Designing Operationally Flexible Diafiltration Membrane Systems for Li/Co Separation

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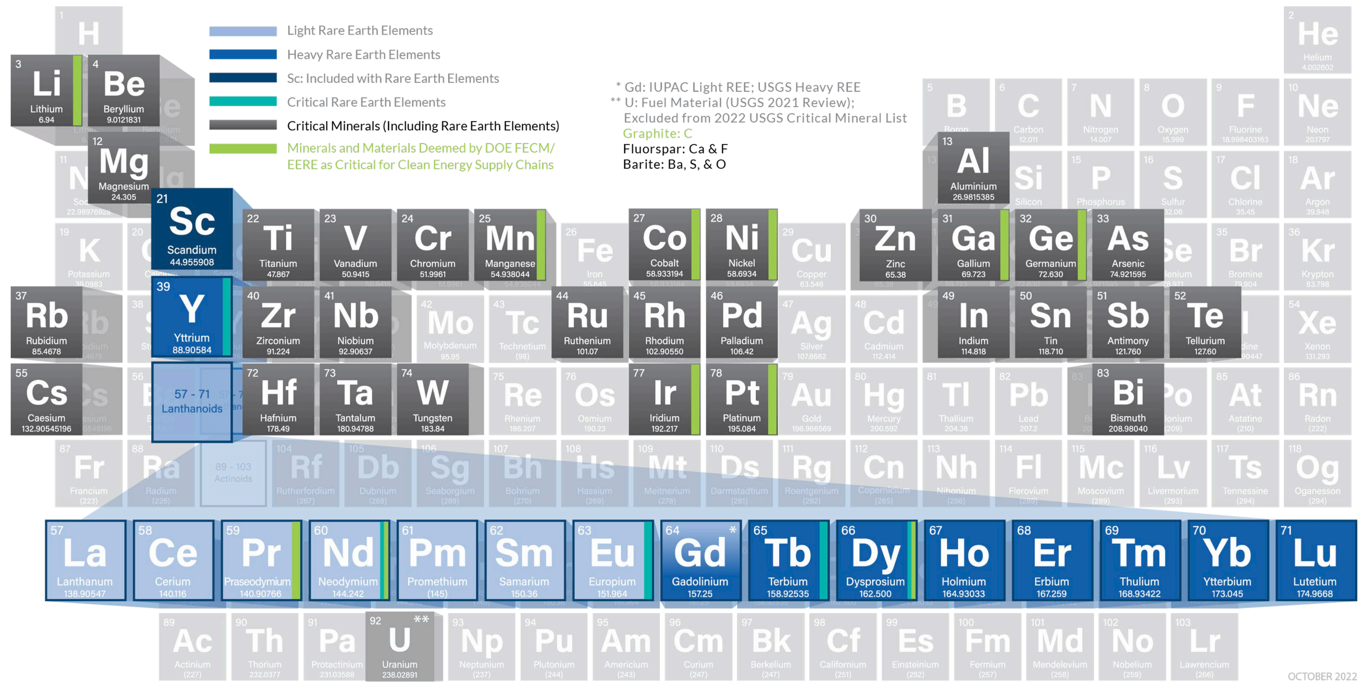
Critical Minerals Overview

The shift to clean energy systems is driving **significant increase in demand for** critical minerals (CMs).



Current Challenges:

– High geographical concentration of CM resources
– Long project times and environmental concerns of mining operations
– Higher vulnerability of supply chains for CMs

Membrane technologies are promising low-energy, aqueous processes with potentially high purity CM recoveries

Multi-Stage Diafiltration Model

(Based on original model from [1])

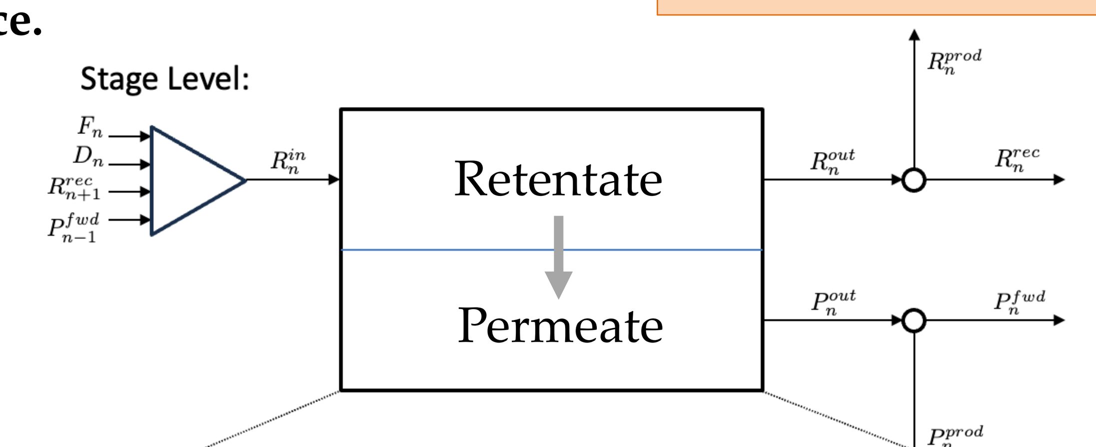
Model extended to:

- Adjustable number of membrane stages (NS) and number of tube elements (NT) using **IDAES unit models**.
- Multi-period applications for changes in process conditions over time.
- Membrane performance parameters **indexed over time and space.**

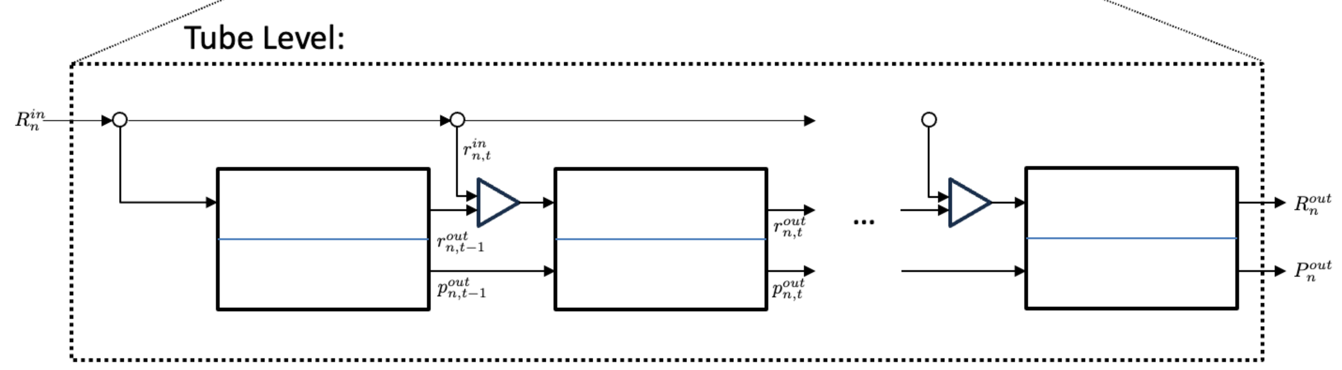
$$\max \quad \mathcal{Cobalt\ Recovery}$$

s.t.
- Stage Connectivity Balances
- Permeate Mass Balances
- Retentate Mass Balances
- Membrane Performance Equations
- Lithium Recovery Bound
- Flow Rate Bounds

Stage Level:



Tube Level:



Process Design Flexibility

Industrial processes must be able to perform under uncertain and changing operating conditions.

Two types of variables in robust process design:

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

Operational flexibility can be added through additional control **degrees of freedom (DoF)**, increasing a system's ability to respond to changes.

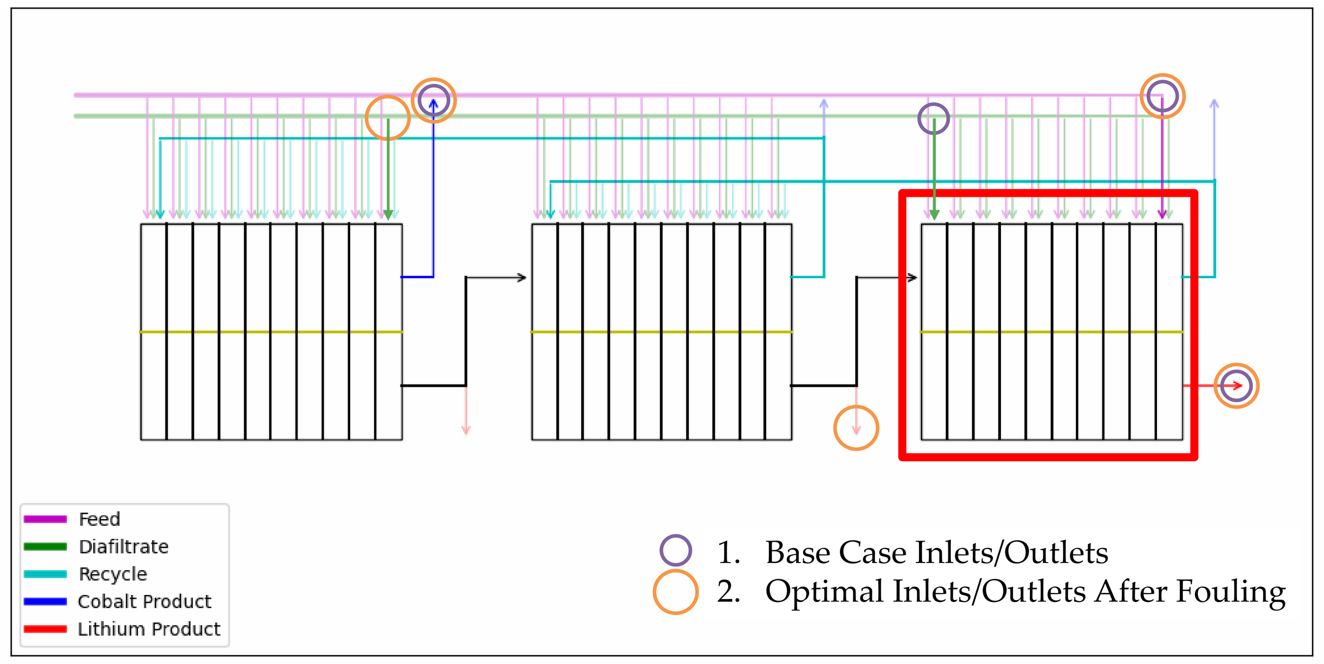
- Stage-Level Mixing: Flows mixed before each stage. The flow of the mixed inlet into each tube can be controlled.
- Tube-Level Mixing: Flows mixed before each tube. This is the most generalized superstructure with greatest capital costs.

Variables	Stage-Level Mixing DoF		Tube-Level Mixing DoF	
	Stage	Tube	Stage	Tube
Length	1	———	1	———
Feed Split	$NS-1$	———	$NS-1$	$NS(NT-1)$
Diafiltrate Split	$NS-1$	———	$NS-1$	$NS(NT-1)$
Recycle Split	———	———	———	$(NS-1)(NT-1)$
Mixed Inlet Split	———	$NS(NT-1)$	———	———
Product Outlets	$2NS-2$	———	$2NS-2$	———
Total DoF	$NS(NT+3)-3$		$3NS \cdot NT + NS - NT - 2$	

Case Studies

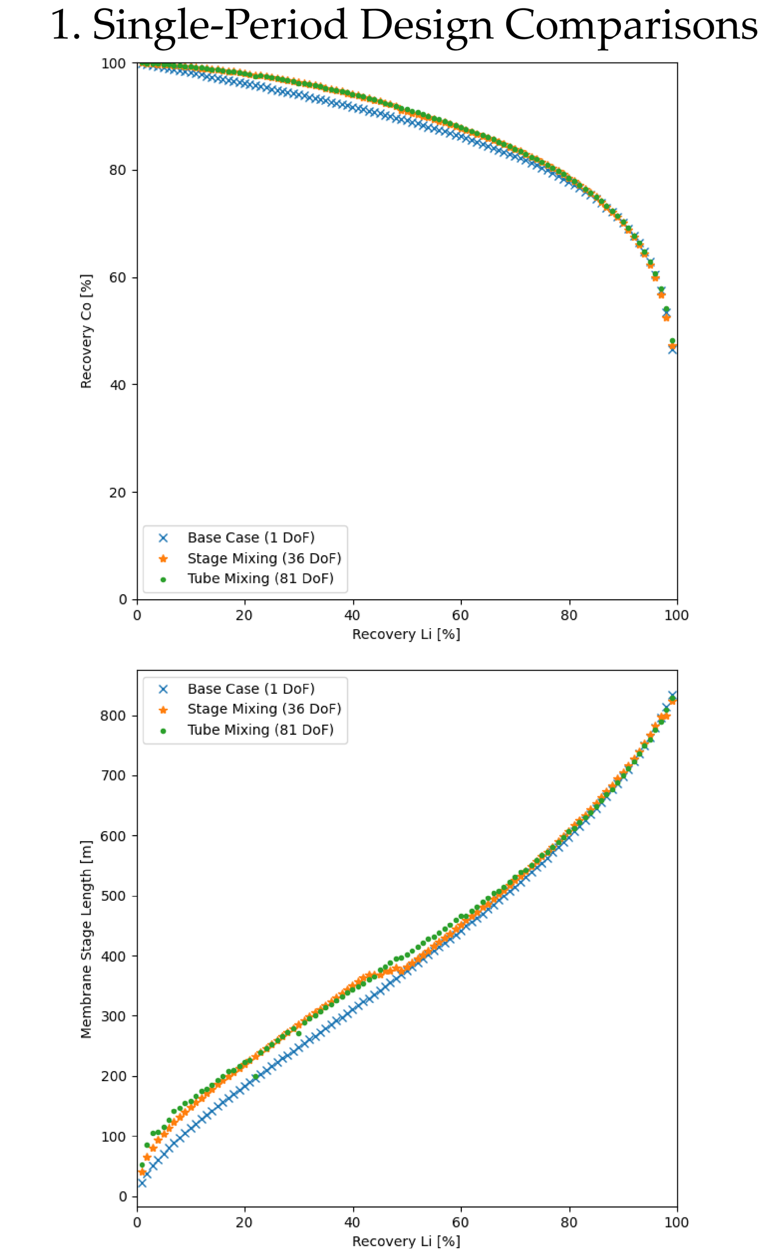
Base Case: Optimal flow configuration for 95% lithium recovery and choice of membrane stage length (1 DoF)

1. Compare base case with flexible design superstructures
2. Investigate effect of decrease in membrane flux over time on process design
   - ➢ Fouling is an inevitable phenomenon in membrane processes and may contribute to a decrease in flux.
   - ➢ We study a **linear decrease** in membrane flux to 50% of its original value over three periods.
   - ➢ **Membrane stage three** is chosen as an important location of process inlets/outlets for the base case.

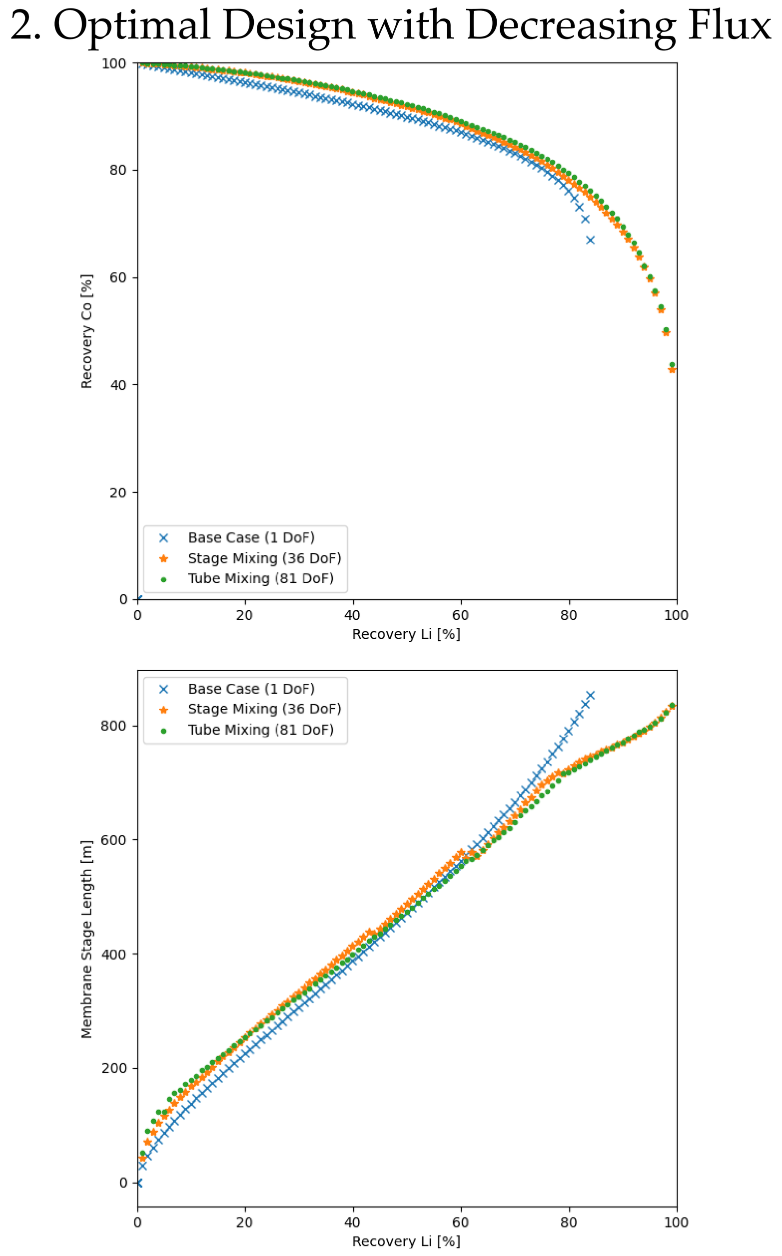


Computational Results

1. Single-Period Design Comparisons



2. Optimal Design with Decreasing Flux



- ✓ Operational flexibility through added DoF (more complex design) obtains **noticeably higher cobalt recoveries.**
- ✓ Decrease in membrane performance results in infeasibility of high lithium recoveries for **base case**.
- ✓ Flexible designs are **feasible across the entire Pareto front** and effectively handle the different operating conditions.

Conclusions and Future Work

Conclusions:

- We developed **operationally flexible, multi-period diafiltration models** for process designs that can adjust to changes in operating conditions and membrane material performance over time.
- Our results allude to the fact that **incorporating flexibility in design is important for minimizing technical risks.**

Future work:

- ❑ Incorporate **uncertainty** into feedstock and membrane performance parameters and **perform robust optimization** using the Pyomo Robust Optimization Solver (PyROS).
- ❑ Add costing into models to allow for **developing diafiltration systems optimized for both cost and performance.**

Acknowledgements

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For more information, please reach out to Thomas Tarka, PrOMMiS Technical Director (Thomas.Tarka@netl.doe.gov)

References

[1] Noah P. Wamble, Elvis A. Eugene, William A. Phillip, and Alexander W. Dowling. Optimal Diafiltration Membrane Cascades Enable Green Recycling of Spent Lithium-Ion Batteries. ACS Sustainable Chemistry & Engineering, 10(37):12207–12225, September 2022.