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Opportunities for Process Intensification with Membranes to Promote Circular Economy Development for Critical Minerals

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ABSTRACT

Critical minerals are essential to the future of clean energy, especially energy storage, electric vehicles, and advanced electronics. In this paper, we argue that process systems engineering (PSE) paradigms provide essential frameworks for enhancing the sustainability and efficiency of critical mineral processing pathways. As a concrete example, we review challenges and opportunities across material-to-infrastructure scales for process intensification (PI) with membranes. Within critical mineral processing, there is a need to reduce environmental impact, especially concerning chemical reagent usage. Feed concentrations and product demand variability require flexible, intensified processes. Further, unique feedstocks require unique processes (i.e., no one-size-fits-all recycling or refining system exists). Membrane materials span a vast design space that allows significant optimization. Therefore, there is a need to rapidly identify the best opportunities for membrane implementation, thus informing materials optimization with process and infrastructure scale performance targets. Finally, scale-up must be accelerated and de-risked across the materials-to-process levels to fully realize the opportunity presented by membranes, thereby fostering the development of a circular economy for critical minerals. Tackling these challenges requires integrating efforts across diverse disciplines. We advocate for a holistic molecular-to-systems perspective for fully realizing PI with membranes to address sustainability challenges in critical mineral processing. The opportunities for PI with membranes are excellent applications for emerging research in machine learning, data science, automation, and optimization.

Keywords: Renewable and Sustainable Energy, Supply Chain, Multiscale Modelling, Process Intensification, Membranes, Machine Learning

INTRODUCTION

As of 2022, there are 50 critical minerals [1] essential to renewable energy, such as lithium and rare earth elements (REEs). Lithium is vital to the function of several different types of batteries. REEs, particularly dysprosium, neodymium, praseodymium, and terbium, have unique properties (e.g., magnetic, fluorescence), which make them essential components of many electronics and clean energy technologies (e.g., displays, hard disk drives, wind turbines, electric vehicles). [2] Further, the term “rare” denotes that REEs are economically difficult to produce or concentrate [3]; although relatively abundant, REEs are generally present in very low concentrations.

Overall, there is a need to diversify the supply of critical minerals, as primary sources (e.g., minerals, clays, and brines) have been declining in quality (i.e., the concentration of critical minerals) [4,5] and the global energy transition (amongst other factors) has increased the demand for critical minerals. The combination of these issues drives a need to develop enhanced recovery processes, including for end-of-life materials, to obtain critical mineral supplies, improve sustainability, and progress

toward circularity goals. [6] These sustainability-driven efforts include moving attention towards alternative feedstocks such as recycled electronic waste and unconventional sources like coal fly ash. Additionally, the concentrations of critical minerals in some alternative and unconventional sources are beginning to surpass those in primary sources. [2,7,8] Regardless of the source, critical mineral processing generally relies on techniques that can use hazardous materials (e.g., acid leaching). [9] One pathway to enhance sustainability and improve the process performance of critical mineral systems may be to integrate membrane technology, which has a track record of success in other industries (e.g., desalination, water treatment, chemical processing, and biomanufacturing). [10]

This brief literature review focuses on opportunities for membrane technologies to optimize and intensify critical mineral processing systems. We emphasize the importance of a molecular-to-systems perspective with close collaborations between process systems engineering (PSE) and other fields (e.g., membrane, data, and computational sciences) to accelerate the development of a circular economy.

CRITICAL MINERAL PROCESSING

Evolving Supply Chains

The continued development of domestic critical mineral infrastructure is vital to decreasing reliance on foreign supply chains. Taking the United States as an example, in 2022, the country produced only 14 critical minerals domestically, relying entirely on net imports for 12 critical minerals and more than 50% on net imports for another 31 critical minerals. [11] Developing domestic supply chains will safeguard against unforeseen insecurities in the global market. For example, the COVID-19 pandemic caused disruptions across all aspects of supply chains, where production of certain critical minerals (e.g., manganese) decreased, and consumption of others (e.g., platinum) increased. [11] Therefore, securing reliable supply chains of critical minerals will be essential to national security and the clean energy sector.

The growing dependence on technology and the decreasing quality of primary ore necessitates a more concerted shift towards harvesting critical minerals from secondary and unconventional sources, including recycled materials. In particular, integrating recycled waste into current infrastructure can promote a circular economy for critical minerals; therefore, developing new and existing processes is essential to achieving global climate goals. There has been some progress in recycling practices; for example, the domestic supply of 7 critical minerals in the United States consisted exclusively of recycled materials [11].

Technology and Challenges

Critical mineral processing systems often contain the four steps presented in Figure 1: mining/extraction, beneficiation/pre-treatment, chemical extraction, and separation/purification. [12] The technology used within these steps depends on the feed stream. For example, mineral ore requires mining techniques (e.g., open-pit, underground, *in situ* extraction) to extract host rocks or the critical minerals [13]; brines frequently need to be pumped from underground [14]; and end-of-life consumer waste (e.g., cell phones) requires diversion from landfills via collecting the products to be recycled (i.e., urban mining). Beneficiation (or pre-treatment) encapsulates the techniques that concentrate the critical mineral feeds by removing unwanted parts (e.g., nonvaluable rock and casings on electronic devices) or physically preconcentrate liquid sources. Typically, both chemical extraction and separation/purification employ hydrometallurgical (i.e., leaching, solvent extraction, and precipitation) or pyrometallurgical techniques (i.e., high temperatures) [7], which obtain critical minerals in usable quantities and purities.

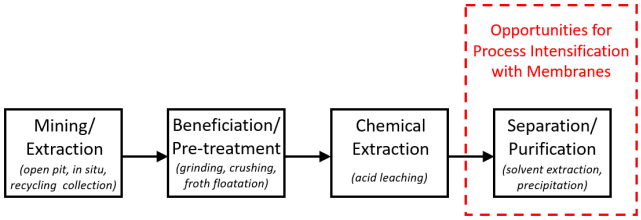

Figure 1. Generalized block-flow diagram for critical mineral processing route.

Overall, there is motivation to revolutionize the processing structure of critical minerals to reduce the environmental impact, physical footprint, or cost of purification. Conventional processing can produce large waste streams, which can be detrimental to the environment, or may have large physical footprints that disturb habitats. For example, acid leaching (hydrometallurgy) dissolves solid critical minerals into a liquid phase, creating acidic waste that requires treatment before disposal. On the other hand, lithium recovery from salt-lake brine has an extensive physical footprint, using large evaporation lakes/ponds to precipitate contaminants out of the solution successively. [15] Separation processes such as solvent extraction use long sequences of settling tanks and separators and have slow process dynamics; thus, they cannot quickly adapt to changes such as new feed concentrations or product specifications. In many of these areas, the focus has shifted to designing processes that reduce the environmental footprint and can address variability in the feed concentrations. Some sustainable solutions address specific environmental concerns (e.g., an

Table 1. A breakdown of different critical mineral sources and 30 references that highlight various membrane technology implementations for each respective feedstock (lithium- or rare earth elements-based).
LIB: lithium-ion battery; SLM: supported liquid membrane; LLM: liquid-liquid membrane; LEM: liquid emulsion membrane; PIM: polymer inclusion membrane
* Industrial waste, mine tailings, and coal leachate
+ Nanofiltration, ion exchange, electrodialysis, electrolysis, capacitive deionization, diffusion dialysis

Feed		Membrane Process	Charged Separations+	SLM, LLM, LEM, PIM	Adsorption	Membrane Distillation
Li	Ore			[51]		
	Brine	[16–18]	[20,52–58]	[59]	[22,31]	[24,60]
	LIB	[19]	[47,61]	[62]		
REEs	Ore			[63]	[23]	
	Magnet		[64]	[65–67]		
	Waste*		[68,69]	[21,70]		

electronic waste recycling process that limits the use of mineral acid leachates [9]); however, the processes are typically bespoke. Replacing certain hydrometallurgical techniques with mass separating agents (e.g., membrane systems) can offer environmental benefits for all critical mineral feed streams and facilitate process intensification (PI).

CRITICAL MINERAL PROCESS INTENSIFICATION

Membrane Opportunities

Membranes are uniquely equipped to aid in PI, as they can potentially improve efficiency, energy consumption, and cost in many chemical engineering systems. [10] Table 1 organizes a non-exhaustive set of references by the lithium- or REE-based feed stream and the corresponding applications of membrane technologies.

Recently, there has been significant work in developing membrane units for critical mineral separations. For example, comprehensive lithium recovery processes from salt-lake brine, primarily relying on nanofiltration (NF), have produced high-purity lithium products. [16–18] Kumar *et al.* [19] developed a process for recycling lithium-ion batteries (LIB) that leverages membranes to obtain battery-grade lithium carbonate. However promising, these processes are limited by their bench-scale design for singular feed streams. Membranes with charge-based separation mechanisms have been extensively applied to lithium extraction. For example, NF membranes have successfully separated lithium and magnesium ions in salt-lake brines by leveraging electrostatic interactions. [20] Similarly, liquid membranes have shown similar separation capabilities with REEs from coal fly ash leachate while utilizing less hazardous solvents than conventional solvent extraction. [21] Adsorption-based membrane techniques have demonstrated enhanced separations for both lithium and REEs. [22,23] Additionally, membrane distillation has been implemented to achieve lithium recovery from brine four times faster than conventional evaporation ponds, with 20 times less surface area, and a corresponding reduction in physical footprint. [24]

PSE can guide future membrane studies like those presented in Table 1. Specifically, membrane cascades, which enable fractionation (i.e., utilize staged separations to isolate single-ion product streams), will be vital within critical mineral processing due to the complex feed streams typical of the industry. For example, batteries in electric vehicles can contain the following critical materials: lithium, cobalt, manganese, nickel, and graphite. [25] While the components are relatively well-defined, the specific material compositions will vary depending on the battery type. [26] Processes to recycle the components of diverse batteries must be able to separate critical minerals from one another for efficient downstream re-manufacture. The optimization of membrane cascades is one of the significant benefits that PSE offers within the critical mineral space.

Multiscale and Interdisciplinary Challenges

The ability to rapidly develop, optimize, and scale up processes can accelerate circular supply chain development and the ability to meet clean energy (and, by extension, critical mineral production) goals. Multiscale optimization can be achieved with bidirectional (bottom-up and top-down) feedback to link technology breakthroughs at materials and device scales with process scale-up, supply chain optimization, and policy development at process and infrastructure scales. We now elaborate on these themes in five specific research opportunities.

Machine Learning to Accelerate Material Design

Due to the number of different membrane materials (e.g., organic, inorganic) [27], materials should be chosen optimally for critical mineral separations and process

development. Membrane optimization is usually inefficient when pursued solely through Edisonian experimentation due to the complexity of the design space (i.e., the parameters needed to describe material properties and reaction conditions) and the physical phenomena (i.e., the parameters within the mathematical model). [27] As such, machine learning (ML's) capabilities with high-dimensional data make it well-suited to tackle membrane problems with many degrees of freedom. [27] Membrane development efforts present an opportunity to further improve and enhance the design, environmental impact, and performance of critical mineral and material production systems, with the performance of membrane materials being the limiting factor in new, more environmentally responsible processes. [28] Recently, there have been significant developments in ML techniques to push the functionality of membrane materials. For example, Bayesian optimization (BO) [29] can search the vast design space (i.e., monomer and fabrication conditions) for NF membranes. [30] The advanced capabilities of BO increased the efficiency of membrane design and allowed for the fabrication of membranes that exceeded the upper limit of the trade-off between water selectivity and permeability. [30]

Mathematical modeling and ML can connect material design with larger length scales to enhance technological success. [27,31] For example, Eugene *et al.* [31] explored adsorptive membranes for removing lithium from water, comparing the properties of several sorbents to identify feasibility ranges. Further, the framework enables analysis of membrane performance after scale-up, emphasizing the importance of characterizing materials within the desired operating range. As another example, Rall *et al.* [32] used artificial neural network surrogate models to optimize membranes at the material and process levels. Testing new materials within the desired system will become vital within critical mineral separations as the feed streams evolve. For instance, process development and optimization must occur as new critical mineral sources emerge in recycled products. Employing similar frameworks for newly identified feed streams can accelerate material testing, process development, and scale-up.

Optimizing Membrane Modules

Computational fluid dynamics (CFD) helps optimize transport and flows in membrane module and device designs. [33] For example, Shirazi *et al.* [34] applied CFD to membrane distillation (MD), a thermally-driven membrane separation process, offering guidance on the physical design of the MD module and improving membrane performance. Recently, Choi *et al.* [35] used CFD with design of experiments (DoE) to identify variables affecting performance and determine the optimal MD module design. Similar optimization strategies using CFD simulations have been applied to membrane bioreactors. [36,37] The success of CFD techniques in optimizing the physical membrane module design can extend to the critical mineral space to enhance overall process development further.

Increasing Experimental Efficiency

PSE paradigms motivate the transition from Edisonian research to optimized and automated experiments.

We posit that membrane science is ripe to benefit from experiment automation and optimization advances. Automating experiments can accelerate material discovery by reducing the required time. For example, Muetzel *et al.* [38] automated a diafiltration experiment, reducing experimentation time by 40% and discovering concentration dependence of transport parameters. Similarly, Ouimet *et al.* [39] dosed a diafiltrate (of higher or lower concentration than the feed) into their automated diafiltration system to evaluate an expansive concentration space for water purification, leading to parameter identification five times faster than traditional filtration methods.

More robust efforts in enhanced experimental automation focus on self-driving laboratories (SDLs), which combine robotics and automated lab work with ML techniques to iterate experiments until the desired objective is reached. [40] SDLs improve computational efficiency (compared to the scientist performing the analysis) and increase the speed and precision of repetitive experimental techniques. [40] Further, SDLs can improve material discovery. For example, MacLeod *et al.* [41] recently developed a SDL for palladium film synthesis to quantify the trade-offs between temperature and conductivity. Their SDL required human action every 40-60 experiments, providing a robust dataset of information and overcoming human limitations. [41] Alternatively to SDLs using data-driven ML models, experimentation can be optimized using model-based design of experiments (MBDoE). MBDoE exploits the mathematical structure of science-based models to identify the experiments that will generate the most informative data efficiently. [42] We anticipate that SDLs driven by MBDoE will be critical to navigating the complex (often competing) phenomena that govern efficient membrane separations.

Process Design and Optimization

Membrane cascades typically have several feasible designs [43], and as the system complexity or size increases, it becomes unfavorable for the researcher to optimize each process individually. Superstructure optimization (SSO) is a popular strategy to assess all configurations using mathematical programming [44], subject to the desired objective (e.g., minimizing energy or cost, maximizing recovery or revenue) and constraints (e.g.,

transport phenomena, number of stages).

The success of SSO for membrane-based processes in other fields (e.g., carbon capture [43,45,46]) can inform future work in the critical mineral space. SSO has optimized membrane cascades within post-combustion carbon capture to identify more efficient designs. [43,45] SSO routinely accommodates multiple objectives (e.g., cost, emissions, water usage). [46] The generalizability of SSO also allows for increased flexibility (e.g., configuration size, separation type, individual module performance). For example, Lee *et al.* [45] found that varying the membrane properties in different stages (higher permeance upstream, higher selectivity downstream) improved process performance and efficiency. The generalized framework of SSO enables the application to diverse applications, allowing adaptation within critical mineral separations. Specifically, diafiltration cascades have used SSO for lithium-cobalt separation systems [47], efficiently optimizing staged separations and evaluating trade-offs in material property targets.

Supply Chain Optimization

Finally, supply chain optimization can identify the best opportunities for PI to maximize the impact at a global scale by promoting resilient and circular supply chains for critical minerals. For example, Canales-Bustos *et al.* [48] considered economic and environmental factors to optimize a mining supply chain subject to decarbonization goals. Fattahi *et al.* [49] investigated uncertainty in the critical mineral supply chain through multistage stochastic programming. Similar studies performing optimization under uncertainty will be essential to developing resilient supply chains, as variability in feed concentration, desired product specifications, market prices, and consumer demand is inevitable. After integrating membranes within process and infrastructure models, PSE methods enable the communication of performance targets back to the materials and device scales. This integrated feedback loop is the key to rapidly optimizing enhanced critical mineral processes within a circular economy.

CONCLUDING REMARKS

We propose a molecular-to-systems perspective of critical mineral processing and process systems engineering to enable process intensification with membranes. Machine learning techniques enable accelerated material discovery by evaluating material properties and process targets across materials, devices, and systems scales. Material discoveries lead to more robust device design, which can be further enhanced using automation and optimization techniques. Superstructure optimization of membrane cascades increases the generalizability and flexibility of process design and can evaluate membrane material property targets and design specifications. Finally, supply chain optimization enables multistakeholder optimization by managing material and energy flows and determining facility siting. [50] The advancements within the device and materials scales inform process design and infrastructure development, and vice versa, emphasizing the need for a holistic approach involving the materials, membrane, data, and computational science communities.

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