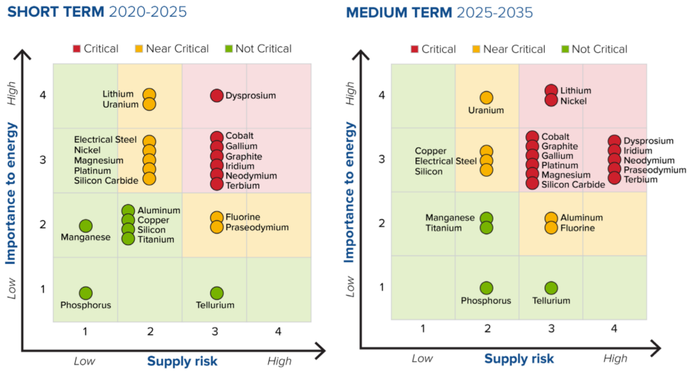
PrOMMiS Model Library

Alejandro Garciadiego[a], Andrew Lee[a], Jinliang Ma[a], Lingyan Deng[a], Marcus Holly[a], Arkoprabho Dasgupta[b], Debangsu Bhattacharyya[b], Soraya Rawlings[c], Bethany Nicholson[c], John Siirola[c], Molly Dougher[d], Alexander W. Dowling[d]

[a] *NETL Support Contractor,* [b] *West Virginia University,* [c] *Sandia National Laboratories,* [d] *University of Notre Dame*

Critical Minerals

- The global effort to curb carbon emissions is accelerating demand for clean energy technologies and critical minerals they rely on
- Provide essential and specialized properties while having no easy substitutes
- Are assigned as critical by the Secretary of the Interior
- The estimated value of rare-earth compounds and metals imported by the United States in 2022 was $200 million[2]



Short and medium-term criticality matrix[1]

Leveraged Existing PSE Infrastructure and Tools

Built of Pyomo, IDAES and WaterTAP:

- Compatible with other IDAES libraries
- Existing unit models
  - Electrodialysis
  - Ion Exchange
  - Nanofiltration
  - Reverse Osmosis

Modeling tools

- Surrogate models and ML:
  - PySMO
  - OMLT
  - ALAMO
- Design of experiments:
  - Pyomo.DoE
- Dynamic modeling:
  - Pyomo.DAE
- Parameter estimation:
  - parmest

References

[1] Bauer D. J., Ruby T. Nguyen R. T., smith B. J., (2023), Critical Materials Assessment, U.S. Department of Energy

[2] U.S. Geological Survey, (2023), Mineral Commodity Summaries

[3] Honaker, R. Q., Zhang, W., Werner, J., Noble, A., Luttrell, G. H., and Yoon, R. H.. (2019) Enhancement of a Process Flowsheet for Recovering and Concentrating Critical Materials from Bituminous Coal Sources. United States: N. p.

[4] Wamble, N.P., Eugene, E.A., Phillip, W.A., Dowling, A.W., 'Optimal Diafiltration Membrane Cascades Enable Green Recycling of Spent Lithium-Ion Batteries', ACS Sustainable Chem. Eng. 2022, 10, 12207−12225

PrOMMiS Unit Model Library

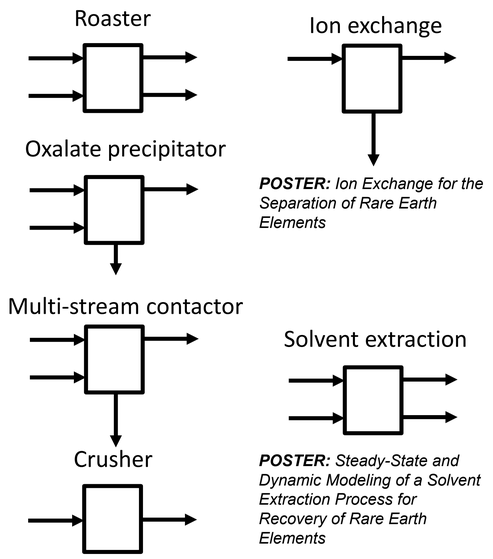
- Open-source
- Multi-hierarchical
- Customizable
- Equation oriented
- Flexible
- Powerful
- Documented

Unit Models

- Calcination and Roasting
- Filter Press
- Grinding and Comminution
- Leaching
- Selective Precipitation
- Solvent Extraction
- Thickening

Property Models

- Leaching and reactions
- Oxalate precipitation
- Solvent extraction
- Lithium-Cobalt diafiltration



POSTER: *Ion Exchange for the Separation of Rare Earth Elements*

POSTER: *Steady-State and Dynamic Modeling of a Solvent Extraction Process for Recovery of Rare Earth Elements*

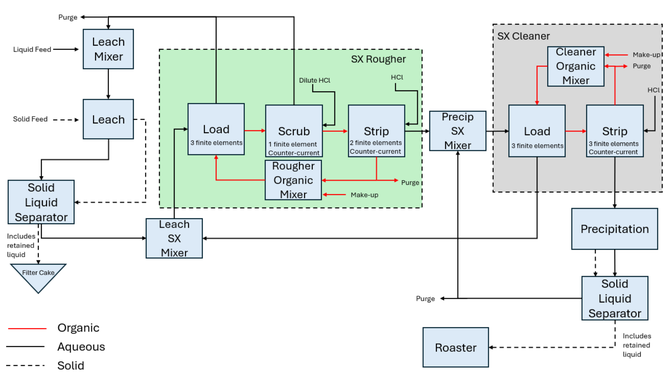
Case Study No. 1: University of Kentucky Pilot Plant

Objective:

- Recovery of Rare earth elements (REE) from coal and coal byproducts in a cost-effective and environmentally benign manner.

Feed:

- Two distinctly different coarse refuse materials (i.e., West Kentucky No. 13 and Fire Clay coal seams).
- Three secondary sources (i.e., heap leach process and naturally formed acid mine drainage system).



Flowsheet of the pilot-sale leaching and solvent extraction circuits[3]

Target capabilities:

- Conceptual Design
- Detailed Process Optimization

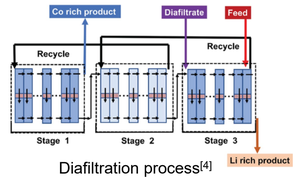
Case study No. 2: Separation of Lithium from Cobalt Via Diafiltration

Objective:

- Separate lithium ions from cobalt ions sourced from recycling Lithium-ion batteries.

Process:

- Membranes are used to selectively separate different components in the feed stream, and a dilute diafiltrate stream is added to the process to avoid solubility-limits.



Diafiltration process[4]

Target capabilities:

- Design of Experiments
- Conceptual Design
  POSTER: *Systematic Design of Complex Processes using GDP: A Comparison of Reformulations*
- Uncertainty Quantification
  POSTER: *Robust Optimization of Critical Mineral Membrane Separations Under Uncertainty*

Takeaways

- Developed a comprehensive unit model library for CMM & REE processing operations including core unit models, property packages, and reaction packages (e.g., solvent extraction, membrane separation, ion exchange).
- Verified unit model library and flowsheet models with available data and simulations (i.e., UKy flowsheet).
- Developed user support and education materials (e.g., demo tutorials, jupyter notebooks, and extensive documentation)

Future Work

- Incorporate external solutions for detailed chemistry models
- Develop additional case studies and related unit operations
- Continue building unit and property model library

Explore the Library and Case Studies

- Documentation: https://prommis.readthedocs.io/en/latest/
- Tutorials for case studies: https://github.com/prommis/prommis/tree/main/docs/tutorials

Acknowledgements

This effort was funded by the U.S. Department of Energy's Process Optimization and Modeling for Minerals Sustainability (PrOMMiS) Initiative, supported by the Office of Fossil Energy and Carbon Management's Office of Resource Sustainability. For more information, please reach out to Thomas Tarka, PrOMMiS Technical Director (Thomas.Tarka@netl.doe.gov)

Contact: Alejandro Garciadiego, alejandro.garciadiego@netl.doe.gov