Yang, Xinbo. **Demonstration of Scaled-Production of Rare Earth Oxides and Critical Materials from U. S. Coal-Based Sources (Final Report).** United States: N. p., 2023. Web. doi:10.2172/1971736.

[5] Garrett, D.E. (1989). Chemical Engineering Economics.

[6] Ames National Laboratory. (2020, March 26). It's all part of the Grind: CMI's new hard drive Shredder serves up plenty of material for recycling science. Ames Laboratory. https://www.ameslab.gov/news/it-s-all-part-of-the-grind-cmi-s-new-hard-drive-shredder-serves-up-plenty-of-material-for

[7] Loh, H.P., Lyons, Jennifer, White, Charles W.. Process Equipment Cost Estimation Final Report. United States: N. P., 2002. Web.

PrOMMiS Costing Library:

$$SC_i = \alpha_i * RP_i^{Exp_i}$$

- SC – scaled cost
- α – reference cost / performance
- RP – reference parameter
- Exp – exponential factor
- i – i^{th} unit operations in the library

Costing results and tutorial

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REE Costing Framework Part 3 - UKy Flowsheet Demo

The purpose of this tutorial is to demonstrate defining, adding, and solving costing for the University of Kentucky flowsheet. It is assumed that the user is already familiar with the flowsheet, which is introduced in detail in the UKy Flowsheet Tutorial. The user should have an understanding of the basic features and structure of the costing framework in PrOMMiS, which is introduced in detail in Part 1 of this tutorial.

The tutorial will take users through the following:

- Adding capital costing to equipment in an existing flowsheet
- Build total plant and operating costs

Useful Links:

- Public GitHub Repository: https://github.com/prommis/prommis/tree/main
- REE Costing Module Code: https://github.com/prommis/prommis/blob/main/src/prommis/uky/costing/re

PrOMMiS Costing Library:

$$SC_i = \alpha_i * RP_i^{Exp_i}$$

- SC – scaled cost
- α – reference cost / performance
- RP – reference parameter
- Exp – exponential factor
- i – i[th] unit operations in the library

1 Import the necessary tools

First, import the required Python, Pyomo, IDAES, and PrOMMiS packages. These will be implemented at variou

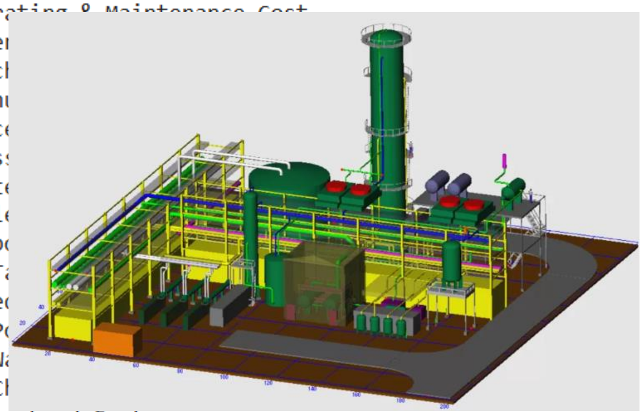
For installation instructions, please refer to the public GitHub repository linked above.

```
Total bare erected cost (MUSD): 49.632
Total overnight (installed) equipment cost:
Total annualized capital cost (MUSD): 16.898

Total annual fixed O&M cost (MUSD): 11.325
Total annual variable O&M cost (MUSD): 4.182
Total annual O&M cost (MUSD): 15.507
Total annual O&M cost per kg REE recovered (USD/kg): 54.127

Total annualized plant cost (MUSD): 32.405
Annual rate of recovery (kg/year): 286493.408
Cost of recovery per kg REE recovered (USD/kg): 113.110
```

```
====================================================================================
costing
------------------------------------------------------------------------------------
                                                                          Value
    Plant Cost Units                                                      MUSD_2023
    Total Plant Cost                                                      147.42
    Total Bare Erected Cost                                               49.632
    Total Installation Cost                                               97.776
    Total Other Plant Costs                                               0.0083065
    Total Fixed Operating & Maintenance Cost                              11.325
    Total Annual Oper                                                     3.8090
    Total Annual Tech                                                     1.8294
    Summation of Annu                                                     5.6384
    Total Maintenance                                                     2.9483
    Total Quality As                                                      0.38090
    Total Sales, Pate                                                     0.12106
    Summation of Sale                                                     2.3570
    Total Admin Supp                                                      0.76181
    Total Property Ta                                                     1.4742
    Total Other Fixed                                                     1.0000e-12
    Total Variable Po                                                     0.38536
    Total Variable Wa                                                     5.1396e-06
    Total Variable Ch                                                     0.0000
    General Plant Overhead Cost                                           2.5845
    Total Plant Overhead Cost, Including Maintenance & Quality Assurance  5.9137
    Total Variable Operating & Maintenance Cost                           4.1823
    Total Land Cost                                                       1.2124
    Total Sales Revenue Cost                                              24.211
    Cost of Recovery (USD/kg REE)                                         113.11
====================================================================================
```

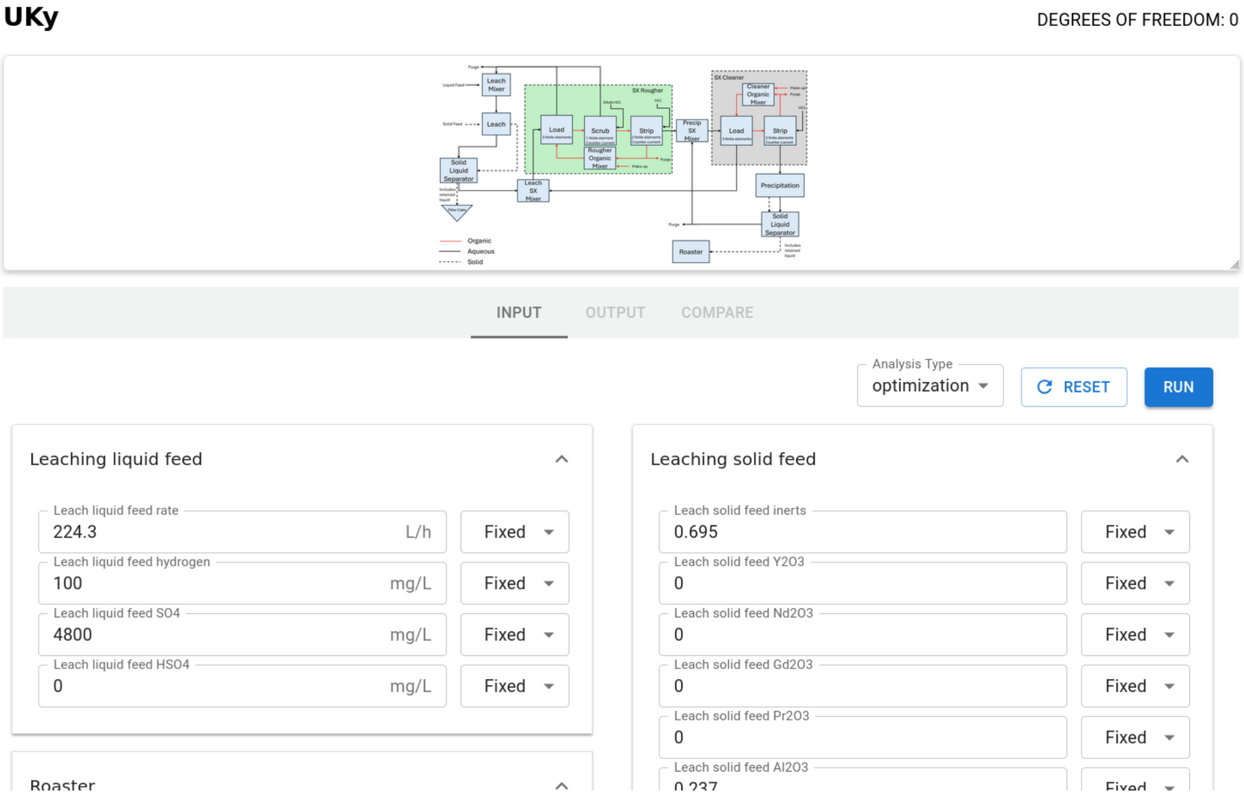


https://github.com/prommis/prommis/blob/ad8ef5e79740ef073f6ce2b797712cb04040ad8b/docs/tutorials/ree_costing_framework_uky_flowsheet_demo-solution.ipynb

Developed flowsheet runner UI

PROMMIS
Process Optimization and Modeling for Minerals Sustainability

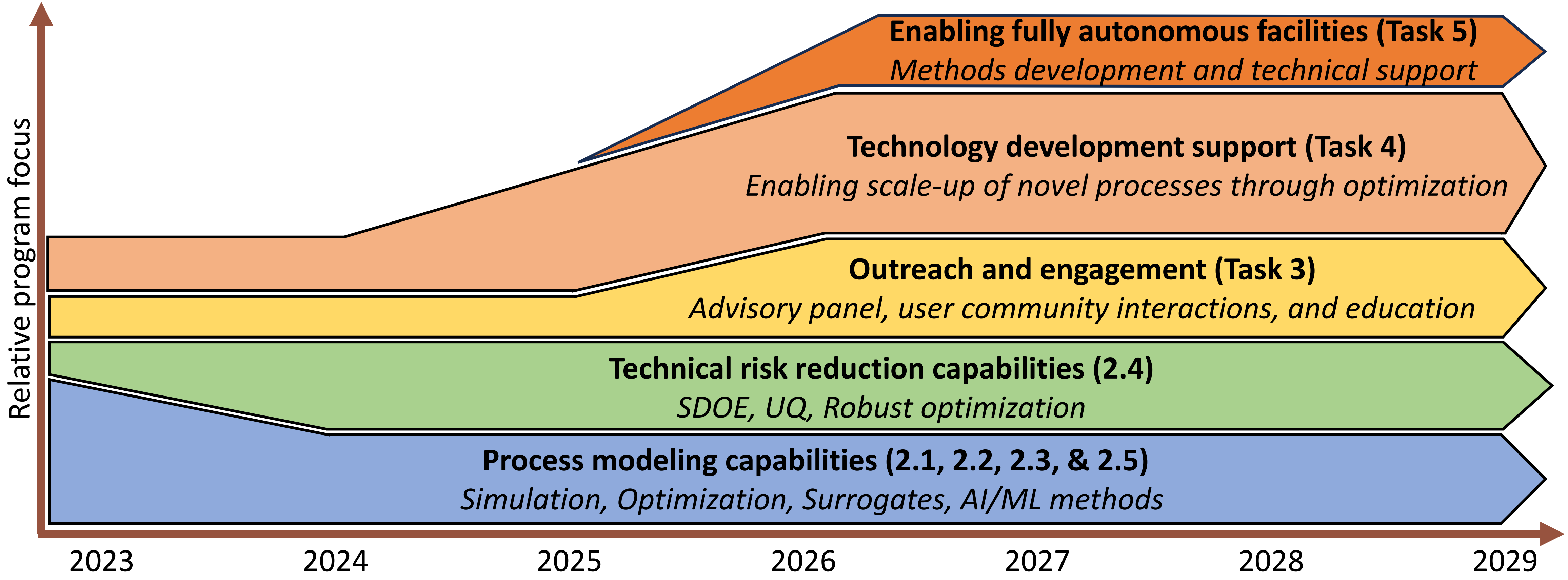
- One-click native install
- Lowers the barrier for new users to run PrOMMiS optimizations
- Provides a vehicle for outreach and tutorials
- Mechanism for facilitating collaboration with partners (without requiring Python-coding expertise)



Flowsheet Processor UI to parameterize and solve existing flowsheets.

PSE+ ecosystem enabled rapid development of PrOMMiS capabilities and focus on application

PROMMIS
Process Optimization and Modeling for Minerals Sustainability



Conclusion

PROMMIS
Process Optimization and Modeling for Minerals Sustainability

- **Accomplishments**
- Empowering industry users with modeling environment
- Accelerate speed of implementation
- Open source for collaboration and extension

- **Future Work**
- Physical/Chemical property model
- Collaboration for pilot plant
- Licensing opportunity

Q & A