# PrOMMiS:
# Applying Novel Modeling Methods to Accelerate CM $RD^3$

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**Carnegie Mellon:** Carl Laird **WVU**: Debangsu **Notre Dame**: Alexander Dowling

**Lawrence Berkeley National Laboratory:** Daniel Gunter **Sandia National Laboratory:** John Siirola

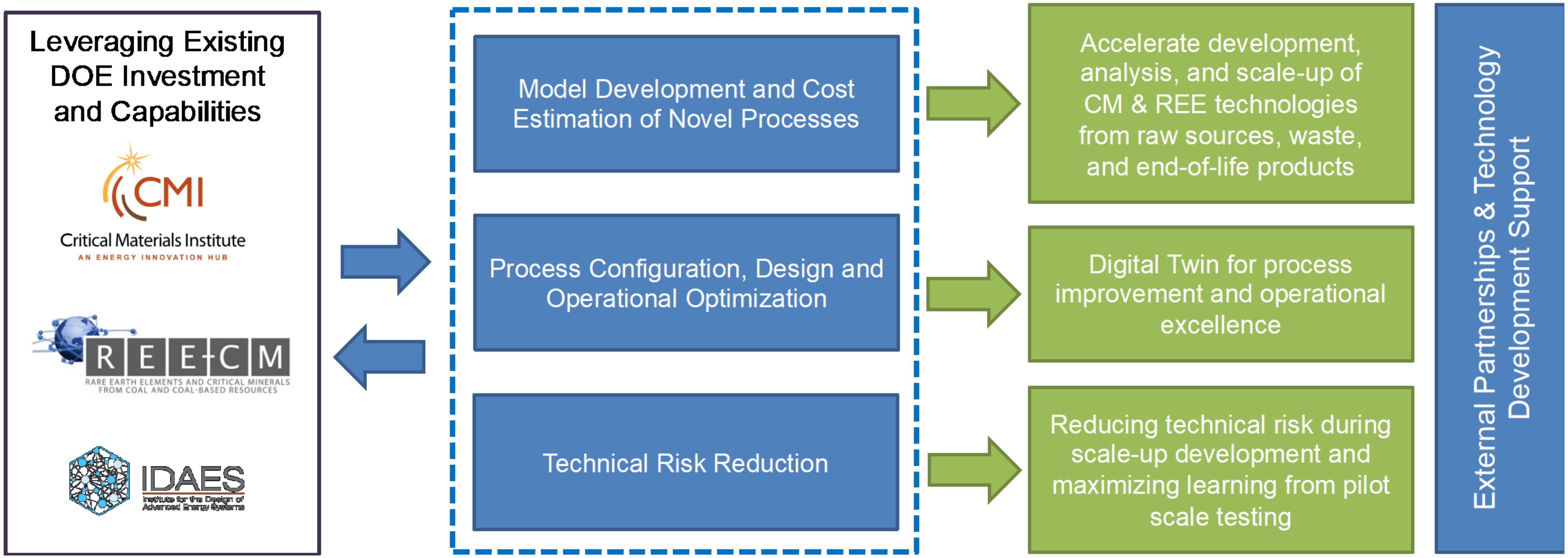
**October 11th, 2023**

# PrOMMiS Overview

- **What is PrOMMiS?**
- **Why is it Important?**
- **PrOMMiS Guiding Principles & Approach**
- **IDAES – A Multi-Scale, Integrated Modeling Framework**
- **Challenges of Applying IDAES to Critical Minerals**
- **PrOMMiS Overview**
  - Objectives
- **PrOMMiS Status**

# PrOMMiS: Process Optimization and Modeling for Minerals Sustainability

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

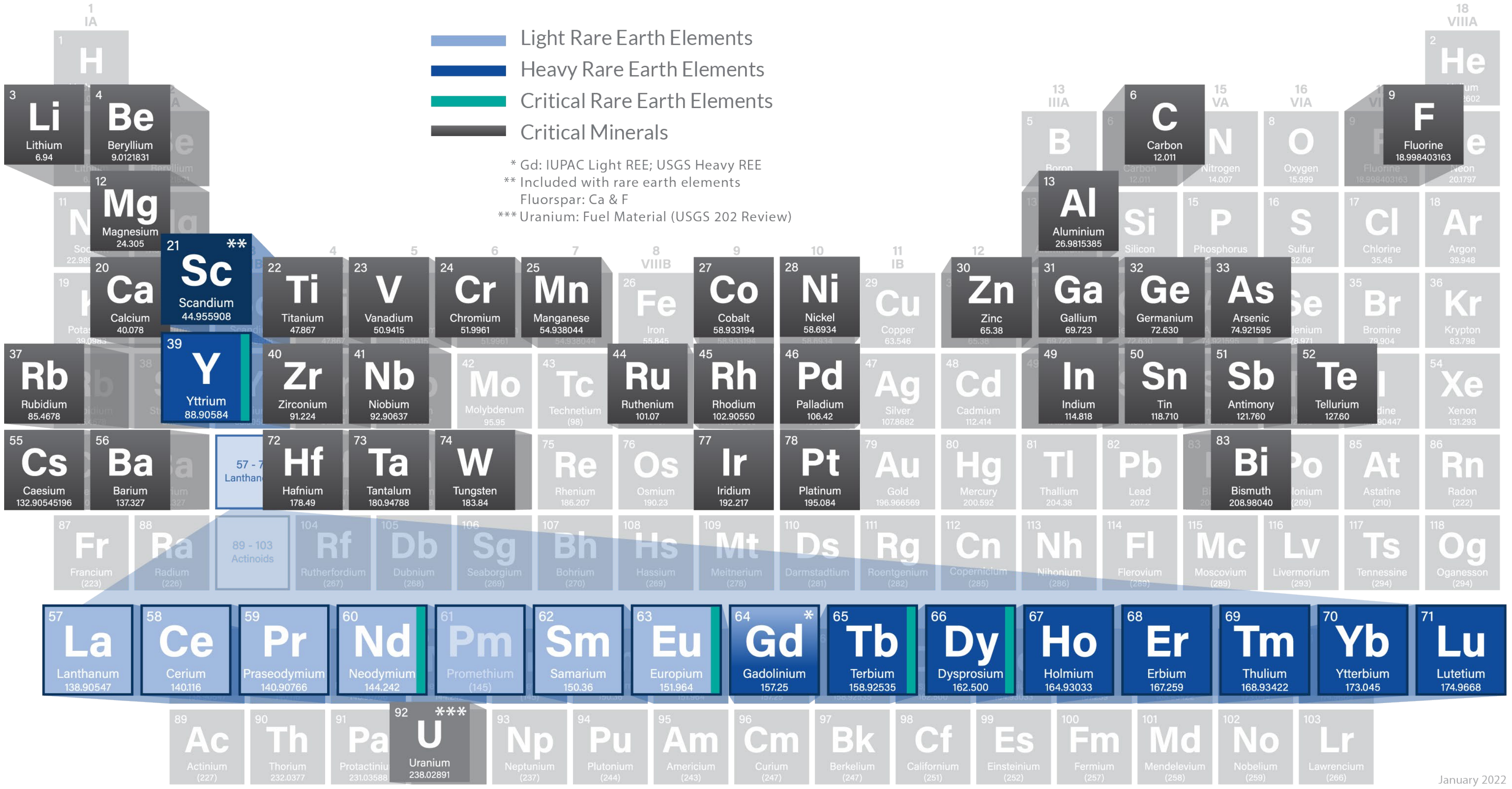


# Critical Minerals & Rare Earth Elements (REE)

NATIONAL ENERGY TECHNOLOGY LABORATORY

## Challenge: Foreign Dependance on Critical Minerals

- Import-dependent on >80% of U.S. rare earth element (REE) demand
- Import-dependent (>50% from foreign source) on >40 of 50* critical minerals
- Import-reliant (100% from foreign source) for at least 12 critical minerals

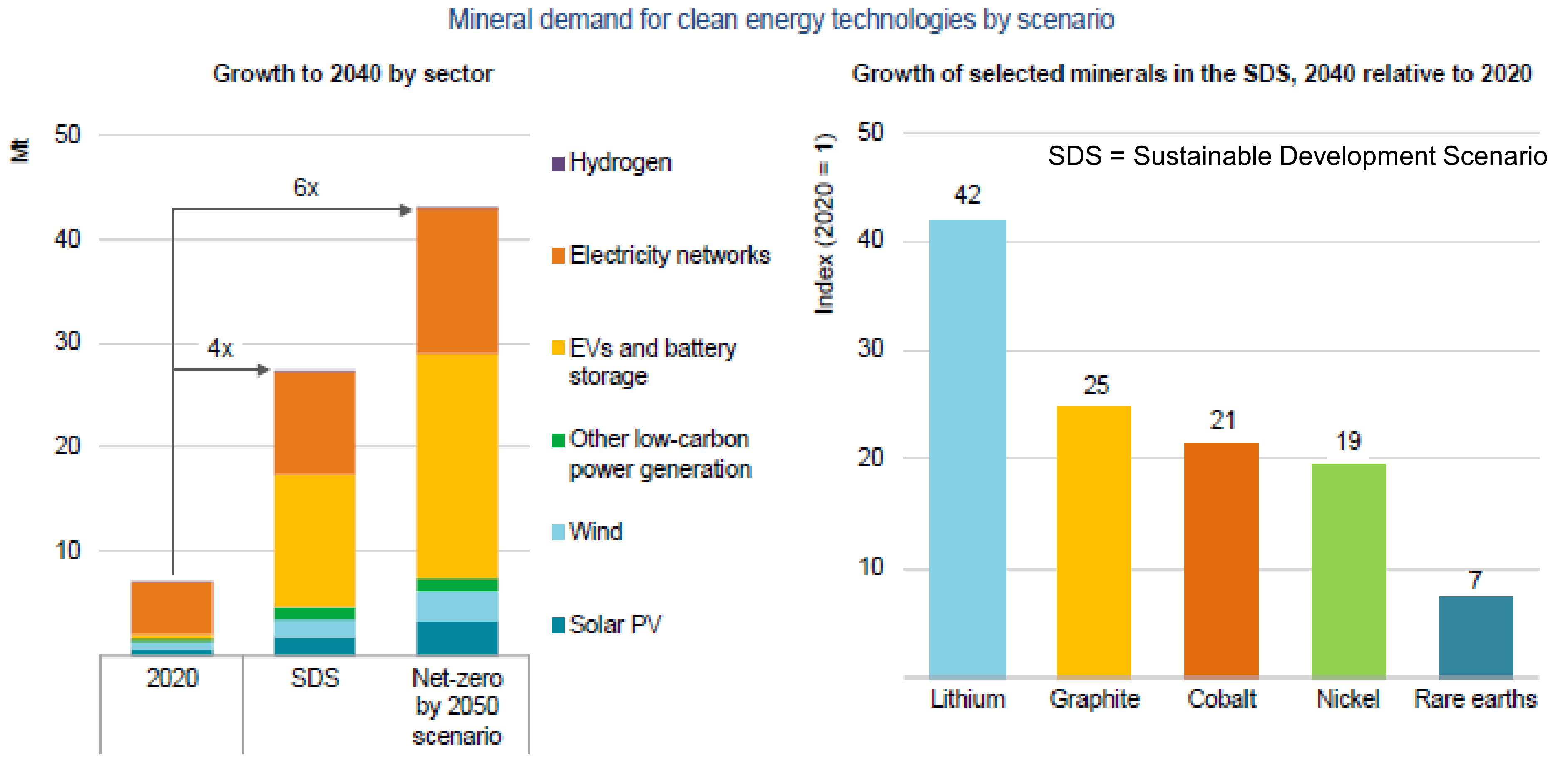



*Critical Minerals – Based on Material's Risk, Supply, & Importance to Clean Energy*

– Federal Register :: 2022 Final List of Critical Minerals: *A Notice by the Geological Survey on 02/24/2022* –

# Critical Minerals & Rare Earth Elements (REE)

## Challenge: Clean Energy Technologies Drive Demand Growth






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

# Understanding the REE Supply Chain

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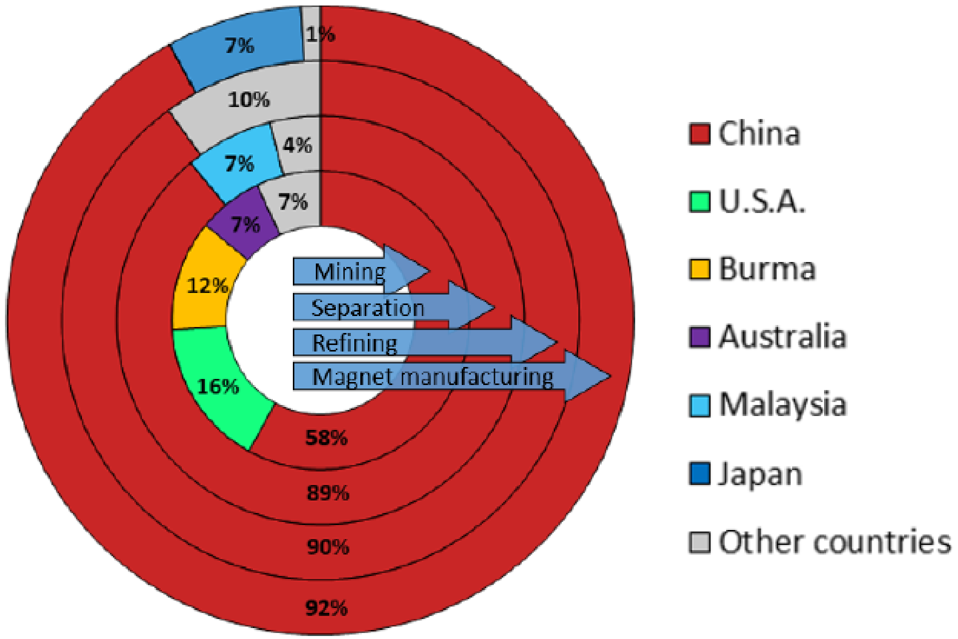
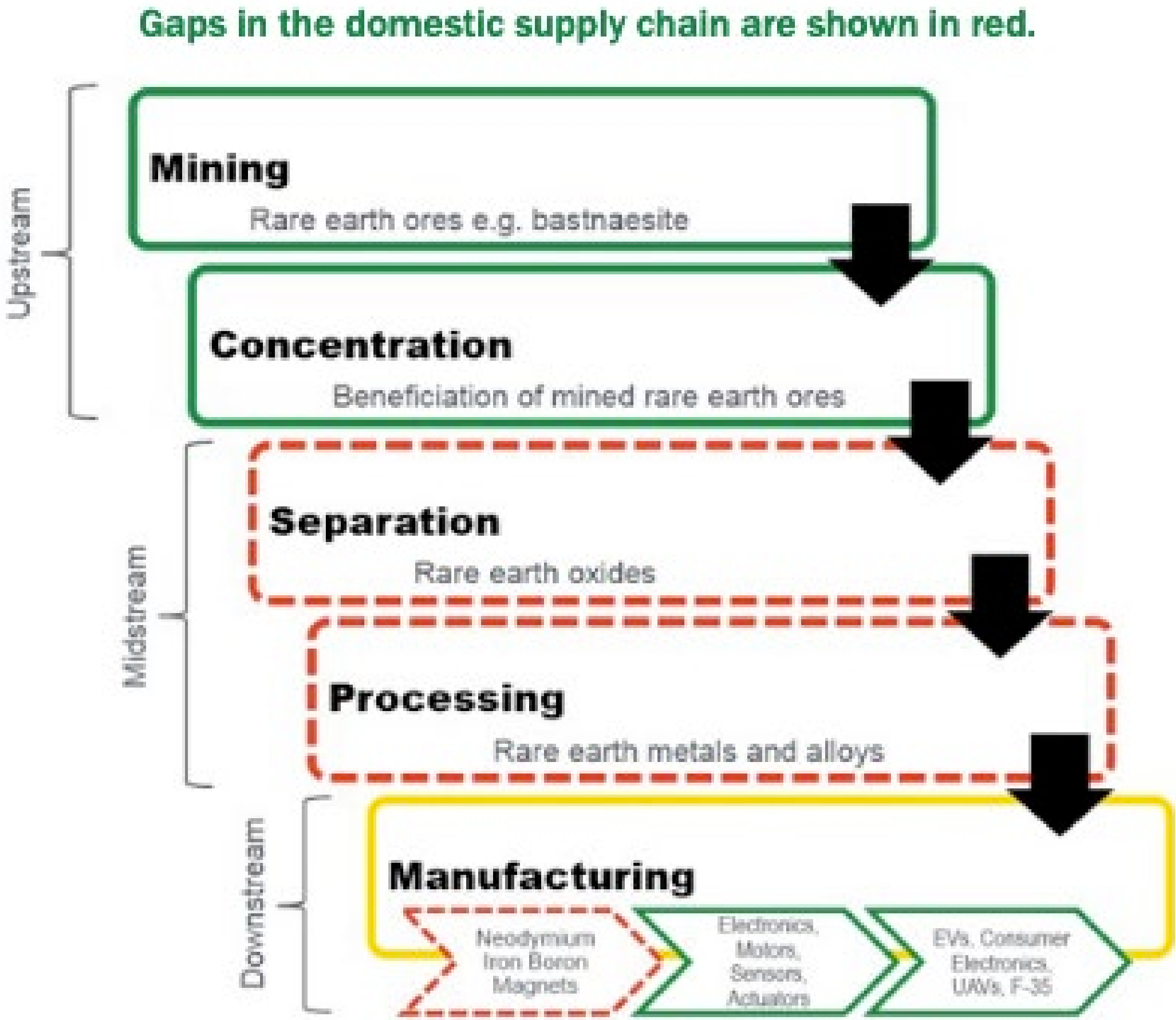
## Challenge: Gaps in Domestic Supply Chain

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




Geographic concentration of supply chain stages for sintered NdFeB magnets



# DOE Critical Minerals & Materials Strategy

NATIONAL ENERGY TECHNOLOGY LABORATORY

All Hands On Deck Approach, Spanning Numerous DOE Offices

## Diversify Supply

Offices: FECM, SC, EERE, NE, ARPA-E, NNSA

**Technologies:** Non-traditional sources; mine tailings; uses for co-products; advanced separations/extraction

**Long-term goals:** Diverse, secure, and resilient domestic sources and supply chains; resource mapping, characterization and fundamental geoscience understanding

## Develop Substitutes

Offices: SC, EERE, ARPA-E, NNSA

**Technologies:** New alloys, phosphors, catalysts; new components and systems

**Long-term goals:** Alternative materials, chemistries, systems, components that provide enhanced functionality for key energy technologies

## Recycling & Reuse

Offices: FECM, SC, EERE, NE, ARPA-E, NNSA

**Technologies:** Recovery from products; chemical/biochemical extraction; additive manufacturing

**Long-term goals:** Economical and energy efficient recovery from products to enable circular economy for critical materials

## Systems Analysis

Offices: FECM, SC, EERE, NE, ARPA-E, NNSA

**Technologies:** Modeling/simulation; systems approach to supply chain; Advanced characterization; techno-economic and life-cycle tools

**Long-term goals:** Integrated suite of systems, TEA, and LCA tools to assess and mitigate future criticality issues and support domestic supply; multi-scale physics/chemistry models

## Demonstrations

Offices: FECM, ARPA-E, EERE, NE, NNSA

**Technologies:** Prototypes and demonstration pilots, including FEED and pre-FEED studies

**Long-term goals:** Accelerate FEED and demonstrations to support commercial scale production

OTT IA LPO

**Stakeholder Engagement:** Access to foreign markets, foreign partners, and financing. Coordinating policy – international and NSC driven

OTT

**Market Analysis:** To support decision making

# Pathways to Commercialization

NATIONAL ENERGY

TRL 7-8 **Demonstration-Scale Facility**
*1-3 tonnes MREO/day – Planned**

**COMMERCIALIZATION**
*Technology available for wide-scale market use*

**DEMONSTRATION**
*System demonstrated in operational environment*

**SYSTEM TESTING**
*System performance confirmed at pilot-scale*

**DEVELOPMENT**
*Technology component validated/integrated*

**DISCOVERY**

*Program Initiated 2014*

PRODUCTION

PROCESSING

PROSPECTING


**FEED Study**
*Released*

**FOA-2404**
Advanced Processing Phase 1

**FOA-XXXX**
Advanced Processing *Phase 2 Planned**

**FOA-2364**
CORE-CM Phase 1

**FOA-XXXX**
CORE-CM *Phase 2 & Phase 3 Planned**

**RFP**
Concept & Feasibility (Pre-FEED) Studies

**FOA-2003**
REE System Optimization & Efficiency Improvements  **CM Production**

TRL 5-7 ***Operational* - First-of-a-Kind Small Pilot-Scale Facilities**

**FOA-1718**
Transformational Separation

TRL 3-5 **FOA-1202**
Conventional REE Separation & Recovery - **80-90% Purity**

**RFP 9067 & RFP 10982**
Field Prospecting

**FOA-2619**
Advanced Process Development

**FOA-3105**
TRL 0-4 through Pilot

2015 2020 2025

*Enabling Technologies -- Sensors, TEA, LCA, REE-URC*

**Planned* means solicitation or future phase(s) may possibly be funded via a future FOA that DOE may or may not issue.

# Commercialization Pathways: Pilot Projects

Producing High Purity MREO & CM (Co, Mn, Ni, etc.) from Coal-Based Sources

NATIONAL ENERGY TECHNOLOGY LABORATORY

UND UNIVERSITY OF NORTH DAKOTA

- Separating MREO concentrate from **lignite**
- August 2022 Pilot Facility Construction Complete
- October 2022 Pilot Facility start-up of Testing

| 2018 | 2019 | 2020 | 2021 |
|---|---|---|---|
| 5 – 10 g<br>5 – 15% purity | 500 g<br>30 – 85% purity | Under Construction | |

WinnerWater SERVICES PSI Physical Sciences Inc.

- Small-Scale Pilot plant cumulatively produced > 1 kg mixed rare earths on an oxide basis from **post combustion coal ash** by 2021. Ended March 2022.

| 2018 | 2019 | 2020 | 2021 |
|---|---|---|---|
| 0.004 kg<br>≥ 10% purity | .057 kg<br>≥ 14% purity | 0.41 kg<br>≥ 67% purity | 0.67 kg<br>≥ 91% purity |

WestVirginiaUniversity

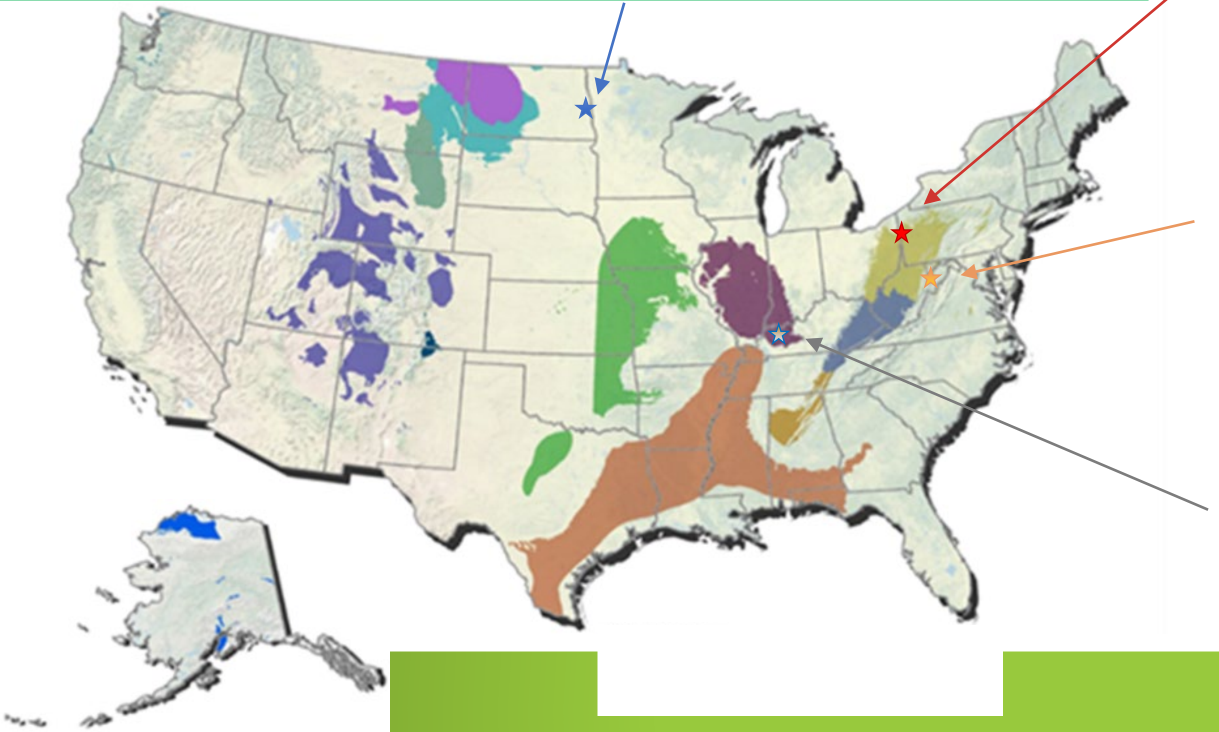
- Produced REE pre-concentrates from **AMD and sludge materials** with ~100% REE recovery, 45% is HREEs

| 2018 | 2019 | 2020 | 2021 |
|---|---|---|---|
| 44 g<br>95 – 99% purity | | Field Pilot-Scale Under Construction to start up June 2022 | |

University of Kentucky

- Pilot plant operation started in Q4 FY21. Produced quantities MREOs in its *modular* pilot-scale facility **from coal refuse materials**

| 2018 | 2019 | 2020 | 2021 | 2022 (Q1) |
|---|---|---|---|---|
| 0.6 kg<br>80% purity | 1.5 kg<br>> 90% purity | 0.41 kg<br>98% purity | 0.4 kg >50% purity<br>& 4 kg 0.5% crude cake | 0.72 kg >95% REE<br>& 0.3 kg (8% Co, 30% Ni)<br>& 0.27 kg (22% Mn) |



# PrOMMiS: Guiding Principles & Approach

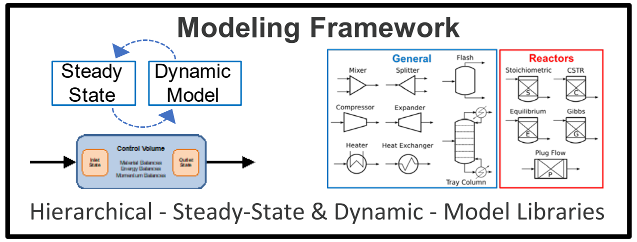
- **Urgency: Rapidly Establish Capability to Get Early Wins**
  - Learn by Doing – Apply to Existing Projects (recently completed or underway)
  - Don't Reinvent the Wheel – Leverage Existing Models & Partnerships
  - Partner with Active Developers

- **Create A Long-Term Capability!**
  - Critical Materials will change over time
  - Flexible, Foundational Platform
  - Early Stakeholder Involvement and Well-Regarded Leadership Board

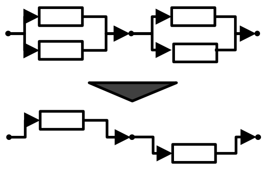
- **Maximize Support & Integration with CM and other DOE R&D Portfolios**
  - CM Related: CMC, CMI, BIL Activities, FECM Awarded Projects
  - Adjacent: Water-related (NAWI, PARETO, WaterTAP)
  - Inter-Agency: DoD Projects, USGS

# IDAES Integrated Platform

Institute for the Design of Advanced Energy Systems

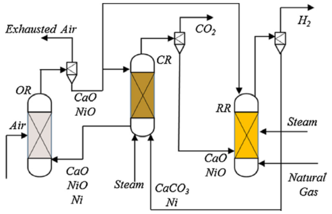



**Conceptual Design**

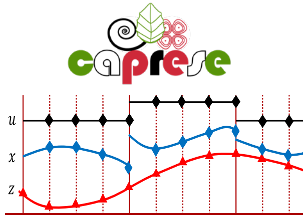


PYOMO GDP

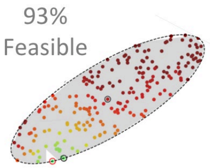
**Plant Design**
**Process Optimization**




**Process Operations**
**Dynamics & Control**




**Uncertainty Quantification**
**Robust Optimization**

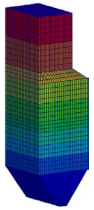



PyROS

**AI/ML**
**Surrogate Modeling**

ALAMO

PySMO



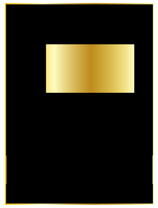
**Enterprise Optimization**
**Grid & Planning**

**Materials**
**Optimization**

MatOpt Nanomaterials optimization

**Open Source: https://github.com/IDAES/idaes-pse**

**Lee, et al., *J. of Adv. Manufacturing and Processing* (2021)**



NATIONAL ENERGY TECHNOLOGY LABORATORY | BERKELEY LAB | Sandia National Laboratories | Carnegie Mellon | West Virginia University | UNIVERSITY OF NOTRE DAME | Georgia Tech

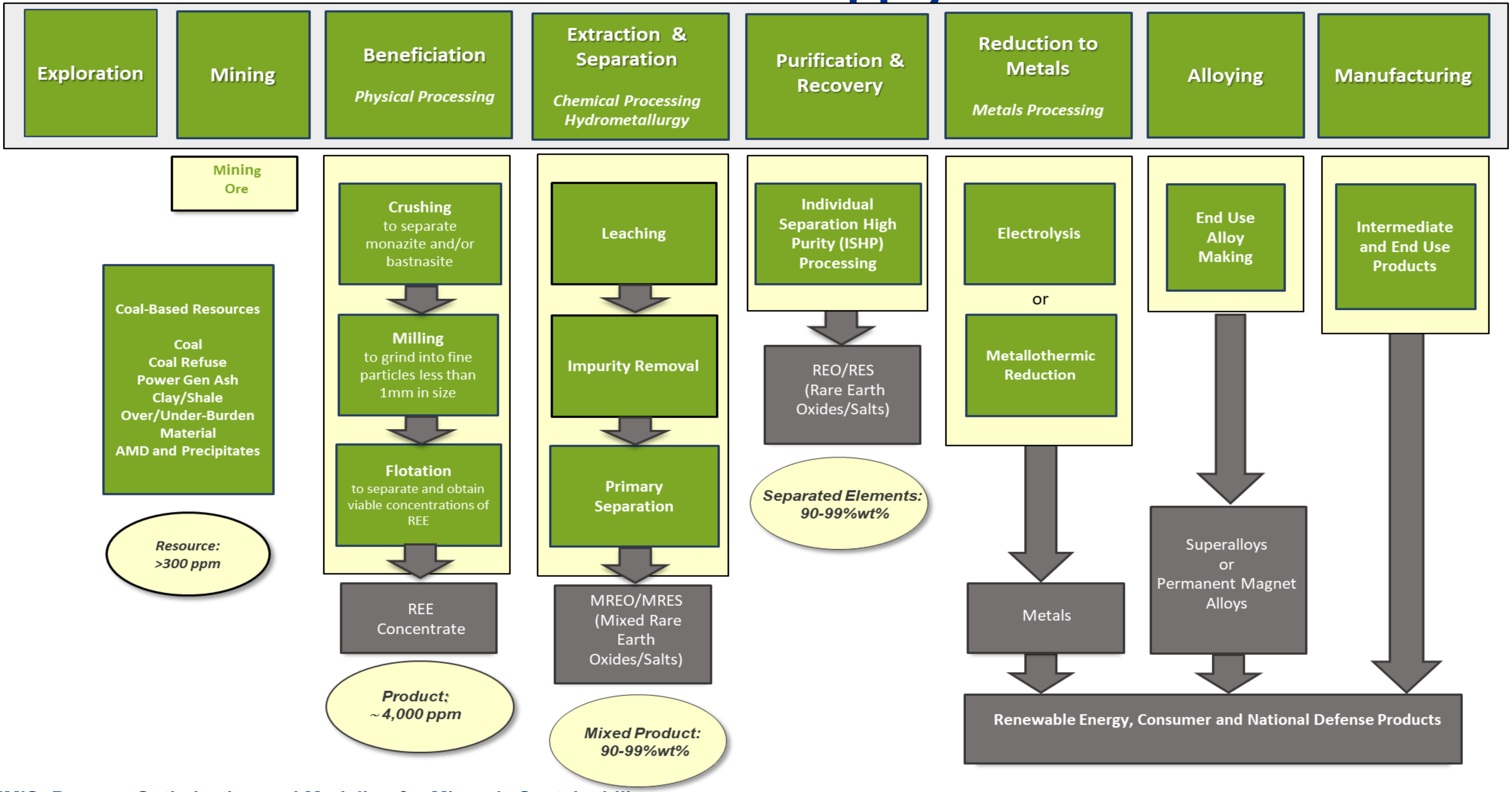
PYOMO

python™

| | | | | |
|---|---|---|---|---|
| Gurobi | CPLEX | Xpress | CBC | Ipopt |
| GAMS | NEOS | Mosek | BARON | GLPK |

PrOMMiS: Process Optimization and Modeling for Minerals Sustainability

# Critical Minerals Supply Chain

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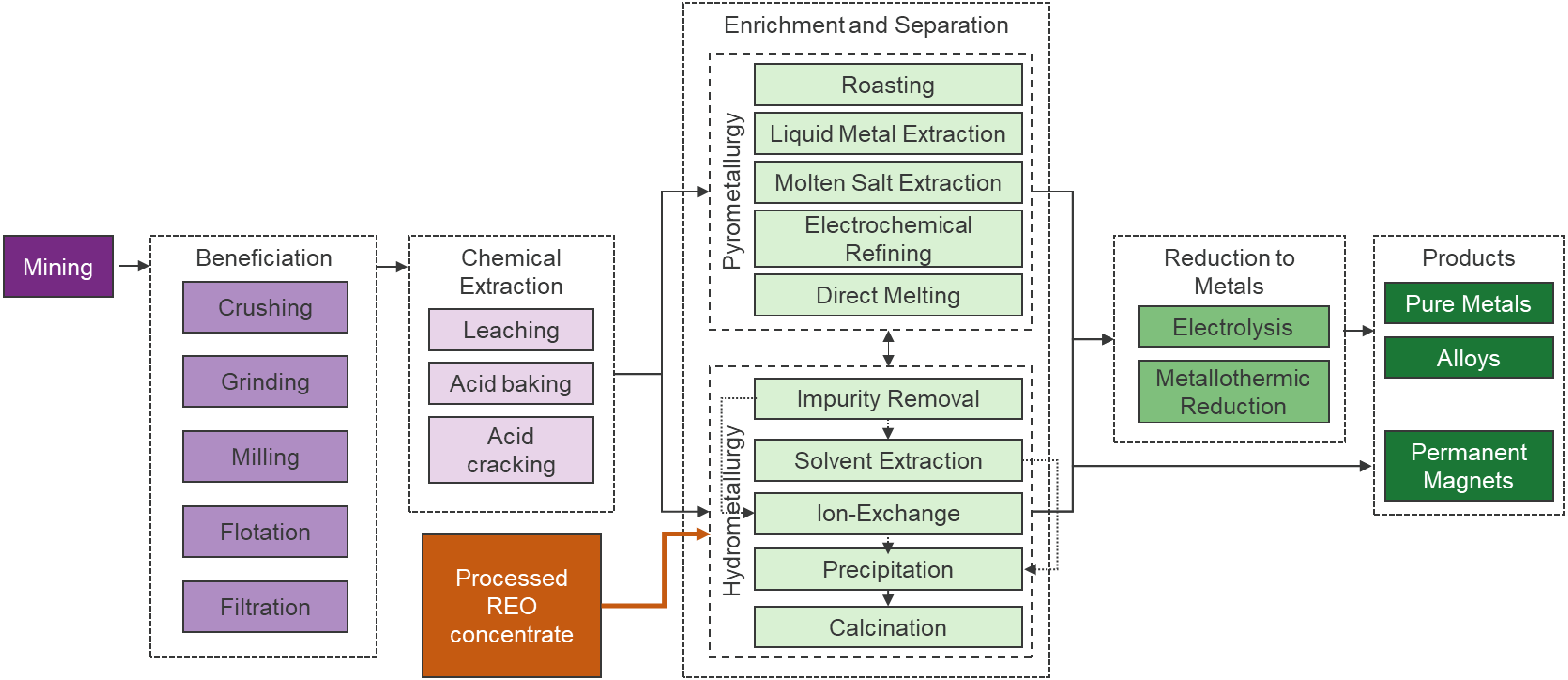
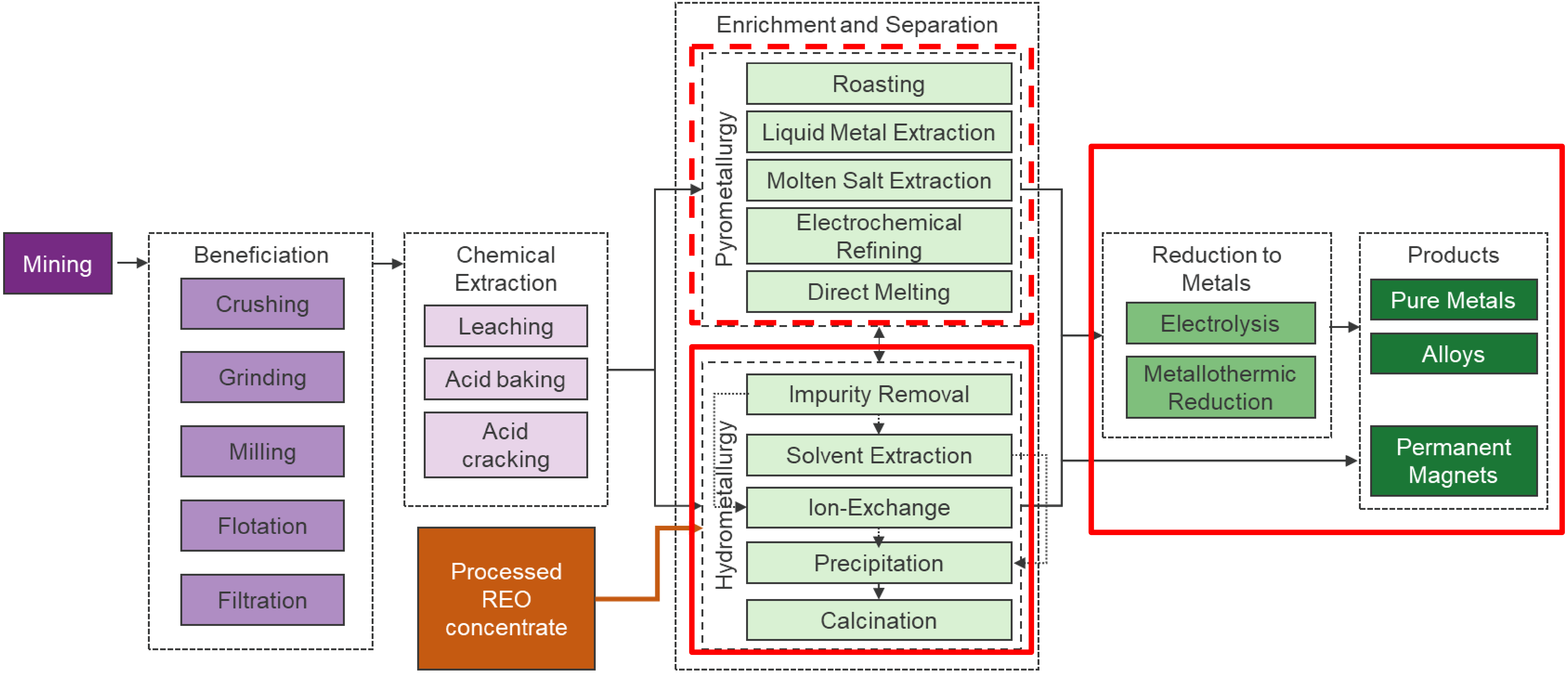



**PrOMMiS: Process Optimization and Modeling for Minerals Sustainability**

# Critical Minerals Supply Chain

## Unit Operations that are Broadly Applicable to Different Feedstocks



# Challenges Associated with Evaluating CM Systems

- **Broad Range of Feedstocks**
  - Conventional Ores: Hard Rock Deposits, Ion-Exchangeable Clays, etc.
  - Unconventional: Produced Water, Mining Refuse, Coal Ash, Acid Mine Drainage, Drill Cuttings, Geothermal Brines, etc.
  - Recycled Materials: Hard Drives, Batteries, Other Magnets, Fluorescent Lights, etc.

- **Wide Range of Potential Products:**
  - Of the X products you could produce from a given feedstock, including multiple individual REE, not all have a market now

- **Lack of Domestic Market for Critical Materials Presents "Chicken/Egg" Problem**
  - Lack of domestic production capacity means "widgets" aren't produced here
  - Lack of offtake means risk for CM producers and uncertainty over what products to actually generate

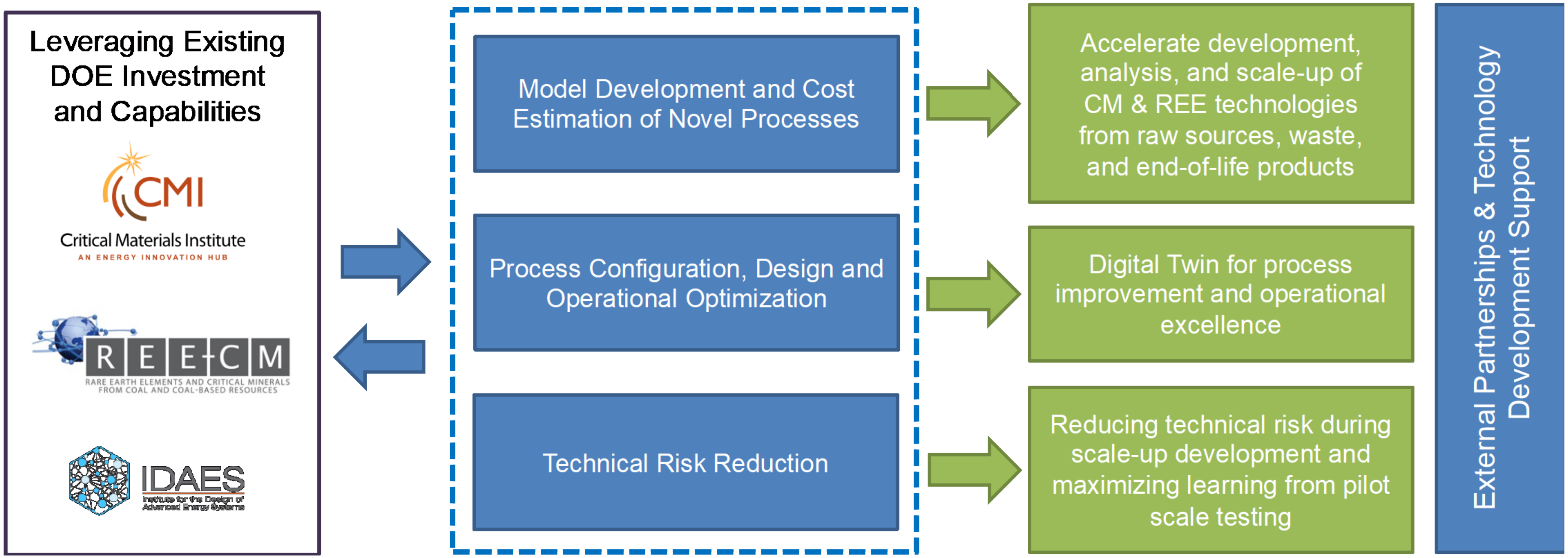
- **Market and Product Uncertainty**
  - Are the CM of today going to be the CM of 5 years from now? Probably not…
  - Market manipulation concerns

# Approach

**How do you eat an elephant?**

# PrOMMiS: Process Optimization and Modeling for Minerals Sustainability

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



# PrOMMiS: Summary of Objectives

**Rapid** & **tangible impacts** by leveraging IDEAS+ & a decade+ of DOE CMM investment.

Breakdown of objectives :

- Development of a **model library** and **costing** capabilities for **simulation, optimization, techno-economic analysis, control, and scale-up** of novel CM & REE processing technologies.
- Integration of **advanced optimization capabilities** for the high-level screening of process configurations to **identify the most promising flowsheets**, followed by **rigorous optimization** of these candidates to **improve performance** and **support scale-up, integration, and deployment**.
- Utilization of **optimization-under-uncertainty** approaches to **de-risk development** and produce designs that are **robust to process variability** (e.g., feedstock characterization).
- Utilization of these capabilities in collaboration with **external partners** to **accelerate** the **development** of viable **novel and intensified processes**, including those used for recovery from raw materials and **recycling** from **end-of-life products**.
- **Maximizing knowledge** gained from budget- and schedule-limited **experimental campaigns** using capabilities for **uncertainty quantification**, including **leveraging models** to inform the design of pilot-scale experiments and data collection requirements.
- Reducing technical risk associated with scale-up, integration, & deployment of novel technologies through the **validation and refinement of models** with bench-, pilot-, and demo-scale **experimental data.**

# PrOMMiS High-level Execution and Capabilities

**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
  - Build on demonstrated track record of solving problems that are intractable with existing commercial tools
- Ensure applicability to range of feedstocks (e.g., mining, waste streams, and recycling end-of-life-products)

**Years 2-5**: Apply PrOMMiS to support development & deployment of specific projects (across a range of feedstocks)

- Establish partnerships with domestic entities who have sufficiently mature (TRL 5+) CM & REE technologies
- Support process design, optimization, control, and scale-up for these novel CM & REE projects
- Reduce technical risk and maximize learning from pilot scale testing to accelerate deployment
- Expand model library and create data warehouse to further accelerate domestic CM & REE RD3 efforts

**Representative projects which can be leveraged to inform initial capability development (year 1)**

- E-Waste Recycling Pilot Facility (CMI/Ames National Laboratory)
- REE Production from Calcium Rich Ash Pilot Facility (NETL's Research & Innovation Center)
- Lithium-Ion Battery Recycling using MSX (CMI/Oak Ridge National Laboratory)

# PrOMMiS Overview

- What is PrOMMiS?
- Why is it Important?
- IDAES – A Multi-Scale, Integrated Modeling Framework
- Challenges of Applying IDAES to Critical Minerals
- PrOMMiS Overview
- **PrOMMiS Status**
  - Modeling: Initial Models Complete
  - Cost & Techno-Economic Analysis (TEA): Under Development
  - Stakeholder Lead Identification: In Progress

# PrOMMiS Status

- **Process Modeling**
  - Gap Analysis to Prioritize Model Development: *Complete*
  - Detailed Literature Review: *Complete*
  - Initiate Development of Unit Operation Models: *Complete*
  - Complete One or More Flowsheets: *Underway*
  - Validate Flowsheet & Perform Optimization Runs: *Calendar Year 2024*

- **Cost Database & Techno-Economic Analysis (TEA)**
  - "Top Down" and "Bottom Up" Approaches: *Complete* / Ongoing*
  - Evaluate public data of REE projects: *Complete* / Ongoing*
  - Initiate development of unit operations cost assessments: *Complete*
  - Complete TEA Framework for One Flowsheet: *Underway*

# PrOMMiS Status (continued)

- **Process Optimization Framework:** *Not Yet Started*
  - Requires one of more working flowsheets
  - **GOAL:** Validate or Build Upon Prior Optimization Efforts
    - Examine projects which have performed on the fly optimization or selected screenings
    - Determine if results can be reproduced
    - Identify additional opportunities for optimization

- **Stakeholder Advisory Board**: *Onboarding In Progress*

# Gap Analysis to Prioritize Model Development

- **Evaluate DOE & Industry Projects to Identify Cases of Interest**
  - High Impact Projects
  - Diversity of Feedstocks Important
  - Prioritize Projects with Willing Collaborators & Good Data Quality

- **Identify High Priority Unit Operations & Property Models**
  - Common Processes Across the Cases of Interest
  - Low-Hanging Fruit: Easy to Model/Models Already Exist
  - Criticality: Necessary for Modeling CM Systems

- **Perform Gap Analysis to Inform Model Development**
  - Qualitative Assessment of Identified Unit Operations & Property Models
  - Literature Review to Determine Availability of Mathematical Representations and Data
  - Brief Stakeholders for Feedback on Prioritization

# PrOMMiS: Overview of Existing Cases

- **FECM Bench- and Pilot-Scale Projects (External Performers)**
  - Bituminous Coal Ash (Physical Sciences, Inc./Winner Water Services)
  - *Coal Refuse (University of Kentucky)*
  - Several others exist

- **IIJA/BIL REE Demonstration Facility Awardees**
  - *Lignite Coal (University of North Dakota)*
  - *Acid Mine Drainage (West Virginia University)*

- **NETL Pilot or Pre-Pilot Projects**
  - *Calcium-rich Fly Ash Technology Commercialization Fund (TCF) Project*
  - Lithium Recovery from Produced Water
  - Critical Mineral recovery from AMD and/or AMD Precipitates

# Literature Review & Model Creation (based on Gap Analysis)

**Modeling Task Status:**

- Identify Cases: Complete
- Gap Analysis: Complete
- Model Creation: In Progress
  - Assign Cases and Unit Operations to Different Teams: Complete
  - Teams perform detailed literature review: Complete
  - Unit operation model creation: In Progress
    - Use existing models or modeling frameworks where feasible
      - IDAES or PARETO models
      - Surrogate models as appropriate
    - Validate with existing models or published data

- **GOAL**: Working Flowsheet by End of 2023

# PrOMMiS TEA Cost Bounding Framework

- **"Top Down" and "Bottom Up" Approaches**
  - Macro data from 43-101 filings to estimate and constrain cost evaluation
  - Equipment cost estimates from the literature or project data, inclusive of rules of thumb
- **Evaluate public data of REE projects**
  - DOE Awardee Final Reports
  - 43-101 and other filings
- **Develop cost & performance assessments for unit operations/processing classes**
  - Unit cost data and metrics
- **Leverage as costing framework for unconventional feedstocks**
  - Learn by doing with a focus on near term results
  - Model fidelity will improve over time

# PrOMMiS Optimization Framework

- **Optimization Framework enables screening & optimization of flowsheets**
  - Identify optimal operating parameters or unit operations (bounded)
  - Screen multiple flowsheets or determine viability of select unit operations
  - Multi-criteria optimization: Cost, Water Use, Energy Use., etc.
- **Requires one of more working flowsheets**
- **GOAL: Validate or Build Upon Prior Optimization Efforts**
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- **Maximize Support & Integration with CM and other DOE R&D Portfolios**
  - <u>CM Related</u>: CMC, CMI, BIL Activities, FECM Awarded Projects
  - <u>Adjacent</u>: Water-related (NAWI, PARETO, WaterTAP)
  - <u>Inter-Agency</u>: DoD Projects, USGS

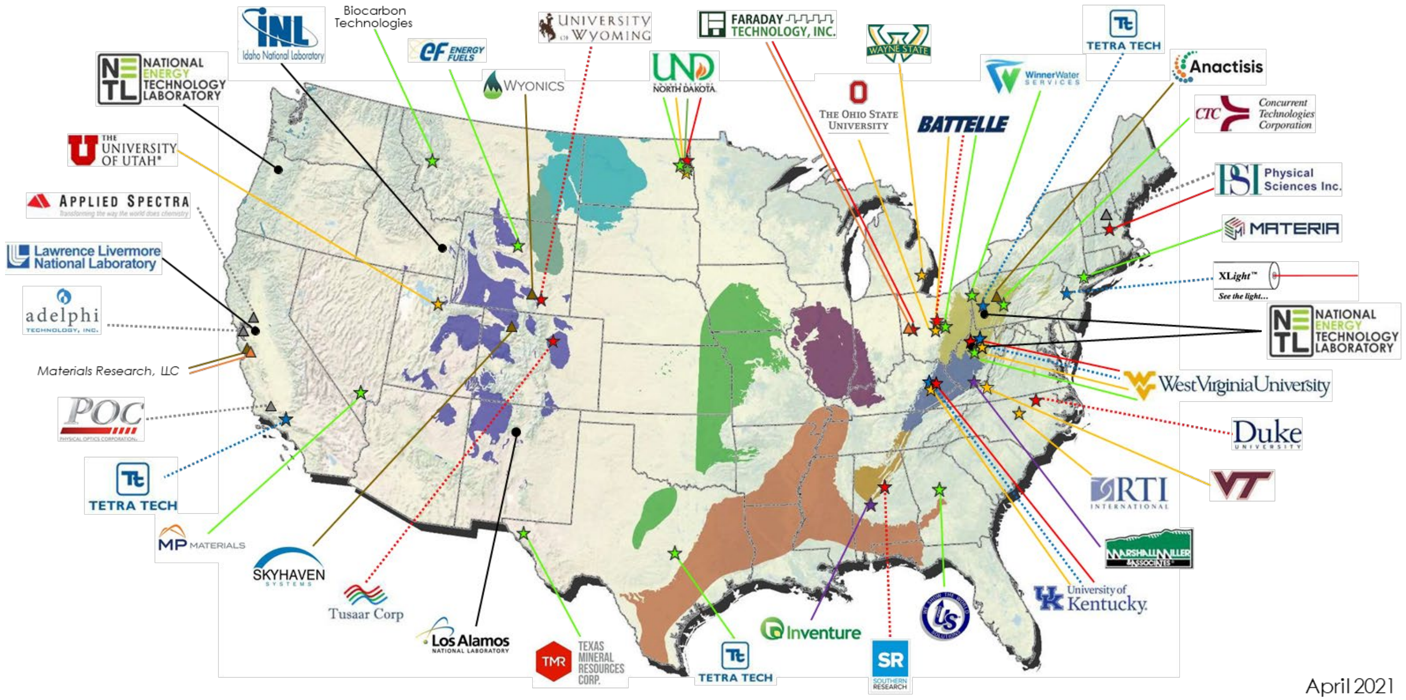
# Acknowledgments

## DOE Office of Fossil Energy & Carbon Management (FECM)

- Grant Bromhal (Division Director, Acting)
- Anna Wendt (Program Manager)
- Mary Anne Alvin (Program Manager)
- W. Morgan Summers
- Traci Rodosta

## NETL MS Leadership & RIC Team

- Jessica Mullen (Technology Manager)
- Burt Thomas (Research & Innovation Center Lead)
- Alison Fritz (SSAE Lead) & Team




## The Entire PSE+ Family

DOE-FECM Personnel, External Stakeholders, NETL TDC Federal Project Managers, NETL RIC & National Lab Scientists and Engineers

# Questions?

VISIT US AT: **www.NETL.DOE.gov**

**@NETL_DOE**

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**@NationalEnergyTechnologyLaboratory**

PrOMMiS

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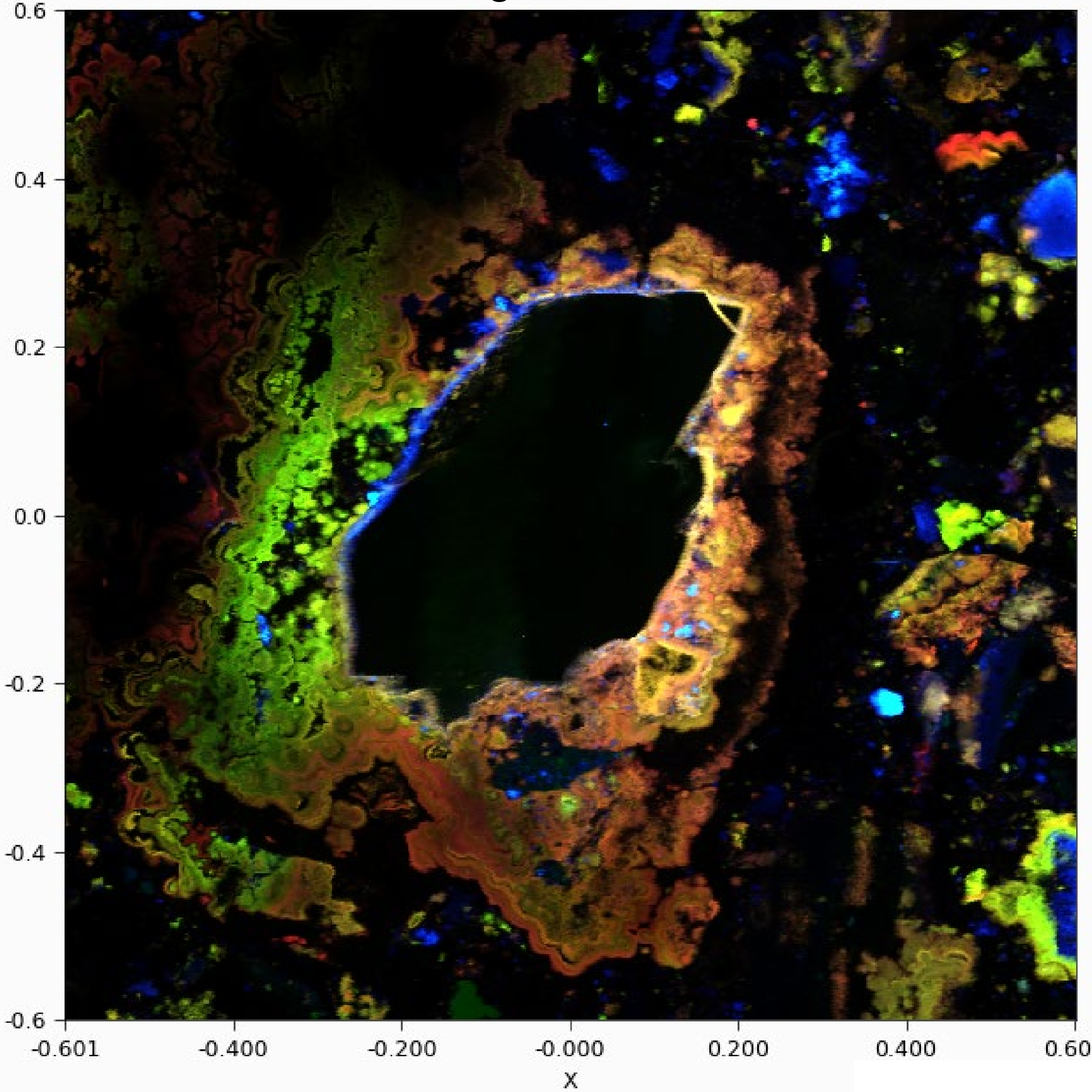
Mn in red, Ni in green, Co/Fe in blue

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Argonne NATIONAL LABORATORY

# PrOMMiS FWP Task Structure

**Task 1. Project Management**

**Task 2. Process Modeling and Optimization Toolset for CM and REE**

**Subtask 2.1 Core Model Development:** Develop library of multi-scale, optimization-ready models of key unit operations in novel CM & REE processes to support technology development activities.

**Subtask 2.2 Cost Estimation of CM & REE Processes:** Establish reliable capital and operating cost frameworks to support technology evaluation, design, and optimization.

**Subtask 2.3 Optimization of Design and Operations:** Demonstrate screening and optimization of process configurations with reduced order models, followed by rigorous optimization of design and operation to support scale-up, integration, and deployment of promising technologies.

**Subtask 2.4 Technical Risk Reduction: Uncertainty Quantification, Robust Optimization, and Sequential Design of Experiments:** Deliver a comprehensive framework for evaluating and reducing the technical risk during development and deployment of novel CM & REE processes.

**Subtask 2.5 Software Engineering and Release Management:** Manage open-source releases of computational tools framework to support modeling and analysis tasks.

# PrOMMiS FWP Task Structure

**Task 3. Outreach and Engagement:**

**Subtask 3.1 Stakeholder Board:** Establish conduit for regular input and feedback on program activities from a variety of partners with strong positions in CM & REE process technology development by creating and maintaining a Stakeholder Board.

**Subtask 3.2 User Community Outreach and Education:** Expand the user community and engagement through increased awareness, advertising, education, and demonstration of software capabilities.

**Task 4. Technology Development Support:** Develop and maintain collaborations with external partners to support their pilot and demonstration projects, improve models with industrial data, and inform system design, optimization, and scale-up through the application of ProMMiS tools.

- 1st year focused on initiating collaborations with industrial partners for technology development support
- Increase effort over initiative to support at least three key pilot projects to de-risk novel technologies and system integration.
- Representative examples of collaboration and technology development opportunities:
    1. E-Waste Recycling Pilot Facility (CMI/Ames National Laboratory)
    2. REE Production from Calcium Rich Ash Pilot Facility (NETL's Research & Innovation Center)
    3. Lithium-Ion Battery Recycling using MSX (CMI/Oak Ridge National Laboratory)

# Gap Analysis to Prioritize Model Development

- **Evaluate DOE & Industry Projects to Identify Cases of Interest**
  - High Impact Projects
  - Diversity of Feedstocks Important
  - Prioritize Projects with Willing Collaborators & Good Data Quality

- **Identify High Priority Unit Operations & Property Models**
  - Common Processes Across the Cases of Interest
  - Low-Hanging Fruit: Easy to Model/Models Already Exist
  - Criticality: Necessary for Modeling CM Systems

- **Perform Gap Analysis to Inform Model Development**
  - Qualitative Assessment of Identified Unit Operations & Property Models
  - Literature Review to Determine Availability of Mathematical Representations and Data
  - Brief Stakeholders for Feedback on Prioritization

# PrOMMiS: Overview of Existing Cases

- **FECM Bench- and Pilot-Scale Projects (External Performers)**
  - Bituminous Coal Ash (Physical Sciences, Inc./Winner Water Services)
  - *Coal Refuse (University of Kentucky)*
  - Several others exist
- **IIJA/BIL REE Demonstration Facility Awardees**
  - *Lignite Coal (University of North Dakota)*
  - *Acid Mine Drainage (West Virginia University)*
- **NETL Pilot or Pre-Pilot Projects**
  - *Calcium-rich Fly Ash Technology Commercialization Fund (TCF) Project*
  - Lithium Recovery from Produced Water
  - Critical Mineral recovery from AMD and/or AMD Precipitates

# PrOMMiS: Overview of Existing Cases (Con't)

- **CMI Pilot Projects**
  - Magnet Recycling
  - *Hard Drive Recycling*
  - REE Recovery during Phosphate Production
- ***Membrane for Lithium Recovery from Produced Water***
- **Others, TBD**
  - REE Recovery from bauxite residues
  - Battery recycling (ReCell)

# PrOMMiS: Overview of Existing Data/Models

- INL Solvent Extraction Optimization Model and Pilot Test-Bed
- PHREEQC/AMDTreat Property Model for Acid Mine Drainage and similar solutions
- Virginia Tech Mineral Processing Optimization Models
- Missouri Science & Technology Optimization Models
- “REESim” spreadsheet model (deliverable from FECM FOA project)
- TEA Cost Bounding Framework (NETL)
- NETL Process Model and Unit Operation Assessment (under development)

# Gap Analysis Process

Identify key metrics

Perform flowsheet evaluation for each pilot process

Quantity metrics on unit processes

Determine final models for development and identify data needs

- List out unit operations
- Identify property models needed for unit operations
- Qualify metrics on unit processes

# Rank and Prioritize with Guiding Principles

**Applicability.**

- Broad modeling context
- Focused property models/ feedstock types

**Realism.**

- Leverage existing models and pilots
- Reasonable computation time

**Impact.**

- Multi-criteria benefits (environmental, energy, cost)
- Critical mineral supply chain impact (filling knowledge gaps for relevant materials)

# Assessment Criteria for Prioritizing Unit Ops & Property Models

## Technical difficulty

Time consuming development ⟷ Simple development

## Performance Impact

Low cost, energy, or environmental impact reduction potential ⟷ High cost, energy, or environmental impact reduction potential

## Data availability

No validation data available ⟷ Existing access to validation data

## Frequency of model use

Highly specific unit process model ⟷ Widely reusable unit process model

## Applicability to stakeholders

Low stakeholder interest ⟷ High stakeholder interest

## Feedstock applicability

Low stakeholder interest ⟷ High stakeholder interest

# Gap Analysis Data Grid – Creation and Screening

## Starting the Gap Analysis:

- Identify relevant cases & Stakeholders

| Process Name | | Source | Product | Data Availability | Process Commonality | Costing | Team Contacts | |
|---|---|---|---|---|---|---|---|---|
| Powder River Basis Coal Byproducts | | Coal Ash | 60% REO | Good | High | Key unit ops missin | Internal | |
| Membrane Separation from Brines | | 3 specific salt lakes | LiCO3 or LiOH, >95% | Limited | Key processes are unique, but many common c | None | Limited for processes studied | |
| HDD Recycling | | Various | | Limited/None | | Some | ? | |
| Phosphates | | Phosphoric acid sludg | 95% pure REO, 46% recovery | Limited in source | High, back end is common with many processes | Some | ? | |
| University of Kentucky | | Coal Ash, AMD | REO, >90% purity | Good | High | Good | Strong | |
| | | | | | | | | |
| **Outreach** | | | | | | | | |
| UND Lignite Coal | | | | | | | | |
| WVU Bench Scale SX | | | | | | | | |
| WVU Acid Mine Drainage | | | | | | | | |
| UWy / Ramaco Carbon carbon products | | | | | | | | |
| | | | | | | | | |

- Qualitative prioritization of Unit Operations

| Supply Chain Area | Operating Unit | Feedstock | Mineral | Exists in Data From | Technical difficulty | Performance Impact | Data availability | Frequency of model use | Applicability to stakeholders | Feedstock applicability |
|---|---|---|---|---|---|---|---|---|---|---|
| Chemical Extraction | Leaching | Low-Rank Coal Fly Ash | REE | FECM Pilot | | | | | | |
| Hydrometallurgy | Solvent extraction | Low-Rank Coal Fly Ash | REE | FECM Pilot | | | | | | |
| Chemical Extraction | Leaching | Acid Mine Drainage | REE | FECM Pilot | | | | | | |
| Hydrometallurgy | Filtration | Acid Mine Drainage | REE | FECM Pilot | | | | | | |
| Hydrometallurgy | Sorbent | Acid Mine Drainage | REE | FECM Pilot | | | | | | |

- Evaluation of needed and existing Property Models

# Data Grid – Diving in!

| | | | | | | | | | | | Technical Difficulty | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | | | Minimum Fidelity | | High Fidelity | |
| Operation Name | No. Cases | Process Data | Performance Data | Sizing/Design Data | Property Data | Costing/TEA Data | Performance Impact | Broader Applicability | Comments | | Unit Op | Properties | Unit Op | Properties |
| **Common Unit Ops** | | | | | | | | | | | | | | |
| Precipitation/Crystallization | 5 | Type Specific | 0 | 1 | 0 to 2 | 2 | 2 | 3 | | | 1 | 1 | 2 | 4 |
| Leaching / Dissolution | 4 | 1 to 2 | 0 | 1 | 2 | 2 | 3 | 3 | | | 1 | 1 | 3 | 5 |
| Solvent Extraction | 3 | 1 to 2 | 0 | Limited | 2 | 2 | 3 | 3 | | | 1 | 1 | 3 | 4 |
| Calcination / Roasting | 3 | 1 to 3 | 0 | 1 | 3 | 2 | 3 | 3 | | | 1 | 1 | 5 | 4 |
| Nanofiltration (NF) | 1 | 1 | 2 | 1 | 0 | 0 | 2 | 2 | Design is likely lab-scale. | | 1 | 1 | 4 | 3 |
| Reverse osmosis (RO) | 1 | 1 | 2 | 1 | 0 | 0 | 2 | 2 | Design is likely lab-scale. | | 1 | 2 | 4 | 3 |
| | | | | | | | | | | | | | | |
| **Application Specific Ops** | | | | | | | | | | | | | | |
| Excavation and transport | 1 | 3 | | 1 | 3 | 2 | 1 | 1 | | | 1 | | | |
| Electrochemical intercalation-deintercalation (El | 1 | 1 | 2 | 1 | 0 | 0 | 3 | 1 | Sizing is likely lab-scale. | | 2 | | | |
| Evaporation | 1 | 1 | 0 | 0 | 0 | 0 | 2 | 2 | | | 1 | | | |
| Electrodialysis | 1 | 1 | 2 | 1 | 0 | 0 to 2 | 2 | 2 | Designs are bench-scale. | | 1 to 2 | | | |
| HDD Disassembly/Shredding | 1 | Type specific | | | | | | 1 | | | | | | |
| Copper valorization tanks | 1 | 1 | 0 | 1 | 1 | 2 | 2 | 1 | | | 1 | | | |
| continuous-flow decanter centrifuge (CFDC) | 1 | 1 | 3 | 0 | 0 | 1 | 3 | 1 | | | 2 | | | |
| Ascorbic acid addition | 1 | | | | | | | 1 | | | | | | |
| Ion Exchange | 1 | 0 | | 0 | 2 | 0 | 0 | 2 | | | | | | |
| Solids Grinding | 1 | | | | | | 2 | 2 | | | 2 | 1 | 3 | 5 |
| Beneficiation (various types) | 1 | | | | | | 3 | 2 | | | 1 | 1 | 4 | 3 |
| | | | | | | | | | | | | | | |
| **Balance of Plant Ops** | | | | | | | | | | | | | | |
| Filtration | | | | | | | | 3 | | | 1 | 1 | 2 | 3 |
| Centrifuge | | | | | | | | 2 | | | 1 | 1 | 3 | 3 |
| Wastewater treatment | | 1 | 0 | 1 | 1 | 2 | 2 | 3 | | | 1 | 2 | 5 | 5 |
| Settlers/Thickeners | | | | | | | | 2 | | | 1 | 2 | 3 | 3 |

# Stakeholder Advisory Board

- **GOAL: Ensure PrOMMiS is meaningful and "Moves the Needle"**
- **Targeted Members**
  - Mineral Process Modeling Experts
  - Critical Material Institute (CMI) Representative
  - Project Leads of existing or upcoming pilot- or demo-scale CMM projects
  - ESG, J40, DEI representative
  - DOE HQ Stakeholders
- **Target Size: 10-15 members**