SLATT UNDERGRADUATE RESEARCH FELLOWSHIP
FINAL REPORT

SCHOLAR NAME:	Noah Wamble
FACULTY ADVISOR:	Dr. Dowling
PROJECT PERIOD:	Winter Term 2020-2021
PROJECT TITLE:	Novel Diafiltration Cascades for Lithium Ion Battery Recycling
CONNECTION TO ONE OR MORE ENERGY-RELATED RESEARCH AREAS (CHECK ALL THAT APPLY):	**(X) Energy Conversion and Efficiency** **( ) Sustainable and Secure Nuclear** **( ) Smart Storage and Distribution** **( ) Transformation Solar** **( ) Sustainable Bio/Fossil Fuels** **( ) Transformative Wind**

MAJOR GOALS AND ACCOMPLISHMENTS

Summarize your research goals and provide a brief statement of your accomplishments (no more than 1-2 sentences). Indicate whether you were able to accomplish your goals by estimating the percentage completed for each one. Use the next page for your written report.

RESEARCH GOALS	ACTUAL PERFORMANCE AND ACCOMPLISHMENTS	% OF GOAL COMPLETED
Finish Analysis of Solutions	Reran and solved model for anisotropic cascades to finish analysis	100%
Create Design Heuristics	Analyzed 1000s of solutions to come up with simple design heuristics	100%
Create Cascade Analysis Videos	Create video plots of the difference cascades to help with design heuristics	100%
Further Education	Participated in MolSSI Coding Best Practices seminar and book study to further educate myself on how to code	100%
Write Paper Outline	Wrote an outline for the paper we intend to write for this research	100%
Write Paper Draft	Currently working on writing the draft as most of the figures are in their final stages now	10%

RESEARCH OUTPUT

Please provide any output that may have resulted from your research project. You may leave any and all categories blank or check with your faculty advisor if you are unsure how to respond.

CATEGORY	INFORMATION
EXTERNAL PROPOSALS SUBMITTED	N/A
EXTERNAL AWARDS RECEIVED	N/A
JOURNAL ARTICLES IN PROCESS OR PUBLISHED	Writing a paper which will be submitted this semester and will count as a senior thesis
BOOKS AND CHAPTERS RELATED TO YOUR RESEARCH	N/A
PUBLIC PRESENTATIONS YOU MADE ABOUT YOUR RESEARCH	Upcoming 2021 AIChE Spring Meeting, April 21st, 2021, Virtual
AWARDS OR RECOGNITIONS YOU RECEIVED FOR YOUR RESEARCH PROJECT	N/A
INTERNAL COLLABORATIONS FOSTERED	William Phillip, WATER Lab, weekly research meetings
EXTERNAL COLLABORATIONS FOSTERED	N/A
WEBSITE(S) FEATURING RESEARCH PROJECT	N/A
OTHER PRODUCTS AND SERVICES (e.g., media reports, databases, software, models, curricula, instruments, education programs, outreach for ND Energy and other groups)	N/A

RESEARCH EXPERIENCE

Please let us know what you thought of your research experience: Did this experience meet your expectations? Were lab personnel helpful and responsive to your needs? What else could have been done to improve your experience or achieve additional results?

I had a wonderful research experience this winter break as this experience met all expectations. It was a great introduction to what conducting computational research full time as a graduate student would be like. All of the lab personnel were helpful and responsive to my needs and were willing to meet with me when I was stuck on an issue. Nothing else could have been done to improve my experience!

FINAL WRITTEN REPORT

With the advent of electric cars, the demand for Lithium is expected to surpass that which can be met from current supply channels. Therefore, new sources of Lithium must be found soon to meet this growing demand. Additionally, with the growing number of electric vehicles, there will be a large number of spent automobile batteries that will create an E-waste boom in the future. However, this work looks at solving both of these problems by recycling these batteries to prevent this E-waste boom from happening and to create a new source to recover Lithium from using a green process. This process will be accomplished by using membrane cascades, as this technology is highly energy efficient.

Membrane processes have been found to be an energy efficient technology that can be used to accomplish separations using greener methodologies. Specifically, diafiltration membrane cascades have been proposed because they have been shown to perform well in lab but have not yet been used much in industry outside of niche applications in the pharmaceutical and food and beverage industries. These membrane cascades are useful at recovering a high value product at high purity and could be applied to this problem of recycling Lithium Ion batteries, where the Cobalt and Lithium ions need to be separated. Typically, these ions are separated by using acid leaching and solvent extraction, where harsh solvents are typically used. This winter break, I am specifically looking at applying advanced process systems methodologies to this separation problem trying to gain insight into how membrane material properties effect the full-scale operation. This work also shows that separations that were once thought to be infeasible and inhibited by material's properties are in fact able to be accomplished, once the entire system has been fully optimized.

To fully optimize this system, this work successfully applies a superstructure model to these diafiltration membrane cascades. In contrast to simulation techniques, superstructure optimization explicitly manipulates configuration parameters such as all feed input locations, recycle strategies, split fractions, number of stages, and membrane area. Thus, this model exploits many more degrees of freedom to search for novel system configurations. An example superstructure model for a three-stage system is shown below in Figure 1.

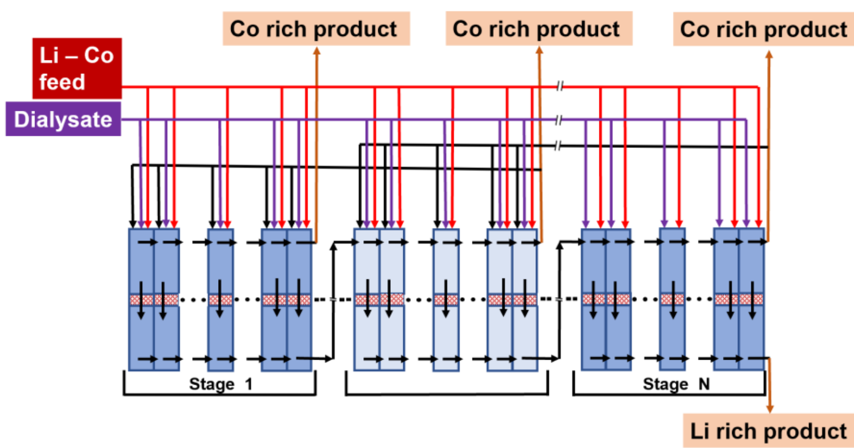
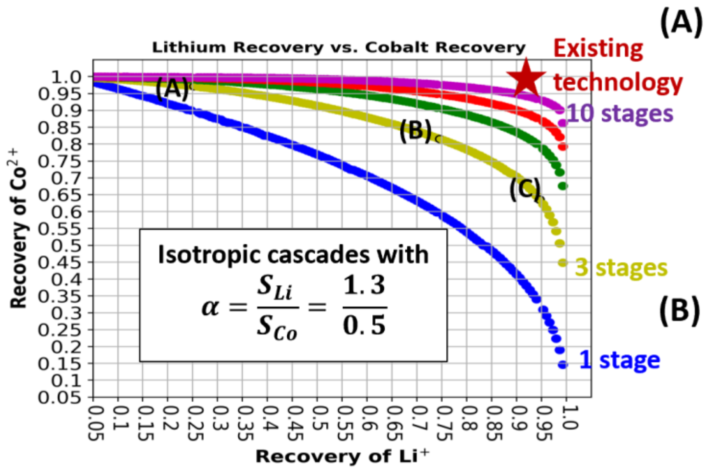
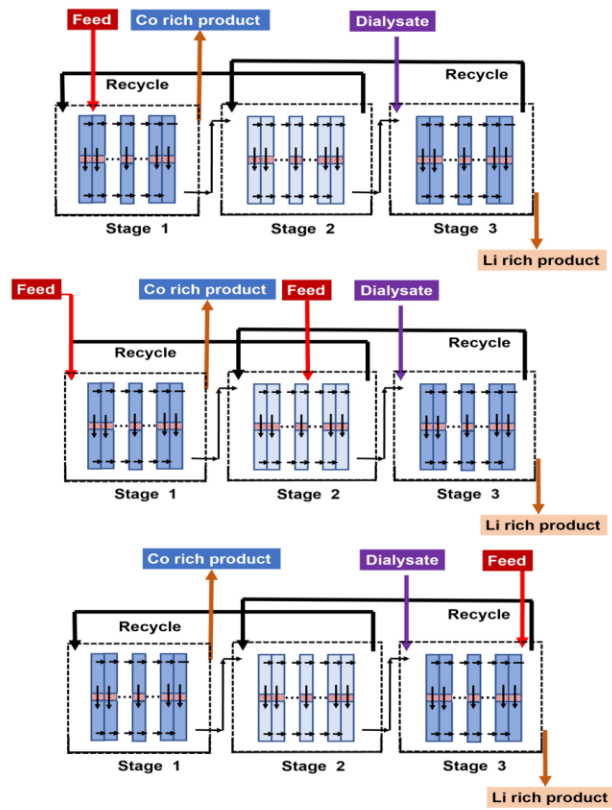


Figure 1. Superstructure Optimization Model where the red box represents the fresh feed into the system and the purple is the fresh dialysate into the stream. These streams are then split into flow streams into each finite element across the cascade. Cobalt product may be drawn from any stage whereas all the lithium product leaves from Stage N.

This Figure reveals how many different solutions this superstructure optimization model can consider as the flow can go to any finite element. Being able to consider such a wide solution set is what allows novel solutions to be found. This model was solved by first maximizing the amount of Cobalt recovered and then fixing this value. In a second optimization step, The amount of impurity in the Cobalt and Lithium product streams is minimized. This model was solved for 1-10 stages, and a sensitivity analysis was performed by varying the amount of Lithium recovered to create Pareto Curves for all of the optimal designs. Please see Figure 2 below which shows these pareto curves, and some sample designs for a three stage system.





	Case A	Case B	Case C
Li^{+} Recovery	25%	75%	95%
Co^{2+} Recovery	97.2%	81.3%	62.9%
Membrane Area (m^2)	96.5	214.7	285.3
Stage Cut 1	0.30	0.66	0.88
2	0.56	0.44	0.47
3	0.56	0.74	0.47

Figure 2. Pareto Curve for isotropic cascades with a selectivity ratio of 2.6 revealing trade-offs between recovery of Cobalt and Lithium and the number of stages used to design the cascade. Three sample designs for a three-stage system are shown on the right side side for (a) low lithium recovery, (b) medium lithium recovery, (c) and high lithium recovery. These designs are also compared with regards to their recoveries, membrane area, and stage cuts in the table above in the figure.

These three sample designs in Figure 2 reveal how the stream input locations are a function of the amount of Lithium recovered. To look at a simpler example, if all of these optimal designs' stream input locations are plotted for just a 2-stage system along the pareto curve, the following plot below in Figure 3 is produced. Each vertical line on Figure 3 corresponds to a single point on the pareto curve as the Lithium recovery is increased.

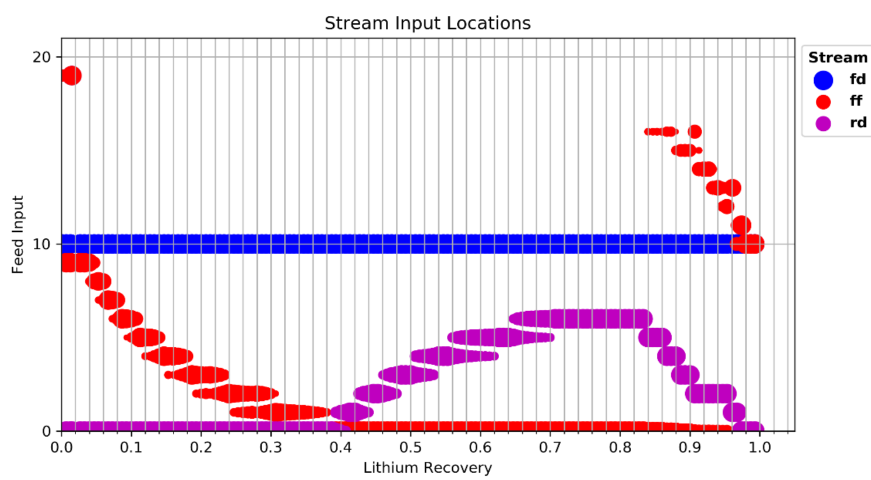


Figure 3. Design Heuristics for a 2 stage system where the blue stream is the fresh dialysate (fd), the red stream is the fresh feed (ff), and the purple stream is the recycle (rd). This figure reveals how the feed input location is a strong function of the amount of Lithium recovered and walks across the cascade which can be explained by the changing concentration gradients. Zero on the y-axis marks the beginning of the first stage, and 10 marks the beginning of the second stage, as there are 10 elements per stage.

By analyzing these solutions, design heuristics were derived, which can help engineers design optimal cascades without needing to go through such a rigorous optimization process. There are four main heuristics that can be used for designing these diafiltration membrane cascades which have been listed below.

1.) Dialysate always enters the beginning of the last stage, as shown by the constant blue line in Figure 3.
2.) Products are pulled off of opposite stages to maximize use of membrane area.
3.) Feed stream walks across cascade in set pattern shown above in Figure 3.
4.) Input streams enter the cascade where the concentration is closest to its own value to minimize entropy mixing losses.