SLATT UNDERGRADUATE RESEARCH FELLOWSHIP
FINAL REPORT

SCHOLAR NAME:	Zachary W. Muetzel
FACULTY ADVISOR:	William Phillip
PROJECT PERIOD:	January – December 2022
PROJECT TITLE:	3D-Printed Crossflow Diafiltration Modules for the Recovery and Recycling of Critical Materials
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
Use computational fluid dynamics software to rapidly guide unit design	COMSOL Multiphysics, a finite element analysis simulation software was used to rapidly enumerate through possible unit designs. Such simulations provided insight into the effect model geometry had on pressure and concentration distributions, flowrates, and membrane performance.	75
Leverage Notre Dame resources to produce chosen designs	The Center for Digital Scholarship and the Engineering Innovation Hub at Notre Dame were used to 3D print several designs. Transferring the designs from simulation to reality yielded valuable information into the feasibility of favorable simulation designs.	25
Validate the separation capabilities of the resulting cascades	3D-printed cascade validation did not occur due to time constraints.	0

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	
EXTERNAL AWARDS RECEIVED	
JOURNAL ARTICLES IN PROCESS OR PUBLISHED	ACS Applied Polymer Materials, *Device for the Acquisition of Dynamic Data Enables the Rapid Characterization of Polymer Membranes*, Zachary W. Muetzel, Jonathan Aubuchon Ouimet, William A. Phillip, Submitted: 9 January 2022, Published: 6 April 2022, 4, 5, 3438-3447
BOOKS AND CHAPTERS RELATED TO YOUR RESEARCH	
PUBLIC PRESENTATIONS YOU MADE ABOUT YOUR RESEARCH	
AWARDS OR RECOGNITIONS YOU RECEIVED FOR YOUR RESEARCH PROJECT	
INTERNAL COLLABORATIONS FOSTERED	Alexander Dowling, Notre Dame CBE Department, consultation on constraining simulation parameters, 2 – 3 Interactions Cara Kilmartin, Notre Dame CBE Department, application of single stage separation model for use in multistage cascades, 4 - 5 Interactions
EXTERNAL COLLABORATIONS FOSTERED	Alexander M. Pérez Reyes, University of Puerto Rico Mayagüez, to allow for insights gained above and below to be continued in future work, 2 – 3 Interactions
WEBSITE(S) FEATURING RESEARCH PROJECT	
OTHER PRODUCTS AND SERVICES (e.g., media reports, databases, software, models, curricula, instruments, education programs, outreach for ND Energy and other groups)	

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?

This research experience combined my interest in 3D printing and modeling with COMSOL Multiphysics, a computational fluid dynamics software that was new to me. Although COMSOL yielded a steep learning curve initially, I realized how powerful the software can be for separations modeling and a variety of other engineering applications. By utilizing a variety of resources internally and externally to Notre Dame, I was able to receive the help I needed to continue making progress toward my research goals. Unfortunately, I largely underestimated the amount of time needed to become technically competent in COMSOL to begin making real progress toward my research goals. Although good progress was made, I felt as though I didn't have enough time to complete my research objective and achieve additional results.

FINAL WRITTEN REPORT

(Please use the space below to describe your research project and objectives, any findings and results you can share, and graphs, charts, and other visuals to help us understand what you achieved as a result of this research experience.)

Society is becoming increasingly reliant on the use of batteries in a variety of applications, but the natural supply of many raw materials required for battery production cannot satisfy the demand. Consequently, for production of the widely used lithium-ion battery to scale with increasing demand, recycling of these batteries, and more specifically the raw materials they contain, will be necessary. At present, cobalt (Co) is the most expensive product of lithium-ion battery recycling, while lithium (Li) is quickly becoming more desired as the supply of natural lithium decreases. Today, harsh solvents are often used in Li/Co separations, which produce toxic byproducts and have unwanted environmental impacts. Fortunately, emerging membrane materials have shown promise as an alternative method for accomplishing this separation because of their flexibility and selectivity.

Clever systems design is required in conjunction with advances in membrane materials to accomplish this challenging separation. Guided by this information, a fellow undergraduate researcher, Cara Kilmartin, developed a model for a single stage diafiltration module (Industrial & Engineering Chemistry Research, **2021,** *60,* (43)). The model was experimentally validated using a physical apparatus that I designed and built. The resulting Acquisition of Dynamic Data (ADD) device is detailed in a paper published in *ACS Applied Polymer Materials*. The ADD device relies on a combination of commercial hardware and custom 3D-printed parts, and this experience prepared me for the proposed research objective below. Specifically, in addition to modeling the performance of a single stage system, Kilmartin et al. extrapolated the results to identify the enhanced performance that can be realized by connecting diafiltration modules in series (i.e., by creating a multi-stage cascade). Unfortunately, there was no experimental apparatus available to probe the performance of multi-stage designs.

The objective of the proposed research was to create crossflow diafiltration cascades that take advantage of the favorable properties of staging and controlling flows to increase the separation efficiency and advance the state-of-the-art in the separation of lithium and cobalt. The created device will be made up of one unit, or stage, that can be combined in sequence with identical units to achieve the desired separation. By allowing identical stages to connect to one another, the cascade has the advantage of having fewer parts and therefore being easier to produce and repair. Using mathematical models, fluid dynamics simulations, and additive manufacturing in an iterative feedback loop, a novel unit design can be created to maximize the separation efficiency and membrane testing capabilities it possesses.

To complete the above objectives, module creation was completed in two stages. First, COMSOL Multiphysics, a computational fluid dynamics software was used to enumerate over possible designs. A favorable design had properties of minimizing the pressure variation inside the module and ensuring the enclosed solution is well mixed, quantified by a maximum of 20% concentration difference within a stream. In parallel with the computational efforts described above, Solidworks, a computer-aided design (CAD) software was used to design physical modules. The resources of the Center for Digital Scholarship and the Engineering Innovation Hub at Notre Dame were then leveraged to 3D print the designed modules to better understand the physical limitations and requirements of future diafiltration cascades. Figure 1 below shows the parallel nature of the two research objectives.

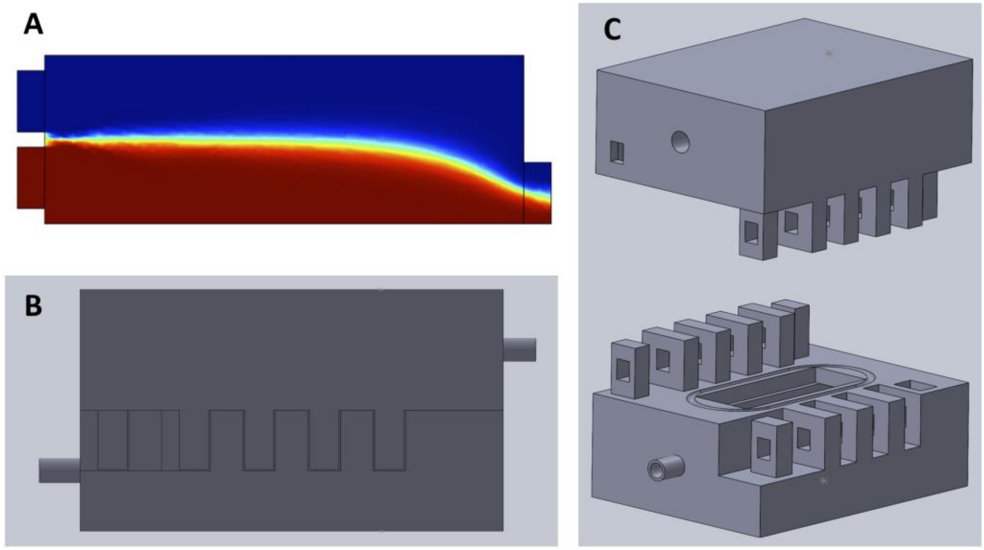

Figure 1. A) The results obtained from a COMSOL Multiphysics simulation shows the concentration gradient within a designed module. B) A physical rendition of the module shown in A, created in the computer aided-design software, Solidworks. C) An exploded view of the module in Solidwork shows how the top and bottom halves can be split apart so a membrane can be placed between the halves to achieve separation.

Panel A in Figure 1 shows a simulation result obtained from COMSOL Multiphysics that illustrates the calculated concentration gradient of solute within the module. Next, Panel B shows an analogous physical rendition, created in Solidworks, of the design simulated in A. Finally, Panel C shows an exploded view of the Solidworks model shown in B, demonstrating how the two halves of the physical rendition can be split apart, accessing a location for the membrane to be placed. The symmetrical nature of the physical model shown in Panels B and C promotes the easy connection of identical modules, allowing such a design to eventually realize the physical creation of a multistage diafiltration cascade.

Ultimately, the creation and optimization of crossflow diafiltration cascades for the recovery and recycling of critical materials is a never-ending process. When combining the computing power of a finite element analysis computational fluid dynamics software like COMSOL Multiphysics, the physical rendition capabilities of Solidworks, and the ultimate flexibility and manufacturing control provided by various 3D printing techniques, further creation, iteration, and optimization are always possible. The research objectives listed above that were not completed are being passed on to future Notre Dame researchers, who will leverage the insights gained from this effort.