Critical Minerals:

Roles for Artificial Intelligence in Support of FECM RDD&D Priorities

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Fossil Energy and Carbon Management

Artificial intelligence (AI) holds the potential to accelerate the transition to a carbon-neutral economy and help achieve the technology research, development, demonstration, and deployment (RDD&D) goals set forth by the DOE Office of Fossil Energy and Carbon Management (FECM) in its *Strategic Vision*. FECM and the National Energy Technology Laboratory (NETL) continuously expand, maintain, and curate extensive scientific data sets and AI tools essential to carbon management, and they are now standing up a robust AI Multi-Cloud Infrastructure to enable the DOE research community to share and leverage a collection of tailored resources to expedite progress toward equitable and sustainable solutions.

As one step toward prioritizing AI development activities, FECM is exploring specific roles for AI in meeting the top RDD&D needs identified in the Vision. This document summarizes a series of discussions in which a range of specialists from FECM, NETL, and the DOE Office of Science suggested potential roles for AI in **Critical Minerals**. This document should be viewed as a representative sample of the types of AI applications that may be needed; it is by no means a comprehensive list.

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AI for Critical Minerals and Rare Earth Elements

Artificial intelligence (AI) holds the potential to enable an affordable domestic supply of the critical minerals[1] (CM) and rare earth elements (REEs) needed to support America's transition to clean energy. As shown in the figure on the following page, AI could play key roles in expediting the location, recovery, processing, and incorporation of critical materials into manufactured products (see inset for main process stages). In the near term, RD&D is focusing on upstream (location and extraction from coal mine waste streams) and midstream (separation and purification) processing. AI trained on evolving technologies, markets, supply chains, and transportation networks may subsequently help determine the most cost-efficient processing routes, infrastructures, and locations to sustainably support clean energy while creating jobs and opportunities in economically stressed regions.

> **Critical Minerals and REE R&D Focus Areas**
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> **Upstream recovery:** Location, assessment, and extraction of CMs from unconventional or novel resources (includes physical separation and beneficiation)
>
> **Midstream processing:** Extraction, separations, recovery, and purification of critical and high-value materials
>
> **Downstream manufacturing:** Incorporation of these materials into commodity or national defense products.
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> Adapted from web page: Critical Minerals and Materials Program (NETL)

Upstream Processes

Upstream Characterization

AI can access extensive existing datasets, legacy records and data, and near real-time sensing to provide new insights on how to locate CM/REE resources; assess their concentrations, species, volume, and value; and select/design optimal recovery technologies.

Locate and characterize resources. AI can use geological, geophysical, geo-chemical, and other data to provide guidance on the likely presence of critical minerals in diverse resources. A myriad of data in open sources (as well as in journals, websites, and other "less friendly" formats) is available for AI-enabled systematic search, acquisition, integration, transformation, and aggregation to enrich the knowledge base. AI tools might continuously evaluate multiple data streams to effectively convert large data resources into useful knowledge, but the tools must be tailored for each end-use case. The most sophisticated current tool, portable x-ray fluorescence (XRF), has marginal detection limits, so the ability to predict the location of REEs and other critical minerals with confidence would be of great interest.

> **Priority REEs and CMs by Use**
>
> - **Magnets:** Neodymium, Praseodymium, and Dysprosium
> - **Energy Storage:** Lithium, Cobalt, Nickel, Manganese, and Graphite
> - **Fuel Cells:** Iridium & Platinum for electrolyzers; Platinum
> - **Wide Bandgap Semiconductors and LEDs:** Gallium
> - **Microchips** (semiconductors): Germanium
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> Briefing by Grant Bromhal, FECM (Bromhal 2022)

AI/ML and deep learning could scale and accelerate *multidimensional analysis* to reduce the work of core sampling and kriging for predicting which minerals are present in conventional and unconventional resources (shale, acid mine drainage, etc.). AI could similarly build insights into the likely co-location, *volumes*, *concentrations,* and specific *compounds or species/forms* (not all are

[1] Critical minerals include any mineral, element, substance, or material designated as critical by the Secretary of Interior (Federal List of CMs), excluding fuel and other specified minerals.

FECM Priority AI R&D for Critical Minerals

Challenge — *AI Assist*

- **Critical Minerals**
  - **Upstream:** Expedite CM location, assessment, and recovery
    - **Characterization**
      - **Locate CM and REE concentrations:** Use nondigital data, trends, colocation patterns to evaluate unconventional resources.
      - **Characterize located resources:** Predict the forms and relative amounts of CMs and REEs in a resource to guide excavation.
      - **Real-time data analysis**: Use near-real-time sensing/rapid characterization and multiple data sources to optimize processes at all stages
    - **Recovery**
      - **Tailor recovery technology:** Use ML and modeling to tailor extraction technologies to the identified resource (spans upstream/midstream)
  - **Midstream:** Expedite efficient assessment, extraction, and processing
    - **Characterization**
      - **Optimize midstream processing:** Characterize CMs during extraction or transport to select best processes/settings at next stage.
    - **Extraction/Separations/Processing**
      - **Tailor processing technology design**: Optimize design of processing technologies/treatments to improve recovery, economics, environment.
      - **Provide decision support for processing:** Conduct risk analyses to ensure long-term viability of infrastructure for CM/REE extraction/processing.

known) of various REEs and CMs to determine whether commercial quantities are present. This capability might eventually be further informed by techno-economic analyses to guide the selection of or improve the cost-effectiveness of raw extraction methods. AI could be particularly helpful in identifying the *secondary colocation* of other REEs and CMs with known deposits (ML may detect patterns if they exist). Multiple REEs and CMs often exist in the same source feedstock, but current processes focus on a single product, often leaving many other CMs and REEs in the waste stream. The aim is to reduce waste from an excavated resource from 99% today to 1% or less.

Predicting mineral species and volumes in geological deposits is sufficiently challenging—but doing so in waste piles is far more complex. Resources come from diverse geological sites and regions and minerals may change or leach over time. Real-time sensing, edge technologies, passive sensing, and in-situ characterization could help AI systems *predict near-surface and subsurface resource availability over time* as climate perturbations and other conditions affect the occurrence of these resources. An opportunity exists for AI to identify trends and anomalies based on the growing body of data.

> "We have so much stockpiled waste from fossil power and industrial sectors that, using this legacy waste, we have significant production potential for rare-earth elements and critical minerals… At the same time, we can create jobs in transition communities and clean up these areas ravaged by mining."
>
> Jennifer Wilcox,
> Principal Deputy Assistant Secretary, DOE/FECM

Real-time data analysis to inform extraction. Certain contaminants are tolerated for some CM/REE applications and not others. AI could assess real-time scans identifying the highly specific characteristics of excavated resources, though this may require more sophisticated scanning tools. AI could then analyze this information and suggest appropriate adjustments to initial extraction methods or techniques.

Upstream Recovery

While CM/REEs are less rare than originally thought, they do not exist in pure form and must be extracted from the ore—making them difficult and costly to mine.

Select extraction method based on resource. After identifying the presence, concentration, and form/species of specific minerals, AI could potentially guide selection of the recovery technologies that would be most cost-effective and likely to yield CMs/REEs of the appropriate quality for the intended application. Focusing on the co-extraction of multiple CMs or REEs from a single resource (many are co-located) could significantly improve productivity and economics.

Midstream Processes

Midstream Characterization

Optimize processing in real time. Better understanding of the presence/nature of CMs/REEs in excavated sources could enable real-time adjustments (e.g., temperature, acidity) to boost processing efficiency. Hundreds of steps may be required to increase the concentration of a single REE, so process optimization and co-production are essential. Additionally, real-time characterization of material variability could help optimize the pre-processing of recovered materials to create uniform material streams.

Midstream In-Facility Extraction/Separations/Processing

Tailor/optimize separations/processing technology design. Based on data from observed CM/REE species extraction, processing, and purification results, AI may suggest novel or tailored processing technologies or combinations thereof to optimize quality and economics. Using thermodynamics, solubility, and other mineral properties, AI could reduce trial and error to expedite discovery of the right mix of physical, chemical, biological, or other treatments to economically yield the highest quantity and quality CMs/REEs for target uses. This capability is likely to increase in accuracy and utility as more data becomes available. Science-based modeling and ML are mutually supportive, but data remains a key challenge.

Provide decision support to maintain flexible processing infrastructure. AI could guide processing decisions to mitigate risk and retain flexibility by considering a range of possible futures as the U.S. processing infrastructure is designed and built. This guidance could help maximize overall productivity and cost effectiveness while minimizing waste over the long term—despite uncertainties.

T*he following section summarizes initial thoughts by AI experts in the Office of Science and the National Energy Technology Laboratory (NETL) on the feasibility of using AI to achieve the stated objectives.*

Feasibility and Challenges

Overall, the suggested CM applications appear suited to AI, but success will depend upon the quantity, quality, consistency, reliability, and accessibility of the relevant data. AI/ML excels at detecting hidden patterns, but each dataset is unique. The reliability of predictions based on algorithms or models generated from data relies on the completeness and level of certainty inherent in that data.

At present, significant human effort is required to physically dig out old ore samples, mine records, waybills, and other documents. AI tools such as optical character recognition (OCR) and natural language processing (NLP) may help with digitizing, but variability in the fields of different types of extracted data (possibly dictated by jurisdiction or company) and the need for data cleaning and context continue to require a human in the loop. That said, this process is underway in numerous projects within many agencies in a wide variety of fields—gradually generating new and better methods. NETL is currently engaged in this type of effort.

Locating concentrations of critical minerals and REEs in specific coal waste streams is an achievable yet particularly complicated undertaking. Supplying context involves identifying the original geophysical characteristics and history of the rock formations from which the raw coal was extracted, figuring out when it was processed and where the waste was placed, then gathering information on the environmental conditions to which the waste pile was subjected over the intervening years. For example, was the pile subsequently moved, covered up by waste from a different source (need to characterize), or subjected to heavy rainfall or flooding that led to leaching or acid mine drainage (AMD)?

To the extent a reliable dataset is developed from a range of existing records and enriched by inferences drawn from samples and other relevant sources, it could serve as a training set for AI. AI predictions can then be explored, providing a feedback loop to incrementally improve the model. A further challenge will come in figuring out if and how that model can then be applied to similar waste streams at other sites within or outside the region.

The outlook is similar for using AI to recover and process needed CMs from other domestic waste streams or more conventional domestic resources. The first steps are to clearly define the specific types of data required for the geographic area, identify the best existing or potential sources and methods, and determine which AI/ML applications are appropriate based on the available data. NETL and other labs can assist in specifying data needs, sources, and filters for each application.

Sources

Bromhal 2022. Dr. Grant Bromhal, briefing on "Overview: Critical Minerals and Materials," Minerals Sustainability Division, Fossil Energy and Carbon Management, U.S. Department of Energy, July 14, 2022. www.energy.gov/sites/default/files/2022-08/Bromhal%20-%20DOE%20CMM%20Overview_July%2014%20Workshop_FINAL.pdf

Griswold 2022. Eliza Griswold, "Could Coal Waste Be Used To Make Sustainable Batteries?" The New Yorker, August 26, 2022. www.newyorker.com/news/us-journal/could-coal-waste-be-used-to-make-sustainable-batteries

NETL. National Energy Technology Laboratory, Critical Minerals and Materials Program webpage. Accessed March 28, 2023. https://netl.doe.gov/resource-sustainability/minerals-and-materials/program-overview/background