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PROMMIS

Process Optimization and Modeling for Minerals Sustainability

PrOMMiS: Applying Novel Modeling Methods to Accelerate CMM RD^3

Thomas J. Tarka, P.E.

CMM R&D Lead

METALLIC Director

PrOMMiS Technical Director

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What is PrOMMiS?

PROMMIS
Process Optimization and Modeling for Minerals Sustainability

Short Answer: Application of the IDAES Integrated Platform to CMM

Platform to Enable Innovation, Inform DOE Research, & Accelerate Deployment

- Process Modeling Software
  - Process performance modeling
  - Perform TEA and enable LCA
- Optimization Package
  - Process Optimization
  - Multi-criteria Optimization
- Support Commercialization

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PrOMMiS: Process Optimization & Modeling for Minerals Sustainability

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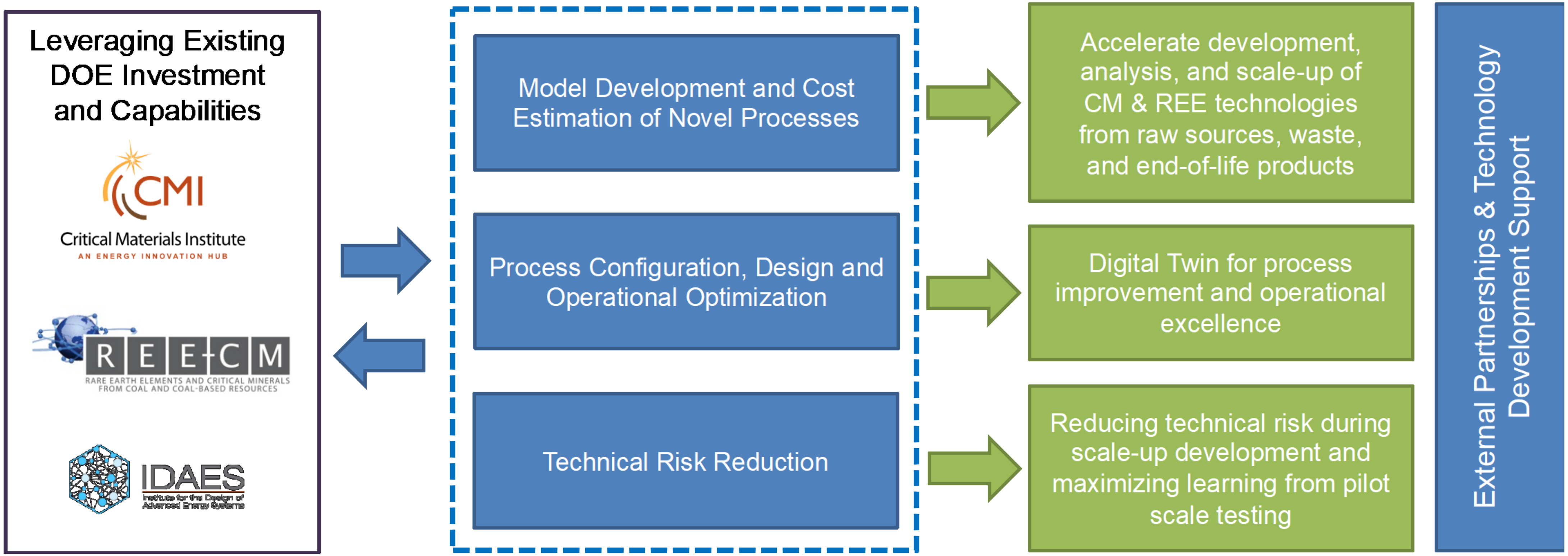
Process Optimization and Modeling
for Minerals Sustainability

Objective: **Accelerate scale-up** and **deployment** of innovative CM & REE processes and establish the toolkit to compress future RD3 timelines by **leveraging IDAES**, **CCSI** and a **decade** of **DOE CM & REE investment**.



Leveraging Existing DOE Investment and Capabilities

Model Development and Cost Estimation of Novel Processes

Process Configuration, Design and Operational Optimization

Technical Risk Reduction

Accelerate development, analysis, and scale-up of CM & REE technologies from raw sources, waste, and end-of-life products

Digital Twin for process improvement and operational excellence

Reducing technical risk during scale-up development and maximizing learning from pilot scale testing

External Partnerships & Technology Development Support

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Presentation Outline

- The Challenge & Context
- PrOMMiS Capabilities & Project Status
- Framework Development
    - Unit and Property Model Libraries
    - Costing Model Libraries
- Case Study: University of Kentucky Coal Waste Pilot Process
- Case Study: Li/Co Recycling Membrane System
    - Nanofiltration / Diafiltration Membrane Cascade Systems
    - Conceptual Design: Flowsheet Screening with Superstructures
    - Technical Risk Reduction: Robust Optimization
    - Technical Risk Reduction: Model-based Design of Experiments

What are Critical Minerals & Materials (CMM)?

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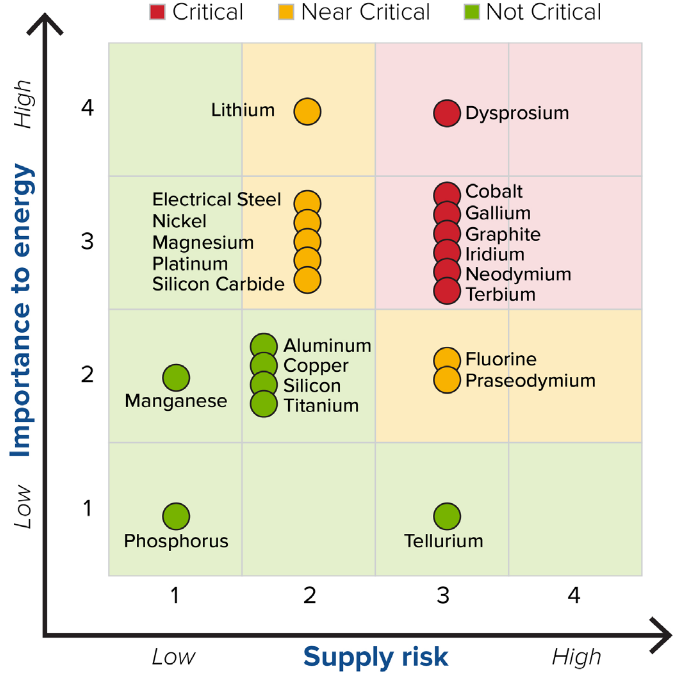
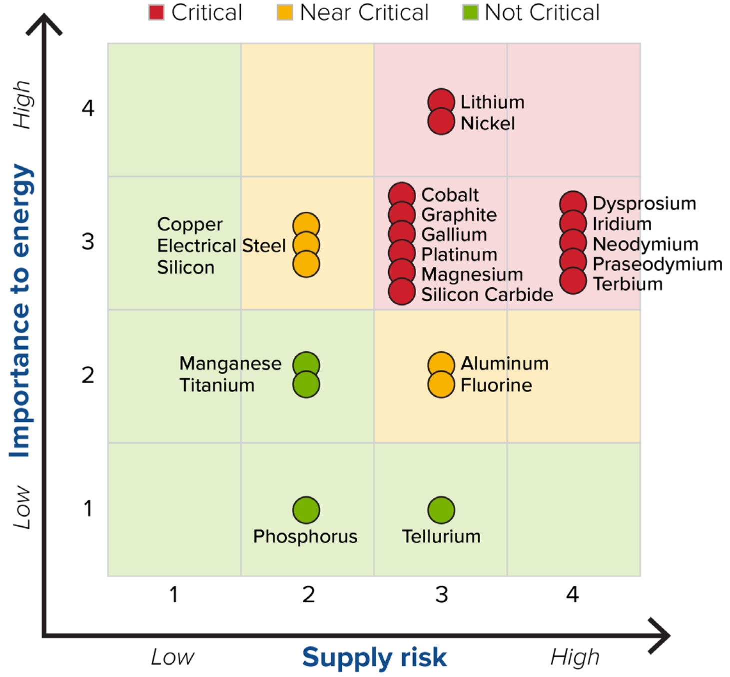
Materials have high risk for supply disruption and serve an essential function in one or more energy technologies

SHORT TERM 2020-2025



MEDIUM TERM 2025-2035



https://www.energy.gov/cmm/what-are-critical-materials-and-critical-minerals

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Challenge:
Clean Energy Technologies Drive Demand Growth

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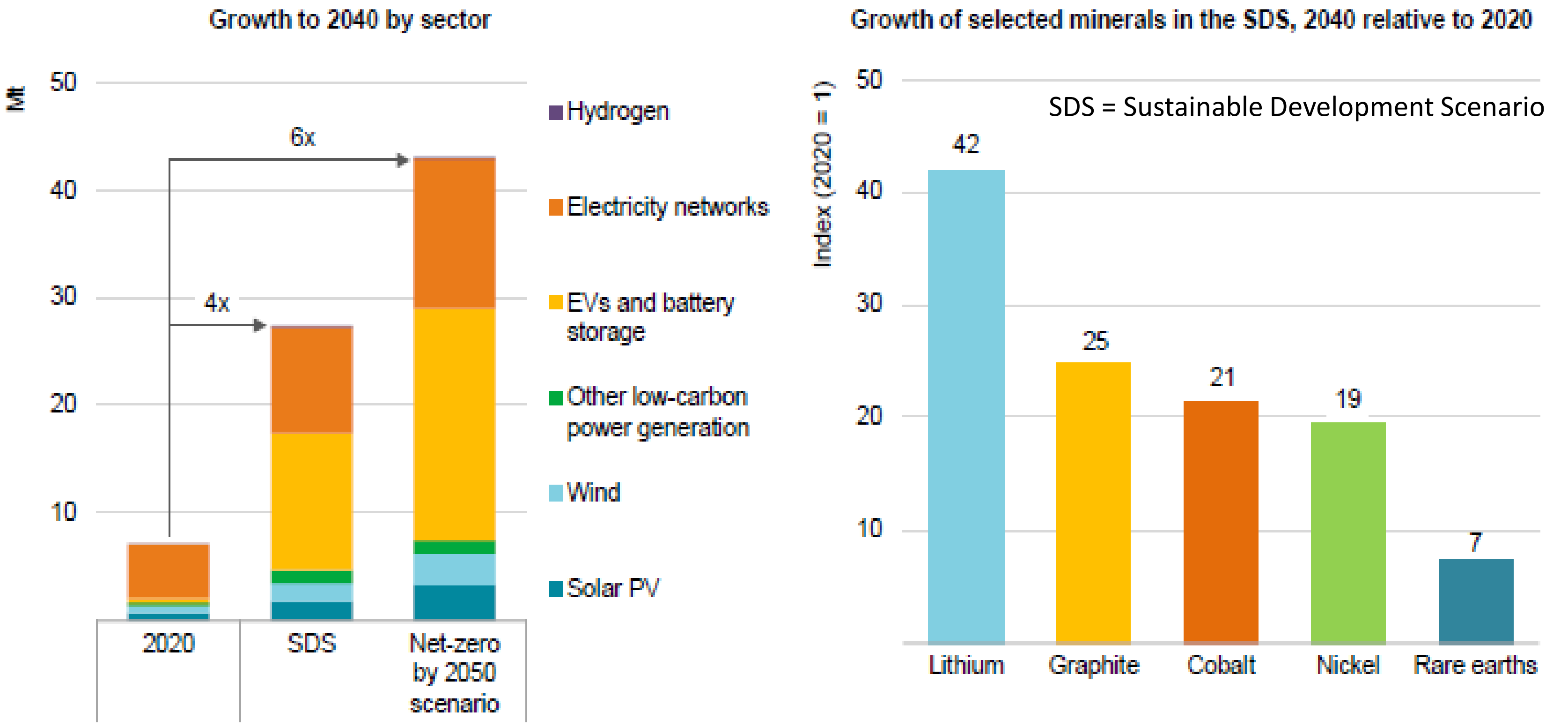
Mineral demand for clean energy technologies by scenario



SDS = Sustainable Development Scenario

IEA. All rights reserved.

Notes: Mt = million tonnes. Includes all minerals in the scope of this report, but does not include steel and aluminium. See Annex for a full list of minerals.

Source: https://www.iea.org/reports/the-role-of-critical-minerals-in-clean-energy-transitions/executive-summary

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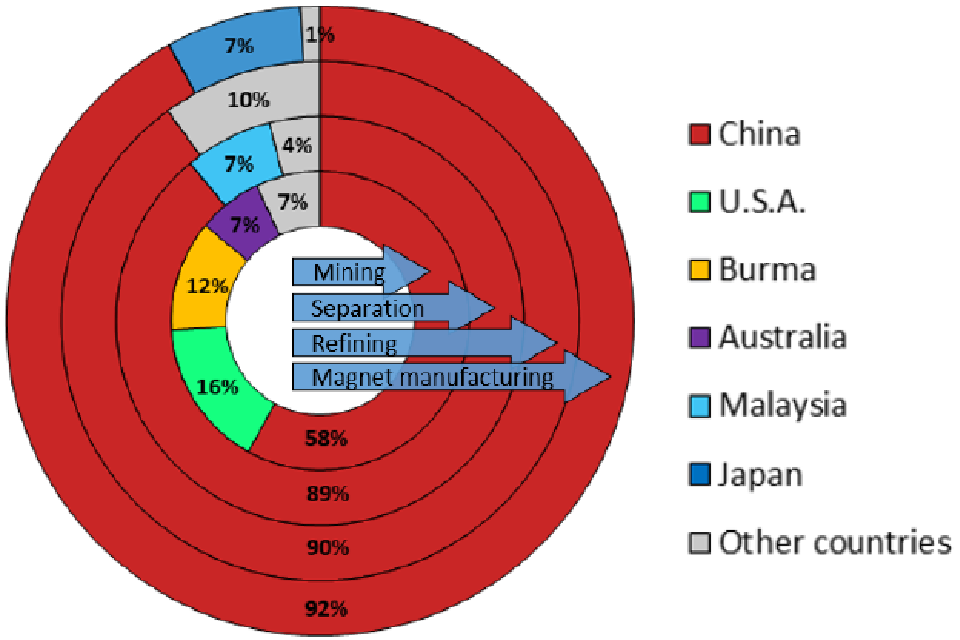
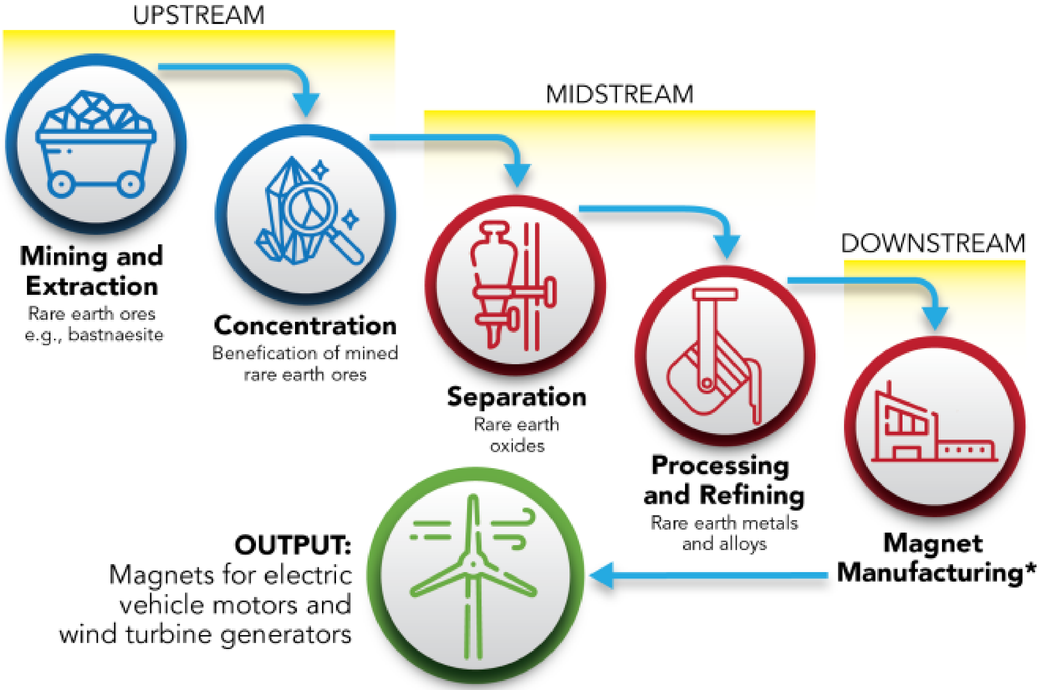
Challenge:
Large Gaps in Domestic Supply Chain - REE

- Up- and Mid-Stream capabilities **are geographically concentrated** in 1-3 countries
- **Lack of midstream capabilities are a gap** that limits
- growth of upstream supply & downstream manufacturing



Geographic concentration of supply chain stages for sintered NdFeB magnets



Red indicates no U.S. commercial capacity

* indicates sintered NdFeB (*neodymium iron boron*) magnets

https://www.energy.gov/policy/securing-americas-clean-energy-supply-chain

Challenge:
Supply Chain Vulnerability – Li-ion Batteries

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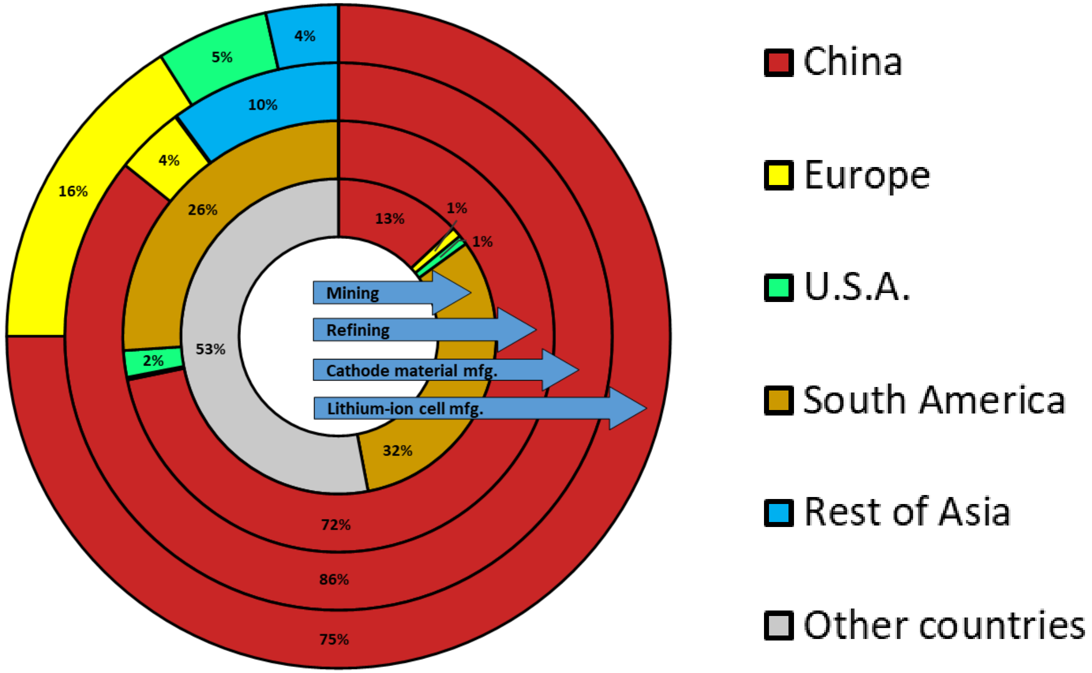

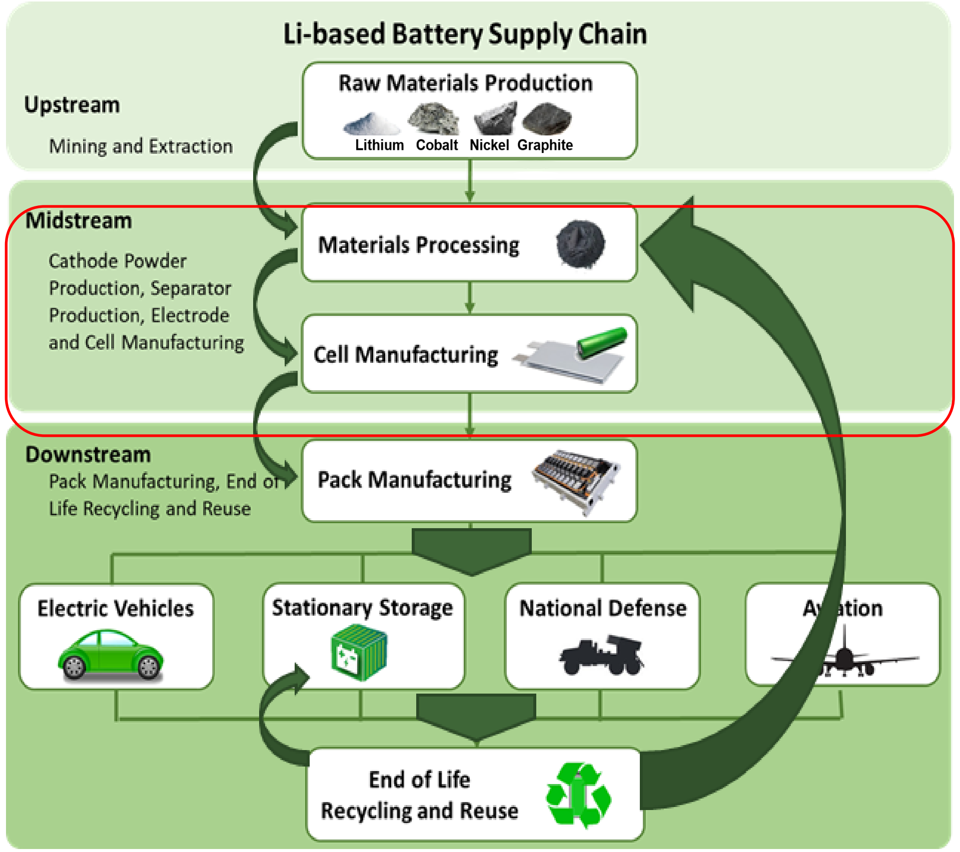

Li-based Battery Supply Chain

Upstream
Mining and Extraction

Raw Materials Production
Lithium Cobalt Nickel Graphite

Midstream
Cathode Powder Production, Separator Production, Electrode and Cell Manufacturing

Materials Processing

Cell Manufacturing

Downstream
Pack Manufacturing, End of Life Recycling and Reuse

Pack Manufacturing

Electric Vehicles

Stationary Storage

National Defense

Aviation

End of Life Recycling and Reuse

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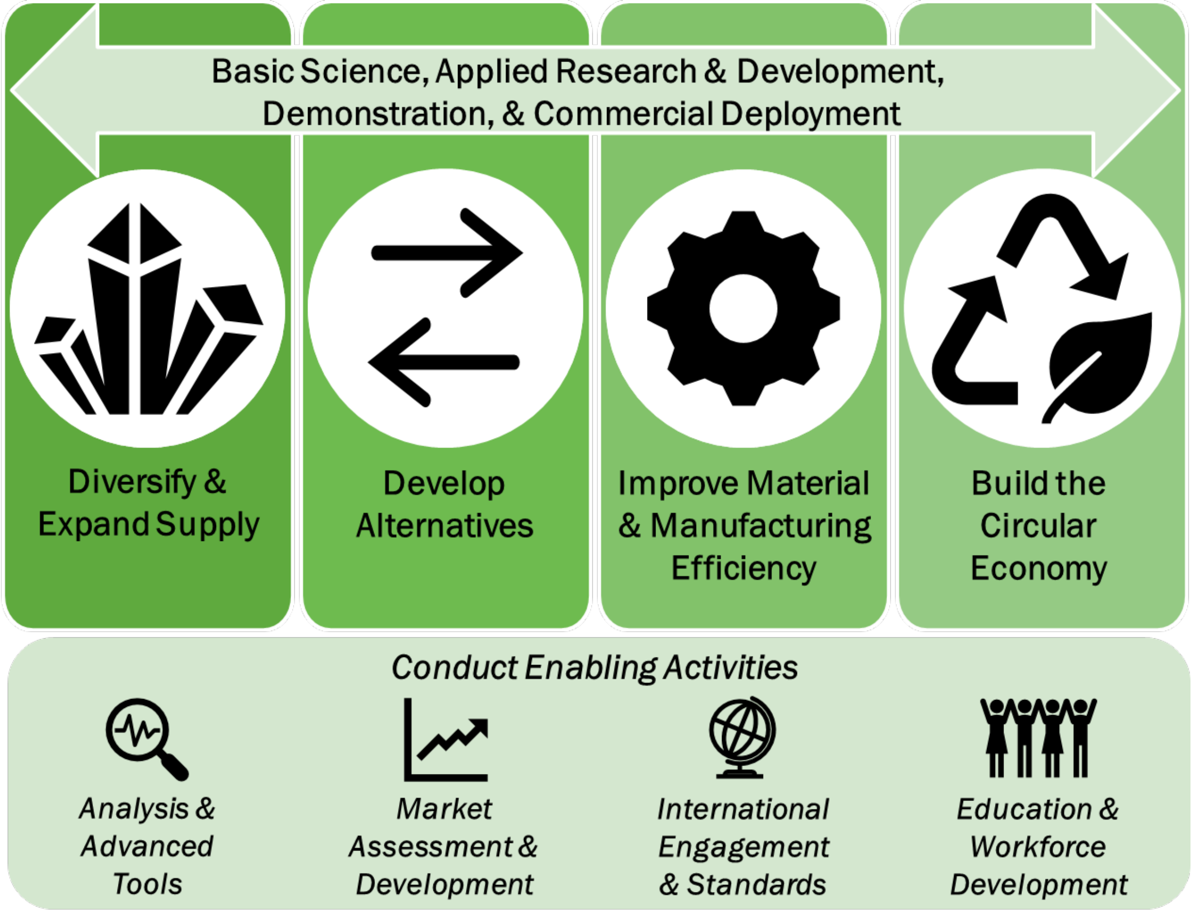
DOE CMM Vision & Strategy

Vision:

- **Build** reliable, resilient, affordable, diverse, sustainable, and secure **domestic critical mineral and materials supply chains**.
- Promote safe, sustainable, economic, and environmentally just solutions to meet current and future needs.
- Support the clean energy transition and decarbonization of the energy, manufacturing, and transportation economies.



Basic Science, Applied Research & Development, Demonstration, & Commercial Deployment

Diversify & Expand Supply

Develop Alternatives

Improve Material & Manufacturing Efficiency

Build the Circular Economy

Conduct Enabling Activities

Analysis & Advanced Tools

Market Assessment & Development

International Engagement & Standards

Education & Workforce Development

https://www.energy.gov/critical-minerals-materials

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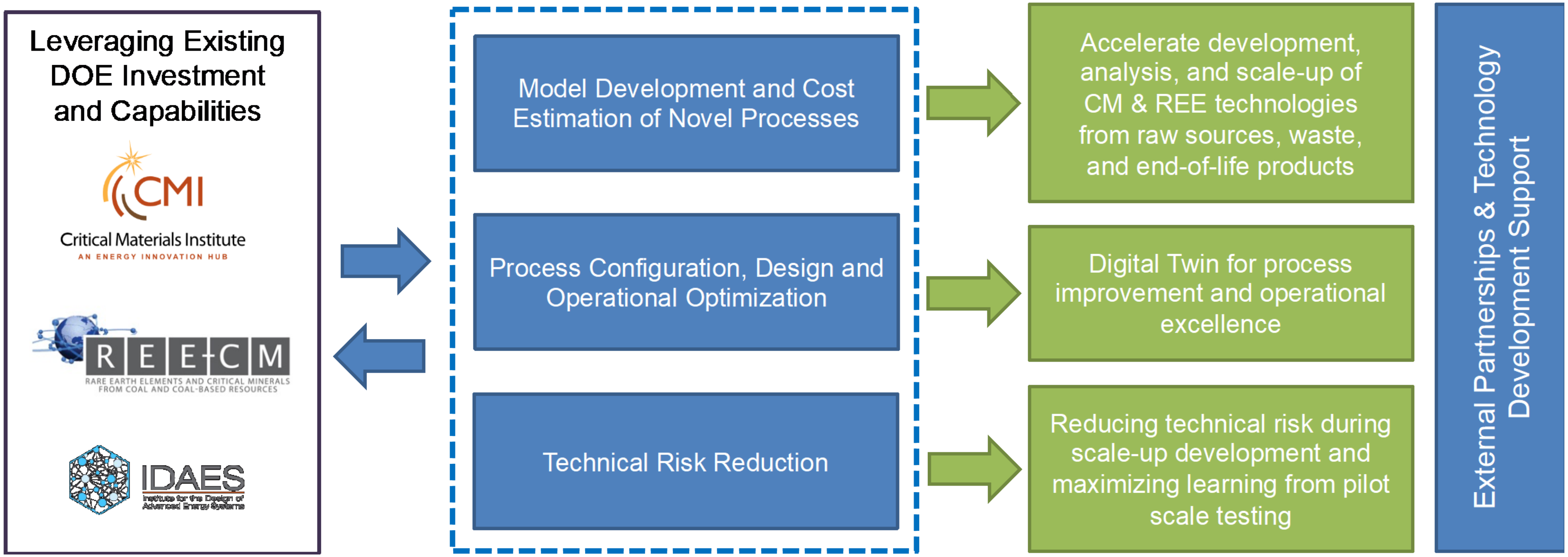

Leveraging Existing DOE Investment and Capabilities

CMI
Critical Materials Institute
AN ENERGY INNOVATION HUB

REECM
RARE EARTH ELEMENTS AND CRITICAL MINERALS FROM COAL AND COAL-BASED RESOURCES

IDAES
Institute for the Design of Advanced Energy Systems

Model Development and Cost Estimation of Novel Processes

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Guiding Principles & Approach

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- **Urgency: Rapidly Establish Capability to Get Early Wins**
  - Learn by Doing – Apply to Existing Projects (recently completed or underway)
  - Don’t Reinvent the Wheel – Leverage Existing Models & Partnerships
  - Partner with Active Developers
- **Create A Long-Term Capability!**
  - Critical Materials will change over time
  - Flexible, Foundational Platform
  - Early Stakeholder Involvement and Well-Regarded Leadership Board
- **Maximize Support & Integration with CM and other DOE R&D Portfolios**
  - CM Related: CMC, CMI, BIL Activities, FECM Awarded Projects
  - Adjacent: Water-related (NAWI, PARETO)
  - Inter-Agency: DoD Projects, USGS

Guiding Principles & Approach

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Process Optimization and Modeling for Minerals Sustainability

The End Goal is…

Guiding Principles & Approach

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The End Goal is…

- **Compress Developmental Timeframes**
- **Innovation Ecosystem**
- **Support DOE Investments & Initiatives**
  - Technology Maturation
  - Unlocking Different Feedstocks
  - Waste Minimization

PrOMMiS High-level Execution & Capabilities

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Year 1:

- ✓ Build capabilities for design, optimization, and scale-up specific to CM & REE processes, enabling technical risk reduction
- ✓ Evaluate landscape of emerging CM & REE production pathways & solicit input on critical industry needs/gaps
- ✓ Leverage existing multiscale modeling and optimization capabilities from CCSI & IDAES
- ✓ Ensure applicability to a range of feedstocks (e.g., mining, waste streams, and recycling end-of-life-products)

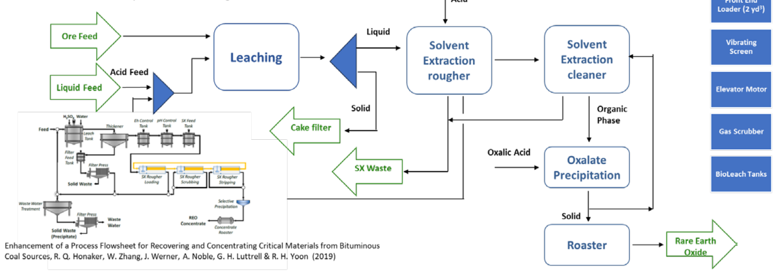
Year 2:

- Expand unit model and costing libraries to include other established technologies to use in different case studies
- PrOMMiS will deploy computational capabilities for advanced process design, scale-up, and analysis of the CMM & REE process: Techno-economic analysis, optimization, control, uncertainty quantification, and technical risk reduction through robust optimization approaches.
- PrOMMiS will work directly with initial technology partners to collaboratively support scale-up and integration of novel technologies.

Major Accomplishments

Created Unit Operation & Property Model library (v1.0) which includes cost data. Successfully developed process flowsheet model for a University of Kentucky REE recovery pilot plant.

Flowsheet of the pilot-scale leaching and solvent extraction circuits

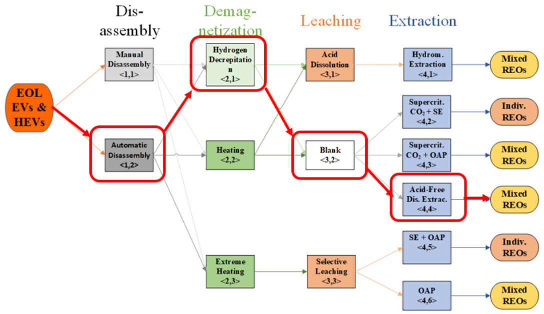


Enhancement of a Process Flowsheet for Recovering and Concentrating Critical Materials from Bituminous Coal Sources, R. Q. Honaker, W. Zhang, J. Werner, A. Noble, G. H. Luttrell & R. H. Yoon (2019)

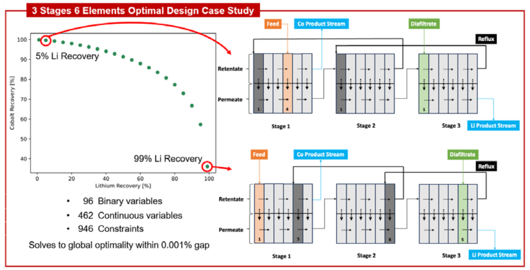
PrOMMiS Costing Library:

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*		

End-of-life magnet recycling model capable of selecting the optimal recovery pathway and most cost-effective technology for different feedstocks.



Demonstrate effective optimization of candidate flowsheet configurations (conceptual design superstructure) for the selected CM & REE case studies.



- 96 Binary variables
- 462 Continuous variables
- 946 Constraints

Solves to global optimality within 0.001% gap

Established collaborations with key partners.

Virginia Tech
CMI Critical Materials Innovation Hub
Wayne State University
University of Kentucky
National Energy Technology Laboratory

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Project Overview - Collaborations

The team has established close **collaborations** with several universities:

	WAYNE STATE UNIVERSITY	University of Kentucky	VIRGINIA TECH	NATIONAL ENERGY TECHNOLOGY LABORATORY	CMI Critical Materials Innovation Hub
Research PI	Tim Dittrich	Rick Honaker, Joshua Werner	Aaron Noble	Nicholas Siefert, Alison Fritz, Ward Burgess, Jon Yang, Bret Howard	Ikenna Nlebedim, Parans Paranthaman, Jason Pries
Research Focus	Sorbent/IX modeling & validation	REE recovery and pilot plant support	Mining and Economics Analysis	Experimental data and modeling support (precipitation, leaching, solvent extraction, etc.)	Acid Free Recycling of Magnets; Membrane solvent extraction

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Framework Development

- What is it?
  - Libraries of models for common unit operations.
  - Includes thermodynamic properties, unit operations and cost estimation.
  - Different levels of rigor to support analyses from conceptual design through to high-fidelity simulations.

- Why do we care?
  - Facilitates rapid assemble of process models from modular components.
  - Will support full optimal design workflow from process synthesis to process control.

A New Domain

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- Need new library of models for minerals processing
  - Need both current and future technologies

- Reviewed literature for REE recovery processes
  - Focus on unconventional resources
    - Coal Waste Products
    - Acid Mine Drainage
    - Brines and Produced Water
    - Phosphates and Gypsum
    - End-of-Life Recycling
      - Batteries
      - Magnets

- Learning by Doing
  - DOE wants immediate results

Unit and Property Model Libraries

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- Goal: Develop a comprehensive library of models for CM & REE processing operations.

- First Year:
  - Identify key unit operations and properties from candidate case studies.
  - Focus on unconventional feedstocks:

- Coal ash and waste
- Acid mine drainage
- Phosphates & gypsum
- Brines
- Battery recycling
- End-of-life magnets

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Core Model Development

- Models (contributed to GitHub)
  - Roaster (calcination)
  - Leaching
  - Solvent extraction
  - Solid liquid separation
  - Precipitation
  - Thickener
  - Crushing and Grinding
  - Evaporation

- Property Packages:
  - Case specific properties
  - Integration of PhreeqC / Mintec

- WaterTAP Models
  - RO
  - Ion exchange
  - Nanofiltration
  - Electrodialysis
  - Membrane Distillation

Process Optimization and Modeling for Minerals Sustainability

Core Model Development

- Case Study Driven
  - External Stakeholders
    - TBD
  - Internal (NETL) Stakeholders
    - Dry Fork Fly Ash (Powder River basin, WY) – REEs from coal byproducts
      - Similar to University of Kentucky process
      - Complex leaching process, but lots of data
    - ABLE Lab – lithium from produced waters
      - Lab scale testing apparatus
      - Includes RO, NF and IX technologies
      - External stakeholders to bring Direct Lithium Extraction technologies for testing
    - Carbon products
      - Complex process involving both pyro- and hydro-metallurgy
      - Stakeholder concerned about releasing outside NETL

REE Costing Framework

https://github.com/prommis/prommis/tree/main/src/prommis/uky/costing

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Current Framework Capabilities

- Capital & Operating Costs
- Annualized Costs & Revenue
- Membrane Capital & Operating Costs via WaterTAP
- Custom Costing Models
- Objectives for TEA – Net Present Value and Cost of Recovery

Ongoing PrOMMiS Integration

- Bottom-Up Costing for Hydrogen Decrepitation (WVU)
- Economy of Numbers (WVU)
- Costing for Li/Co diafiltration (ND)
- Superstructure UI integration (LBNL)
- Tutorial development (NETL)

Planned Capabilities

- For March 2025:
  - Operation Labor Estimation
  - Tax & Environmental Incentives
  - Byproduct Recovery Value
- For EY25:
  - TEA of at least two processes
  - Cost & Price UQ to supplement task 2.4 tools

PrOMMiS Costing Library

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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 Furnace*
- Diafiltration (Li/Co Separation)*
- Nanofiltration**
- Reverse Osmosis**
- Ion Exchange**
- Membranes**

* Bottom-up Cost Models (users can write their own custom models)

** WaterTap library

PrOMMiS Costing Library:

$$SC_i = RC_i * \left(\frac{RP_i}{SP_i}\right)^{Exp_i}$$

- SC – scaled cost
- RC – reference cost
- SP – scaled parameter
- RP – reference parameter
- Exp – exponential factor
- i – ith unit cost account

References:

[1] 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.

[2] 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.

[3] 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.

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

[5] 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

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

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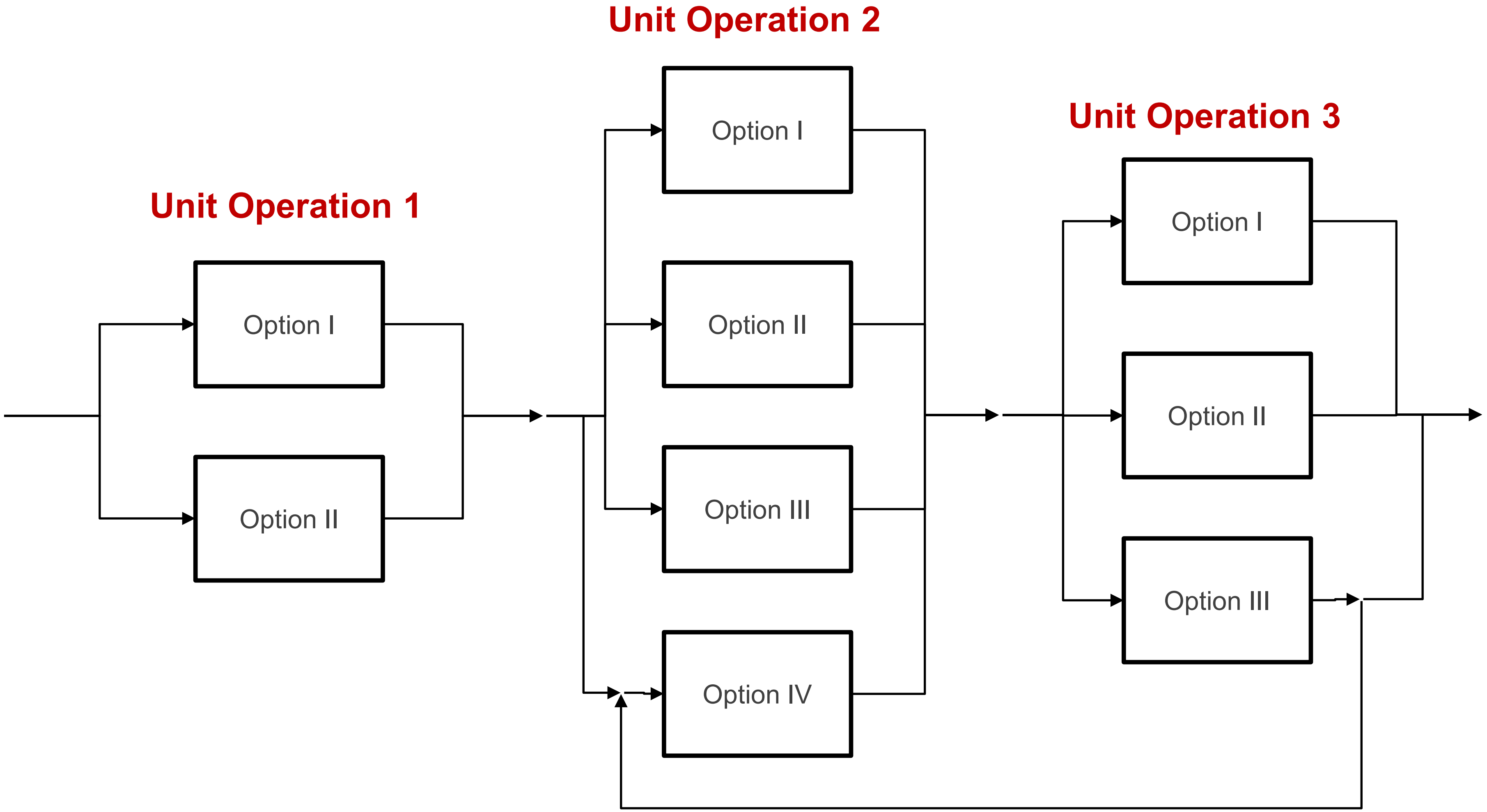
Case Study:
University of Kentucky Coal Waste Pilot Process

UKy Coal Waste Pilot Process

- What is it?
  - Integrated flowsheet for extraction and separation of REEs from West Kentucky No. 13 coal waste.
  - Integrates unit and costing models into single model of leaching and separation train.
- Why do we care?
  - Proof-of-concept example of integrating model libraries to simulate real world process.
  - FECM funded project with easily available data.
  - Capable of optimizing process for cost and/or chemical consumption.

Superstructure Optimization for Conceptual Design



Unit Operation 1

Option I
Option II

Unit Operation 2

Option I
Option II
Option III
Option IV

Unit Operation 3

Option I
Option II
Option III

Optimal Design and Configuration

Rapid screening

9 disjunctions
18 binary variables
→ 315 choices

+ PYOMO GDP

Superstructure Optimization for Conceptual Design

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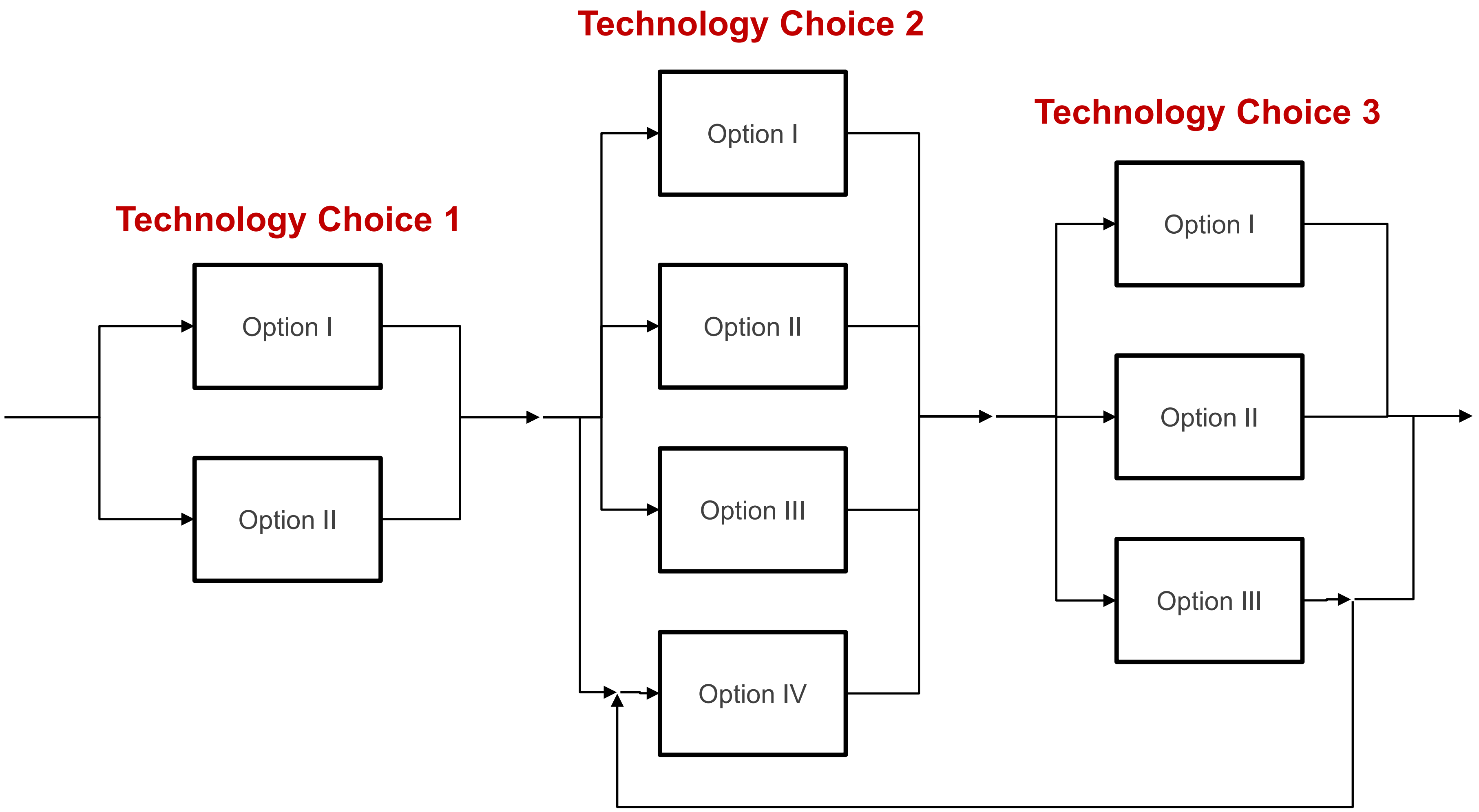


Technology Choice 1

Option I
Option II

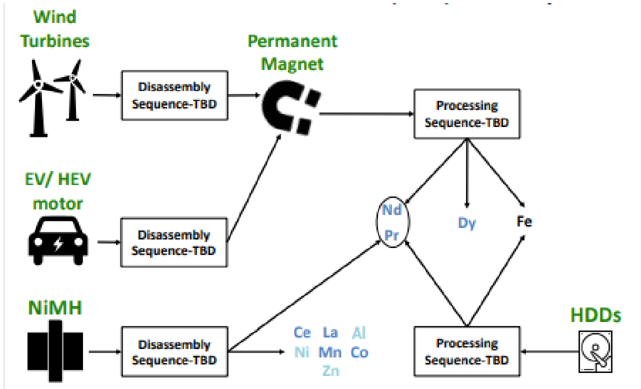
Technology Choice 2

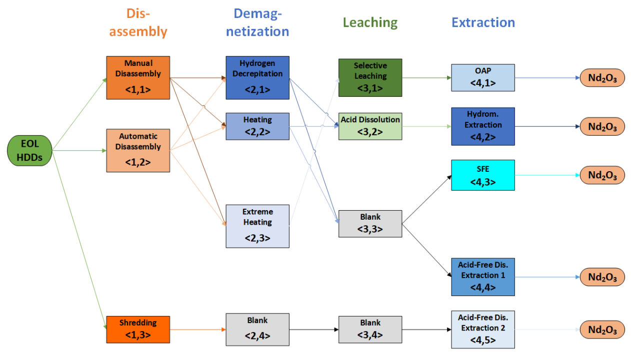
Option I
Option II
Option III
Option IV

Technology Choice 3

Option I
Option II
Option III

Superstructure optimization and technology selection for end-of-life-products (Prof. Torres)





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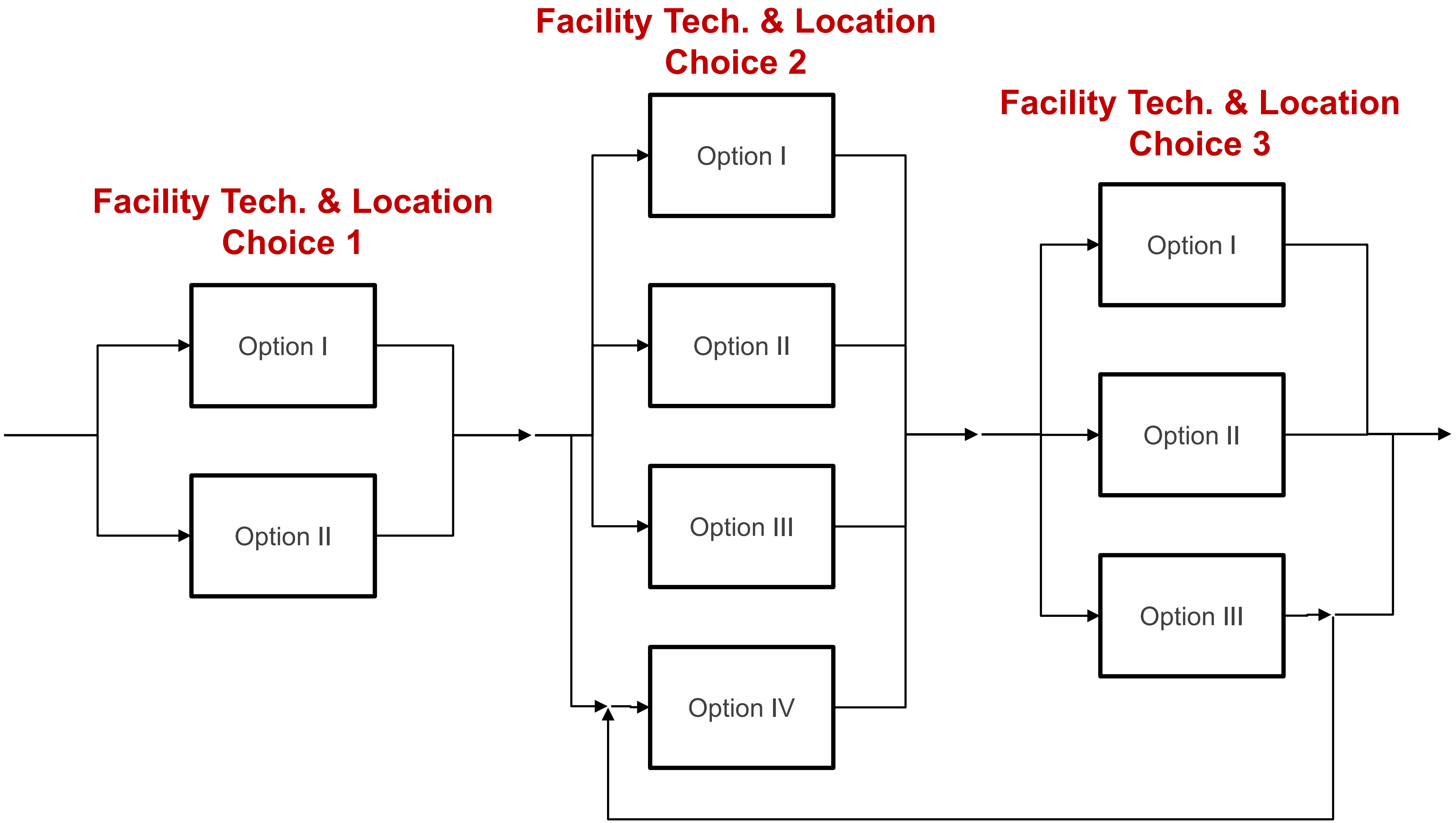

IDAES Conceptual Design Framework

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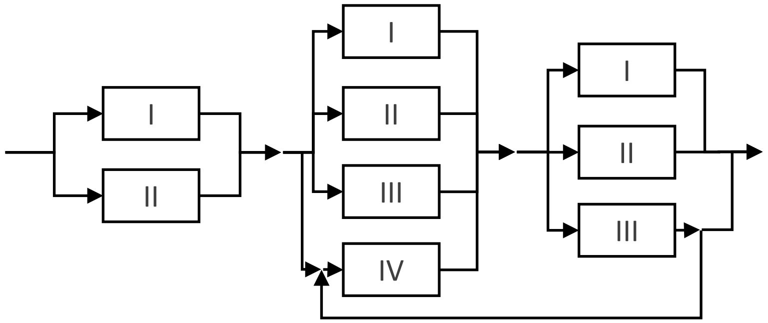
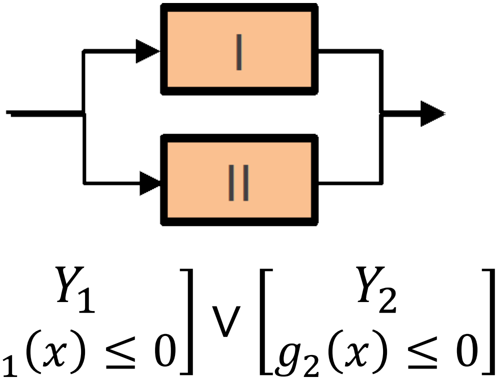
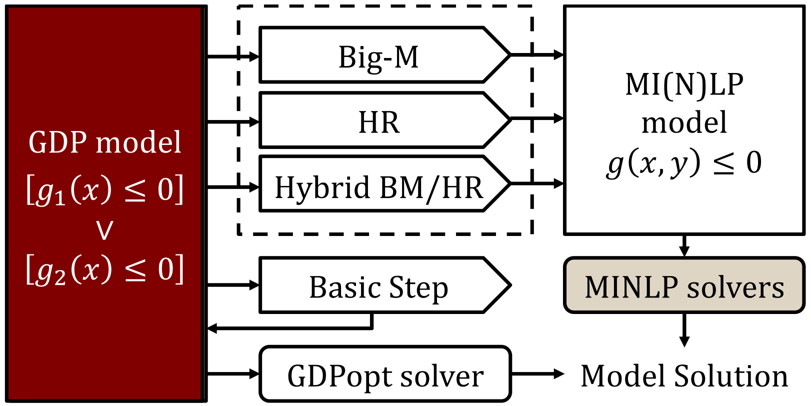


PrOMMiS Modeling Framework



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

Pyomo.GDP Disjunctive Modeling



GDP model
$[g_1(x) \leq 0]$
$\vee$
$[g_2(x) \leq 0]$

Big-M
HR
Hybrid BM/HR
Basic Step
GDPopt solver

MI(N)LP model
$g(x, y) \leq 0$

MINLP solvers

Model Solution

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

IDAES
Institute for the Design of Advanced Energy Systems

PYOMO GDP

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Case Study:
End of Life Product Recycling

Case Study – End of Life Product Recycling

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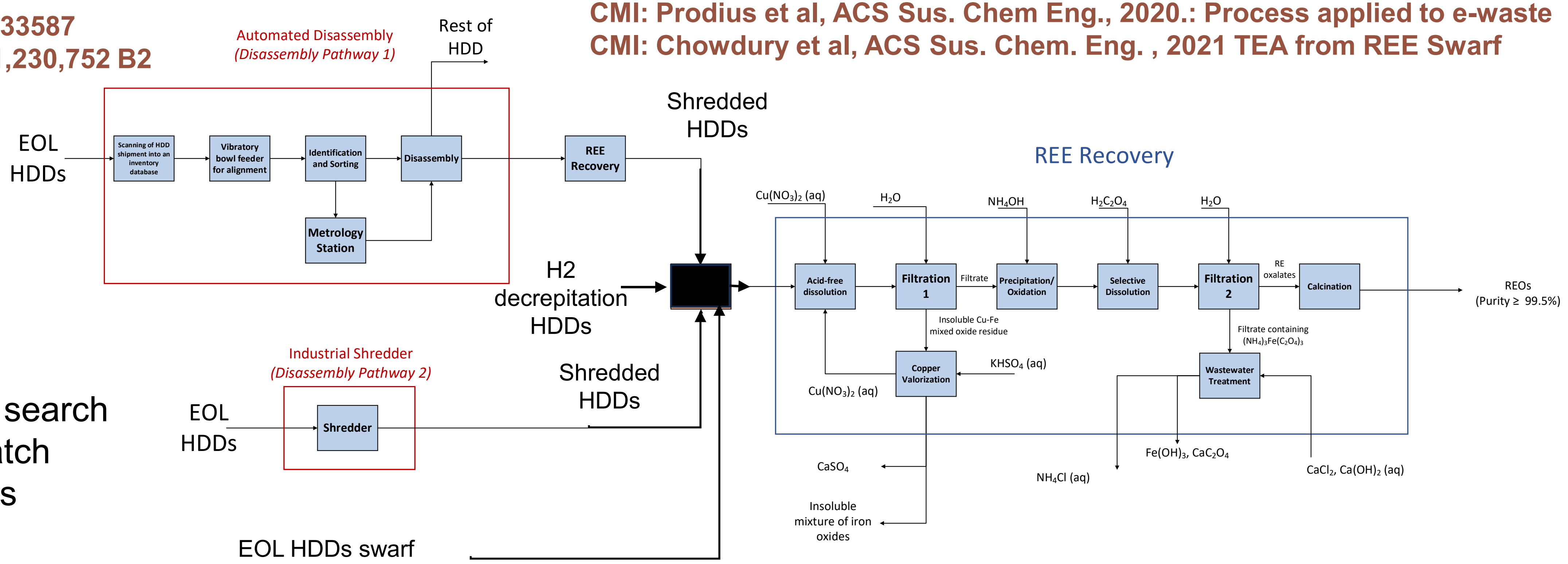
Process Optimization and Modeling for Minerals Sustainability

- Data: Literature, Oak Ridge National Labs, Critical Minerals Innovation Hub
- Example for HDDs:

ORNL- Pub133587
Patent US 11,230,752 B2

Iowa U: Patent US 10,648,063 B2 Dissolution and separation of rare earth metals
CMI: Prodius et al, ACS Sus. Chem Eng., 2020.: Process applied to e-waste
CMI: Chowdury et al, ACS Sus. Chem. Eng. , 2021 TEA from REE Swarf



- Expand literature search
- Mix & Match processes

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2. Literature search: Processing Pathways

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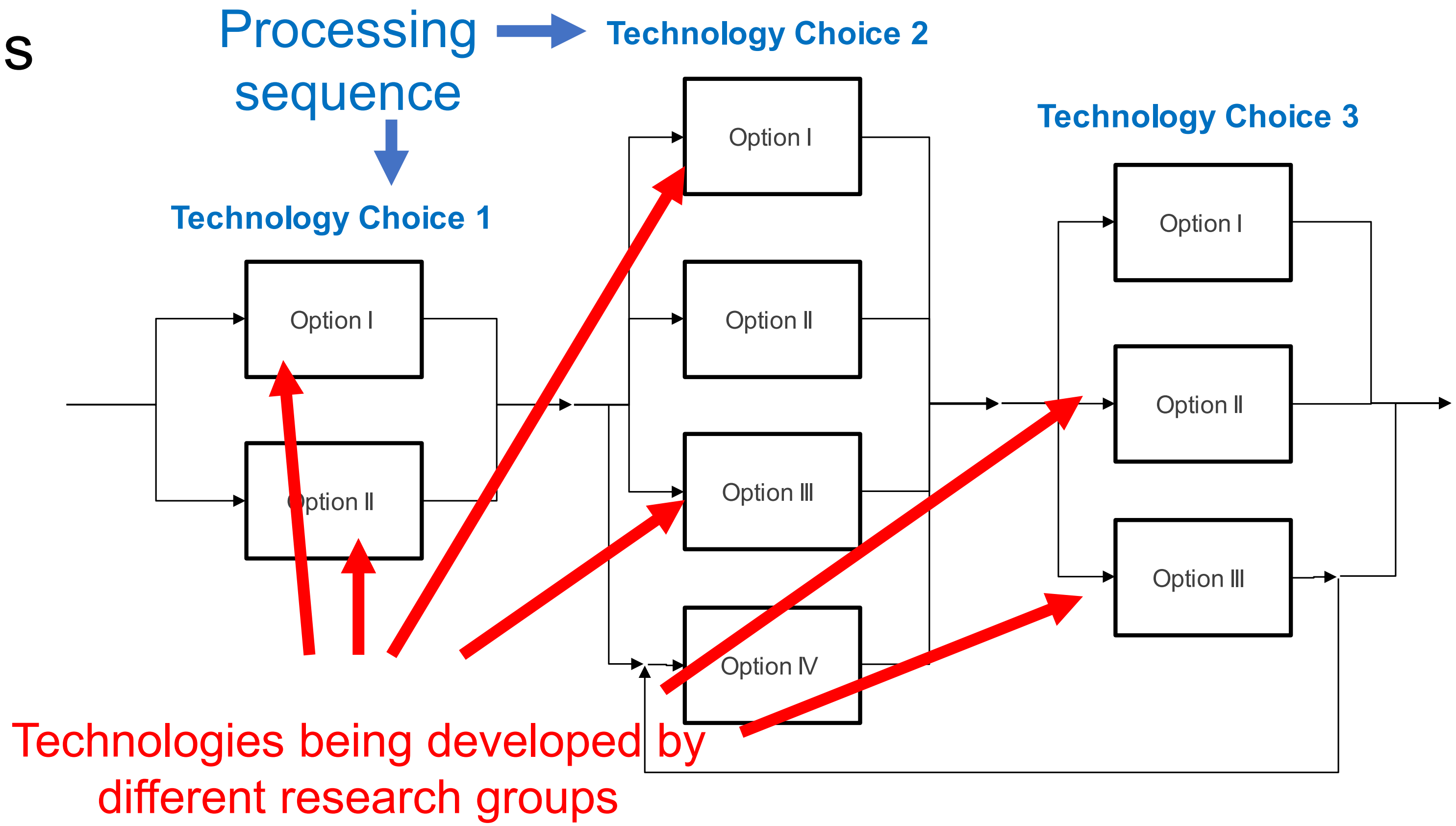
- Most (experimental) efforts focus on advancing part of the REE processing
- How to combine efforts from different groups to find the best processing pathway?

=> Screening via superstructure optimization for conceptual



(Figure: courtesy Prof. Laird)

3. EoL Superstructure

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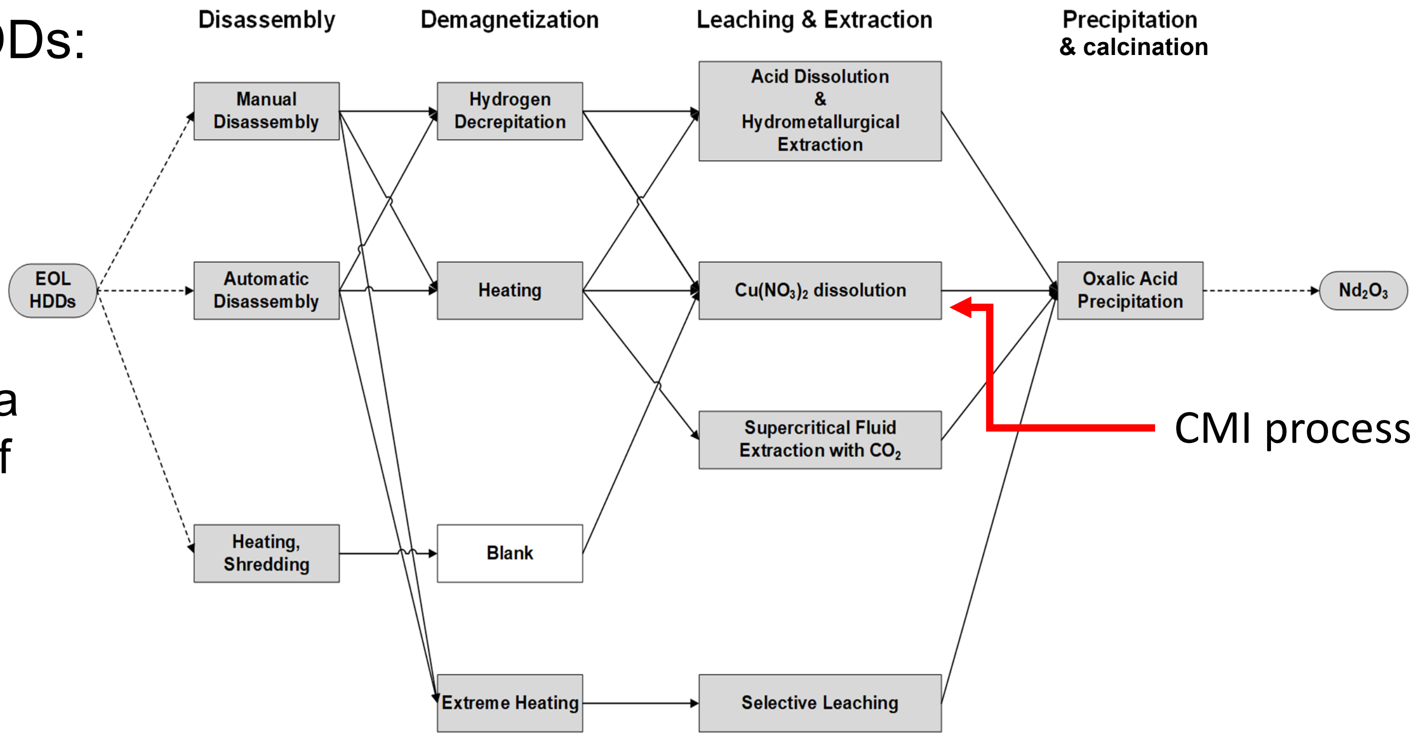
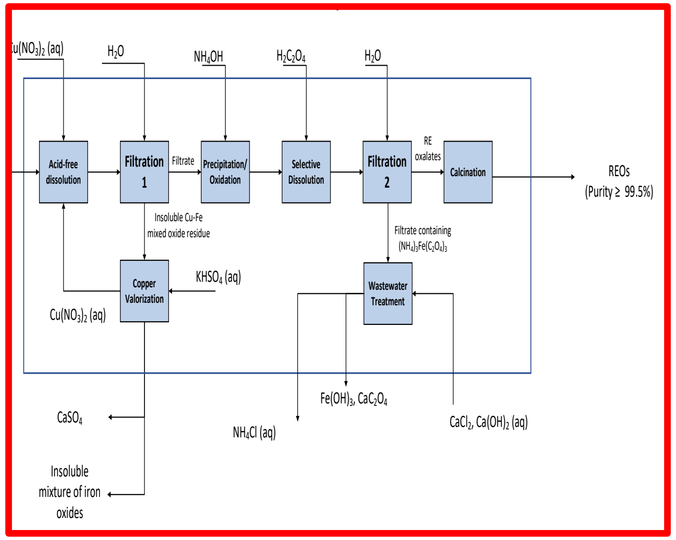
- Organize existing data in processing stages, identify competitive technology options at each stage
- Identify new connections
- Example for HDDs:
  - Each block is a flowsheet itself





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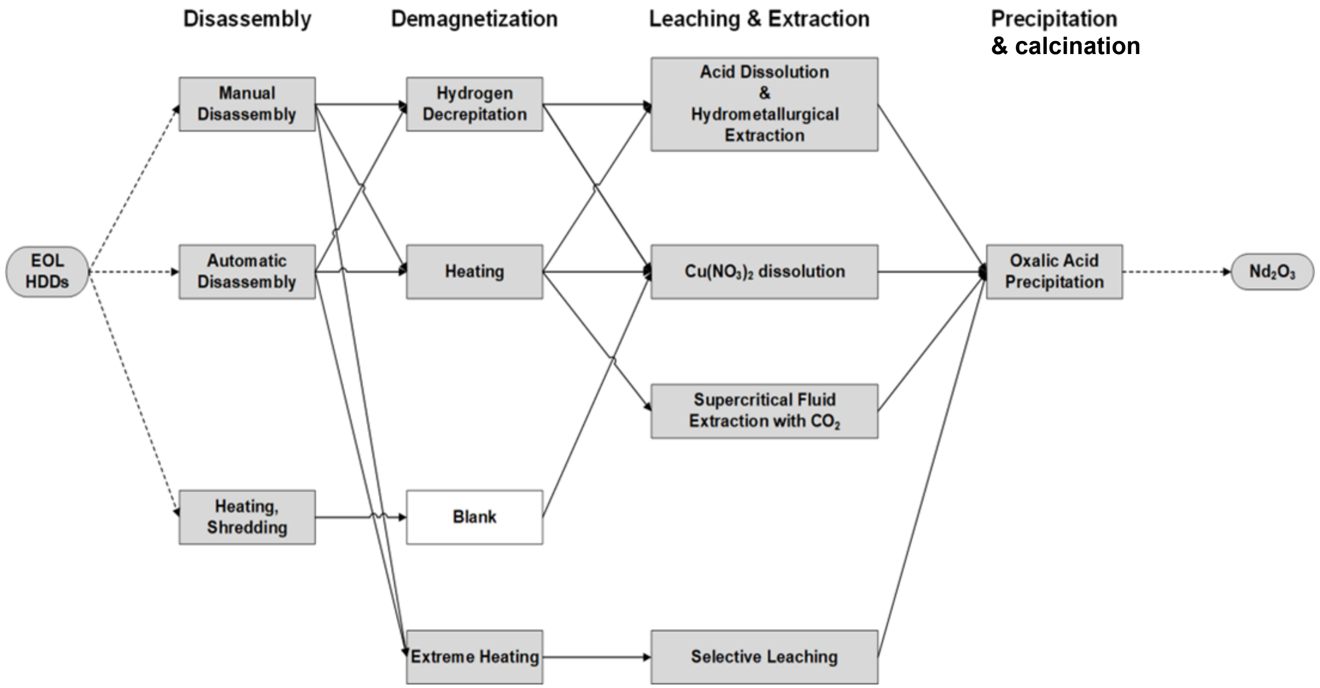
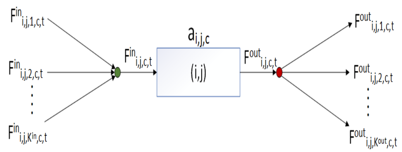
3. EoL Superstructure Modeling

- Superstructures are modeled as networks



- Technology options → nodes → binary variable *y =1* if in optimal pathway
- Arcs: flows of each species
- Inlet/ Outlet flows → MB from simulations



$$\sum_{k=1}^{K^{in}} F^{in}_{i,j,k,c,t} = F^{in}_{i,j,c,t} \qquad F^{out}_{i,j,c,t} = \sum_{k=1}^{K^{out}} F^{out}_{i,j,k,c,t}$$

$$F^{out}_{i,j,c,t} = a_{i,j,c} * F^{in}_{i,j,c,t}$$

- Allowed connections: logical constraints
- Objective function: NPV
    - CAPEX/OPEX: TEA in the literature or own: APEA, Bhattacharya's group
    - Framework: Seider et al.
- Currently updating withTask 2.2 developments

4. Process flowsheet development and costing- Example

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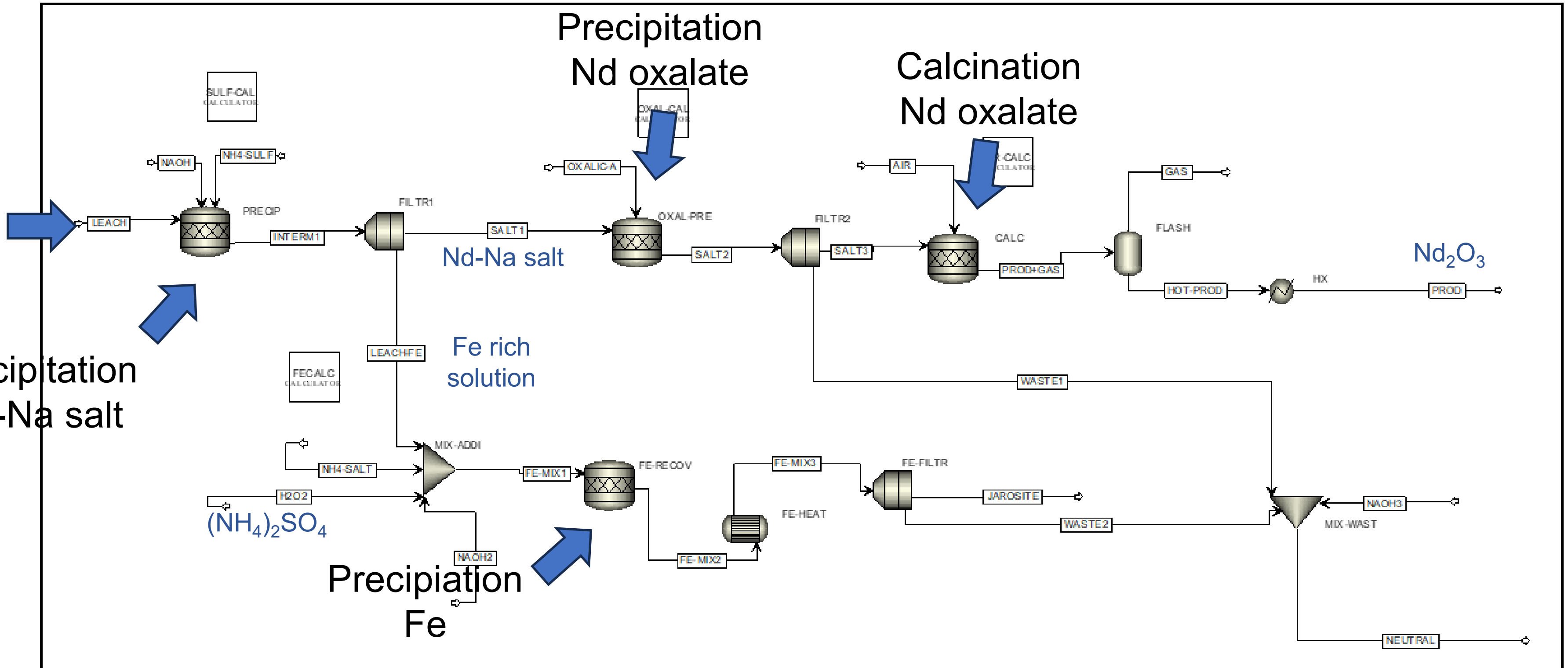


Leachate from previous (acid) dissolution

Precipitation Nd-Na salt

Nd-Na salt

Fe rich solution

$(NH_4)_2SO_4$

Precipitation Fe

Precipitation Nd oxalate

Calcination Nd oxalate

Nd_2O_3

Figure 5: Aspen simulation built for the hydrometallurgical process built using reaction yield data from [24].

- Initial simulations in Aspen Plus

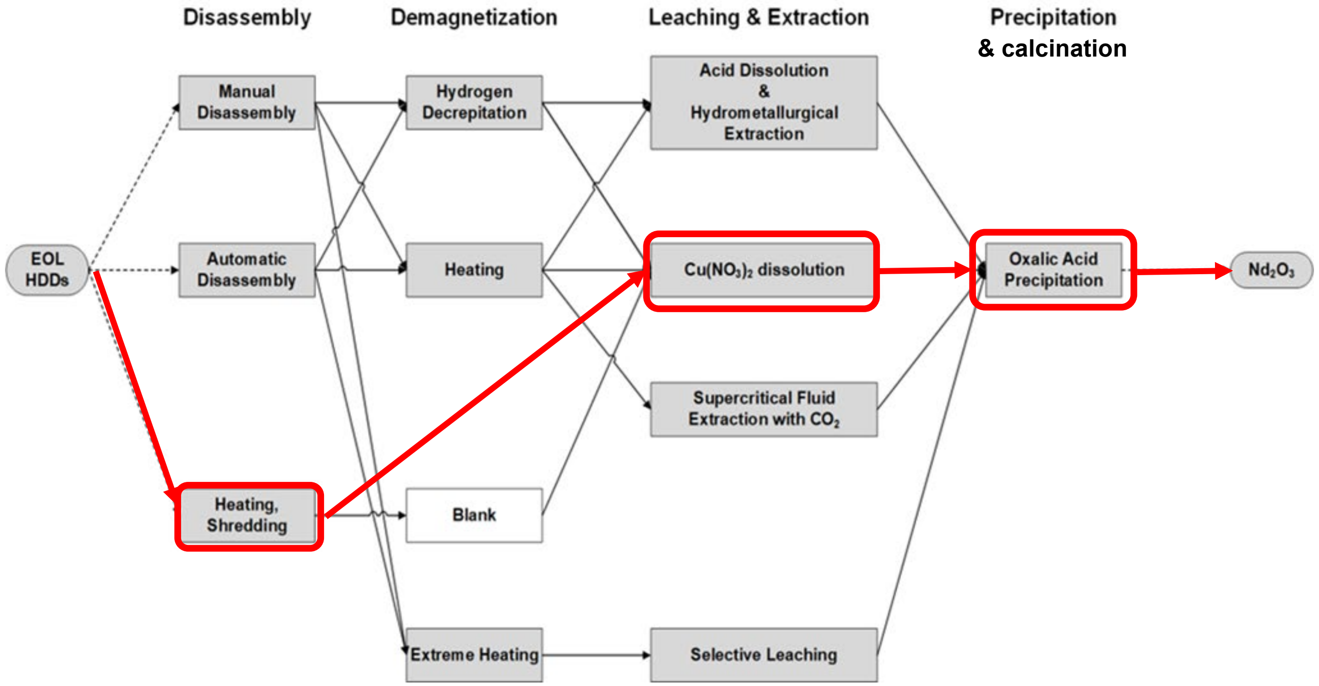
24. Lyman, J.W., Palmer, G.R.: Recycling of Rare Earths and Iron from NdFeB Magnet Scrap. High Temperature Materials and Processes. 11, 175–188 (1993). https://doi.org/10.1515/HTMP.1993.11.1-4.175

Process Optimization and Modeling for Minerals Sustainability

5. Case Study: Recovery REO from HDDs

(C. Laliwala, Al Torres, proceedings FOCAPD 2024)

- Optimal pathway



- Base case: plant recycles 60 % of all available EOL HDDs in the U.S. each year.
- Optimal pathway:
  - Shredding
  - Acid Free dissolution
- NPV negative

5. Case Study: Recovery REO from HDDs

(C. Laliwala, Al Torres, proceedings FOCAPD 2024)

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- Optimal solution for different collection rates (from future and past wastes) and REO prices;

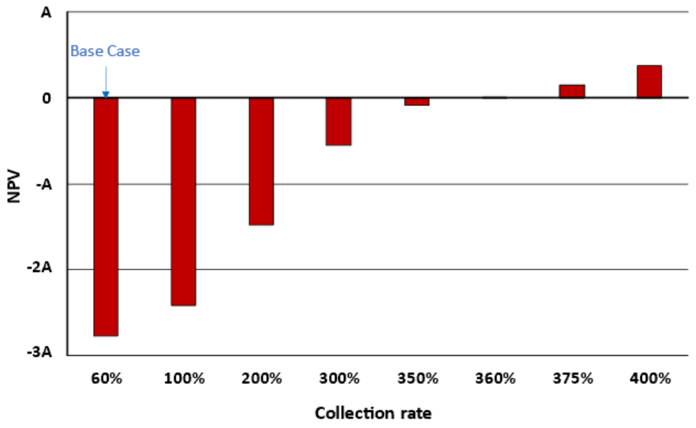


Figure 6: NPV for a varying collection rate. The base case is a collection rate of 60% and no recycling of EOL HDDs generated prior to plant production. The NPV break-even point was found to occur at ~360%. Numerical values are not reported to preserve confidentiality.

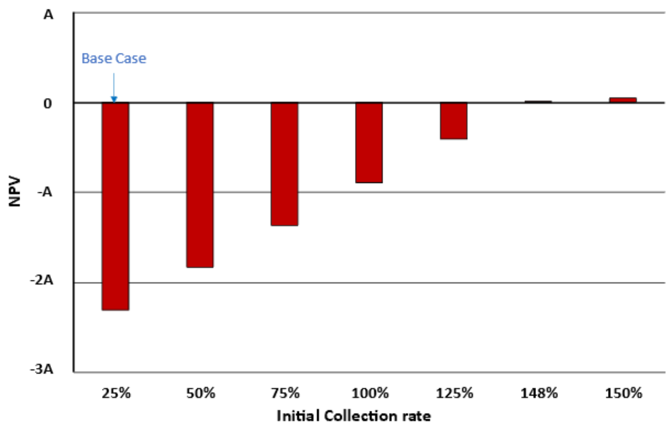


Figure 7: NPV for a varying initial collection rate. The base case has a collection rate of 60% and an initial collection rate of 25%. The NPV break-even point was found to occur at ~148%. Numerical values are not reported to preserve confidentiality.

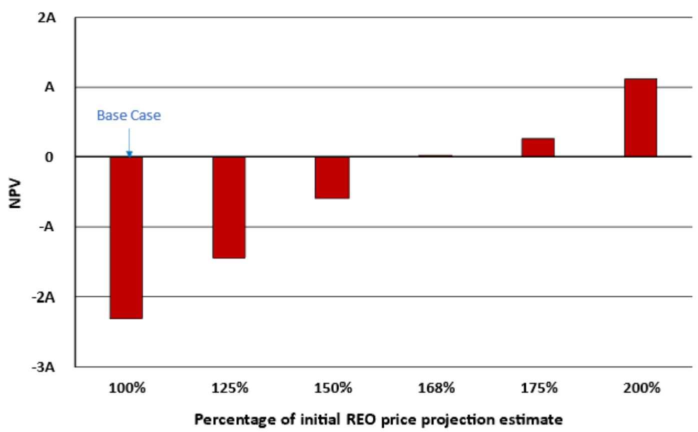


Figure 8: NPV for varying percentages of the initial REO price projection estimate. The NPV break-even point was found to occur at ~168%. Numerical values are not reported to preserve confidentiality.

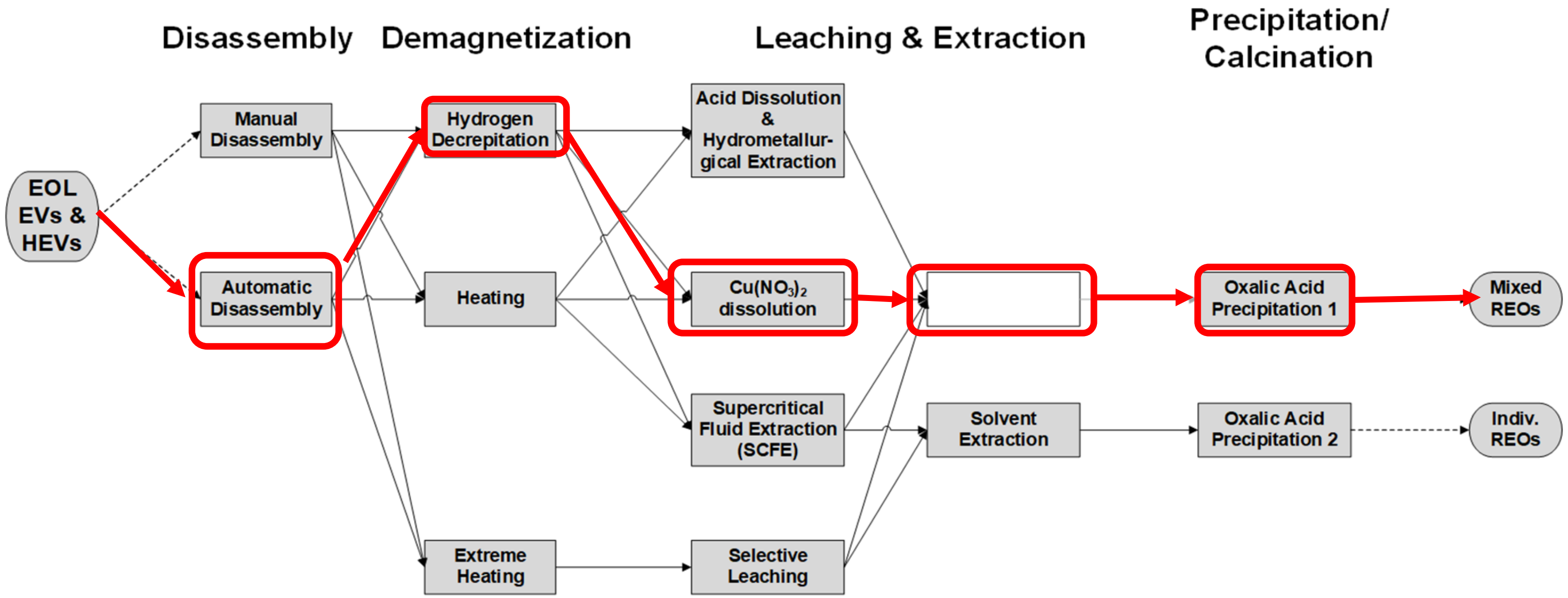
- ONL Shredding + CMI acid-free dissolution always optimal pathway

Process Optimization and Modeling
for Minerals Sustainability

5. Case Study: Recovery REO from EV/HEV

(C. Laliwala, Al Torres, proceedings ESCAPE/PSE 2024)

- Slightly different superstructure;



- Base case: plant recycles 10 % of all EOL EVs and HEVs in the U.S. each year.
- Optimal pathway:
  - Automatic disassembly
  - Hydrogen decrepitation
  - Acid Free dissolution
- NPV positive

5. Case Study: Recovery REO from EV/HEV

(C. Laliwala, Al Torres, proceedings ESCAPE/PSE 2024)

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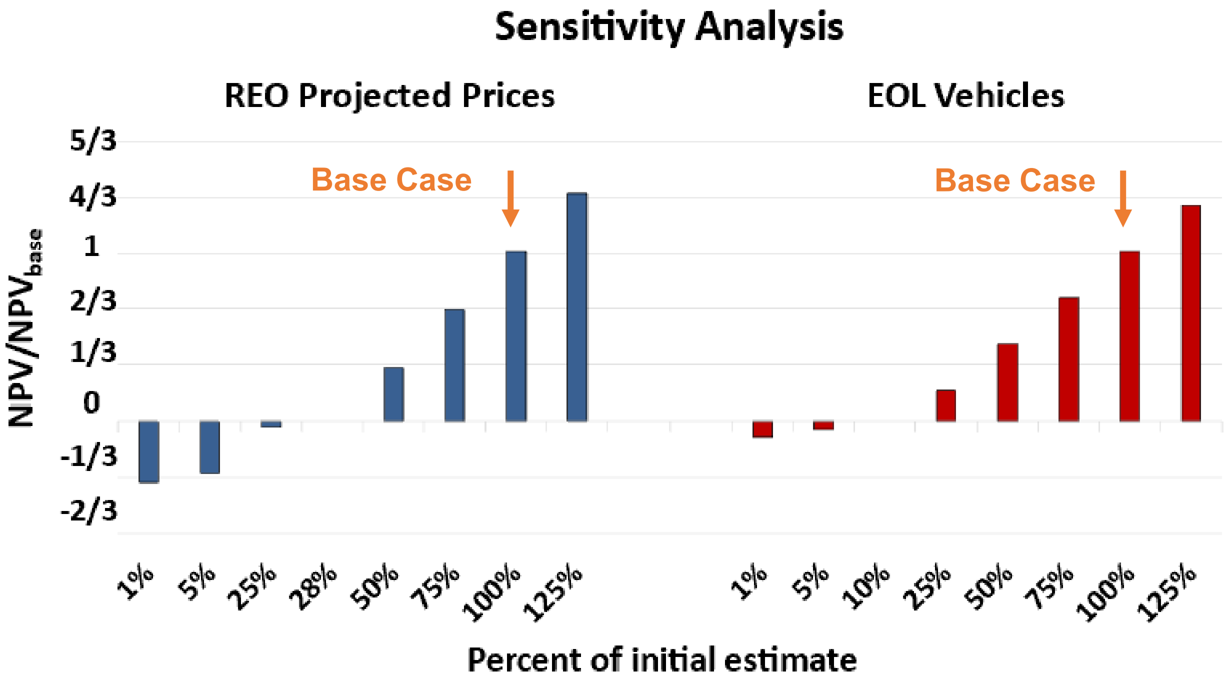

Figure 3. Sensitivity analysis for the product projected prices, and amount of EOL vehicles available for recycling. Values are reported normalized to the base case optimal solution to preserve confidentiality.

- Automatic disassembly, hydrogen decrepitation, acid-free dissolution were always selected as optimal

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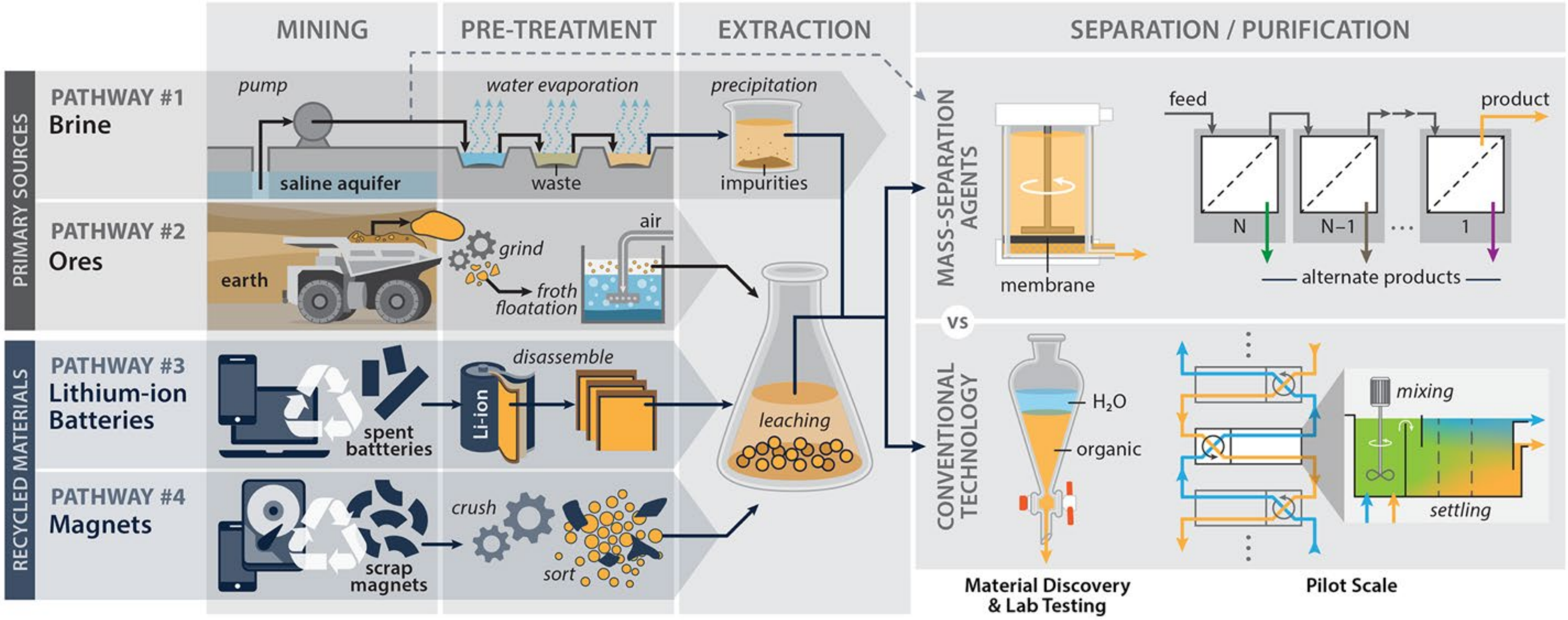
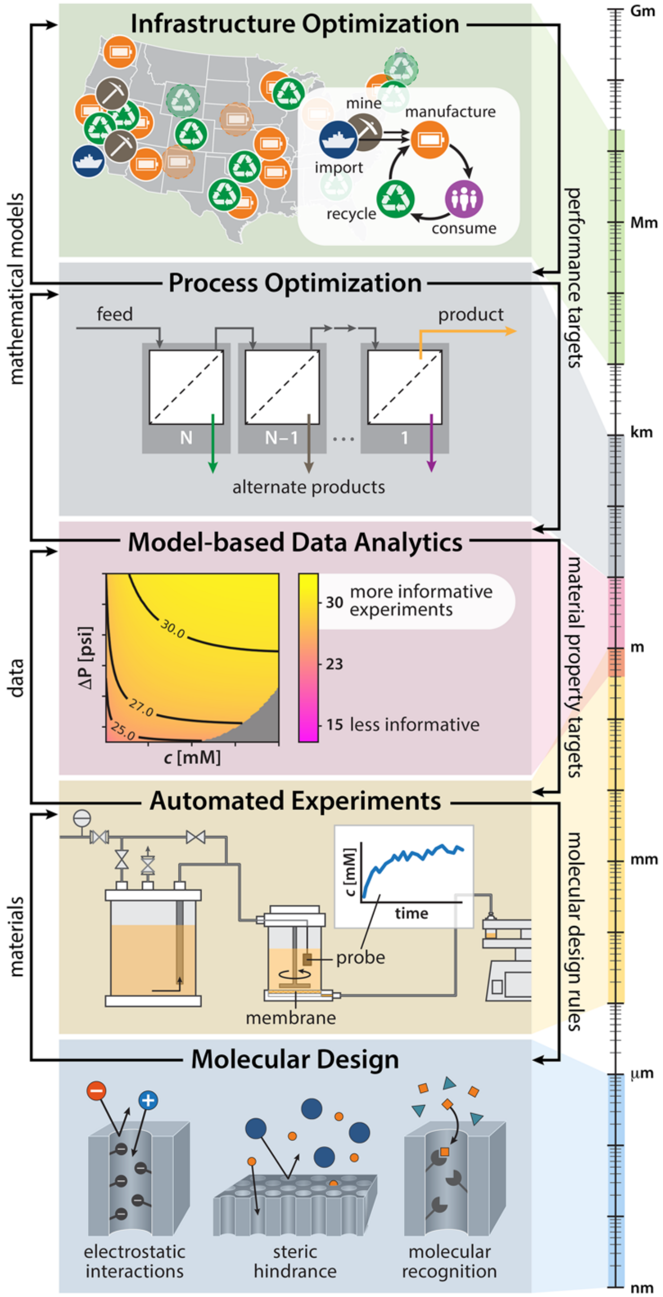
Process Optimization and Modeling for Minerals Sustainability

Advanced Optimization Capabilities

FWP subtask 2.3

How to systematically explore CM process intensification with membranes?





Lair, Ouimet, Dougher, Boudouris, Dowling, Phillip, *Annual Reviews in Chemical Engineering (2024),* accepted.

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Case Study: Li/Co Membrane System

What is it? Optimization membrane separation cascade to fractionate Li and Co ions (e.g., battery recycling) as an alternative to extraction cascades

- Reduce the use of environmentally challenging solvents
- More flexible and efficient separations

Why do we care? Highlights benefits of optimization

- Identifies new designs and design rules
- Accelerates process scale-up
- Quantifying separation trade-offs, informs materials and device targets

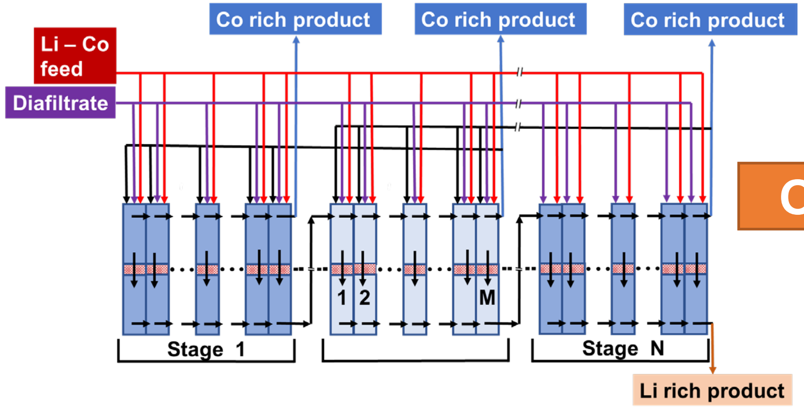
Motivation: Lithium/Cobalt Fractionation

Wamble, Eugene, Phillip, Dowling (2022), *ACS Sustainable Chemistry & Engineering*

performance data & specifications

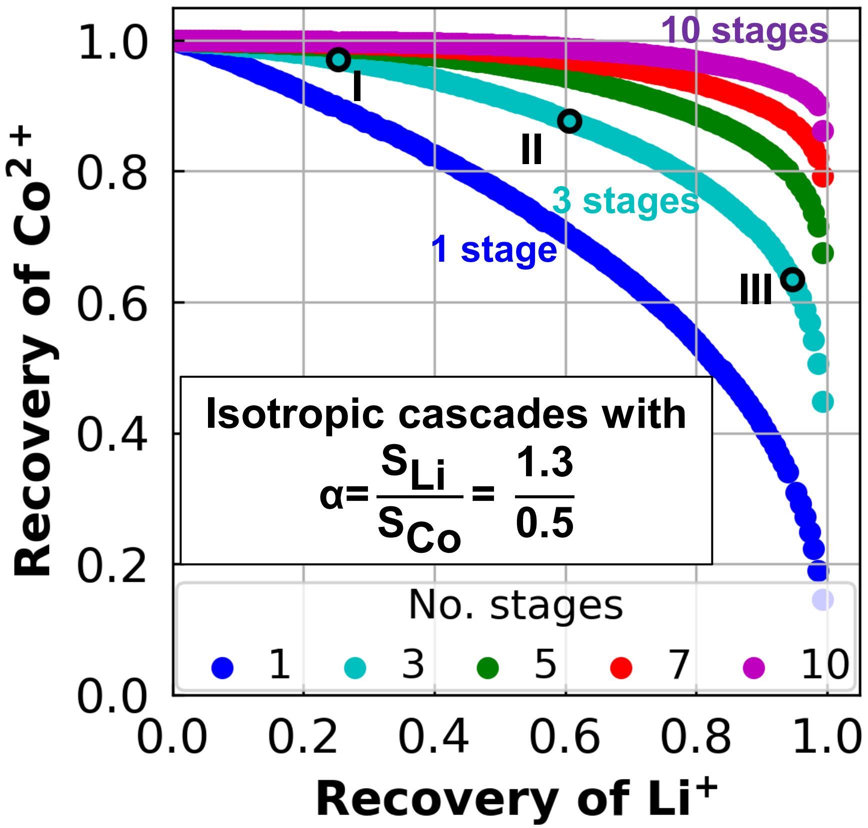
Model

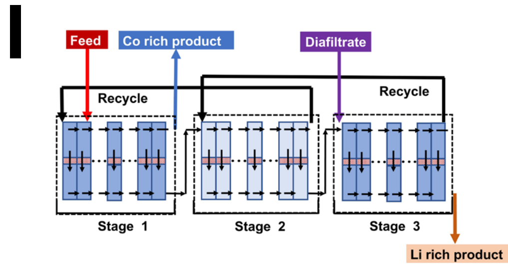
superstructure

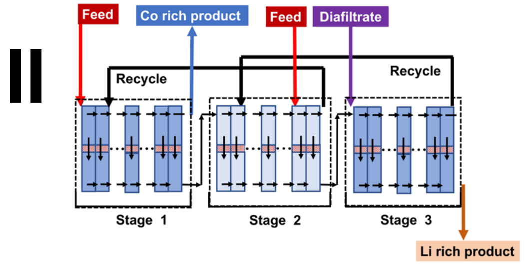


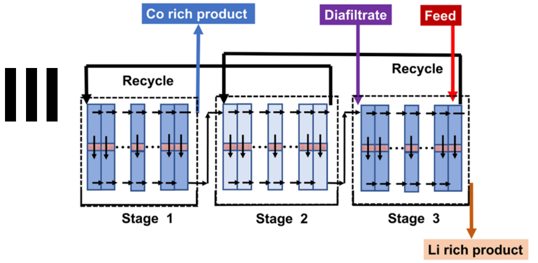
Optimize

optimal trade-offs, material property targets









Case Study: Li/Co Membrane System

Prior work:
- Demonstrates how optimization identifies new designs, informs material targets
- Bespoke and one-off implementation, 2+ years of student effort

Optimization-based flowsheet screening with superstructures:
- Automated mixed integer flowsheeting screening, demonstrated on Li/Co example
- [Ongoing] U. Kentucky flowsheet extraction with multiple products and sequencing

Technical risk reduction:
- Designed processes that are robust to uncertainty (e.g., membrane performance, feed variability)
- [Ongoing] Extend to U. Ky. components, improve design realism, incorporate detailed costing
- [Ongoing] Integrate uncertainty quantification and DoE with robust optimization

Example: Membrane Separation of Li-Co

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- Given known (maybe uncertain) feed characteristics and desired product specifications
- Superstructure formulation to rapidly determine the optimal configuration (# of stages, feed, diafiltrate, reflux connectivity)
- Advantage of framework
  - Intuitive to modeler
  - Avoid zero-flow issue
  - Solution with existing framework

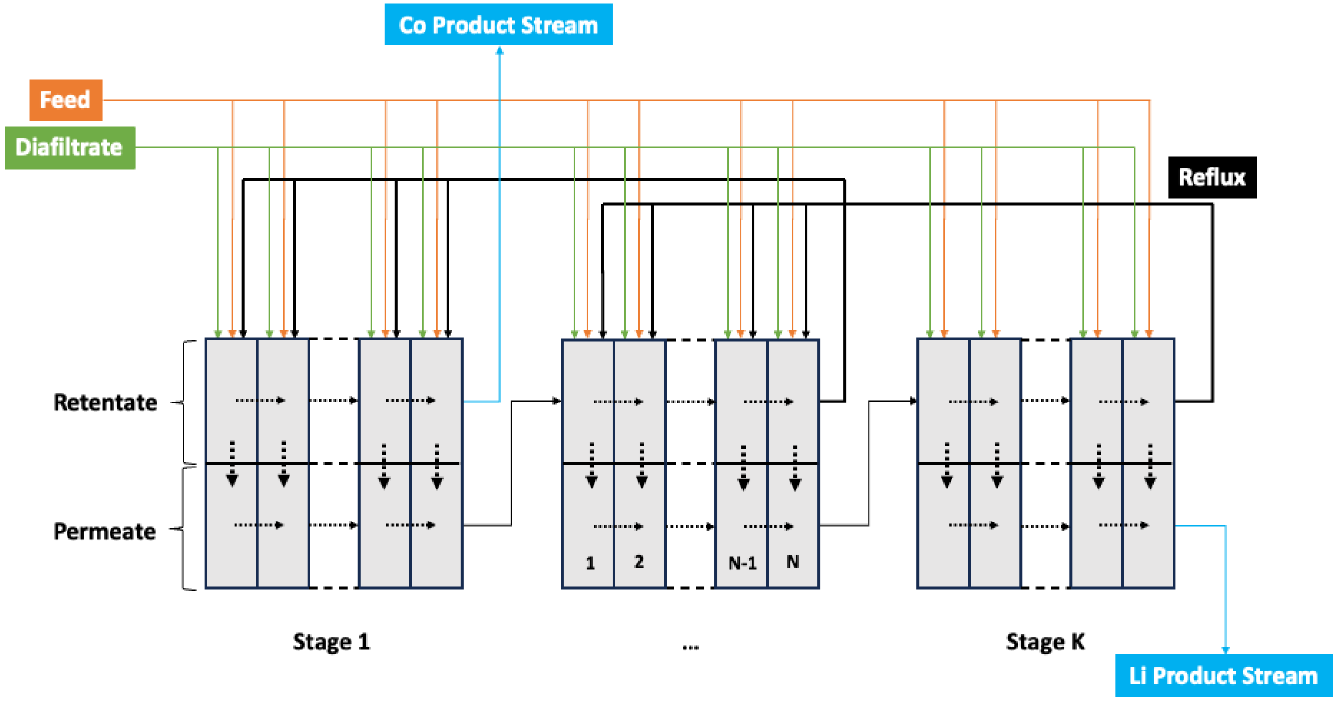

Figure 2: Superstructure of a generalized membrane cascade

Source: Ovalle D, Tran N, Laird CD, Grossman IE. Optimal Membrane Cascade Design for Critical Mineral Recovery Through Logic-based Superstructure Optimization. FOCAPD (2023)

Case Study: Li/Co Membrane System

Prior work:
- Demonstrates how optimization identifies new designs, informs material targets
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Technical Risk Reduction

Chrysanthos Gounaris, Alex Dowling, Anca Ostace

FWP subtask 2.4

Multi-Stage Diafiltration Model

(Based on original model from [1])

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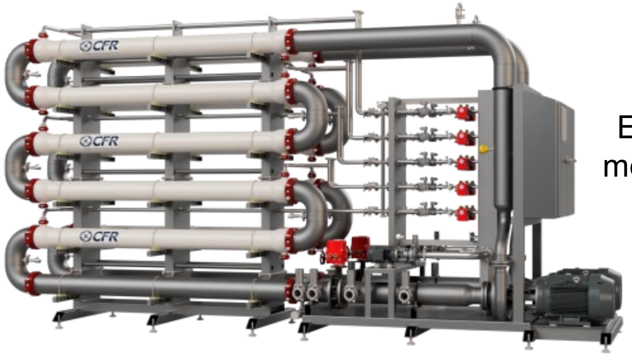
Model extensions:

- **Adjustable number of membrane stages and tube elements** using IDAES unit models
- **Added precipitator units** to isolate Co/Li products and recycle diafiltrate streams
- **Multi-period** model to handle varying process conditions over time
- **Alternative superstructures for mixing of flows** before each stage versus before each tube



Example membrane stage

[2]

Problem Formulation

max Cobalt Recovery

s.t. Lithium Recovery ≥ Spec

Permeate Mass Balances

Retentate Mass Balances

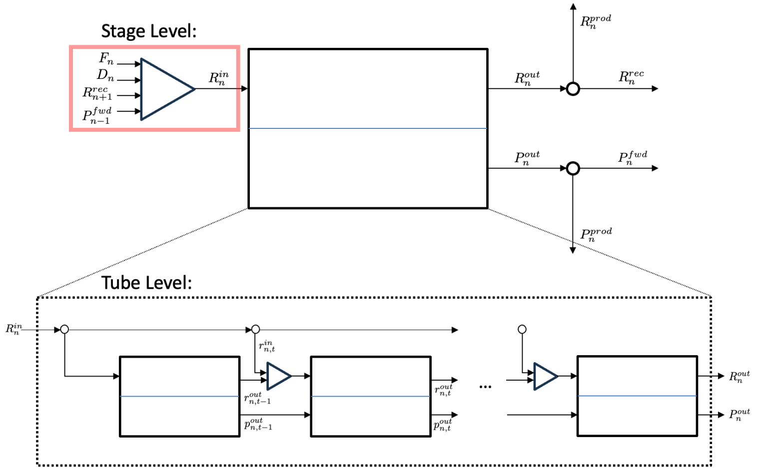
Membrane Performance Equations

Stage Connectivity Balances

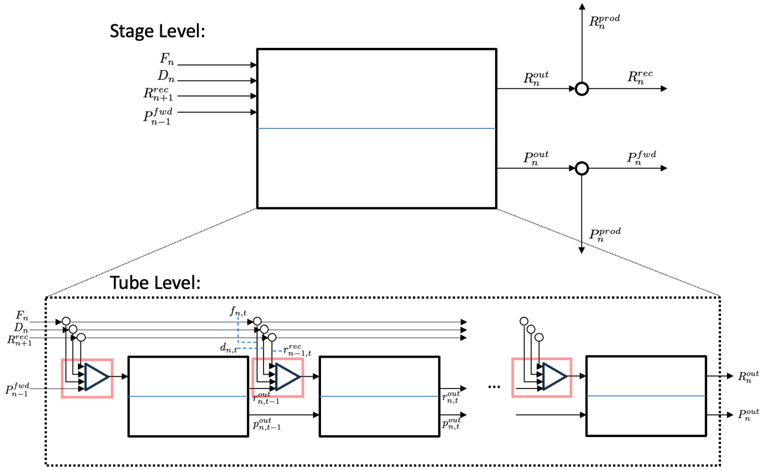
Flow Rates ≥ 0

Interchangeable objectives

Mixing before each stage



Mixing before each tube



[1] Wamble, NP, Eugene, EA, Phillip, WA, Dowling, AW. Optimal Diafiltration Membrane Cascades Enable Green Recycling of Spent Lithium-Ion Batteries. *ACS Sustainable Chemistry & Engineering*, 10(37):12207–12225, 2022.
[2] Ultrafiltration Membrane Skids. Complete Filtration Resources. https://www.gotocompletefiltration.com/wastewater-treatment/ultrafiltration-membrane-skids-2/

Robust Optimization

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

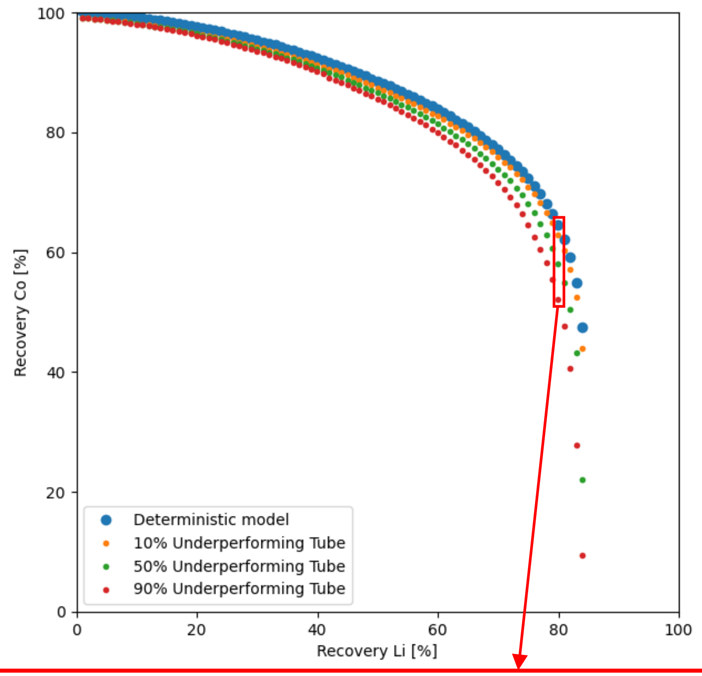
Potential Sources of Uncertainty

- Location and rate of **membrane fouling**
- **Feedstock** flow rate and solute concentrations
- Membrane **manufacturing variation**
  - Seek to ensure optimal performance for up to *N* membrane tubes underperforming

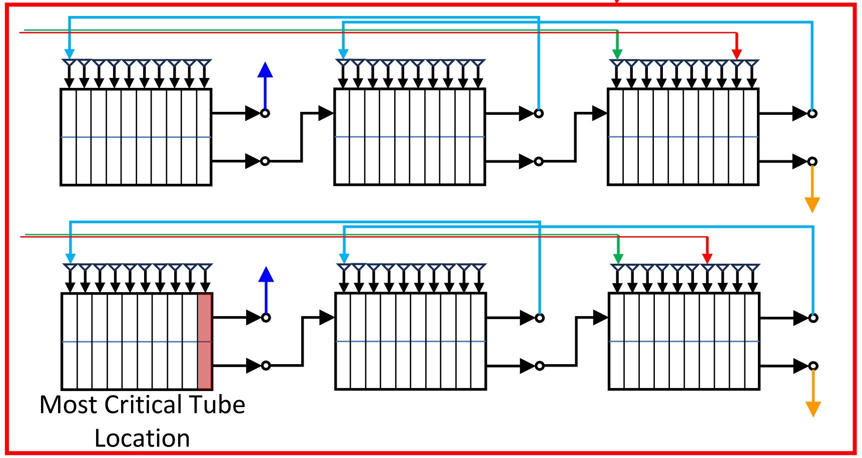
Two types of DoF in robust process design:

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

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



Pareto Front Comparisons of Robust Feasible Designs
(3 Stages x 10 Tubes/Stage)



Deterministic Model Flowsheet
(Stage Length: 753m)

Robust Feasible for 50% Underperforming Tube Flowsheet
(Stage Length: 785m)

---

[3] Isenberg, NM, Akula, P, Eslick, JC, Bhattacharyya, D, Miller, DC, Gounaris, CE. A generalized cutting-set approach for nonlinear robust optimization in process systems engineering. *AIChE Journal,* 67(5):e17175. 2021.

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

Robust Optimization Across System Sizes

Model Size	Worst-Case Cobalt Recovered		
	1 Underperforming Tube	2 Underperforming Tubes	3 Underperforming Tubes
Small (1 stage x 3 tubes)	51.1%	30.1%	Rob. Inf.
Medium (2 stages x 5 tubes)	69.5%	62.6%	55.4%
Large (3 stage x 10 tubes)	81.4%	79.4%	77.4%

Increasing size of membrane cascades allows for more cobalt to be recovered

Increasing number of underperforming tubes for robust feasible designs comes with a cost of reduced cobalt recovery

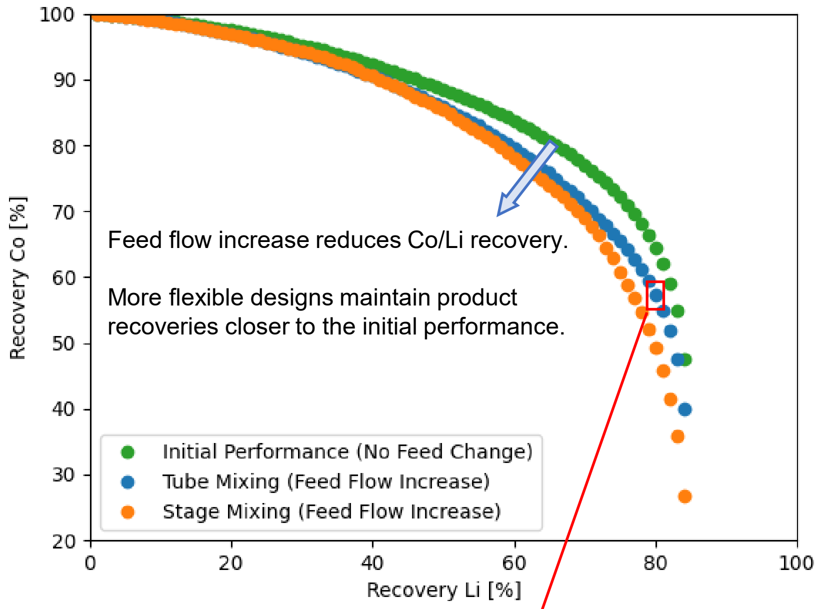
Model Settings:
- Tube-mixing configuration
- ≥ 60% lithium recovery requirement
- 50% flux decrease in underperforming tubes

Operational Flexibility Over Multiple Periods

Operational flexibility to achieve requirements under **changing operating conditions**.

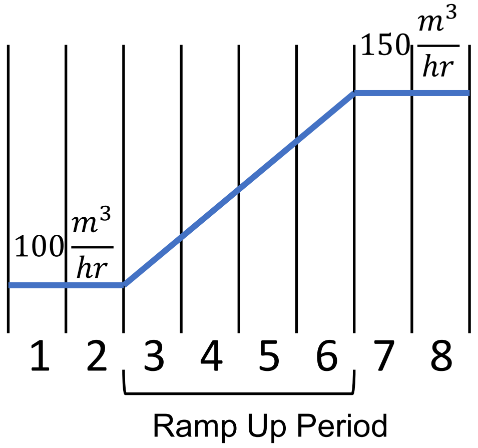
Case Study: Upstream plans to increase feed flow rate by 50%. Can we cope with it?

- Base case design does not possess sufficient operational DoF to adjust product/recycle flows and cannot maintain lithium recovery requirements
- Stage-Level Mixing and Tube-Level Mixing configurations can adjust feed/product stream locations to adapt to change.

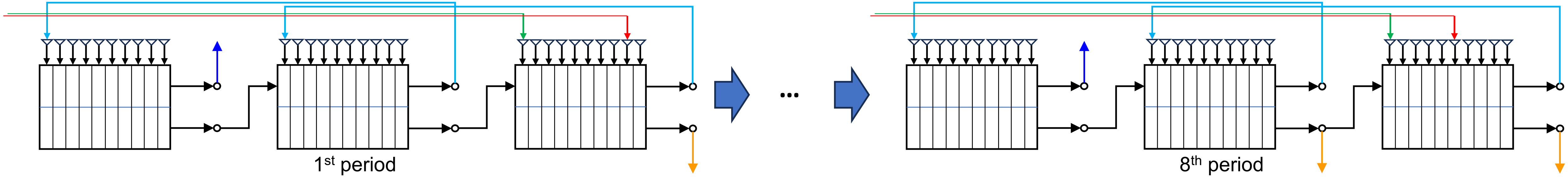


Feed flow increase reduces Co/Li recovery.

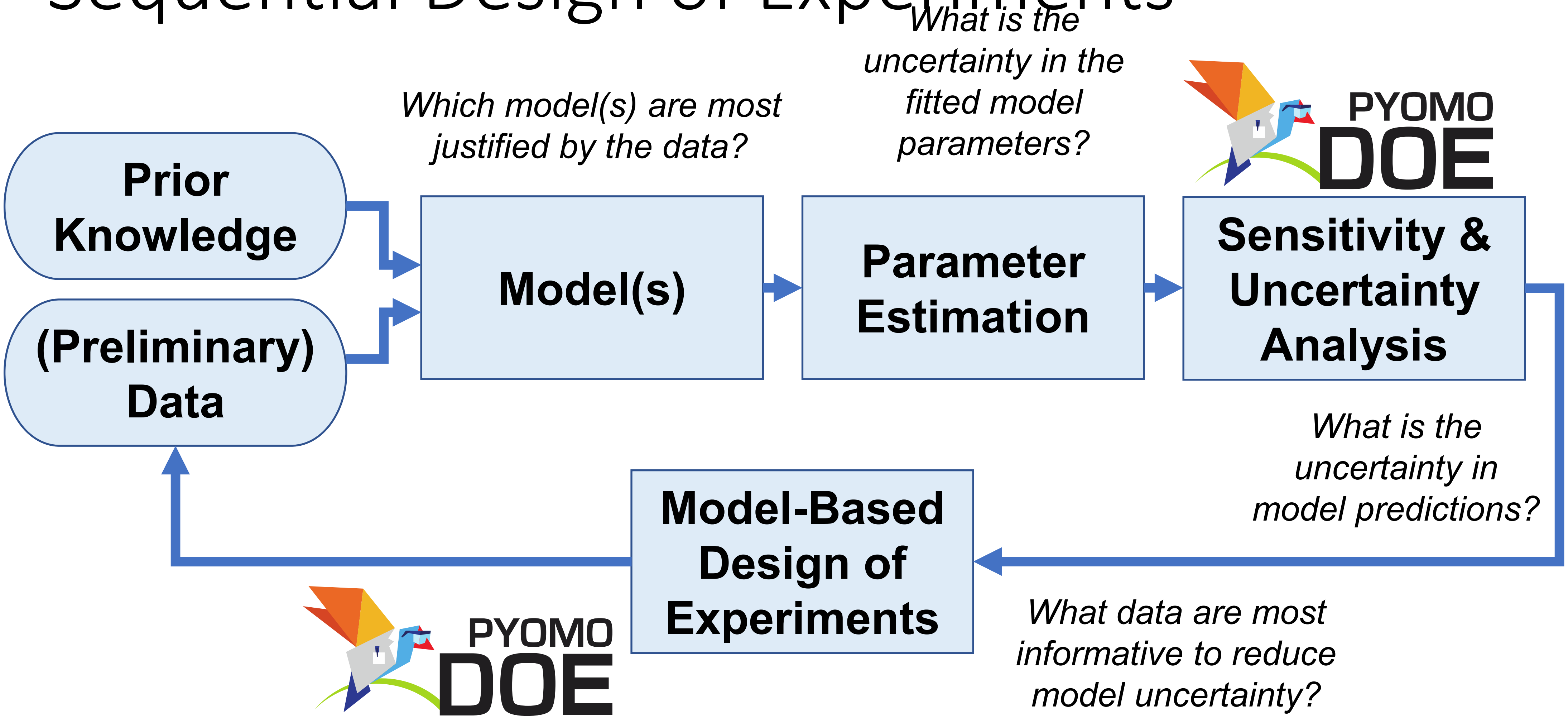
More flexible designs maintain product recoveries closer to the initial performance.



Evolution of Operation
(80% Li Recovery)



Sequential Design of Experiments



Prior Knowledge

(Preliminary) Data

Which model(s) are most justified by the data?

Model(s)

What is the uncertainty in the fitted model parameters?

Parameter Estimation

PYOMO DOE

Sensitivity & Uncertainty Analysis

What is the uncertainty in model predictions?

Model-Based Design of Experiments

What data are most informative to reduce model uncertainty?

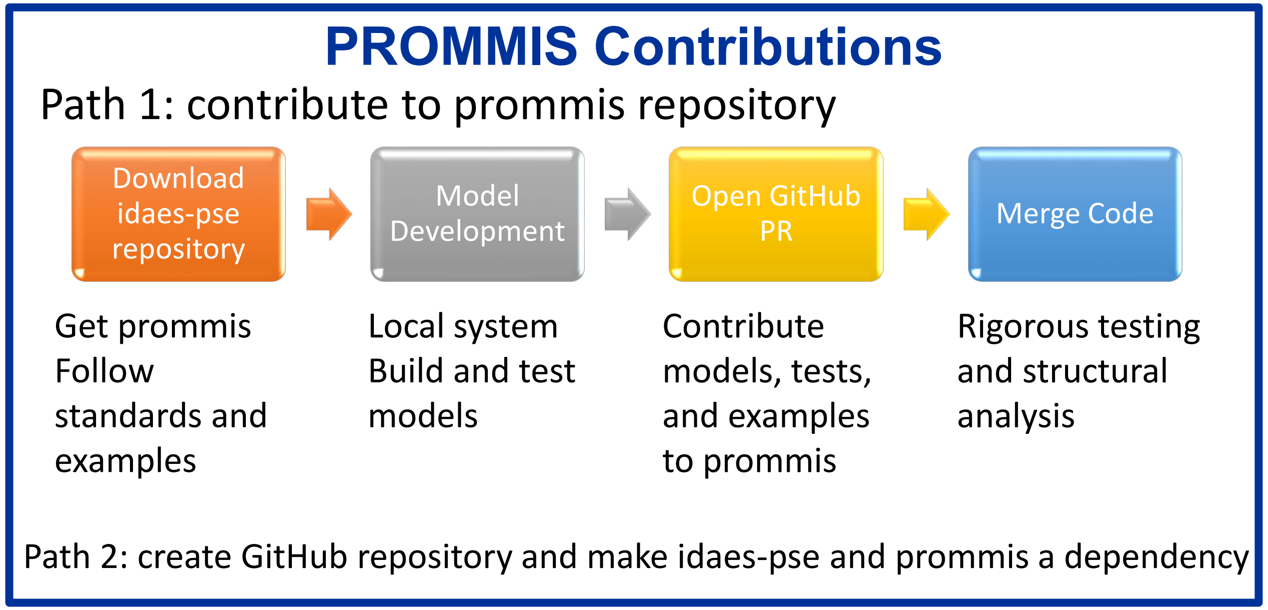
PYOMO DOE

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

Open-Source Platform

PROMMIS
Process Optimization and Modeling for Minerals Sustainability

- Website: https://idaes.org/research/application-areas/
- GitHub repository:
  - https://github.com/prommis/prommis
- Documentation:
  - https://prommis.readthedocs.io/en/latest/
- Bi-Weekly Software Engineering teleconferences coordinating development
- Targeting quarterly internal/public releases
- IPMP in progress for fully open-source license
- Overview video: coming soon!



PROMMIS Contributions

Path 1: contribute to prommis repository

Get prommis
Follow standards and examples

Local system
Build and test models

Contribute models, tests, and examples to prommis

Rigorous testing and structural analysis

Path 2: create GitHub repository and make idaes-pse and prommis a dependency

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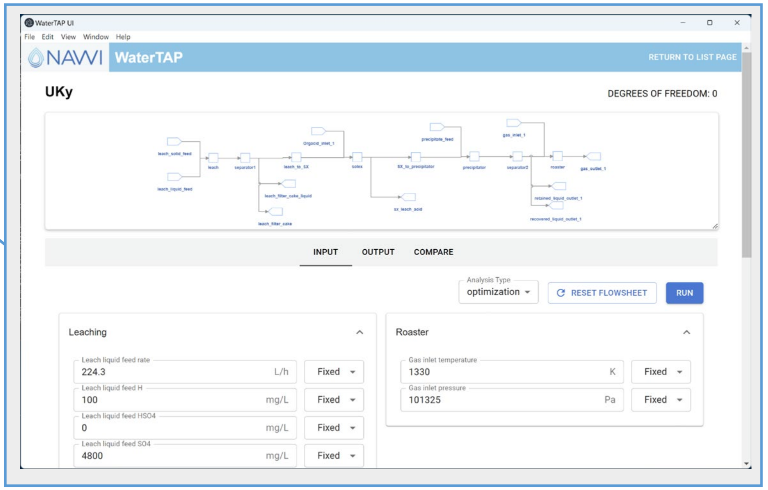
Usability

Leverage NAWI/WaterTAP UI infrastructure
- Define key model inputs and outputs
- Distribute UI with PROMMIS flowsheets
- Parallel parameter sweeps (sensitivity analysis)



UKy

DEGREES OF FREEDOM: 0

Analysis Type: optimization

Leaching

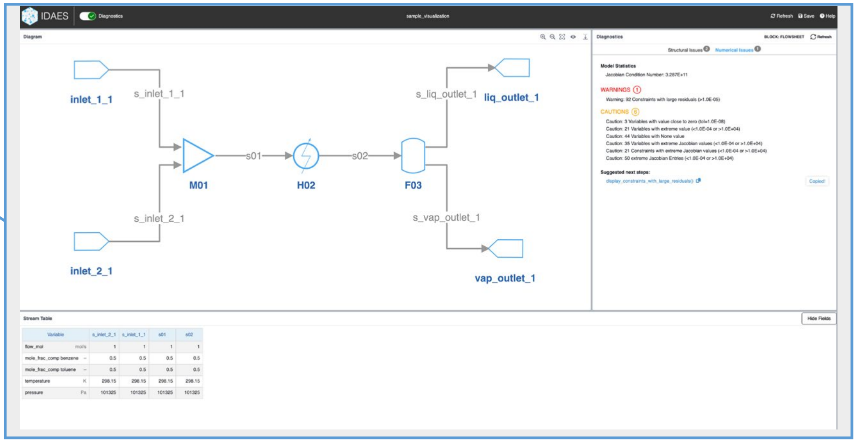
Leach liquid feed rate	224.3 L/h	Fixed
Leach liquid feed H	100 mg/L	Fixed
Leach liquid feed HSO4	0 mg/L	Fixed
Leach liquid feed SO4	4800 mg/L	Fixed

Roaster

Gas inlet temperature	1330 K	Fixed
Gas inlet pressure	101325 Pa	Fixed

Gather requirements for UIs specific to WT
- E.g., conceptual design model configuration

Leverage IDAES core flowsheet visualization
- View flowsheet diagrams
- PROMMIS models <- new diagnostics capabilities



Model Statistics

Jacobian Condition Number: 3.287E+11

WARNINGS ①

Warning: 92 Constraints with large residuals (>1.0E-05)

CAUTIONS ⑥

Caution: 3 Variables with value close to zero (tol=1.0E-08)
Caution: 21 Variables with extreme value (<1.0E-04 or >1.0E+04)
Caution: 44 Variables with None value
Caution: 35 Variables with extreme Jacobian values (<1.0E-04 or >1.0E+04)
Caution: 21 Constraints with extreme Jacobian values (<1.0E-04 or >1.0E+04)
Caution: 50 extreme Jacobian Entries (<1.0E-04 or >1.0E+04)

Suggested next steps:

display_constraints_with_large_residuals()

Stream Table

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
pressure	Pa	101325	101325	101325	101325

Assist team with Jupyter Notebooks and online documentation

Acknowledgements:

The PROMMIS team gratefully acknowledges support from the U.S. DOE's Fossil Energy and Carbon Management Office of Resource Sustainability.

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For questions and comments, please contact our Technical Director, Thomas Tarka (Thomas.Tarka@netl.doe.gov).

Office of Fossil Energy and Carbon Management: Grant Bromhal, Gabby Intihar, Morgan Summers.

National Energy Technology Laboratory: Thomas Tarka, Tony Burgard, Steve Zitney, Andrew Lee, Miguel Zamarripa, Alison Fritz, Alejandro Garciadiego, Brandon Paul, Anca Ostace, Radhakrishna Gooty, Jinliang Ma, Lingyan Deng, Marcus Holly, Elmira Shamlou, Javal Vyas.

Sandia National Laboratories: John Siirola, Bethany Nicholson, Michael Bynum, Edna Soraya Rawlings.

Lawrence Berkeley National Laboratory: Dan Gunter, Keith Beattie, John Shinn, Oluwamayowa Amusat, Sarah Poon, Ludovico Bianchi.

Carnegie Mellon University: Larry Biegler, Ignacio Grossmann, Carl Laird, Chrysanthos Gounaris, Ana Torres, Jason Yao, Christopher Laliwala, Daniel Ovalle.

West Virginia University: Debangsu Bhattacharyya, Quang-Minh Le, Akintomiwa Ojo, Arkoprabho Dasgupta.

University of Notre Dame: Alex Dowling, Molly Dougher, Hailey Lynch.

Georgia Tech: Nick Sahinidis, Dimitros Fardis.

2023 Joint PROMMIS/CCSI$_2$/IDAES Technical Team Meeting
Lawrence Berkeley National Lab

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Older Slides

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Technical Risk Reduction

Chrysanthos Gounaris, Alex Dowling, Anca Ostace

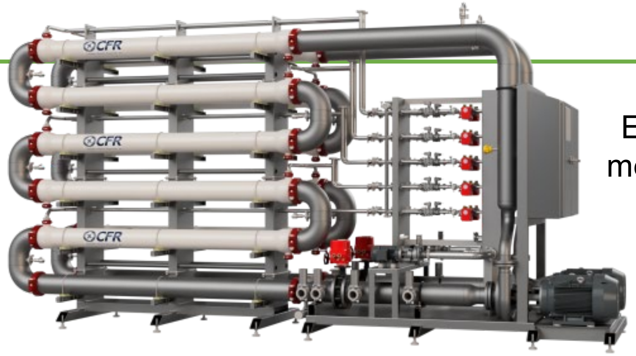
FWP subtask 2.4

Multi-Stage Diafiltration Model

(Based on original model from [1])

Model extensions:

- **Adjustable number of membrane stages and tube elements** using IDAES unit models
- **Added precipitator units** to isolate Co/Li products and recycle diafiltrate streams
- **Multi-period** model to handle varying process conditions over time
- **Alternative superstructures for mixing of flows** before each stage versus before each tube



Example membrane stage

[2]

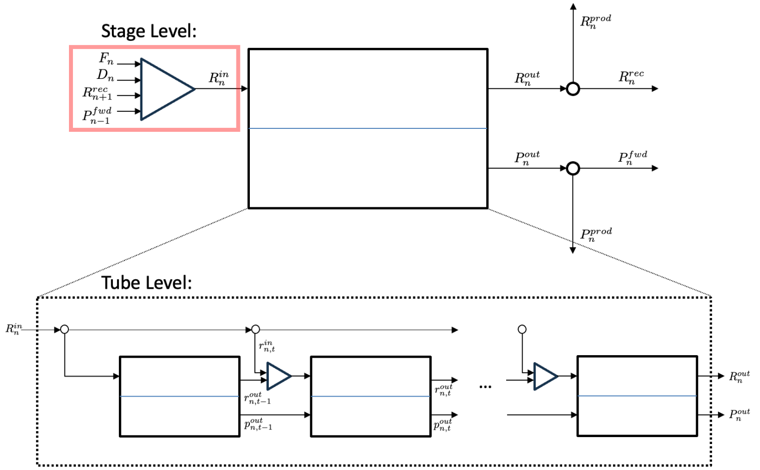
Problem Formulation

max
Cobalt Recovery

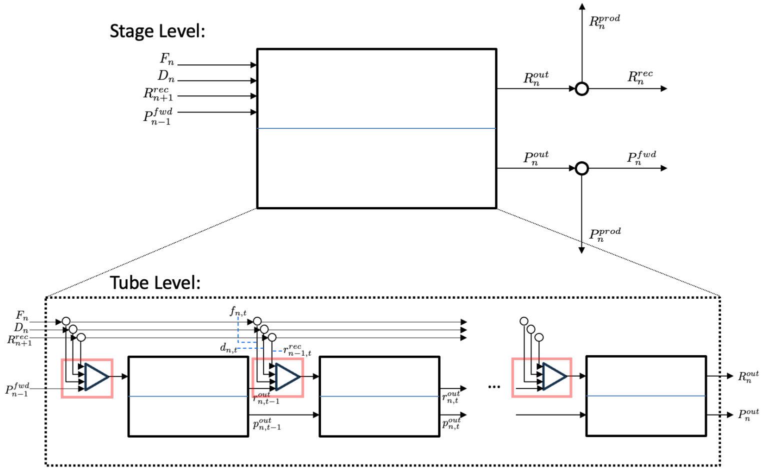
s.t.
Lithium Recovery ≥ Spec
Permeate Mass Balances
Retentate Mass Balances
Membrane Performance Equations
Stage Connectivity Balances
Flow Rates ≥ 0

Interchangeable objectives

Mixing before each stage



Mixing before each tube



[1] Wamble, NP, Eugene, EA, Phillip, WA, Dowling, AW. Optimal Diafiltration Membrane Cascades Enable Green Recycling of Spent Lithium-Ion Batteries. *ACS Sustainable Chemistry & Engineering*, 10(37):12207–12225, 2022.
[2] Ultrafiltration Membrane Skids. Complete Filtration Resources. https://www.gotocompletefiltration.com/wastewater-treatment/ultrafiltration-membrane-skids-2/

Robust Optimization

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

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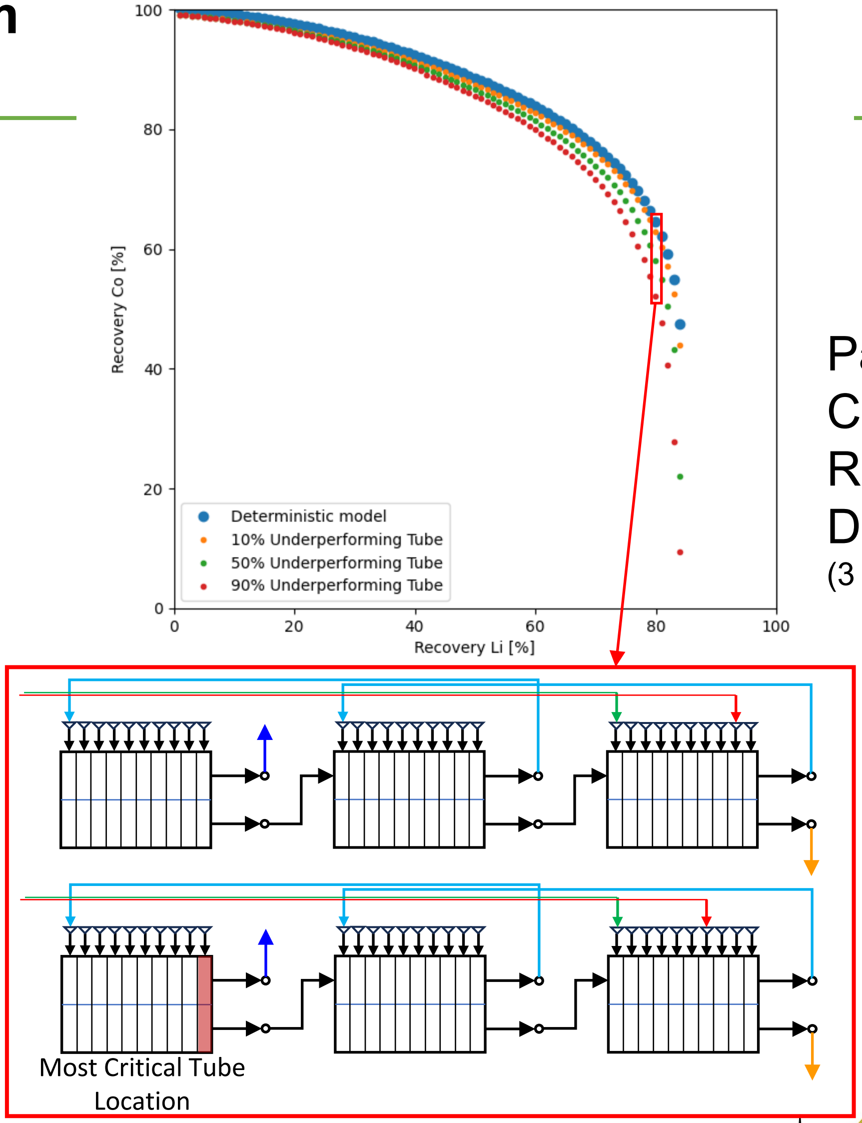
Potential Sources of Uncertainty

- Location and rate of **membrane fouling**
- **Feedstock** flow rate and solute concentrations
- Membrane **manufacturing variation**
  - Seek to ensure optimal performance for up to *N* membrane tubes underperforming

Two types of DoF in robust process design:

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

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



Pareto Front Comparisons of Robust Feasible Designs
(3 Stages x 10 Tubes/Stage)

Deterministic Model Flowsheet
(Stage Length: 753m)

Robust Feasible for 50% Underperforming Tube Flowsheet
(Stage Length: 785m)

[3] Isenberg, NM, Akula, P, Eslick, JC, Bhattacharyya, D, Miller, DC, Gounaris, CE. A generalized cutting-set approach for nonlinear robust optimization in process systems engineering. *AIChE Journal*, 67(5):e17175. 2021.
[4] Isenberg, NM, Sherman, JA, Siirola, JD, & Gounaris, CE. PyROS: The Pyomo Robust Optimization Solver. *Forthcoming*. 2024.

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Robust Optimization Across System Sizes

Model Size	Worst-Case Cobalt Recovered		
	1 Underperforming Tube	2 Underperforming Tubes	3 Underperforming Tubes
Small (1 stage x 3 tubes)	51.1%	30.1%	Rob. Inf.
Medium (2 stages x 5 tubes)	69.5%	62.6%	55.4%
Large (3 stage x 10 tubes)	81.4%	79.4%	77.4%

Increasing size of membrane cascades allows for more cobalt to be recovered

Increasing number of underperforming tubes for robust feasible designs comes with a cost of reduced cobalt recovery

Model Settings:
- Tube-mixing configuration
- ≥ 60% lithium recovery requirement
- 50% flux decrease in underperforming tubes

Operational Flexibility Over Multiple Periods

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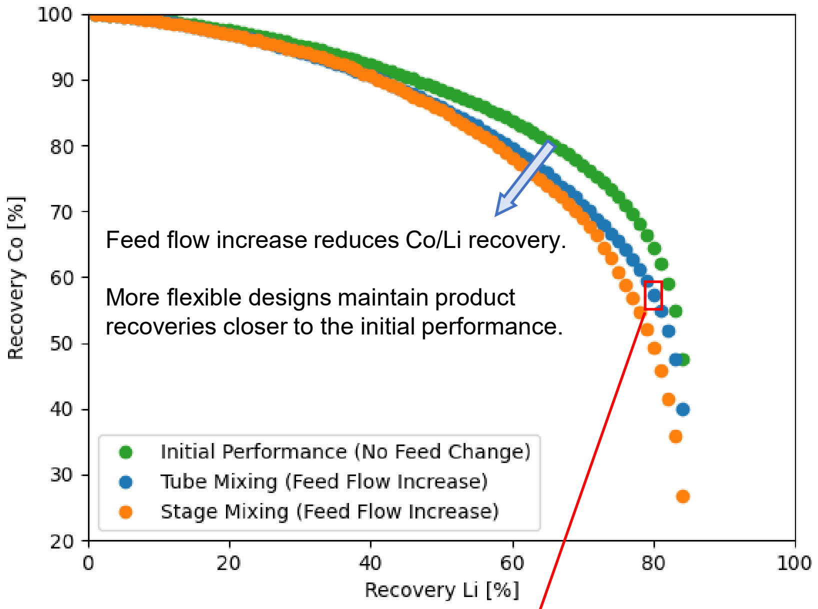
Operational flexibility to achieve requirements under **changing operating conditions**.

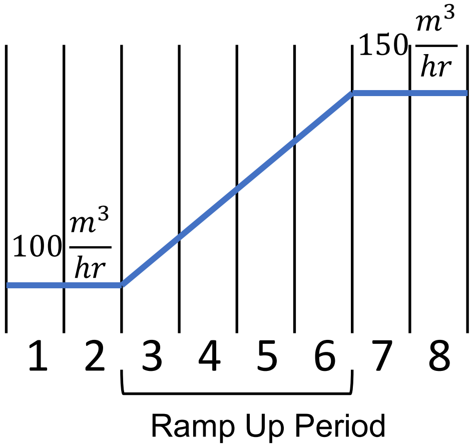
Case Study: Upstream plans to increase feed flow rate by 50%. Can we cope with it?

- Base case design does not possess sufficient operational DoF to adjust product/recycle flows and cannot maintain lithium recovery requirements
- Stage-Level Mixing and Tube-Level Mixing configurations can adjust feed/product stream locations to adapt to change.

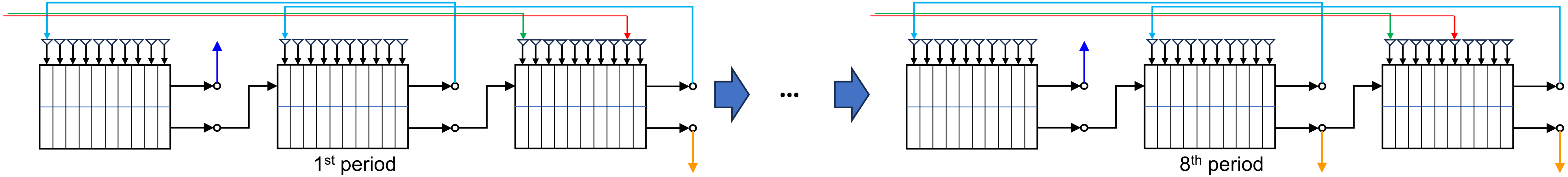


Feed flow increase reduces Co/Li recovery.

More flexible designs maintain product recoveries closer to the initial performance.



Evolution of Operation
(80% Li Recovery)



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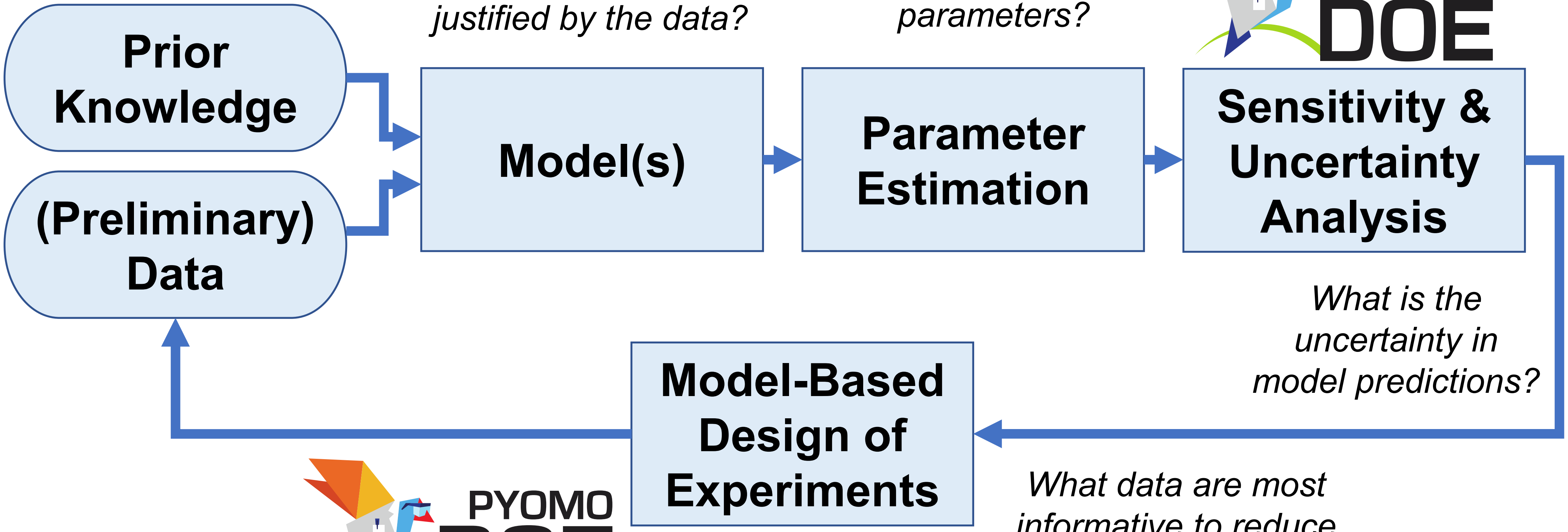
Sequential Design of Experiments



Prior Knowledge

(Preliminary) Data

Which model(s) are most justified by the data?

Model(s)

What is the uncertainty in the fitted model parameters?

Parameter Estimation

Sensitivity & Uncertainty Analysis

What is the uncertainty in model predictions?

Model-Based Design of Experiments

What data are most informative to reduce model uncertainty?

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

Open-Source Platform

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- Website: https://idaes.org/research/application-areas/
- GitHub repository:
  - https://github.com/prommis/prommis
- Documentation:
  - https://prommis.readthedocs.io/en/latest/
- Bi-Weekly Software Engineering teleconferences coordinating development
- Targeting quarterly internal/public releases
- IPMP in progress for fully open-source license
- Overview video: coming soon!

PROMMIS Contributions

Path 1: contribute to prommis repository

Download idaes-pse repository →	Model Development →	Open GitHub PR →	Merge Code
Get prommis Follow standards and examples	Local system Build and test models	Contribute models, tests, and examples to prommis	Rigorous testing and structural analysis

Path 2: create GitHub repository and make idaes-pse and prommis a dependency

Usability

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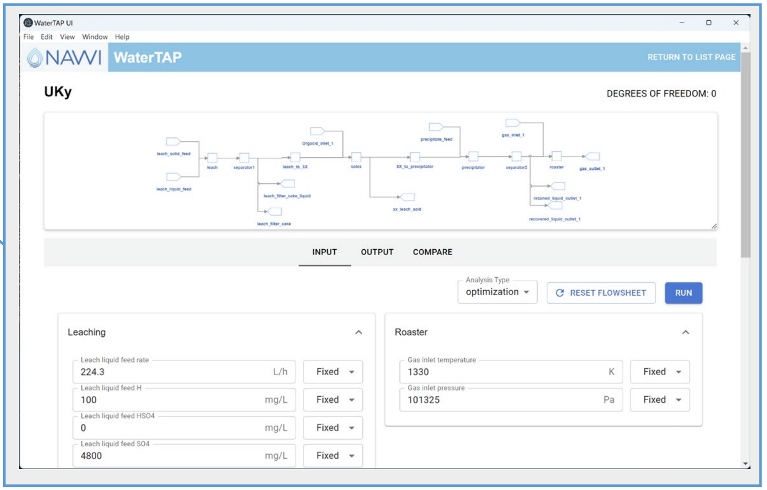
Leverage NAWI/WaterTAP UI infrastructure
  - Define key model inputs and outputs
  - Distribute UI with PROMMIS flowsheets
  - Parallel parameter sweeps (sensitivity analysis)

Gather requirements for UIs specific to WT
  - E.g., conceptual design model configuration



UKy

DEGREES OF FREEDOM: 0

Analysis Type: optimization

Leaching

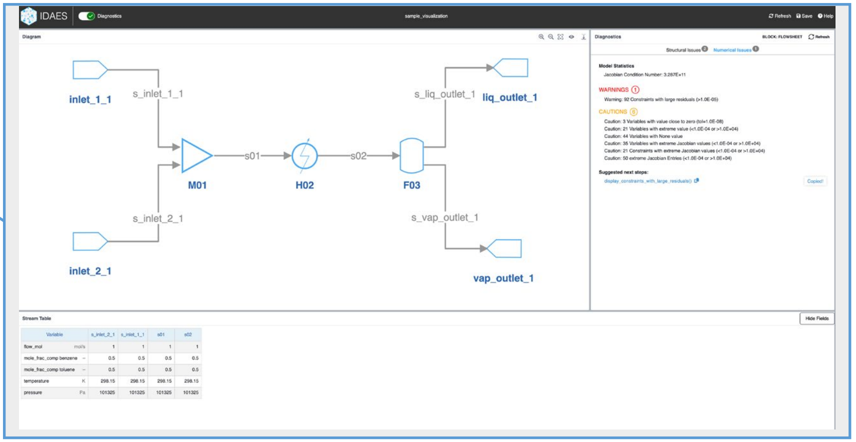
Leach liquid feed rate: 224.3 L/h Fixed
Leach liquid feed H: 100 mg/L Fixed
Leach liquid feed HSO4: 0 mg/L Fixed
Leach liquid feed SO4: 4800 mg/L Fixed

Roaster

Gas inlet temperature: 1330 K Fixed
Gas inlet pressure: 101325 Pa Fixed

Leverage IDAES core flowsheet visualization
  - View flowsheet diagrams
  - PROMMIS models <- new diagnostics capabilities

Assist team with Jupyter Notebooks and online documentation



Model Statistics
Jacobian Condition Number: 3.287E+11

WARNINGS (1)
Warning: 92 Constraints with large residuals (>1.0E-05)

CAUTIONS (6)
Caution: 3 Variables with value close to zero (tol=1.0E-08)
Caution: 21 Variables with extreme value (<1.0E-04 or >1.0E+04)
Caution: 44 Variables with None value
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Suggested next steps:
display_constraints_with_large_residuals()

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
pressure	Pa	101325	101325	101325	101325

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Leaching Summary

Feed Composition Data Used

- Coal Composition: UKy Final Report Appendix E, Tables 2 & 6

Model Equations and Data for Unit Process

- Shrinking Core kinetic model
- Operating Conditions: UKy Final Report Tables 3.7.1 & 3.7.2
- Elemental Recovery: UKy Final Report Figures 3.7.4, 3.7.5, & 3.7.6a

Validation Data Used

- None available

Additional Data Required

- Additional experimental data for fitting and validation

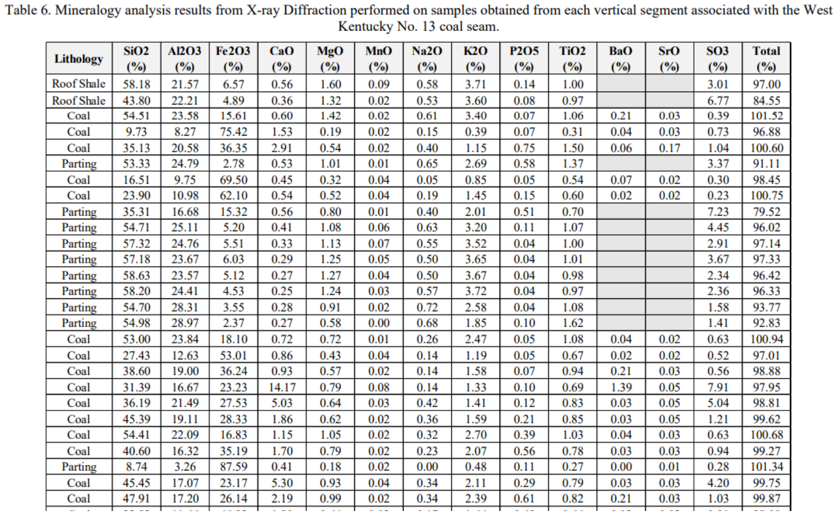

Table 6. Mineralogy analysis results from X-ray Diffraction performed on samples obtained from each vertical segment associated with the West Kentucky No. 13 coal seam.

Lithology	SiO2 (%)	Al2O3 (%)	Fe2O3 (%)	CaO (%)	MgO (%)	MnO (%)	Na2O (%)	K2O (%)	P2O5 (%)	TiO2 (%)	BaO (%)	SrO (%)	SO3 (%)	Total (%)
Roof Shale	58.18	21.57	6.57	0.56	1.60	0.09	0.58	3.71	0.14	1.00			3.01	97.00
Roof Shale	43.80	22.21	4.89	0.36	1.32	0.02	0.53	3.60	0.08	0.97			6.77	84.55
Coal	54.51	23.58	15.61	0.60	1.42	0.02	0.61	3.40	0.07	1.06	0.21	0.03	0.39	101.52
Coal	9.73	8.27	75.42	1.53	0.19	0.02	0.15	0.39	0.07	0.31	0.04	0.03	0.73	96.88
Coal	35.13	20.58	36.35	2.91	0.54	0.02	0.40	1.15	0.75	1.50	0.06	0.17	1.04	100.60
Parting	53.33	24.79	2.78	0.53	1.01	0.01	0.65	2.69	0.58	1.37			3.37	91.11
Coal	16.51	9.75	69.50	0.45	0.32	0.04	0.05	0.85	0.05	0.54	0.07	0.02	0.30	98.45
Coal	23.90	10.98	62.10	0.54	0.52	0.04	0.19	1.45	0.15	0.60	0.02	0.02	0.23	100.75
Parting	35.31	16.68	15.32	0.56	0.80	0.01	0.40	2.01	0.51	0.70			7.23	79.52
Parting	54.71	25.11	5.20	0.41	1.08	0.06	0.63	3.20	0.11	1.07			4.45	96.02
Parting	57.32	24.76	5.51	0.33	1.13	0.07	0.55	3.52	0.04	1.00			2.91	97.14
Parting	57.18	23.67	6.03	0.29	1.25	0.05	0.50	3.65	0.04	1.01			3.67	97.33
Parting	58.63	23.57	5.12	0.27	1.27	0.04	0.50	3.67	0.04	0.98			2.34	96.42
Parting	58.20	24.41	4.53	0.25	1.24	0.03	0.57	3.72	0.04	0.97			2.36	96.33
Parting	54.70	28.31	3.55	0.28	0.91	0.02	0.72	2.58	0.04	1.08			1.58	93.77
Parting	54.98	28.97	2.37	0.27	0.58	0.00	0.68	1.85	0.10	1.62			1.41	92.83
Coal	53.00	23.84	18.10	0.72	0.72	0.01	0.26	2.47	0.05	1.08	0.04	0.02	0.63	100.94
Coal	27.43	12.63	53.01	0.86	0.43	0.04	0.14	1.19	0.05	0.67	0.02	0.02	0.52	97.01
Coal	38.60	19.00	36.24	0.93	0.57	0.02	0.14	1.58	0.07	0.94	0.21	0.03	0.56	98.88
Coal	31.39	16.67	23.23	14.17	0.79	0.08	0.14	1.33	0.10	0.69	1.39	0.05	7.91	97.95
Coal	36.19	21.49	27.53	5.03	0.64	0.03	0.42	1.41	0.12	0.83	0.03	0.05	5.04	98.81
Coal	45.39	19.11	28.33	1.86	0.62	0.02	0.36	1.59	0.21	0.85	0.03	0.05	1.21	99.62
Coal	54.41	22.09	16.83	1.15	1.05	0.02	0.32	2.70	0.39	1.03	0.04	0.03	0.63	100.68
Coal	40.60	16.32	35.19	1.70	0.79	0.02	0.23	2.07	0.56	0.78	0.03	0.03	0.94	99.27
Parting	8.74	3.26	87.59	0.41	0.18	0.02	0.00	0.48	0.11	0.27	0.00	0.01	0.28	101.34
Coal	45.45	17.07	23.17	5.30	0.93	0.04	0.34	2.11	0.29	0.79	0.03	0.03	4.20	99.75
Coal	47.91	17.20	26.14	2.19	0.99	0.02	0.34	2.39	0.61	0.82	0.21	0.03	1.03	99.87

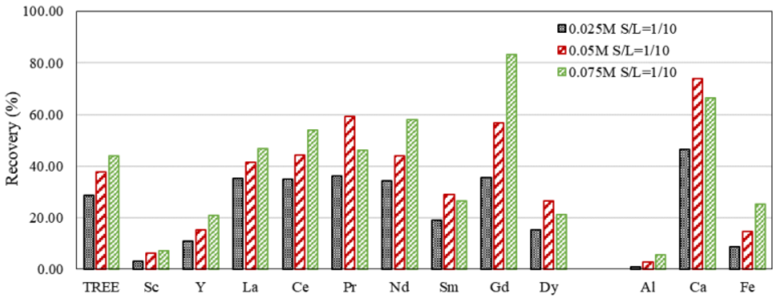

Figure 3.7.4. Effect of acid concentration on major REE and contaminants leaching recovery.

WVU Team (Prof. Debangsu Bhattacharyya)

Solvent Extraction Summary

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Feed Composition Data Used

- Aqueous feed: REESim excel file, buffer tank of cleaner circuit, concentration of components
- Organic feed: REESim excel file, stripping operation of cleaner circuit, concentration of components
- Components considered: Al, Ca, Fe, Sc, Y, La, Ce, Pr, Nd, Sm, Gd, Dy
- Extractant considered: DEHPA

Model Equations and Data for Unit Process

- Komulanein et. al., Hydrometallurgy, 81, 52-61, 2006, Lyon et. al., Industrial and Engineering Chemistry Research, 56, 1048-1056, 2017, and several other papers
- REESim excel file, Phase-1 report, Final phase report,
- Extraction percentage, extractant dosage and pH variation data, feed and product concentration, etc.

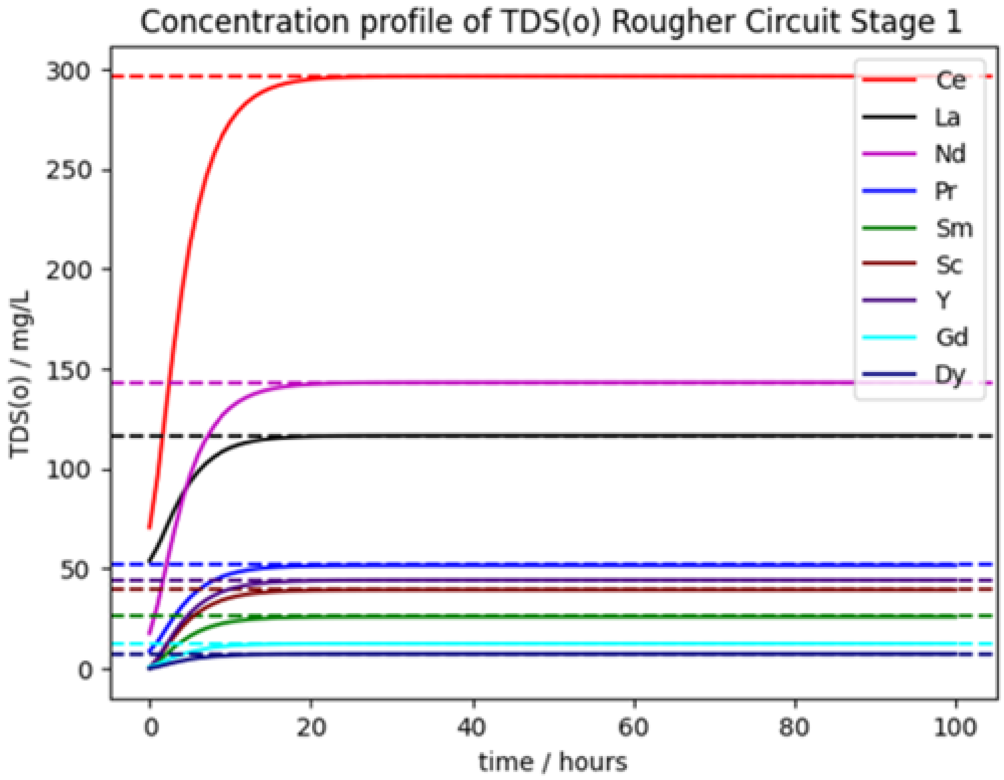
Validation Data Used

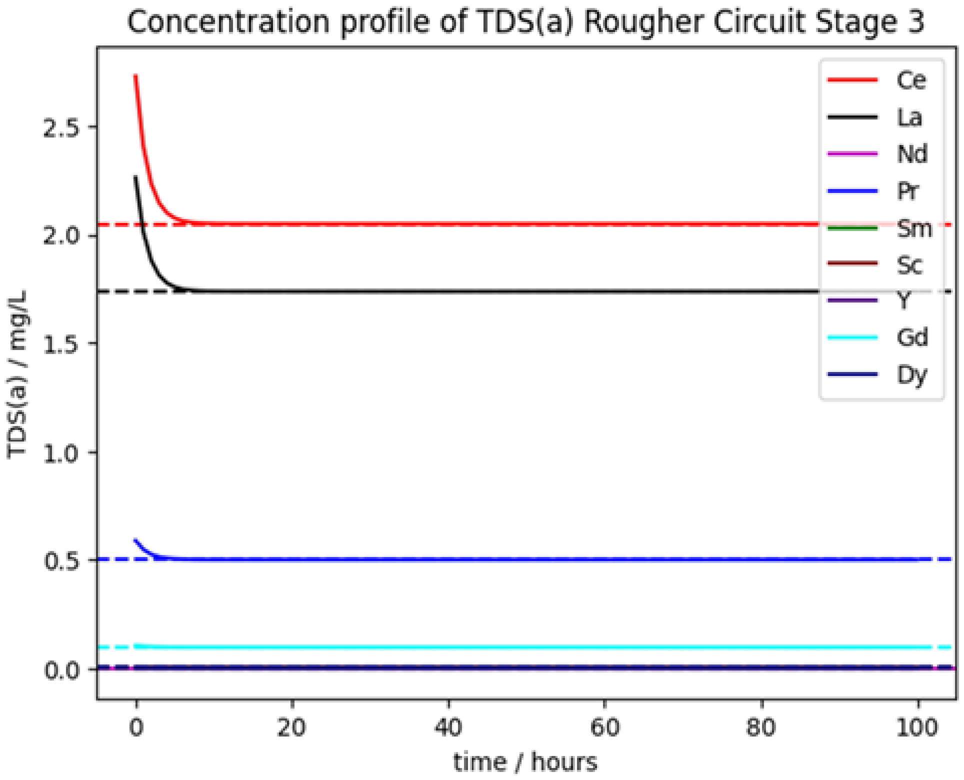
- Aqueous and organic streams concentration values from REESim excel file, Phase-1 report, and final phase report

Additional Data Required

- Following data are lacking in general in the literature in this area including UKy literature- studies on emulsification, if any, density gradients in the mixer/settler, axial and radial mixing, mass transfer rate, studies on interfaces and continuous and dispersed phase distributions, and ion concentration variation, also dynamic data are mostly lacking.

Solvent Extraction Summary

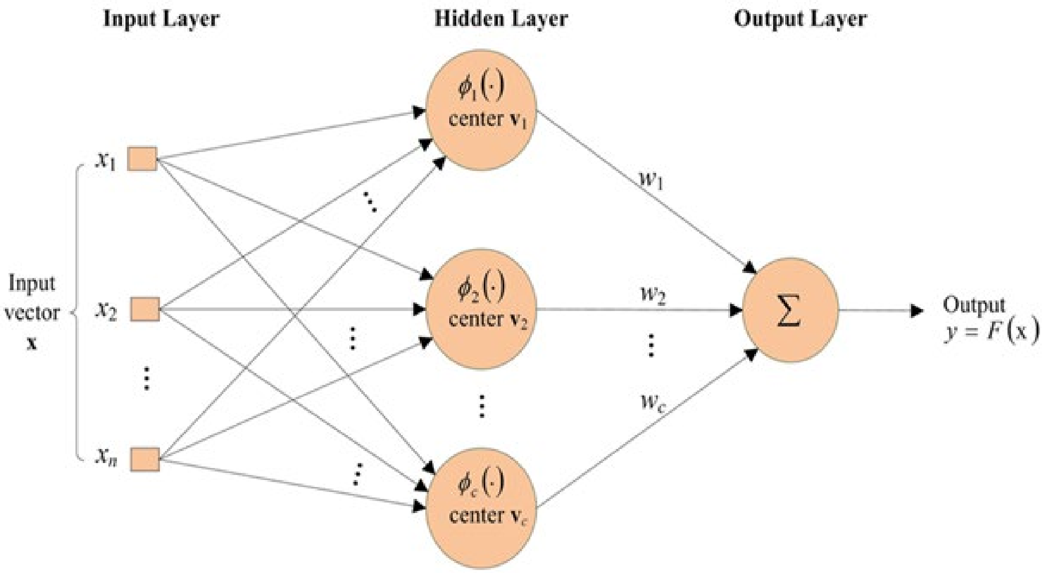

Concentration profile of TDS(o) Rougher Circuit Stage 1

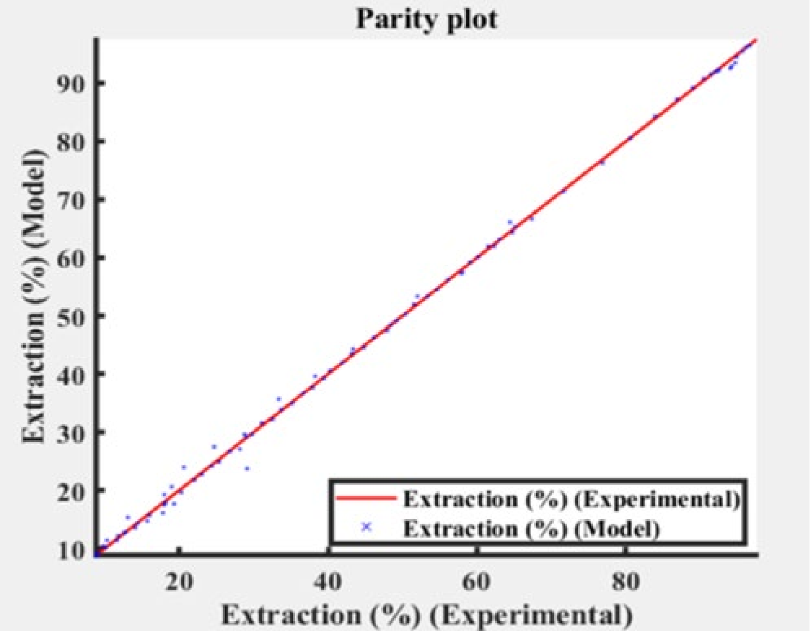

Concentration profile of TDS(a) Rougher Circuit Stage 3

- First-principles, dynamic model of the counter-current multi-stage, multi-component solvent extraction system followed by stripping
- Model results compare well with the data from the UKy pilot plant data.

Solvent Extraction Summary

- Using the UKy pilot plant data, a data-driven model for the distribution coefficient as a function of pH and extractant concentration.
- Future work will include development of higher fidelity models of the solvent extraction system, inclusion of more solvent materials in the database, validation of the dynamic model of the solvent extraction system, control system development for feed and other disturbance rejection, and development of a model for the membrane solvent extraction system with validation using the NETL in-house data.





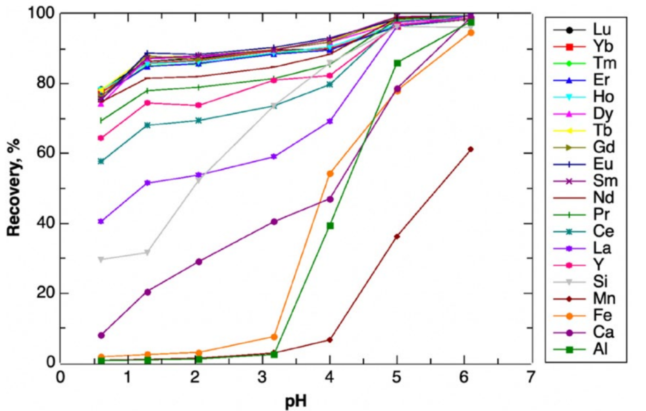
Precipitation Summary

Feed Composition Data Used

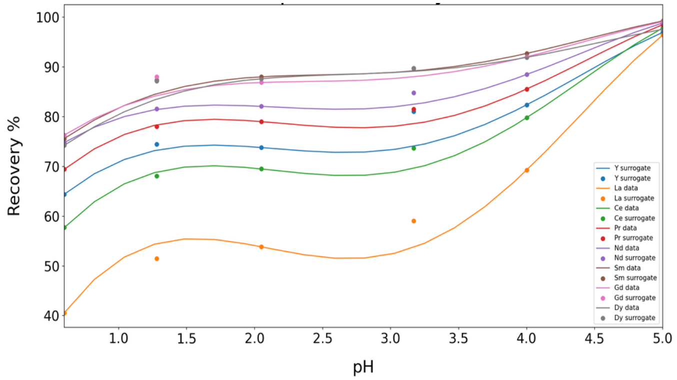
- Input is fed from the solvent extraction system
- Output would need to be validated from inputs and specific pH, acid dosage, and reaction time

Model Equations and Data for Unit Process

- Equilibrium reactor with fixed partition coefficients
- Partition coefficients calculated from data in the literature
- A Hybrid Experimental and Theoretical Approach to Optimize Recovery of Rare Earth Elements from Acid Mine Drainage Precipitates by Oxalic Acid Precipitation, Y. Wang, P. Ziemkiewicz, and A. Noble, Minerals 2022, 12, 236
- One problem is that since it is not a multivariable study, the surrogate model can only be created for one variable



A Hybrid Experimental and Theoretical Approach to Optimize Recovery of Rare Earth Elements from Acid Mine Drainage Precipitates by Oxalic Acid Precipitation, Y. Wang, P. Ziemkiewicz, and A. Noble, Minerals 2022



Surrogate model results

Precipitation Summary (Model Validation)

Validation Data Used

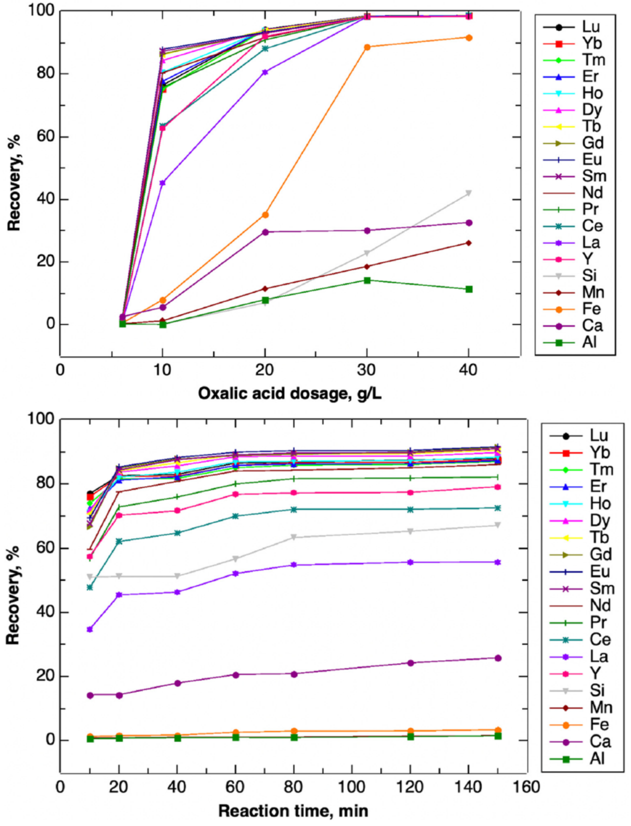
- The validation test are based on partition calculated from data
- The model is validated with this data as the surrogate model being built will be based on this data as it is a full data base
- Paper recovery %

Additional Data Required

To build the surrogate and test with UK data, we will require data for:

- recovery vs pH,
- recovery vs acid dosage
- recovery vs reaction time

Need multivariable data set where (pH, dosage, reaction time, contaminants) are varied



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NETL Team (Jinliang Ma)

REE Oxalate Roaster Summary

Feed Composition Data Used

- Solid feed: PrecipitateParametersData, with optional moisture content
- Gas feed: Generic ideal gas mixture (N_2, O_2, CO_2, H_2O)

Model Equations and Data for Unit Process

- Currently 100% conversion to oxides
- Full species mass balance and energy balance
- User specified solid recovery (default 95%)

Validation Data Used

- UKy REESim excel spreadsheet

Additional Data Required

- Conversion and recovery for individual species as functions of temperature and other operation conditions, if available

- $RE_2(C_2O_4)_3 \cdot xH_2O + 1.5O_2 \rightarrow RE_2O_3 + 6CO_2(g) + xH_2O(g)$
- **Impurities:**
  - $Fe_2(C_2O_4)_3 \cdot 2H_2O \rightarrow Fe_2O_3$
  - $Al_2(C_2O_4)_3 \cdot H_2O \rightarrow Al_2O_3$

Ion Exchange Summary

Feed Composition Data Used

- Leaching process outlet from UKy flowsheet

Model Equations and Data for Unit Process

- Modified version of unit model from WaterTAP platform
- Data for unit operation and resin from references [1] and [2]

Validation Data Used

- No validation available, but model was tested using batch experimental data from literature (references in unit model)

Additional Data Required

- No additional data required

References:

[1] S. Mondal, A. Ghar, A.K. Satpati, P. Sinharoy, D. K. Singh, J.N. Sharma, T. Sreenivas, and V. Kain, Recovery of rare earth elements from coal fly ash using TEHDGA impregnated resin, Hydrometallurgy 185, 2019, 93-101.

[2] Dupont Amberlite XAD(TM)7HP Polymeric Adsorbent. Product Data Sheet Polymeric Adsorbent. February 2023. URL:

https://www.dupont.com/content/dam/dupont/amer/us/en/water-solutions/public/documents/en/IER-AmberLite-XAD7HP-PDS-45-D00782-en.pdf

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PrOMMiS Subtask 2.2: CM & REE Process Cost Estimation

Brandon Paul, Miguel Zamarripa, Debangsu Bhattacharyya, Alison Fritz

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Bottom-Up Costing Approach

- Missing data or capital costing correlations not available for required equipment sizes and process performance.
- New technologies – TRL < 3, process technology/process do not exist.
- Leverage existing data to build capital cost based on unit operations in the process or manufacturing steps (i.e., Solvent extraction: vessel, column hydraulics, etc.)

Cost for processing components and core equipment

Penalize materials of constructions and design factors.

Calculate indirect costs (based on existing vendor quotes)

Bottom-Up Costing Approach: Economy of Numbers

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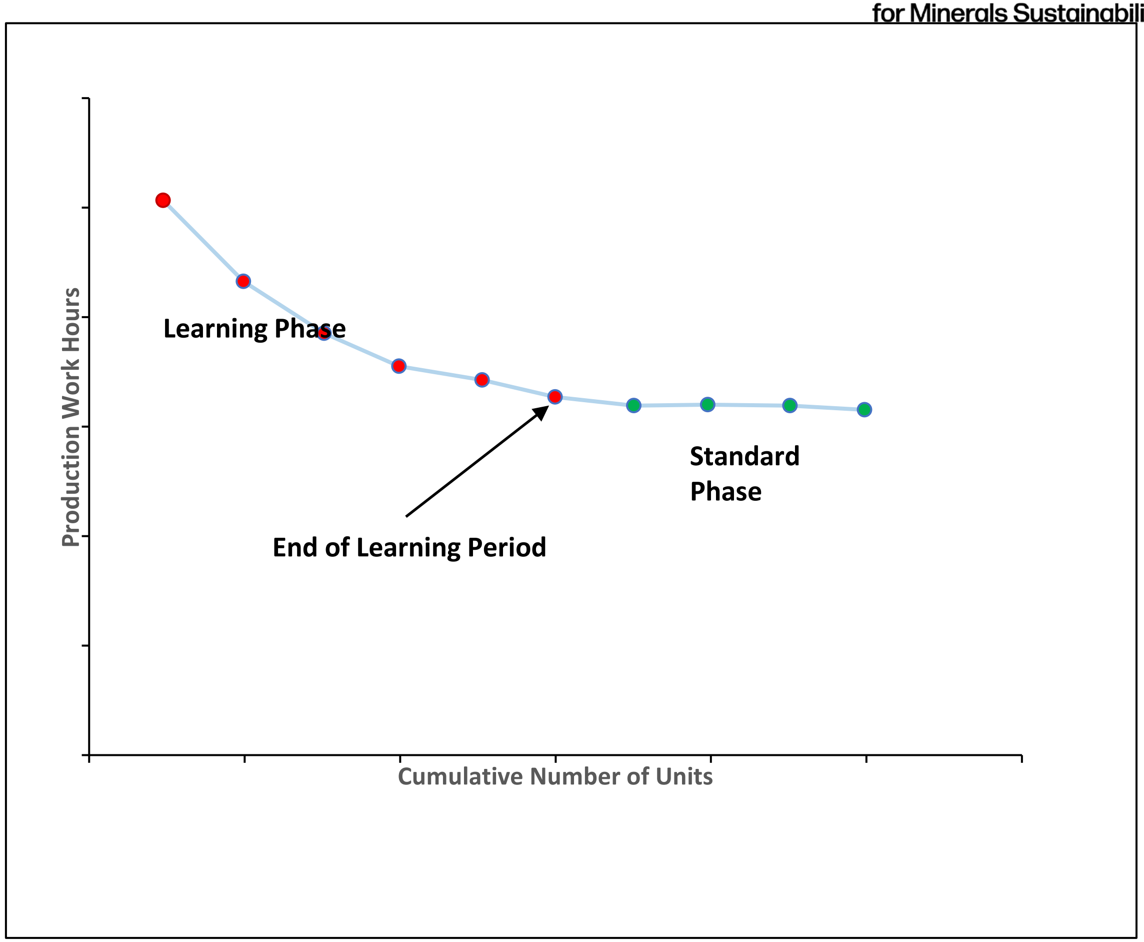
- For a comprehensive cost estimate and future profitability of novel/First-Of-A-Kind (FOAK) equipment, it is imperative to factor in the economy of number which affects the labor costs.
- Due to consistent proficiency improvement, labor hours reduce as the cumulative production quantity rises.
- Following a preliminary CAPEX and OPEX estimate for a hydrogen decrepitation furnace unit, a comprehensive bottom-up cost estimate is underway.



CM/REE Costing Framework

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Capital Cost and Project Cost Calculations

https://github.com/prommis/prommis/tree/main/src/prommis/uky/costing

Variable	Definition	Expression	Units
BEC	Bare Erected Cost	$scaled\ cost = no.equipment * reference\ cost * \left(\frac{scaled\ parameter}{reference\ parameter}\right)^{\alpha} * \left(\frac{flowsheet\ cost\text{–}year\ factor}{reference\ cost\text{–}year\ factor}\right)$	Million $
TPC	Total Plant Cost	$TPC = BEC + installation\ costs + other\ costs$	Million $
TOC	Total Overnight Capital	$TOC = TPC + Owner's\ cost$ (e.g. royalties, preproduction, inventory, financing)	Million $
TASC	Total As Spent Capital	$TASC = TOC * 1.144$	Million $
Annualized Cost	Annualized Capital Cost	$Annualized\ Cost = 0.1002 * TASC$	Million $/yr

O&M Cost Calculations

Fixed O&M Cost [MM$/yr]	Notes
Annual Labor (split into Operating and Technical labor)	$labor\ rate * operators\ per\ shift * shifts\ per\ day * operating\ days\ per\ year * (1 + labor\ burden)$
Maintenance & Gen. Materials	2% of TPC
Quality Assurance & Control	10% of Annual Operating Labor
Sales, Patenting & Research	0.5% of Total Revenue
Admin & Support Labor	20% of Annual Operating Labor
Property Taxes & Insurance	1% of TPC
Membrane Materials	Function of area; calculated by WaterTAP

Variable O&M Cost [MM$/yr]	Notes
Consumables	$flowrate * price$ OR $waste\ flowrate * disposal\ cost$
- Power requirements	$0.07/kWh; can specify efficiency %, defaults to 85%
- Waste disposal costs	Solid waste, precipitate waste, dust & volatiles
- Other chemicals	Water, diesel, bioleaching solution, H2SO4, natural gas for roasting, reagents for precipitation
Land Ownership	Leasing costs per year
Plant Overhead	20% of Total Fixed + Consumables + Land Ownership

Levelized Cost of Recovery ($\frac{\$}{kg-year}$) = Levelized capital cost + Levelized annual fixed O&M cost + Levelized annual variable O&M cost + Levelized REE transport cost

Supported Unit Operations

Equipment Type	Coefficient	Exponent	Process Parameter	Units	Source
Front End Loader (2 yd^3)	147400	1	Number of Units	dimensionless	3
Front End Loader (10 yd^3)	945700	1	Number of Units	dimensionless	3
Bucket Elevator	322000	1	Number of Units	dimensionless	2
Jaw Crusher	651	1.25	Power Draw	hp	2
VSI Crusher	3247	0.68	Power Draw	hp	3
Roll Crusher	1120	0.8484	Power Draw	hp	2
Vibrating Screen	1002	0.9093	Screen Area	ft^2	2
Storage Bins	4441	0.6185	Storage Capacity	ton	2
Dry Ball Mill	35000	0.556	Power Draw	hp	2
PE Tanks	1.3812	0.9492	Storage Capacity	gal	2
Steel Tanks	179	0.5624	Storage Capacity	gal	3
Tank Mixer	10640	0.564	Power Draw	hp	2
Elevator Motor	1719.5	0.6592	Power Draw	hp	2
Process/Slurry Pump	2152	0.3814	Feed Rate	gal/min	2
Thickener	280	0.8023	Thickener Area	ft^2	2
Filter Press	6068	0.72	Filter Volume	ft^3	2
Conveyor	2092	0.5491	Throughput	ton/hr	2
Roaster	390000	0.48	Heat Input	MBTU/hr	2
Gas Scrubber	6.6039	0.9414	Gas Rate	ft^3/min	2
Spray Chamber Quencher (7000-60000 cfm)	23835	0.11400	Gas Rate	ft^3/min	5
Spray Chamber Quencher (60000-230000 cfm)	914.53	0.4108	Gas Rate	ft^3/min	5
Chiller	97585	0.6	Heat Input	MBTU/hr	2
Solution Heater	25929	0.953	Heat Input	MBTU/hr	2
Belt Filter	207819	0.249152	Throughput	ton/hr	3
BioLeach Tanks	2405	0.4203	Storage Capacity	gal	4
Blower	197	0.4625	Gas Rate	ft^3/min	4
Mixer Settler	9182	0.45	Volume	gal	2
HDD Recycling Shredder (2700 drives/hour)	50000	1	Number of Units	dimensionless	6
HDD Recycling Furnace (Hydrogen Decrepitation)	64723	0.6197	Heat Input	MBTU/hr	7

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- Sourced from Uky REE Recovery Reports [2,3,4] and literature[5,6,7]
- Fit capital cost correlations in the form

$$Cost = Coefficient * Parameter^{Exponent}$$

- Membranes (e.g. nanofiltration, reverse osmosis, ion exchange) costed via WaterTAP

[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.

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PrOMMiS Subtask 2.3: Advanced Optimization Capabilities for End-of-Life Products

Ana Torres, Christopher Laliwala

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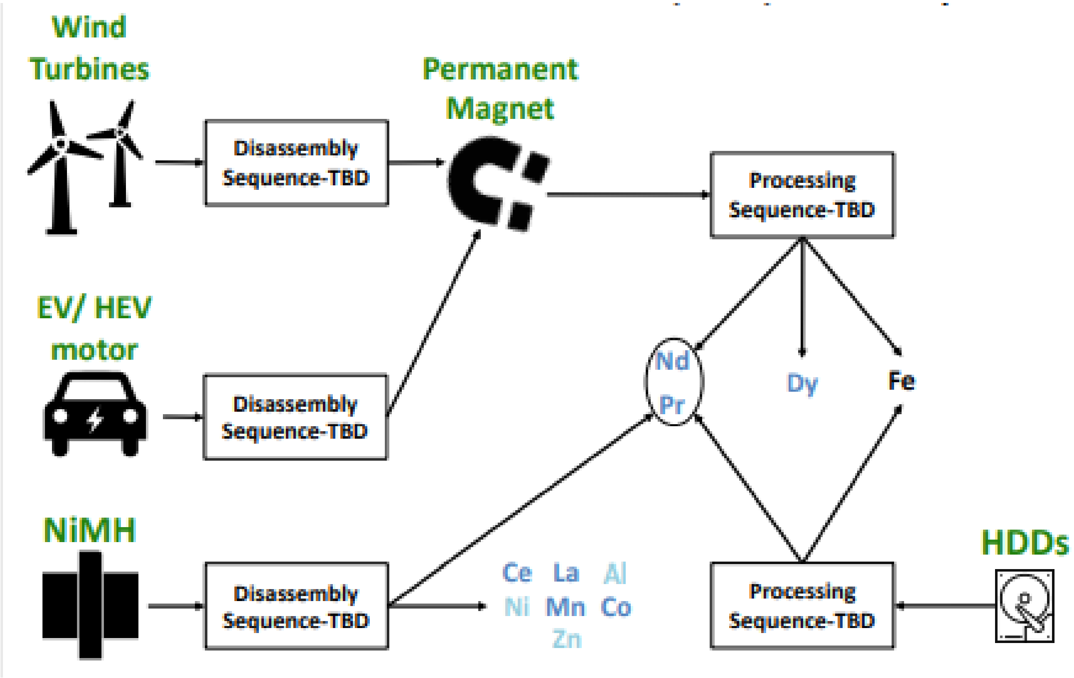
End Of Life Products - Introduction

- Approach: superstructure-based conceptual design EoL to REO
- Long term goal: EoL feedstock agnostic process

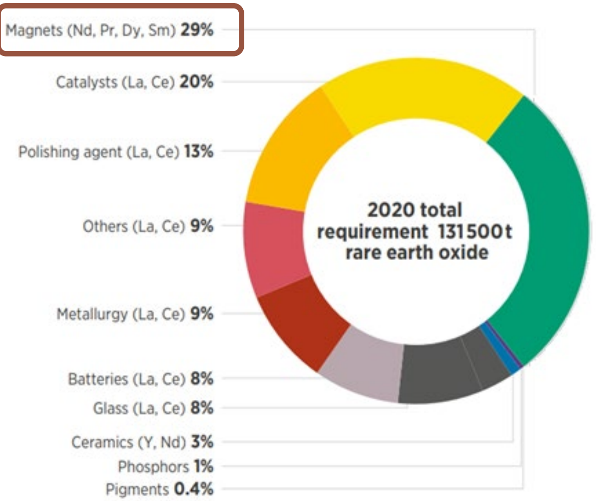


Activities

1. Prioritization of EoL; Quantification of feedstock potential
2. Literature Search: processing pathways
3. Superstructure development, modeling, and optimization
4. Process flowsheet development, simulation, and economic analysis (if not available in literature)
5. Application to 2 case studies: Permanent magnets from HDD EV/HEV

EoL Products – (1) Prioritization

- Setting priorities



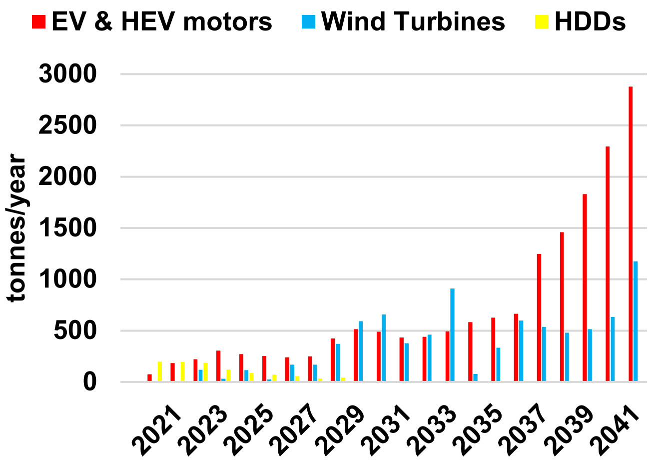
REO	Price (USD/KG)	
	2018	2021
La	2	2
Ce	2	1.5
Nd	50	143
Dy	179	452
Pr	63	140

Figure: Dolf Gielen, & Martina Lyons. (2022). *Critical Materials For The Energy Transition: Rare Earth Elements.*, IRENA

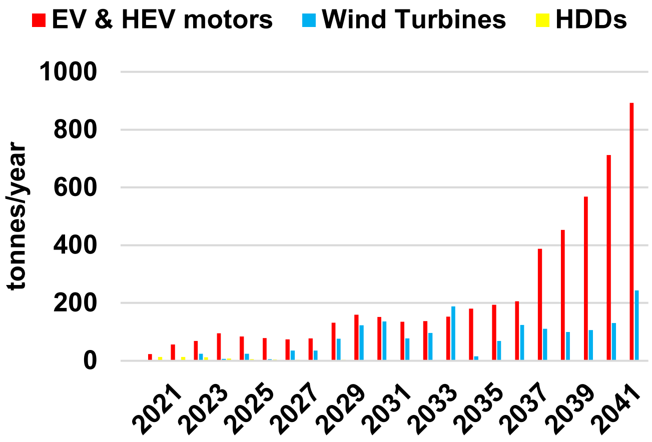
=> Permanent Magnets

- Quantification of feedstock potential in the USA

Nd/Pr Available for Recycling



Dy Available for Recycling



Figures made on the basis of sale projections/ technology adoption/ lifetime/ composition. Lower and upper estimates were obtained.

References:

- Blast et al. (2014). Recycling von Komponenten und strategischen Metallen aus elektrischen Fahrantrieben.
- Alves Dias, P., Bobba, S., Carrara, S., Plazzotta, B. (2020), The role of rare earth elements in wind energy and electric mobility, EUR 30488 EN, Publication Office of the European Union, Luxembourg, ISBN 978-92-79-27016-4.
- Sprecher, B., Kleijn, R., & Kramer, G. J. (2014). Recycling Potential of Neodymium: The Case of Computer Hard Disk Drives. Environmental Science & Technology, 48(16), 9506–9513. https://doi.org/10.1021/es501572z
- Dolf Gielen & Martina Lyons. (2022). Critical Materials For The Energy Transition: Rare Earth Elements.
- LDV Total Sales of PEV and HEV by Month (updated through May 2023). (2023). https://www.anl.gov/esia/reference/light-duty-electric-drive-vehicles-monthly-sales-updates-historical-data

EoL Products – (2) Processing Pathways

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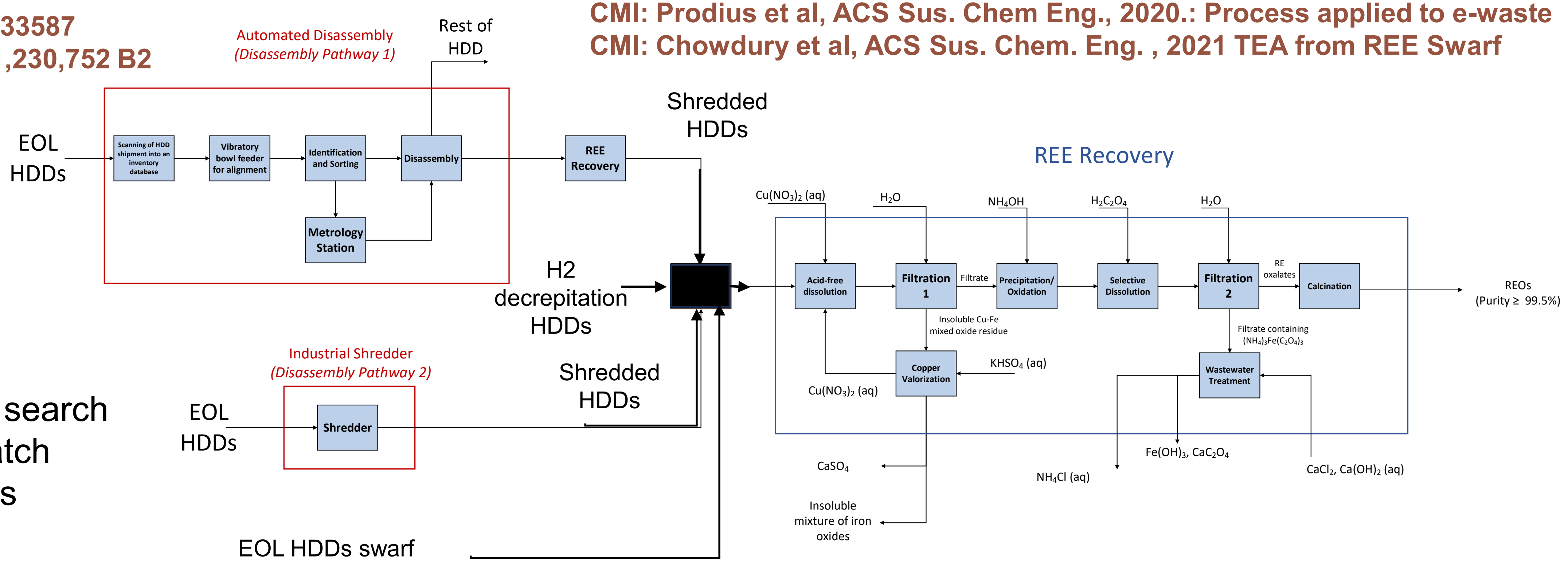
- Data: Literature, Oak Ridge National Labs, Critical Minerals Innovation Hub
- Example for HDDs:

Iowa U: Patent US 10,648,063 B2 Dissolution and separation of rare earth metals
CMI: Prodius et al, ACS Sus. Chem Eng., 2020.: Process applied to e-waste
CMI: Chowdury et al, ACS Sus. Chem. Eng. , 2021 TEA from REE Swarf

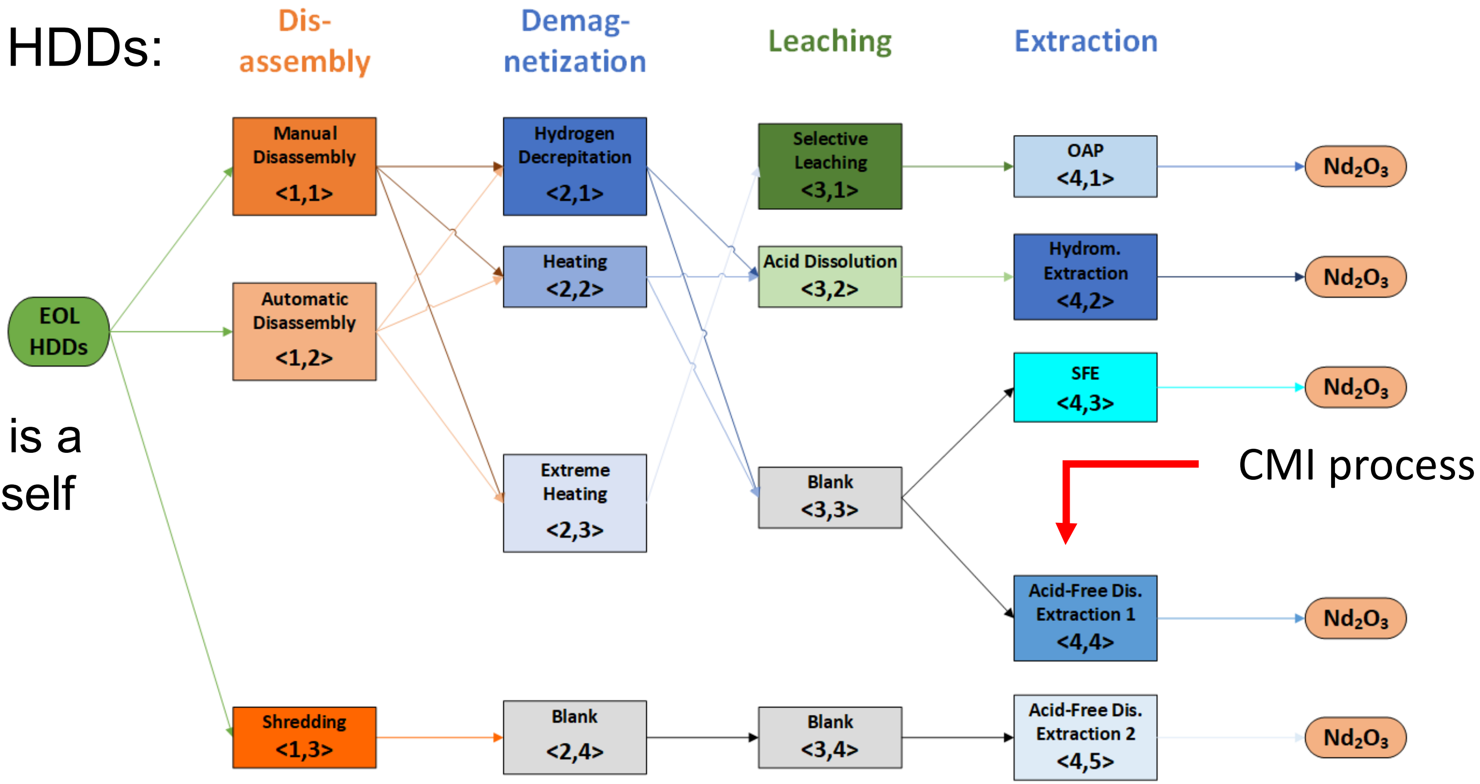
ORNL- Pub133587
Patent US 11,230,752 B2



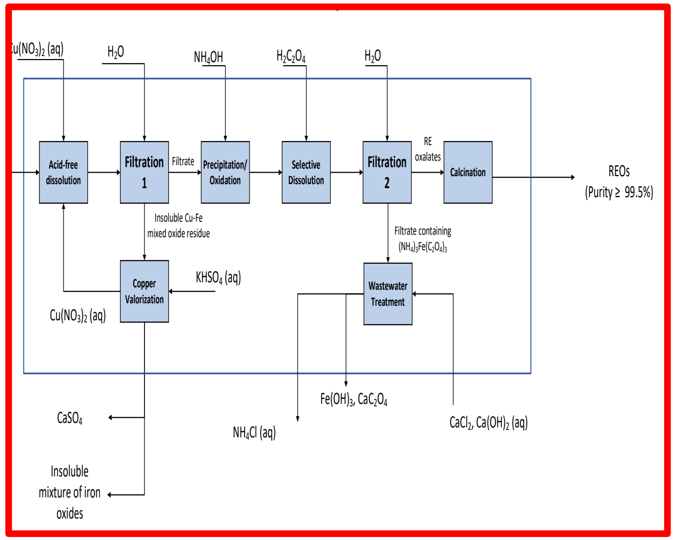
- Expand literature search
- Mix & Match processes

EoL Products – (3) Superstructure

- Organize existing data in processing stages, identify competitive technology options at each stage
- Identify new connections
- Example for HDDs:



- Each block is a flowsheet itself



EoL – (3) Superstructure Modeling

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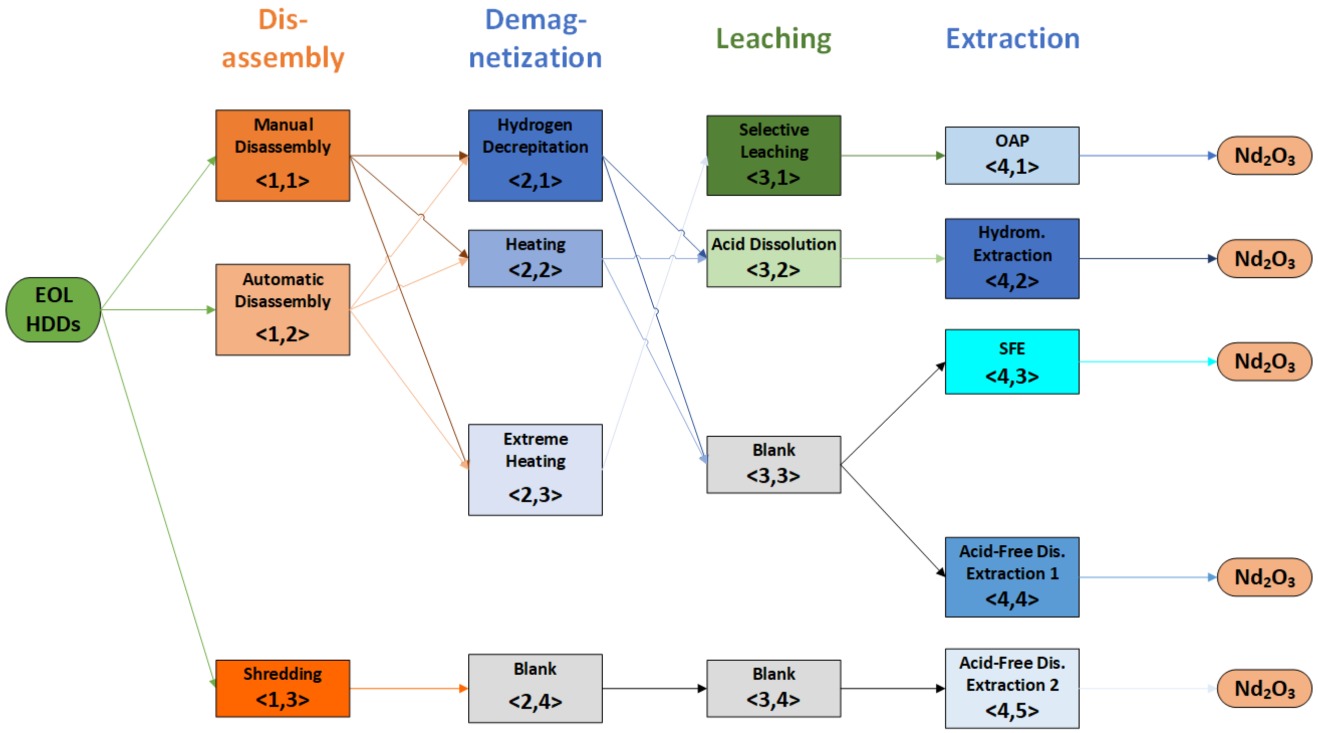
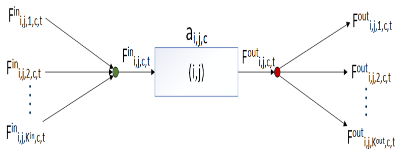
- Superstructures are modeled as networks



- Technology options → nodes → binary variable *y =1* if in optimal pathway
- Arcs: flows of each species
- Inlet/ Outlet flows → MB from simulations



$$\sum_{k=1}^{K^{in}} F^{in}_{i,j,k,c,t} = F^{in}_{i,j,c,t} \qquad F^{out}_{i,j,c,t} = \sum_{k=1}^{K^{out}} F^{out}_{i,j,k,c,t}$$

$$F^{out}_{i,j,c,t} = a_{i,j,c} * F^{in}_{i,j,c,t}$$

- Allowed connections: logical constraints
- Objective function: NPV
  - Installed equipment cost and OPEX data: from TEA: existing in the literature or our own (via Aspen Tech)
  - Framework: Seider et al.

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EoL – (4) Process flowsheet development and costing

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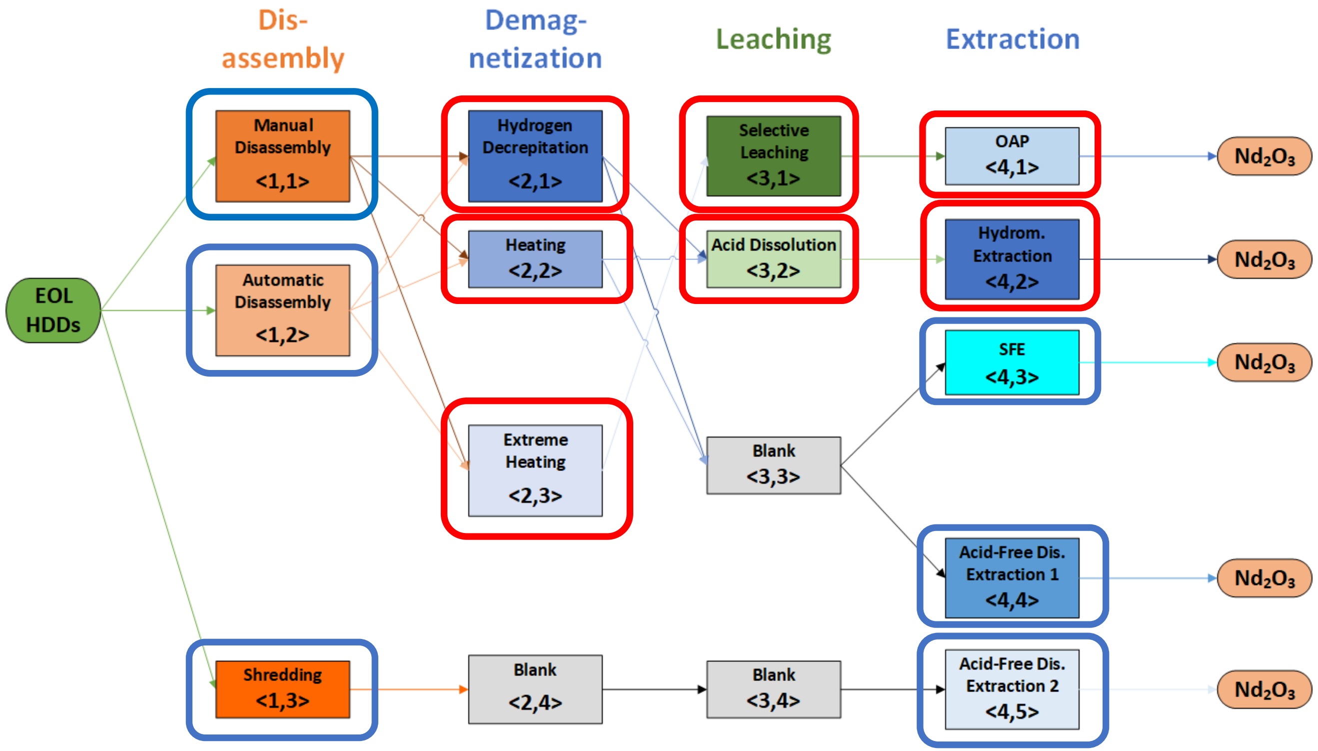
- Only for those for which we could not find TEA in the literature published data



- OPEX and CAPEX in literature
- Required OPEX and CAPEX estimation

- **Estimations:**
  - **Aspen Plus flowsheet development**
  - **Aspen Economics: Equipment cost**

EoL – (4) Process flowsheet development and costing- Example

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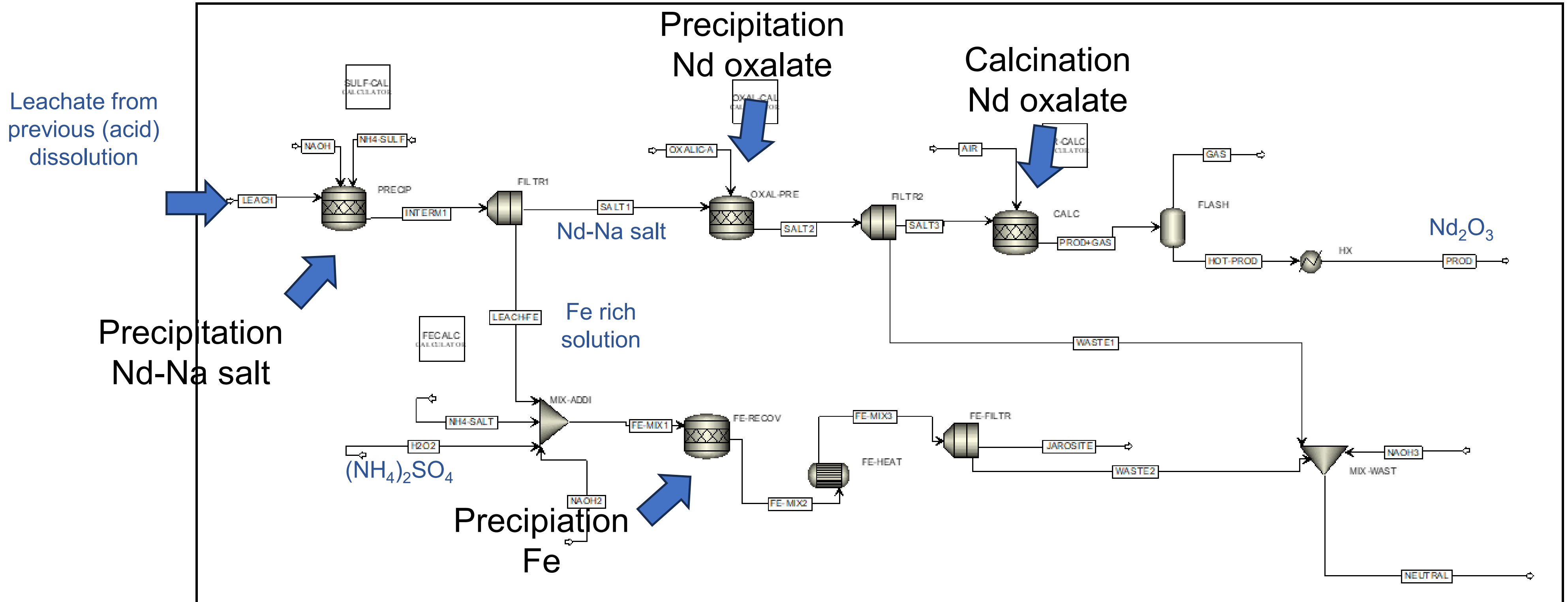

Leachate from previous (acid) dissolution

Precipitation Nd-Na salt

Precipitation Nd oxalate

Nd-Na salt

Calcination Nd oxalate

Nd_2O_3

Fe rich solution

$(NH_4)_2SO_4$

Precipitation Fe

Figure 5: Aspen simulation built for the hydrometallurgical process built using reaction yield data from [24].

24. Lyman, J.W., Palmer, G.R.: Recycling of Rare Earths and Iron from NdFeB Magnet Scrap. High Temperature Materials and Processes. 11, 175–188 (1993). https://doi.org/10.1515/HTMP.1993.11.1-4.175

EoL (5) Case Study: Recovery REO from HDDs

(C. Laliwala, AI Torres, submitted FOCAPD 2024)

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- Optimal solution for different collection rates (from future and past wastes) and REO prices;

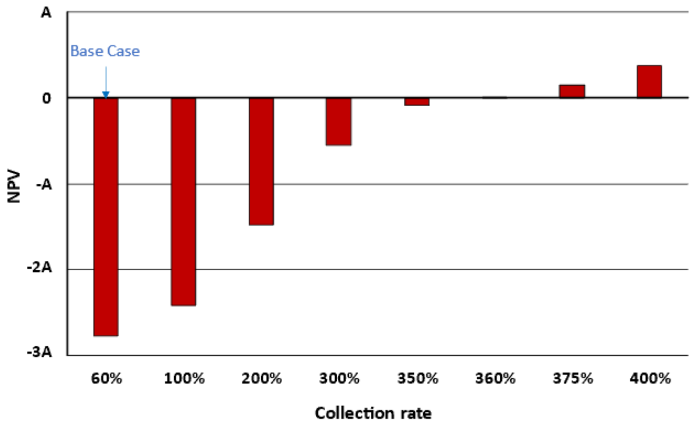


Figure 6: NPV for a varying collection rate. The base case is a collection rate of 60% and no recycling of EOL HDDs generated prior to plant production. The NPV break-even point was found to occur at ~360%. Numerical values are not reported to preserve confidentiality.

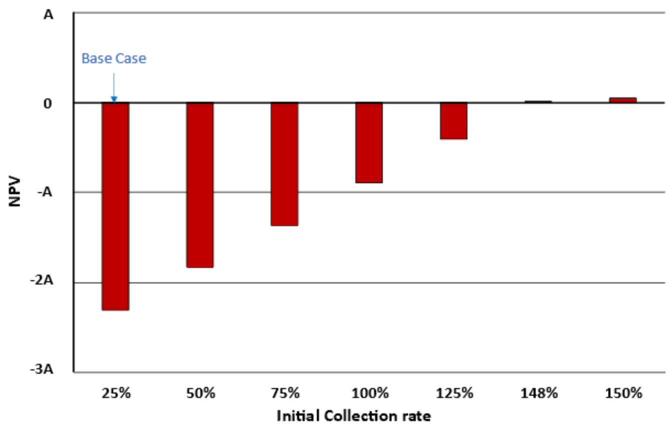


Figure 7: NPV for a varying initial collection rate. The base case has a collection rate of 60% and an initial collection rate of 25%. The NPV break-even point was found to occur at ~148%. Numerical values are not reported to preserve confidentiality.

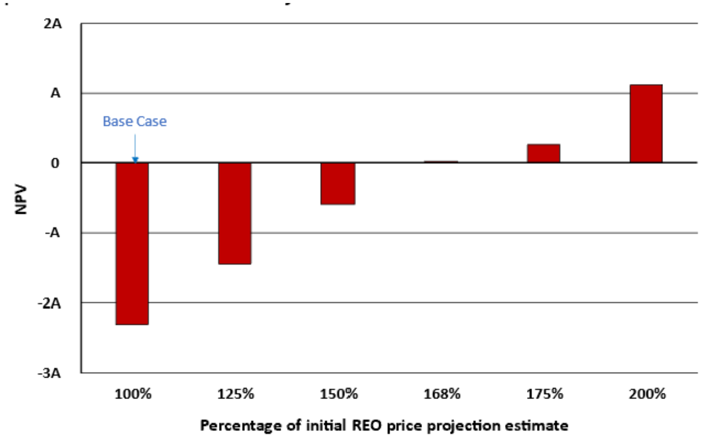


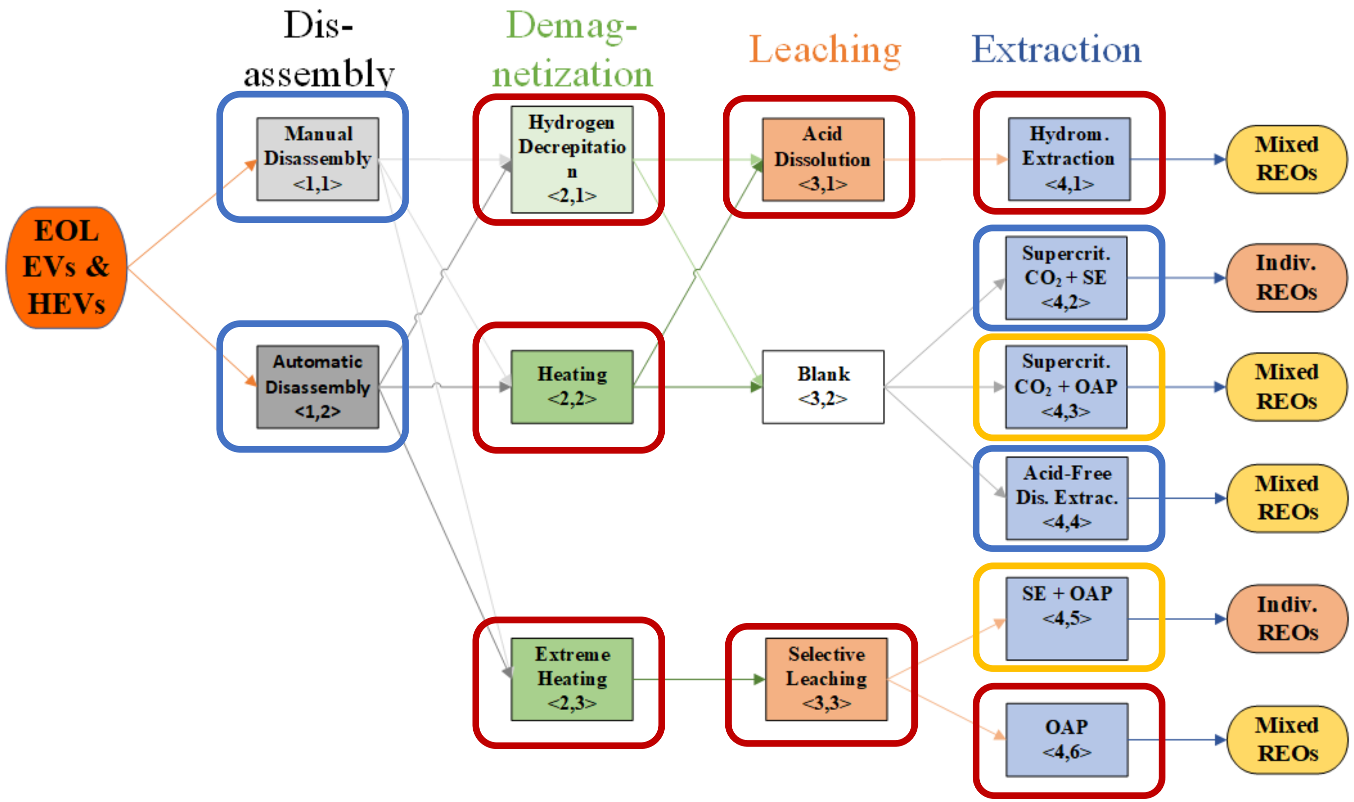
Figure 8: NPV for varying percentages of the initial REO price projection estimate. The NPV break-even point was found to occur at ~168%. Numerical values are not reported to preserve confidentiality.

- ONL Shredding + CMI acid-free dissolution always optimal pathway

EoL (5) Case Study: Recovery REO from HDDs

(C. Laliwala, Al Torres, ESCAPE 2024, accepted)

- Slightly different superstructure;



- **OPEX and CAPEX in literature**
- **Required in house estimation**
- **Mix of literature and estimation**

EoL (5) Case Study: Recovery REO from HDDs

(C. Laliwala, Al Torres, ESCAPE 2024, accepted)

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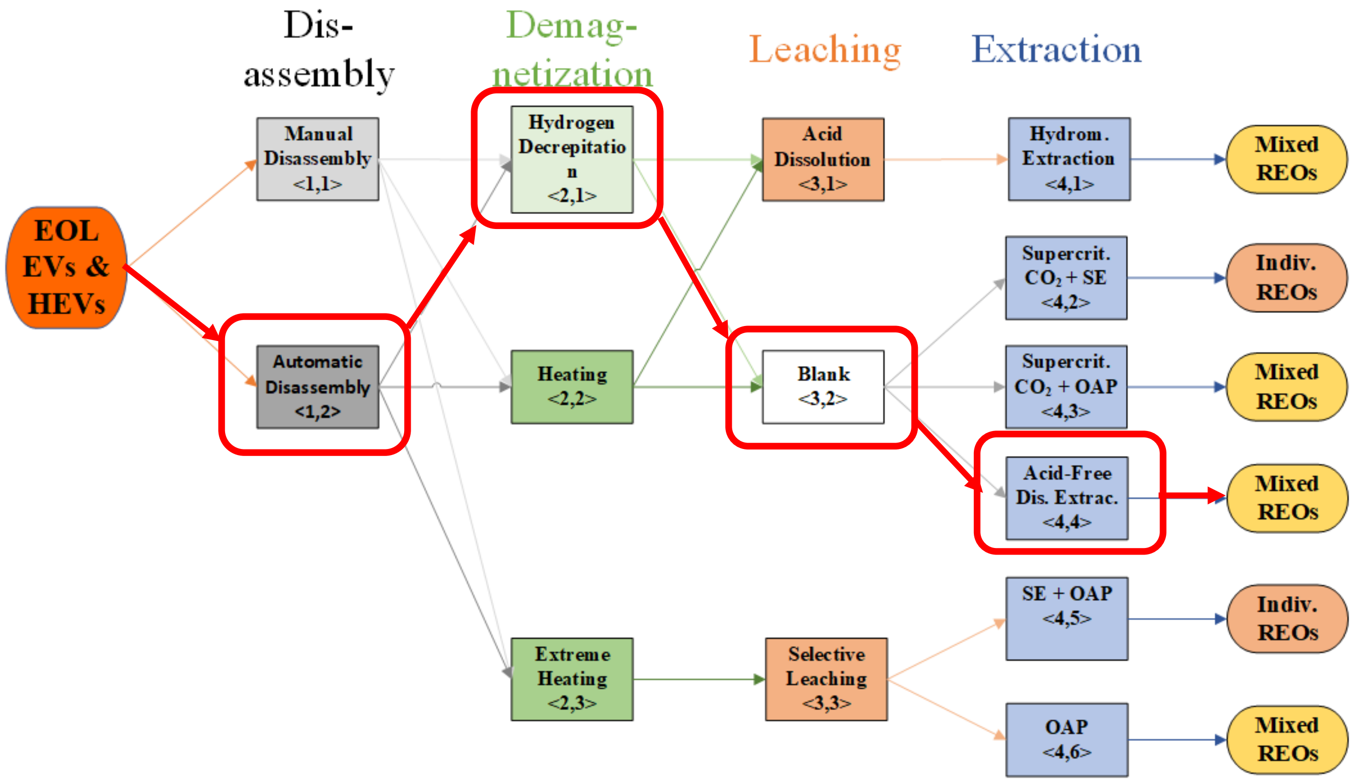
- Slightly different superstructure;



- Base case: plant recycles 10 % of all EOL EVs and HEVs in the U.S. each year.
- Optimal pathway:
  - Automatic disassembly
  - Hydrogen decrepitation
  - Acid Free dissolution
- NPV positive

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EoL (5) Case Study: Recovery REO from HDDs

(C. Laliwala, AI Torres, ESCAPE 2024, accepted)

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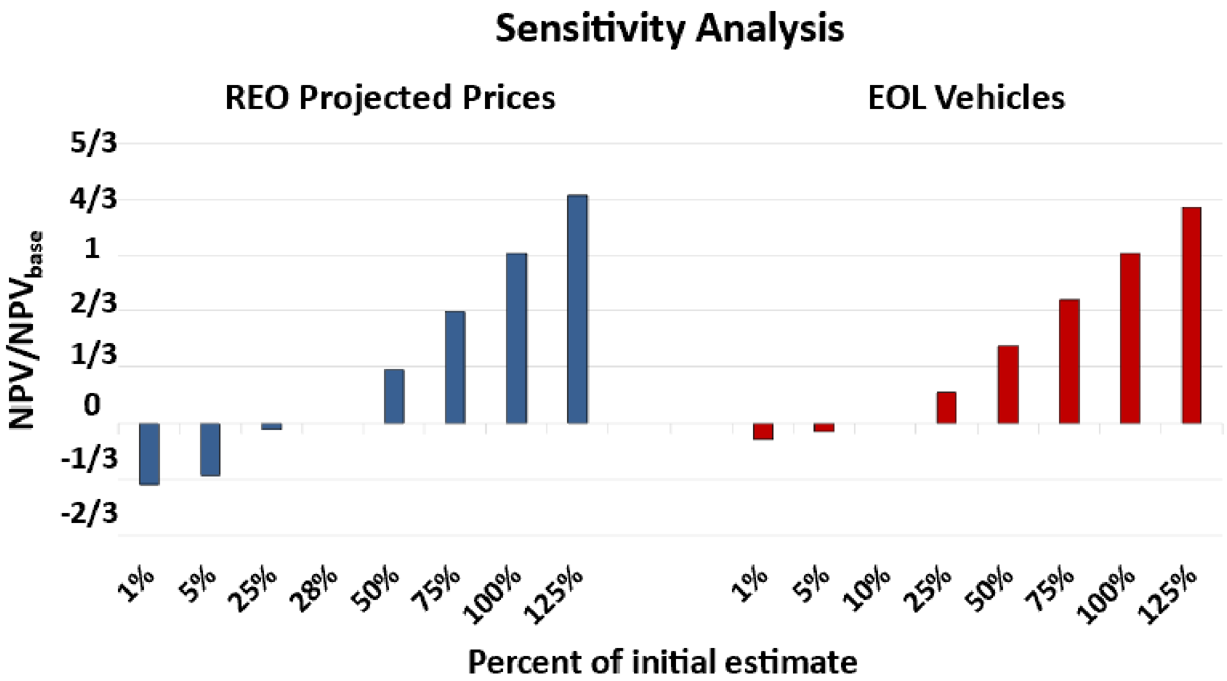

Figure 3. Sensitivity analysis for the product projected prices, and amount of EOL vehicles available for recycling. Values are reported normalized to the base case optimal solution to preserve confidentiality.

- Automatic disassembly, hydrogen decrepitation, acid-free dissolution were always selected as optimal

Benchmark Surrogate Modeling Approaches

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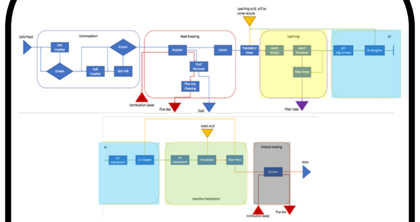
Predictability | **Solvability**



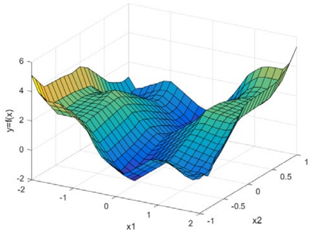
Process simulator/data
- Complex units (columns, reactors)
- Superstructure

⇨

Interact with CPU/GPU clusters for computation

Train surrogate models
Machine learning

⇨



Trained models

⇨

$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & g(x) = 0 \\ & x \in [x^l, x^u] \end{aligned}$$

Embed in optimization

⇨

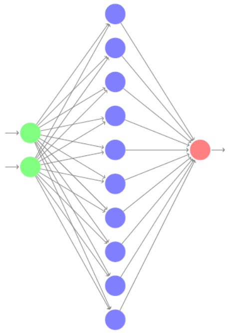
x^*, f^*

Optimal solutions found

ALAMO

PySMO

OMLT



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Future Work

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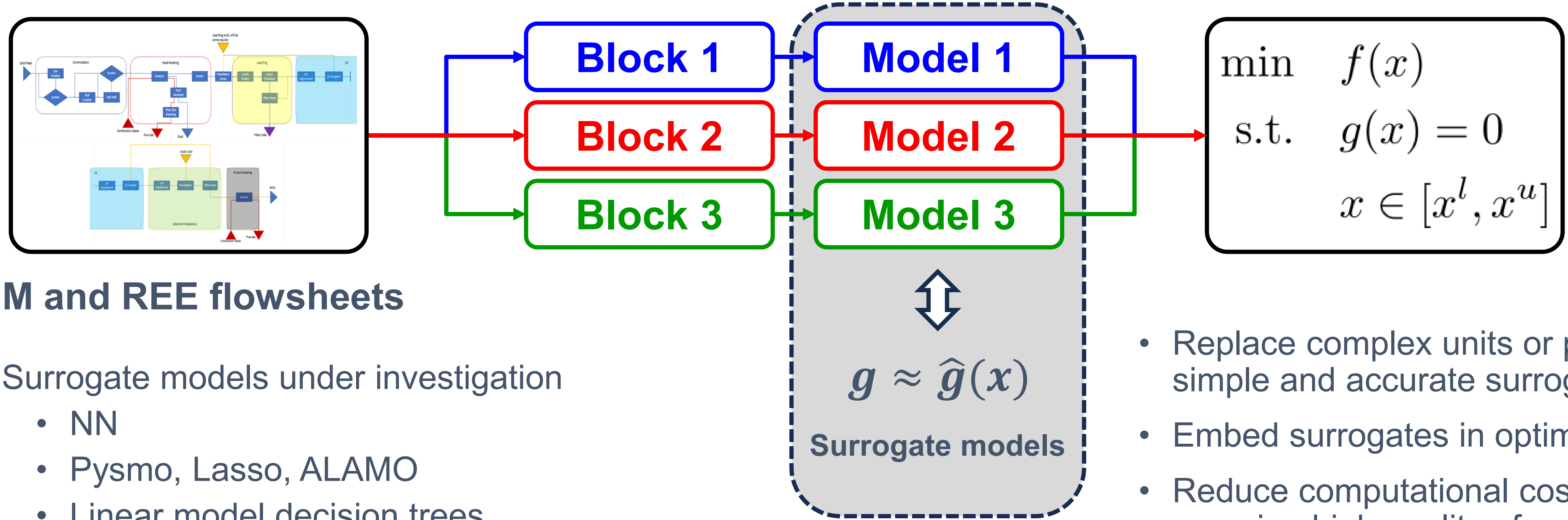
System simulation

Disaggregation and modeling

Optimization



$$\min \quad f(x)$$
$$\text{s.t.} \quad g(x) = 0$$
$$x \in [x^l, x^u]$$

$$g \approx \hat{g}(x)$$

Surrogate models

CM and REE flowsheets

- Surrogate models under investigation
  - NN
  - Pysmo, Lasso, ALAMO
  - Linear model decision trees
  - Symbolic regression

- Replace complex units or parts with simple and accurate surrogates
- Embed surrogates in optimization
- Reduce computational cost while ensuring high quality of solutions

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Overview – What You'll Hear

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Process Optimization and Modeling for Minerals Sustainability

- Coal to Rare Earth Elements – University of Kentucky
  - Process Model & Unit Operations
  - Cost Model Development
- Membranes
  - Process Model Development & Application Summary
  - Optimization Cases Studies
  - Enabling Scale-Up: Model-Design of Experiments
- End of Life Pathways – Magnets & Hard Drives
  - Process Model
  - Cost Model
  - Superstructure Optimization & Findings
- Ongoing / Parallel Efforts
  - Identifying Model Uncertainty
  - Benchmark Surrogate Modeling Approaches
- Model Usability & Distribution

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Open-Source Platform

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- Website: https://idaes.org/research/application-areas/
- GitHub repository:
  - https://github.com/prommis/prommis
- Documentation:
  - https://prommis.readthedocs.io/en/latest/
- Bi-Weekly Software Engineering teleconferences coordinating development
- Targeting quarterly internal/public releases
- IPMP in progress for fully open-source license
- Overview video: coming soon!

PROMMIS Contributions

Path 1: contribute to prommis repository

Download idaes-pse repository → Model Development → Open GitHub PR → Merge Code

Download idaes-pse repository	Model Development	Open GitHub PR	Merge Code
Get prommis Follow standards and examples	Local system Build and test models	Contribute models, tests, and examples to prommis	Rigorous testing and structural analysis

Path 2: create GitHub repository and make idaes-pse and prommis a dependency

Usability

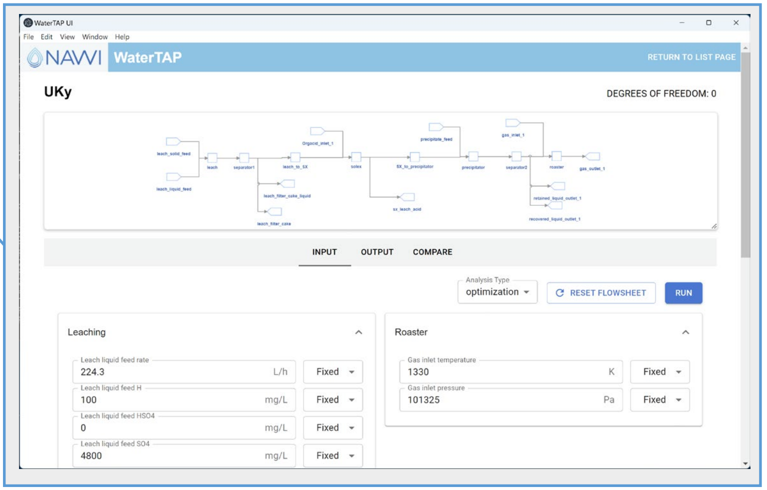
PROMMIS
Process Optimization and Modeling for Minerals Sustainability

Leverage NAWI/WaterTAP UI infrastructure
- Define key model inputs and outputs
- Distribute UI with PROMMIS flowsheets
- Parallel parameter sweeps (sensitivity analysis)

Gather requirements for UIs specific to WT
- E.g., conceptual design model configuration

Leverage IDAES core flowsheet visualization
- View flowsheet diagrams
- PROMMIS models <- new diagnostics capabilities

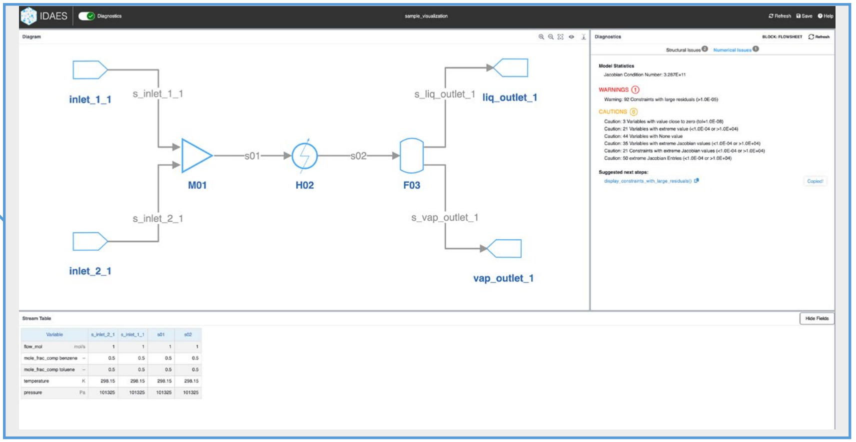
Assist team with Jupyter Notebooks and online documentation



Analysis Type: optimization

Leaching
- Leach liquid feed rate: 224.3 L/h — Fixed
- Leach liquid feed H: 100 mg/L — Fixed
- Leach liquid feed HSO4: 0 mg/L — Fixed
- Leach liquid feed SO4: 4800 mg/L — Fixed

Roaster
- Gas inlet temperature: 1330 K — Fixed
- Gas inlet pressure: 101325 Pa — Fixed



Model Statistics
Jacobian Condition Number: 3.287E+11

WARNINGS ①
Warning: 92 Constraints with large residuals (>1.0E-05)

CAUTIONS ⑥
Caution: 3 Variables with value close to zero (tol=1.0E-08)
Caution: 21 Variables with extreme value (<1.0E-04 or >1.0E+04)
Caution: 44 Variables with None value
Caution: 35 Variables with extreme Jacobian values (<1.0E-04 or >1.0E+04)
Caution: 21 Constraints with extreme Jacobian values (<1.0E-04 or >1.0E+04)
Caution: 50 extreme Jacobian Entries (<1.0E-04 or >1.0E+04)

Suggested next steps:
display_constraints_with_large_residuals()

Stream Table

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
pressure	Pa	101325	101325	101325	101325

Capital Cost Estimation Approach

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for Minerals Sustainability

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

$$\mathrm{SC} = \mathrm{RC}\left(\frac{\mathrm{SP}}{\mathrm{RP}}\right)^{\mathrm{EXP}}$$

$$\mathrm{EXP} = \frac{\ln\left(\frac{\mathrm{RC1}}{\mathrm{RC2}}\right)}{\ln\left(\frac{\mathrm{RP1}}{\mathrm{RP2}}\right)}$$

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

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

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

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PrOMMiS Costing Library (to date)

PROMMIS
Process Optimization and Modeling for Minerals Sustainability

- 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

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 – ith unit operations in the 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.