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A GWEN Symposium

Graduate Women in Engineering Network

February 7, 2022
Abstract Booklet

WOMEN IN ENGINEERING PROGRAM

Contents

Effects of mix design and cement chemistry on flow and strength of mortar internally cured with superabsorbent polymers

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Keywords: superabsorbent polymers, cement chemistry, mortar flow, mechanical properties

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Superabsorbent polymer (SAP) hydrogel particles serve as internal curing agents in cementitious mixtures via the mechanisms of initial absorption and subsequent desorption of water throughout the cement matrix. Internally cured cementitious mixtures exhibit increased degree of hydration and reduced shrinkage and cracking, which can increase service life. SAP is added to cementitious mixtures in its dry form and absorbs water from the fresh cementitious mixture itself. If no mix adjustments are made to compensate for water absorbed by SAP during the swelling stage, the inclusion of SAP has the potential to decrease the mixture's flow. The effects of two different SAPs on the percentage flow of mortars were investigated using the mortar flow table test. Three approaches for modifying mix design were tested with respect to their effect on percentage flow and on compressive and flexural strength. Approach I: Extra water was introduced at a flat dosage or at a dosage equivalent to the SAP's equilibrium swelling capacity to compensate for the mixing water initially absorbed by the SAP. Approach II: (High range) water reducing admixture (HRWRA) was introduced at a dosage sufficient to produce mortar with a target percentage flow. Approach III: HRWRA was added to the SAP-containing mortars at a dosage sufficient to produce a SAP-free mortar of the same water to cement ratio (w/c) with a target percentage flow. Approach III was then tested using cements of different types and chemistries to evaluate the influence of SAP-binder chemical interaction on mortar flow and strength. We will present flow and strength results from these approaches to modifying mortar consistency when internally curing with SAP and results on the effect of SAP on strength at a given w/c.

Developing a Conceptual Framework to Understand Chemical Engineering Students' Learning Process in a Materials and Energy Balances Course

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Keywords: chemical engineering education, student success, learning, qualitative research

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Students are typically introduced to the chemical engineering curriculum through a materials and energy balances (MEB) course. Therefore, this course prepares students for future chemical engineering coursework, and students' learning experiences and outcomes in this introductory engineering classes impact their degree pathways. Notably, approximately 50% of engineering students leave their engineering program within the first two years. To begin to address this concern in a chemical engineering context, a framework that considers students' cognitive (i.e., knowledge), behavioral, and affective (i.e., feelings and emotions) processes within a sociocultural context is necessary.

This paper builds on the existing theoretical framework of self-regulated learning (SRL) to describe a systems approach to understanding the multifaceted context of learners in an MEB course. SRL was developed as a general learning framework that frames learning as a regulatory process with feedback mechanisms. Here, learners set learning goals and make decisions relevant to these goals constrained by personal and contextual factors. A learner's environment and larger context are inextricably linked with their learning development as individuals learn through collaborative dialogues with peers and instructors. SRL aids in addressing why some students achieve the desired learning outcomes and how the learning environment influences the learning process; however, it does not consider the unique sociocultural factors that affect systematically minoritized students (i.e., women and Black, Indigenous, and Latinx students).

This paper reports on the development of a conceptual framework to determine how chemical engineering students navigate their learning in an introductory MEB course, which will be informed by qualitative data from five focus groups. The focus groups will consist of four to eight students and will be formed considering self-identified gender, race/ethnicity, and international student status. By considering students' identities, we plan to build rapport within each focus group and intentionally capture students' experiences different from the norm in chemical engineering. The focus group will ask questions about students' experiences within the course context, challenges to learning and success in the course, how they navigate those challenges (including support infrastructure), and feelings of motivation and support for succeeding in the class and their future careers. The results will produce a conceptual framework that considers students' cognition, motivation, and behavior in the context of students' identities and environmental factors. This framework will be helpful for chemical engineering education researchers studying how students learn new chemical engineering concepts and stakeholders interested in understanding how chemical engineering students navigate the discipline.

Subcutaneous Drug Delivery Methods for Increased Bioavailability

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Keywords: drug delivery, bioavailability, cellular interactions

Diverse biologic therapeutic compounds such as monoclonal antibodies (MAbs) are medicines derived from living organisms as opposed to chemically synthesized small molecules. They are traditionally protein based and therefore cannot be orally administered. Therefore, Subcutaneous (SC) drug delivery is the future of at-home therapies for biotherapeutics--it reduces invasive hospital visits, cost of drugs, and pain associated with administration. However, SC drug delivery is limited by a reduction in bioavailability of some drugs following injection. Bioavailability refers to the fraction of drug that reaches the vascular system post-injection. The factors causing low bioavailability range from molecule size and molecule charge to uptake transporter affinity and formulation. The drug formulation is challenged by different components of the SC space such as collagen causing entanglement and increased viscosity, hyaluronic acid (HA) reacting with charged drugs, preferential lymphatic uptake of drugs larger than 16 kDa, among other issues. Although some methods have included changing the drug's formulation, this is not always possible. Methods covered in this review encompass the use of different mechanical and chemical means of increased drug bioavailability. The approaches include electricity-based methods, ultrasound-based methods, and permeation enhancement methods, which take advantage of reactions in the body. In the case of most existing methods, either the potential for at-home therapies is not possible, larger molecules are not aided in increased bioavailability, or they don't target both increased blood and lymphatic vessel uptake. These methods have the potential to increase the subcutaneous bioavailability of previously problematic drugs with some providing promising at-home capabilities.

Geospatial and social factors affecting heating electrification in the U.S.

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Keywords: environmental equity, heating electrification, geospatial analysis

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As the climate crisis grows, nearly every sector of civilization is under pressure to quickly decarbonize. The heating sector in particular accounts for almost half of total global energy consumption, with only 1/10th of heat produced from renewables (IEA, 2021). The adoption and technological advancement of heat pumps is key to electrifying heating and introducing more renewable sources. Heat pumps use electricity to transfer heat from a reservoir (usually air, water, or geothermal) to an indoor space, while more conventionally used furnaces and boilers generate heat with fossil fuels. This study aims to review literature on the sociological and geospatial factors related to consumers' ease of transition to electric heating. Such topics will include issues of energy justice and equity, grid access, energy poverty, and other possible barriers to heat pump installation and use. Furthermore, the study will present multiple maps of Illinois as a case study, combining existing NASA climate data and demographic information from the US Census to identify the most disadvantaged regions of consumers. We will focus first on social metrics of income and race as key identifiers for energy inequity. In addition, we will explore factors of living arrangements (i.e. persons per household), age, gender, and health. As for climate factors, we will focus on weather in various parts of the state to determine which regions have higher heating demands compared to others. Eventually, we would like to develop this study into a full model of the United States to better understand and communicate gaps in energy policy and research.

Investigation of Lamination Approaches of SiC Ceramic-Filled Polymer Blends for Heat Excahnger Applications

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Keywords: silicon carbide, co-extrusion, heat exchangers

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Silicon carbide (SiC) is a ceramic material that retains its high strength at elevated temperatures, is corrosion-resistant, and has a high thermal conductivity. These properties make SiC desirable for high-temperature heat exchangers for use in airplane gas turbine engines. One of the ways to improve the efficiency of heat exchangers, thus reducing CO2 emissions of the aircraft, is to increase the amount of porosity in the heat exchanger. Ceramic co-extrusion is a process of shaping ceramic powders where a feedrod of a ceramic/polymer mixture is heated and extruded through a reduced cross-section, reducing the size but retaining the symmetry of the original feedrod. The co-extrusion process is useful in creating the micro-porosity needed for better heat exchanger efficiency. One of the disadvantages of the co-extrusion process is the lamination step that is required to mate two extrudates together. The lamination step is often where delaminated regions occur. These delaminations cause a decrease in the strength of the heat exchanger. This presentation will focus on processing methods used to mitigate the delamination of extrudates. Some of the methods that will be discussed are using mechanical abrasion to remove any excess polymer and using a bimodal powder distribution to enhance particle interaction. Through a combination of techniques, the amount of delamination has been significantly reduced leading to improved heat exchanger strength. Delamination is an overarching issue when trying to mate two ceramic-polymer blends pieces together. This research provides insight into solutions to delamination that can be applied to various other applications besides high-temperature heat exchangers.

Design of Coupled Composite Plate Shear Walls for Seismic Applications

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Keywords: Seismic Design, Composite Systems, C-PSW/CF

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Coupled Composite Plate Shear Walls - Concrete-Filled (CC-PSW/CF) are an innovative seismic force-resisting system recently adopted in building codes. CC-PSW/CFs consist of composite plate shear wall - concrete filled (C-PSW/CF) and composite coupling beam components. C-PSW/CFs are composed of parallel steel faceplates connected by steel tie bars. These modules are prefabricated, shipped to the construction site, and erected. Once on site, the empty modules are filled with plain concrete. Composite action between the steel plates and concrete is ensured through steel tie bars and steel shear studs. Composite coupling beams are steel box sections with concrete infill. The CC-PSW/CF system is an alternative to conventional concrete core wall systems widely used in mid- and high-rise building design. CC-PSW/CFs have shown promise at decreasing on-site construction time compared to reinforced concrete core walls as they do not require the formwork, falsework, or wait time due to curing concrete typically walls do. This presentation will discuss the capacity design philosophy for CC-PSW/CF systems and design requirements enforced to ensure the system behavior follows this philosophy. The core concept of CC-PSW/CF design is enforcing a strong wall-weak coupling beam philosophy. This design philosophy results in the desired structural collapse progression of: (1) yielding in coupling beams, (2) yielding in walls, (3) plastic hinge formation in all coupling beams, and (4) plastic hinge formation in walls. After presenting the design philosophy and provisions, an example structure is presented which implements the design procedure. Nonlinear pushover and time history analysis is performed to explore if the structural collapse milestones are achieved. This performance is evaluated against relevant performance standards, ultimately showing that, when the design provisions are implemented, the resulting structure can be proportioned such that the behavior follows the desired collapse mechanism.

System Dynamics Model of STEM Retention Rates in Higher Education

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Keywords: System Dynamics, System Feedback Modeling, Data Collection, Policy

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A decline in the number of STEM candidates entering the workforce has been observed, and there is reason to believe this could lead to a shortage of STEM candidates within the US education system [1]. In an effort to better understand the various influences of students' pathways to STEM careers and what can be done to reverse the decline of STEM candidates, a System Dynamics model of the "STEM pipeline" has been created. The STEM pipeline describes the system encompassing a student's journey to a career in STEM and consists of K-12 education, higher education, and the STEM workforce. System Dynamics modeling has been used historically to study the STEM pipeline, but previous studies have lacked emphasis on the higher education portion of the system. This research attempts to model the impact of various policies made in institutions of higher education that affect retention rates in STEM fields.

My presentation will be focused on the general use of System Dynamics modeling, my methods used while creating the model of the STEM pipeline, verification and validation performed on the model, results gathered from the model, as well as plans for future research. I would prefer to give this presentation as a traditional conference talk. Giving a conference talk would give me the opportunity to convey to the audience the power of system dynamics modeling, any results of the model I have gathered, and gain experience presenting this material before future conferences I attend.

The model of the STEM pipeline is in its preliminary stages, and the majority of the current efforts are focused on data collection. A preliminary functional model has been created, and data gathering efforts are underway. Once data is collected, it will be cleaned, processed, and incorporated into the model. Results are expected to be implicative of trends seen in retention rates within STEM fields as various policies (such as scholarship opportunities, tutoring availability, program diversity, etc.) are adjusted within the model. The goal of this research is to identify which policies institutions of higher education can leverage with the goal of increasing overall STEM retention rates. Preliminary results of the model are expected to be available at the time of the presentation, with clear goals outlined for future research.

[1] Kelic, Andjelka, and Aldo A. Zagonel. Science, Technology, Engineering, and Mathematics (STEM) career attractiveness system dynamics modeling. No. SAND2008-8049. Sandia National Lab.(SNL-NM), Albuquerque, NM (United States), 2008.

First-Principles Analysis of Ammonia Decomposition Reaction on High Entropy Alloy Catalysts

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Keywords: High Entropy Alloys, Density Functional Theory, Heterogeneous Catalysis,

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The development of periodic Density Functional Theory (DFT) calculations combined with advanced synthesis techniques has accelerated the understanding of multimetallic alloy catalysts. A new class of materials namely high entropy alloys (HEAs) recently introduced, constituting a whole new paradigm in catalysis. HEAs comprise multiple principal elements, with completely mixed atomic structures, generating millions of unique chemical environments around active sites, considerably more than conventional alloys. These materials have advantages such as improved stability, tunable active sites that offer possibilities for favorable binding energetics and kinetics. However, there are fundamental challenges associated with HEAs. The complex materials space cannot be navigated exhaustively using first-principles methods. Additionally, the theories and models proposed for the traditional alloys may not be translatable directly to HEAs.

In this study, we develop a model for a high entropy bimetallic alloy catalyst, that can be flexibly extended to incorporate multiple elements. Additionally, we develop tools to sample different binding sites and investigate the free energy landscape for simple adsorbates on these sampled sites. To illustrate our approach to modeling HEAs, we choose the ammonia decomposition reaction as a probe reaction and Co-Mo as the model catalyst, based on the promising activity demonstrated by our collaborators (Wang group) using a HEA catalyst. Using our simple model, we investigate the binding energies of various reaction intermediates on the HEA surfaces using DFT and generate a free energy landscape. We hypothesize that these binding energies are linearly correlated with the elemental identity of nearest neighbors around the adsorption site. We also identify the rate-determining step in the reaction mechanism and further, hypothesize that the rate-determining remains constant for varying surface arrangements.

We find that while there is a qualitative linear relationship between the mean binding energies and elemental identity of the nearest neighbors, there is no clear quantitative correlation, motivating efforts to develop more complex, non-linear models involving machine learning. For the sampled surfaces, linear scaling relationships appear to be weak. To confirm this, we will sample more surface arrangements and compositions. Lastly, we deduce that the rate-determining step for the ammonia decomposition reaction is recombinative nitrogen desorption and it remains constant across the different considered surface arrangements, but this result could change when larger alloy space is ultimately considered. We will expand on our analysis in the future by incorporating more elements in the HEA and developing a microkinetic model.

Attack-Resilient Distributed Optimization-based Control ofMulti-Agent Systems with Dual Interaction Networks

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Keywords: Urban Air Mobility, Cybersecurity, Autonomy

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The vision for the Urban Air Mobility airspace is a highly automated, cooperative, passenger and/or cargo carrying air transportation service for economic purposes. Comprised of highly complex, safety critical cyber-physical systems (CPSs), the integration of a UAM network within the National Airspace (NAS) requires the development of robust human-machine decisionmarking and control paradigms that are resilient to cyberattacks. Consequently, cybersecurity of CPSs has emerged as one of the most important issues for UAM general operation. In this paper, we consider Denial-of-Service (DoS) cyberattacks and its effects on maintaining separation for agents within the UAM airspace. We propose a novel distributed optimizationbased control framework that adopts a primal-dual Lagrangian subgradient approach that uses mixed information from two Laplacian interaction networks to ensure convergence to a global minimizer despite the presence of DoS cyberattacks and constraints on agent separation. This algorithm can be implemented over time-varying networks, and allow agents to asymptotically agree on optimal solutions.

Predicting learning outcome in a first-year engineering course: a human-centered learning analytics approach

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Keywords: educational data analytics, first-year engineering, human-centered

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First-year engineering programs allow students to explore the fields of engineering before students finalize their engineering major. Often these courses are relatively large with several sections, thus, it can be rather difficult for an individual instructor to recognize when an individual student begins to lose engagement. Learning management systems (LMS) (e.g., Canvas, Blackboard, Brightspace, etc.) can be useful tools to both provide consistent curriculum across several sections of a courses, as well as for generating data regarding students' engagement with course materials.

The problem of predicting learner outcomes more quickly to inform educational interventions has been studied from a variety of learning analytic approaches. However, common approaches tend to neglect the role of the data quality in terms of data transformation and human intervention necessary to predict learning outcomes and return valuable insights to instructional teams. This is further aggravated when working under complex conditions such as those of FYE classes.

The purpose of this Complete Research paper is to explore the following research questions: What type of LMS objects contain more information to explain students' grades in a first-year engineering course? and Is the inclusion of a human operator during the data transformation process significant to the analysis of learning outcomes?

The context of this study is in a large first-year engineering course at a midwestern research institution. We collected student interaction data from an LMS on students' in two sections of the course, with a total of 187 students. We use two different datasets differentiated by the involvement of human operators with contextual knowledge of the course. Mainly, coding of the content in the LMS platform is performed by a person with knowledge of the class. A generalized linear mixed model (GLMM), use to predict the grade in the final exam, along with prediction capability, evaluated by the accuracy and precision of the model, is used to compare both results.

The preliminary findings indicate that students' engagement with career exploration curriculum were the strongest predictors of students' final grade in the course. That is a particularly interesting finding because the amount weight the career assignments contributed to the overall course grade was rather low. Additionally, while both models produced adequate fit indices, the human-informed model performed significantly better and resulted in more clearly interpretable results.

Looking through the lens of a human center learning analytics perspective, we find that while prediction is an automatable process that might not require a human involved, the insights returned to FYE classrooms would most likely remain hidden without the involvement of human operators in the data transformation and analysis process. The human-informed model provides results that are directly applicable to instructional teams in the identification of a low-weight category of assignments (i.e., career exploration) that was a more useful indicator of students' engagement and outcome in the course. The full paper will discuss the practical implications for FYE instructional teams, as well as recommendations for future research.

Reproducibility of a Chemical and Microbiological Environment Among Replicate Building Plumbing Systems.

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Keywords: drinking water, building plumbing, reproducibility

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In the midst of the COVID-19 pandemic, public health concern over stagnated tap water within building plumbing was brought to light as commercial and campus buildings were shut down across the nation. In response to this concern, major research efforts were conducted to test the microbial and chemical environments within the plumbing of unoccupied buildings as well as the efficacy of preventative and remedial methods. Water quality degradation was noticed in buildings that experienced extended stagnation. However, it was also noticed that results varied across studies due to the diversity of building infrastructure (i.e. pipe material and water disinfectant type). Due to these studies having mostly been conducted on variable, existing infrastructure, it is difficult to make generalizations from these results and thus further research is needed to be conducted using more controlled environments. A team of Purdue engineering graduate and undergraduate students along with faculty and staff collaboratively built 4 large plumbing wall systems here at Purdue that will represent 4 standard building plumbing infrastructure. Each plumbing wall has been built the same, made of copper pipes in triplicate and are equipped with a water heater storage tank and a water softener. These walls create a much more controlled environment as opposed to existing infrastructure and the multiple replicates allow for better comparison of results. In order for the data of multiple replicates in a large-scale experiment to be comparable, reproducibility of these replicates must first be proven. My first experiment with these walls has been on determining if replicate plumbing systems undergoing the same water quality conditions will result in reproducibility (i.e have equivalent or similar results). In order to do this, I have collected samples to measure certain parameters such as pH, temperature, chlorine, turbidity, total and dissolved organic carbon, total and dissolved metals, cell counts, and so on over a 5 week period. Tests for these parameters are still being run and data is still in the process of being collected.

What The Next Generation Thinks About Manufacturing

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Keywords: Manufacturing, STEM initiatives, Career perceptions, industry-led summer camps

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Manufacturing continues to be an important industry in the United States and one that is critical to the nation's economy. However, the industry faces increasing difficulty in finding skilled workers to fulfill their workforce needs. It is estimated that within the next decade there will be 3.5 million available manufacturing jobs and of those, at least 2 million will go unfilled [1]. Currently, up to 89% of manufacturers cannot find skilled workers to fill open job positions [2]. One potential cause of this skills gap is thought to be the poor perceptions of manufacturing careers held by the general public. A Deloitte study showed that while a majority of American's have positive perceptions about the future workforce in manufacturing, less than 50% believe manufacturing to be a rewarding career, and one-third would not encourage their children to pursue a career in manufacturing [3]. The same study, however, shows that parents who work in manufacturing are twice as likely to encourage their children to pursue a manufacturing career as compared to the average American [3]. This can indicate that exposure to manufacturing may help to enhance the public perception of the industry, and ultimately show manufacturing as a good career choice. As a result, there have been several attempts to demystify manufacturing through educational efforts, especially at the K-12 level. While these efforts are typically designed to engage young students in manufacturing, research attempts focused on better understanding their impacts on children's perceptions of related careers seem to be lacking. Therefore, this study focused on investigating children's perceptions of manufacturing before and after a summer camp titled Robotics in Manufacturing, that was co-hosted by several manufacturers in one midwestern town. The research question that guided this study was "What impact, if any, does an industry-led manufacturing summer camp have on children's perceptions of careers in manufacturing?"

Transport and lymphatic uptake of biotherapeutics through subcutaneous injection

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Keywords: Lymphatic uptake, Biotheraupeutics, Subcutaneous injection

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Drug transport and uptake in the subcutaneous tissue receives increasing attention in biomechanical and pharmaceutical researches, as subcutaneous administration becomes a common approach for the delivery of biotherapeutics, such as monoclonal antibodies. In this paper, high-fidelity numerical simulations are used to investigate the mechanisms governing drug transport and absorption in the subcutaneous tissue, which is expressed as a porous medium modeled by Darcy's law. The effects of tissue properties (permeability and porosity), the injection flow rate, and the vascular permeability of lymphatic vessels on the lymphatic uptake are studied. Additionally, an empirical formula for the lymphatic uptake during the injection is developed based on the numerical results. The roles of lymphatic drainage, blood perfusion, osmotic pressure, and the drug binding to the cells and the extracellular matrix in the lymphatic uptake are systematically studied. Furthermore, the drug distribution and absorption in a multi-layered porous medium are investigated to illustrate the effect of heterogeneity of permeability, as the permeability varies over a wide range in different layers of the tissue (such as dermis, subcutaneous tissue, muscle). While the interstitial pressure plays an essential role in the mechanisms regulating the absorption of free monoclonal antibodies, the binding and metabolism of drug proteins also affect the drug absorption by reducing the total free monoclonal antibodies.

Fabrication and testing of a powder rheometer using model-directed design

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Keywords: particles, flow, simulations, sensors

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Powders are made of solid particles and have fluid-like flow properties, which is useful for transporting material and shaping the powder into products for manufacturing. There is a lack of understanding in how the particle properties influence the bulk flow behavior. A model-directed approach was used to design and fabricate a tilted Couette cylinder power rheometer for measuring bulk flow behavior. The rheometer applies a shear force to the powder and various sensors are used to measure the powder response. These sensors can only measure properties at the boundary conditions, so discrete element method (DEM) computational modeling was used to simulate the rheometer prototype. The simulations were used to visualize the dynamic internal structure of the particles and gain understanding how these structures influence the observed flow response. Using the DEM simulations early in the design process proved helpful in identifying and solving issues in the prototype design before experiments were conducted.

Four main sensors were used to collect data during the experiments: an internal motor position encoder to measure the rotor positional velocity, a load cell to measure outlet mass flow rate, a tactile pressure map sensor to measure the location and magnitude of force chains along the stator wall, and a high-speed camera to capture the cross-sectional view of particles moving inside the device. Three materials were investigated: microcrystalline cellulose, carbon steel, and zirconia. All samples were made of spherical particles but had various mean particle size.

The rotor velocity of the rheometer was found to directly influence the mass flow rate of particles exiting the system, and the equation to describe this relationship for the various samples tested was found using dimensional analysis. The wall pressure data showed a repeating pattern in the pressure peak location and magnitude in cases where the rotor had an oscillatory velocity. Particle tracking performed on the videos recorded was used to calculate the velocity profile across the flow gap. The particle tracking results showed that the shape and size of the velocity profile curve is influenced by the particle size and material.

Overall, the use of modeling has been helpful in giving insight into the design of the rheometer, and the experimental results have shown that using a system of various sensors can give information about different aspects of the particle flow behavior. Future work will include increasing the sensor capabilities of the rheometer, investigating a larger variety of particle types, and connecting the results from the experiments to the simulations.

In silico model characterizing in vitro M. tuberculosis Granuloma Dynamics

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Keywords: tuberculosis, computational modeling, host-pathogen dynamics

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Prior to the COVID-19 pandemic, tuberculosis (TB) was the leading cause of death due to a single infectious agent. TB is caused by the inhalation of Mycobacterium tuberculosis (Mtb). The hallmark of Mtb infection is the formation of granulomas - dense structures composed of macrophages and lymphocytes that encapsulate infected macrophages, extracellular bacteria, and dead cell debris. These granulomas are unique microenvironments orchestrated by the immune response to contain Mtb and localize host-pathogen interactions. Approximately 90% of individuals infected with Mtb harbor granulomas that control bacterial spread, resulting in asymptomatic disease known as latent TB infection (LTBI). In vitro studies with human primary cells infected with Mtb have shown that cells from LTBI individuals can better control Mtb growth compared to cells from naive individuals (those who have never had TB before). But identifying mechanisms behind these differences is challenging.

My research uses a complementary approach that incorporates computational modeling to help analyze, interpret and guide these complex in vitro granulomas. We have developed an agent-based model that generates virtual versions of in vitro granulomas to help elucidate the differences between LTBI and naive host cell responses. Our computational model mimics Mtb infection through interactions between virtual macrophages, CD4+ T cells and Mtb. Mechanisms include Mtb growth, macrophage phagocytosis resulting in Mtb death or macrophage infection, macrophage and T cell activation, T cell proliferation, and cytokine/chemokine diffusion and degradation.

Preliminary model results showed that LTBI-like cells had more TB-specific T cell proliferation, more activated macrophages leading to more Mtb killing compared to naive-like cells. However, within naive and LTBI groups, results showed, somewhat counterintuitively, that more proliferation of TB-specific T cells does not always result in better Mtb control despite resulting in more activated macrophages. A possible explanation is that parameters governing a macrophage’s ability to kill such as phagocytosis, resting and active killing probabilities, and cellular dysfunction threshold have an influence on Mtb control in addition to macrophage activation. Taken together, this suggests that variations between and within LTBI and naive groups could be attributed to T cell proliferation and macrophage killing abilities, respectively.

Our model will advance our understanding of host-pathogen interaction mechanisms in Mtb infection through fundamental discoveries using a combined computational/experimental approach. Our findings will help analyze, interpret and guide Mtb granuloma exploration with the ultimate goal of developing new TB treatment strategies.

The effect of nano-additives on the hydration behavior and durability of concrete containing fly ash

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Keywords: concrete durability; hydration; nano-additives; scaling.

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Incorporating fly ash in cementitious systems containing ordinary portland cement (OPCs) increases their long-term strength and durability. However, the inclusion of fly ash also reduces the heat of hydration of such systems and their hydration rate. Thus, its use slows the development of strength at early ages. The reduced rate of hydration, and the associated lower early-age strength, can increase the risk of durability problems such as early surface deterioration (scaling) if young concrete is exposed to challenging environmental conditions.

The purpose of this research was to assess the influence of nano-additives (titanium dioxide nanoparticles/nano-TiO_2) on the hydration process and the durability of fly ash concrete. The experiments were performed on cementitious composites containing class C fly ash (24% by weight of cement) and various levels of nano-additives.

The isothermal calorimetry (IC), thermogravimetric analysis (TGA), and Vicat setting time tests were carried out to investigate the effect of nano-additives on the hydration process of fly ash pastes. The influence of nano-additives on the permeability of concrete containing fly ash was determined by a water absorption test using different methods of sample conditioning. Furthermore, the scaling test was performed to evaluate the influence of the nano-additives on the scaling resistance of concrete containing fly ash. Preliminary results indicated that the addition of nano-additives can accelerate the hydration process, reduce water permeability, and improve the scaling resistance of concrete containing fly ash.

My presentation will cover the introduction and background of this research, experimental campaigns, details of my findings, and discussion regarding the future work.

The Influence of Engineering Students' Extracurricular Involvement on Career Aspirations and Professional Development

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Keywords: engineering student support, extracurricular involvement, career preparation

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This research study investigates engineering students' motivation for pursuing different types of extracurricular involvement, factors that influence this choice, and connections to engineering career aspirations. In exploring the connection between extracurricular involvement and student career aspirations, this study explores the potential of extracurricular involvement to support persistence in engineering. This study further seeks to characterize significant aspects of undergraduate engineering students' involvement based on perceived importance and impact to students.

This study investigates the following research questions: 1) What motivates engineering students to join extracurricular involvements? 2) What is the relationship between engineering students' extracurricular involvement choices and career aspirations (career expectations and certainty of career choice)?

This study analyzes survey data from two cohorts of undergraduate engineering students at a large Midwestern university, collected before (N=212) and during the covid-19 pandemic (N=279, additional responses currently being collected). The survey was developed from a conceptual framework of the mechanisms that influence student involvement and its impact. Survey participants responded to open- and closed-ended questions about the types of organizations in which they are involved, the extent of their involvement, activities in which they have participated through their involvement, and factors that influenced their involvement choices. The survey also collected information about students' career aspirations, including their career plans and certainty in career choice. Open-ended responses about students' current involvement and perceived significance were coded to develop a categorization of involvement types based on their perceived significance and role to students. Then, regression analysis was used to investigate 1) how motivation for involvement is predictive of type of involvement and career expectations and 2) how type of involvement is predictive of career certainty and expectations.

This study builds on existing studies of engineering student involvement to examine different measures of extracurricular involvement and how different aspects of involvement may uniquely influence students' experiences. By better understanding the influence of different types and activities of involvement, students can make more informed choices to pursue involvement options suited to their interests and goals. Additionally, this study's examination of factors that influence students' choice of extracurricular involvement can help inform university programming and advising to support students in these choices. This study extends current work by connecting extracurricular involvement to career expectations and preparation, offering the potential to develop interventions to support students in choosing extracurricular involvement

and to retain graduates in their transition to the workforce through partnerships with student services, policymakers, and stakeholders.

Impact of Epoxy Manufacturing and Installation Conditions on Chemical Leaching in Drinking Water Infrastructure

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Keywords: Infrastructure, drinking water, epoxy

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The aging of potable water infrastructure systems and the need to replace lead service lines has increased public discussion and utilization of epoxy linings. Epoxy linings are installed by the chemical manufacture of the new material inside an existing damaged pipe or tank. The in-situ manufacture of this plastic poses unique challenges to utilities and consultants as post-installation performance verification practices are not available. Furthermore, field installations of epoxy lining are completed at various temperatures, and contractors may have different methods. A literature review was conducted to review existing knowledge gaps and best practices associated with the practice of epoxy installation, which revealed that very little information currently exists in the United States pertaining to chemical leaching from epoxy linings in potable water applications. From the information that does exist, analysis has revealed leaching of organic carbon, bisphenol compounds, and potential interactions with chlorine disinfectant for potable water in contact with epoxy linings. Moreover, the NSF International Standard 61 is often invoked, but data from these studies and the condition of the materials tested are not disclosed. Therefore, considering the various installation techniques by contractors, environmental conditions, and differences in the resins themselves, best practices and long-term leaching impacts are not fully understood. Bench-scale testing was completed to evaluate the effects of epoxy lining conditions (specifically, curing time and resin to hardener ratio) on chemical and microbiological water quality impacts. Experiments were being conducted during Fall 2021 and will be completed in Spring 2022. Water quality is being analyzed for volatile organic compounds, semi-volatile organic compounds, and total organic carbon concentrations using gas chromatography mass spectrometry and an organic carbon analyzer. Bisphenol compounds are a specific target analyte, and assimilable carbon is also being investigated. Thermal and physical properties using thermogravimetric analysis and soxhlet extraction of the composites are also being investigated to assess volatile material content and crosslink density, respectively. Preliminary evidence shows high organic carbon leaching, as well as variations in leaching for different installation conditions as compared to manufacturer instructions.

Engineering Education Graduate Students' Perceptions of Academic Writing Norms

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Keywords: engineering education, graduate education, writing, qualitative

Academic writing is an important aspect of graduate education. To succeed in their programs, graduate students must learn to communicate their research in a way that resonates with other scholars in their field. In other words, they must write in a way that aligns with the expectations of their field. In the field of engineering education, graduate students come from varied disciplines, and many are new to the field. They may find that the expectations around academic writing in engineering education differ from their prior experiences in other disciplines.

This study uses academic literacies theory to understand how graduate students in engineering education experience the social norms of academic writing. Academic literacies theory adopts a social and cultural perspective to writing, as opposed to a cognitive approach, and views writing as a social activity deeply connected to institutional and disciplinary contexts. Thus, writing skills are not necessarily transferable from previous contexts; instead, they adapt based on expectations in new disciplines and departments. Expectations around academic writing are tied to epistemologies of the field and dictate what counts as knowledge. These expectations may be explicitly or implicitly communicated to students and likely influence their writing practice.

To understand how these academic writing norms manifest in graduate engineering education, this qualitative study addresses the research questions: What do engineering education graduate students perceive as norms in academic writing? How do these norms inform their own writing practices?

To address this research question, I interviewed seven graduate students in the School of Engineering Education about their practices around writing and their perceived expectations of academic writing in the field. I focused on one department so I could understand the expectations around writing embedded within the localized context of a single department and more broadly within the field of engineering education. In alignment with academic literacies theory, my data sources include interviews rather than writing excerpts. I am less interested in students' writing skill and more interested in their perceptions of scholarly writing and publishing in their field and how these perceptions inform their own writing practices.

I transcribed the interviews and analyzed them using an inductive approach. I focused on students' comments and perceptions around three areas: (1) norms and expectations around academic writing, (2) what constitutes good academic writing, and (3) where they received these messages. In the presentation, I will share the findings from these analyses. I hope these findings can inform ways to support graduate students' development as writers and scholars in engineering education.

Does your place of residence affect your opportunities to engage in active travel and be healthier?

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Keywords: Built environment, Access to Infrastructure, Physical Activity, Structural Models

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Background: The relationship between active travel behavior and health has been acknowledged to differ across geographic settings (i.e., urban, suburban, and rural areas) in the U.S. These differences are specially related to links that involve the built environment and infrastructure characteristics of those areas. Simultaneously, the built environment and access to infrastructure are frequently associated with different levels of physical activity that are thought to variate in these areas and are related to the likelihood of developing non-communicable diseases such as obesity.

Methods: In this paper, we explore the difference between those three geographic settings in terms of the built environment, access to infrastructure (connectivity), and levels of physical activity in the U.S. Using individual-level survey data complemented with publicly available secondary data, we perform an ANOVA to see whether access to supermarkets, physician, pharmacies, metabolic equivalent of task (METs) and body mass index (BMI) differ across four different geographic settings: urban, suburban, large rural towns, and isolated rural areas; that surrounded survey respondents. After, we estimate a multi-group structural equation model to disentangle the differences across the areas of study.

Results: The analysis of variance showed that distance to supermarkets, pharmacies, and physician offices are statistically different across the four settings. However, the difference is only slightly significant for METs and BMI across these four geographic locations. The factor analysis results demonstrate that the most important factors to be considered in terms of the built environment are density, design, and mix land use. The built environment has a lower effect on respondents' physical activity in isolated rural and suburban areas compared to urban areas and large towns, which are more compact and promote higher levels of physical activity. The two areas might offer better ways to reach a desire destination (i.e., grocery store, pharmacies) by other means than driving.

Conclusions: This study's results add further evidence of how different the impact can be depending on the area where a person resides. From the results, it can be concluded that access to opportunities does not have a linear relationship with the level of rurality a place has. The results provide guidance for policymakers on which factors and strategies could be the focus to better promote physical activity in each of the geographic settings.

ON THE HAUSDORFF DISTANCE BETWEEN A PARETO SET AND ITS DISCRETIZATION

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Keywords: multiobjective simulation optimization, Pareto Set Approximation

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We consider the problem of multi-objective simulation optimization (MOSO), that is, nonlinear multi-objective optimization in which the objective functions can only be observed with stochastic error. MOSO problems exist at the interface of two well-developed research fields: deterministic multi-objective optimization and simulation optimization. There are different flavors of the MOSO problems based on the decision variables [1]. Our broad goal is to develop an approach to compare MOSO algorithms in the context of continues variables. Thus, we consider the following problem,

Problem M: min $f(x)=(f_1(x),f_2(x),\ldots,f_d(x))$ s.t. $x\in X$. where $f:R^q\rightarrow R^d$ is a vector-valued function, the feasible set X is compact and, $f_i(x) := E[F_i(x,\xi)]$ is an expected value where ξ is a random variable. The solution to a MOSO problems is the set of points whose images are non-dominated, called the efficient set, $\mathcal{E}$. The image of $\mathcal{E}$ is called the Pareto set, P. Let us follow a simple procedure: select m distinct points $X_m := \{\tilde{x}_1,\tilde{x}_2,\ldots,\tilde{x}_m\}\subset X$. This set becomes handy in the formulation of defining discretized efficient and Pareto sets.

Let $\mathcal{E}_m$ and P_m is the respective efficient and Pareto sets for Problem M solved over the discretized feasible set X_m. Due to randomness in MOSO problems, we cannot find the efficient set and Pareto set directly for Problem M, we need to estimate the solution set by solving the following problem,

Problem $\hat{M}_m(n)$: min $\{\tilde{F}(\tilde{x},n)=(n^{-1}\sum_{i=1}^{n} F_1(\tilde{x},\xi_i),\ldots,n^{-1}\sum_{i=1}^{n} F_d(\tilde{x},\xi_i))\}$ s.t. $\tilde{x}\in X_m$.

Problem $\hat{M}_m(n)$ estimates the solution to Problem M and solution of it is $\hat{\mathcal{E}}_m(n)$, which estimates $\mathcal{E}$.

To quantify the error in this solution approach, we consider the following expected Hausdorff distances, where the bounds on the right-hand sides follow from the triangle inequality, $E[H(\mathcal{E},\hat{\mathcal{E}}_m(n))]\le H(\mathcal{E},\mathcal{E}_m)+E[H(\mathcal{E}_m,\hat{\mathcal{E}}_m(n))]$ $E[H(P,f(\hat{\mathcal{E}}_m(n)))]\le H(P,P_m)+E[H(P_m,f(\hat{\mathcal{E}}_m(n)))]$

There are two main components of the error: the discretization error and the selection error. We can decrease the selection error by increasing the number of replication number (n) and the discretization error by increasing the number of sampled points (m) [2].

Toward quantifying the discretization error, we provide an upper bound on the deterministic error term in the context of bi-objective convex quadratic optimization with spherical level sets. Our bound implies that if t is the dispersion of the observed points measured in the decision space, then the Hausdorff distance between the Pareto set and its discretization is $O(\sqrt{t})$ as t decreases to zero. Our future work includes relaxing assumption of circular level sets to generalize our results to all bi-objective quadratic problems, obtaining the required bound on the selection error term E[$\mathbb{H}(\mathcal{E},\mathcal{E}\_m\ (n))$] as a function of n and, extending the results to higher number of objectives to cover all MOSO problems.

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Theoretical perspectives from organizational psychology on the role of family-work balance in women's departure from the engineering profession.

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Keywords: family-work balance, engineering profession, women in engineering, career pathways

The recent and sudden changes in the workplace that have resulted from the COVID-19 pandemic have further exacerbated the already existing work-life balance challenges of women in the engineering profession. Many professionals have suddenly found themselves working at home, often without childcare. Women have been disproportionally impacted by this pandemic, as even in dual-earning families, women frequently take on a higher percentage of the responsibilities for home and childcare. Family-work balance influences women's engineering career pathways, including their decision to leave the engineering profession.

In this study, a three-pronged approach is used to develop a framework for understanding the role of work-life balance in women's decision to leave the engineering profession. First, I explore what is currently known about the influence of family-work balance on women's engineering career journeys, particularly their decisions to leave the engineering profession after having worked in industry. Next, to broaden our perspective on the topic, I integrate related literature on women's experiences in engineering, STEM, and other male-dominated professions. Finally, to expand our understanding of the work-life challenges of women in engineering, I incorporate concepts from organizational psychology, such as job burnout, resource allocation/ job-demands-resources, work-family boundary management, and contemporary issues.

The resulting theoretical framework contributes to our understanding of the work-life balance challenges of women in engineering, increasing our awareness of the influence of culturally defined roles, non-linear career paths, and extreme jobs on women's decisions to leave the engineering profession. Using this framework to study women's engineering career decisions allows the identification of creative and proactive solutions to retain those who feel pushed out of engineering due to the challenges of family-work balance.

Seismic stability of lunar lava tubes

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Keywords: Moonquakes, seismic stability, lunar lava tubes

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The potential existence of lunar lava tubes has been studied for over half a century. The improvement of high-quality image technologies became a great asset for space investigation facilitating the mapping and analysis of the Moon surface. In addition to that, space explorers are reaching new territories with the help of advanced technology and engineering; the Mars surface is being explored, and the information collected is the first step towards bringing human life to the red planet.

Government agencies and now private commercial companies are carefully looking to the potentials of space exploration. The Moon brings interest from different industries. Mining, science, tourism, possible water existence in the form of ice, and the ultimate goal of a permanent extraterrestrial settlement are among a few trend topics. The Moon is also strategically located between Earth and Mars, which could be helpful for future explorations of the red planet. However, it is necessary to protect future explorers against the Moon's hazards to accomplish this goal. The Moon has many inhospitable characteristics, but the most studied ones are the threats stemming from the lack of air pressure, oxygen, extreme temperature fluctuations, and hazards such as meteorite impacts and intense particle radiation.

Another Moon hazard is related to the Moonquakes, and those are divided into four important categories. As previously mentioned, the seismicity from meteorite impacts, thermal quakes from contraction and expansion due to thermal differences of lunar materials, and deeper and shallow quakes. According to the Nasa data from Apollo missions, shallow quakes have been registered only a couple of times. However, shallow quakes can be as strong as 5.0 on the Richter scale and could have a long duration compared with Earthquakes (Watters et al. 2019; science.nasa.gov), and could represent the biggest threat to a permanent human settlement on the Moon.

All those environmental threats on the Moon bring the necessity of human shelter. Building a shelter requires extra materials, and the transportation of those materials to the Moon can be incredibly costly. A good alternative is to use structures already existent on the lunar underground, the lava tubes. Like on Earth, lava tube formation occurs due to volcanic activity; after the eruption is ceased and the lava is not inside the tubes anymore, the underground structures remain available.

The stability of the lava tubes is the main point of this research. To use the lunar underground structures as human shelter, it is essential to evaluate how stable those structures are in the face of the Moon hazards. Numerical models and finite element analysis will be used for this evaluation. Data analysis is not concluded yet. For this symposium, the objective is to present the goals of this research.

Computational Modeling of Host-Pathogen Interactions to Compare Experimental Models of Tuberculosis Infection

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Keywords: computational modeling, agent-based modeling, tuberculosis

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Tuberculosis (TB) continues to be global public health crisis. In 2020, an estimated 1.3 million people died from TB. TB is a curable, but treatment can be challenging as it requires 6-12 months of treatment with up to 4 drugs, even with drug-susceptible strains. One limiting factor in our ability to improve TB treatment is an incomplete understanding of the interactions between the bacteria, M. tuberculosis (Mtb), and the host immune system. Specifically, interactions within the site of infection, the granuloma, remain unknown. Granulomas are organized, spherical clusters of immune cells that form around bacteria.

Interactions between host cells and Mtb are often explored with models in a laboratory setting. Traditional culture methods combine Mtb and host cells on a plate where they grow and interact at the bottom of a culture well. There has been recent interest in developing 3-dimensional spheroid models that can represent the TB granuloma environment more closely. Our previous work has shown that spheroid models using peripheral blood mononuclear cells have better bacterial control than traditional culture equivalents. However, the cause of these differences between culture methods remains unclear and difficult to identify with experiments alone.

We use a computational model to simulate both spheroid and traditional culture to test whether the difference in Mtb control can be explained by differences in spatial organization alone. We construct an agent-based model tracking individual Mtb, macrophages, CD4+ and CD8+ T cells. Model mechanisms include phagocytosis of Mtb by macrophages and activation of macrophages through two pathways, $NF_{\kappa}B$ and STAT1. Parameters include cytokine secretion rates, activation thresholds, and probabilities of killing and movement. We iteratively refine the parameter space using Latin hypercube sampling, experimental Mtb counts to filter, and alternative density subtraction to adjust parameter ranges.

Our results suggest that spatial differences alone can account for the differential Mtb control between traditional and spheroid cultures. We hypothesized that the poorer Mtb control in the traditional model is due to lower levels of macrophage activation compared to spheroids. However, preliminary results suggest that the traditional model has more macrophage activation initially, while the spheroid model has a slower increase in macrophage activation. Notably, the spheroid model has more activation of infected macrophages. The difference in infected macrophage activation is specifically due to STAT1, implying more T cell activation in the spheroid model. But the opposite was seen, with traditional model having more activated T cells.

Together, our results suggest that the spatial organization of spheroids allows for more specific and effective activation of macrophages. Our model will be used to answer further questions about the dynamics of early Mtb infection in granulomas and to potentially “3-dimensionalize” results from traditional models.

Bioinspired structures with fast shape change via 3D printing

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Keywords: programmable structures, smart materials, 3D printing, shape memory polymers, multistability

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Despite lacking muscular and nervous systems to provide actuation and sensing, several species of plants are capable of very fast motion. In particular, the Venus flytrap can snap its leaves closed in less than one second to trap prey. This speed is due to the leaves' bilayer architecture of cells with contrasting, curvilinear pre-strain fields. Pre-strain-based fast shape change is of increasing interest in engineering industries as a method of creating structures that adapt to different operating conditions without the need for conventional actuation and sensing systems. This enables increased efficiency and unique functionalities, combined with decreased weight and part count. However, conventional methods of creating pre-strained synthetic structures are unable to replicate the complex geometry and pre-strain fields found in the Venus flytrap and typically require expensive, specialized manufacturing equipment.

Using the geometric freedom of 3D printing and the pre-strain generated in shape memory polymers (SMPs) by extrusion, we achieve bioinspired, fast morphing structures with complex curvatures and geometries. During printing, the SMP filament is stretched in the direction of extrusion. By cooling the printed filament quickly, we freeze this stretch in the SMP, thereby encoding directional pre-strain in each layer of the structure. When the printed structure is heated to above the SMP's glass transition temperature, this pre-strain is released, and the structure becomes compliant. In this compliant phase, the structure is multistable, meaning it can snap quickly and reversibly between multiple, pre-determined stable configurations. When cooled again, the structure regains stiffness and is monostable in its most recent configuration. This activation process is reversible and repeatable; the multistability may be turned on and off by temperature change. Because 3D printing allows for highly complex geometries with little corresponding increase in manufacturing difficulty, we can easily print bioinspired designs with complex curvatures, including recreating the Venus flytrap leaf. We also demonstrate the use of specialized SMP filaments to enable magnetic actuation of multistable structures. This accessible and low-cost manufacturing method for complex multistable structures has potential applications in smart buildings, advanced packaging, and robotics.

Inter-scanner reproducibility for validation of multi-site studies in magnetic resonance spectroscopy at 3T

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Keywords: MRI, Neuroscience, multi-vendor

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Multi-site magnetic resonance imaging (MRI) studies are often performed due to their benefits of large dataset collections as well as the ability to sample geographically diverse populations for better generalization, as well as to provide sufficient statistical power to detect significant associations in research. However, they also introduce considerable sources of variance to the studies, especially variance across the scanners at different sites. The Purdue University MRI facility houses two 3T scanners, which provides the unique opportunity for comparison of the two scanners while limiting multiple sources of variance such as operators, subjects, data acquisition, and analysis. In this study, we compare magnetic resonance spectroscopy (MRS) results on identical subjects, expecting high reproducibility across both scanners, which would validate the use of different scanners in multi-site studies. The goal of MRS is used to analyze the chemical composition of tissues by excluding the overwhelming signals from water and fat, MRS can detect small metabolites existing in millimolar (mM) concentrations. These metabolites can be differentiated because they resonate at slightly different frequencies based on their local chemical environments. The commonly studied metabolites are N-acetyl-asparate (tNAA), molecule present in healthy neurons. Creatine (Cr), an energy metabolism molecule. Choline compounds (Cho) which are markers in the synthesis and breakdown of cell membranes. Myo-inositol (mI) which is only found in glial tissue. Glutamine-Glutamate-GABA complex (Glx) which is a primary neurotransmitters and lactate (Lac- which is a product of anaerobic metabolism. For this MRS study, seven healthy subjects (age 27±3) were scanned on a Siemens Prisma scanner, with a 64-channel head coil, then on a GE Discovery scanner, with a 32-channel Nova head coil. Due to its limited chemical shift displacement error, MRS was performed using identical semi-adiabatic localization by adiabatic selective refocusing (sLASER) sequences with a 30ms echo time, in five brain regions: anterior cingulate cortex (ACC), frontal white matter (FWM), left insula, left- and right- dorsal lateral pre-frontal cortex (DLPFC). These brain regions were chosen due to their roles in multiple neurological disorders, including addiction, PTSD, and traumatic brain injury. The results for intrascanner variability show that the 3T Siemens Prisma scanner produced slightly smaller variability amongst seven subjects with the CV ranging from 3.654% to 17.989%. On the other hand, 3T GE Discovery scanner revealed CV from 4.917% - 20.782%. For interscanner variability, extensive statistical analysis revealed that 70% (146 out of 210 datasets) of GE data had increased metabolite concentrations compared to the Siemens data. Across different brain regions, the least variance was observed within ACC (1.847%), while the most variance was within rDLPFC (13.211%). Overall, CV between the scanners is well within recommended values. The highest reported variance between the two scanners is

19.130% for Glx in FWM, while the lowest is 3.478% for tNAA in lDLPFC. This study used a closely matched methodology to compare the MRS measurements made at 3T. Most of the metabolite concentrations, calculated using tissue water as an internal intensity reference and corrected for CSF effects, showed no statistically significant difference between the two scanners.

Simultaneous Colorimetric and Electrochemical Detection of Trace Hg2+ Using a Portable and Miniaturized Aptamer-Based Sensor

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Keywords: Biosensors, biomaterials, colorimetric detection, electrochemical detection, user-friendly

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Heavy metals are significant environmental pollutants that are naturally found in the earth's crust. Among them, mercury is considered the most toxic due to its nephron and neurotoxicity to humans, but unfortunately, it is still widely distributed in the environment. According to the World Health Organization, elemental mercury vaporizes readily and can stay for up to a year in the atmosphere, where it ultimately settles in the sediment of water bodies. Other major sources include anthropogenic activities such as agriculture, mining, incineration, and discharges of industrial wastewater. For that reason, the detection and monitoring of trace amounts of mercury have gained attention in the past decades. Current detection methods include ICP-MS, HPLC, and ICL-AES and despite their high sensitivity and selectivity, they are still complex, required trained personnel, and are not suitable for On-Site detection. Therefore, the development of rapid, user-friendly, and reliable sensors is necessary. In this study, we developed a µ-PAD paper device incorporated into a miniaturized three-electrode system for the simultaneous colorimetric and electrochemical detection of mercury through Ps-AgNPs and Ps-AuNPs aggregation (as a result of ssDNA-Hg2+ interaction) and impedance spectroscopy. The portable and miniaturized device is a simple, rapid, and highly selective sensor for the sensitive detection of Hg2+ down to 0.5 ppm. The resulting paper-based microfluidic device (µ-PAD) assembled with a PCB system, consists of a cost-effective, portable, and versatile aptasensor (ssDNA) that serves as a basis for the fabrication of universal paper-based colorimetric and electrochemical platforms with the capability of multiplex and multi-replicates and it is promising for On-site applications in agriculture and environmental safety.

An Agent-Based Model to Assess the Efficacy of Targeting Biofilms in Mycobacterium avium Reinfection

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Keywords: computational modeling, agent-based model, lung infection, biofilm

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OBJECTIVES: Mycobacterium avium complex (MAC) pulmonary disease is caused by ubiquitous environmental microbes, notoriously difficult to treat and prone to recurrence, and increasing inboth incidence and prevalence [1]. The high rates of reinfection indicate a potential for non-antibiotic prophylactic treatments.

MAC are well known to form biofilms in the environment, which in vitro have been shown to aid in epithelial cell invasion [2], cause premature apoptosis in macrophages [3], and inhibit antibiotic efficacy [4]. We developed an agent-based model that shows the interactions between bacteria, biofilm and immune cells. This model has allowed us to explore both the intracellular scale (bacterial phenotypes and macrophage killing), and tissue scale (biofilm formation and epithelial invasion). We hypothesize that biofilms are key to establishing recurring infections in the lung, and will use our model to perform virtual knock-outs to better understand the effects targeting biofilms in prophylactic treatment to reduce reinfection rates.

METHODS: We used Repast Simphony to develop a three-dimensional ABM of in vivo MAC colonization to infection within the first 14 days post-deposition. The model environment represents a length of lung airway with a layer of mucus/epithelial lining fluid (ELF). Bacteria agents are deposited in the lung airway, while macrophages patrol. Biofilm is represented by continuous variables in each grid compartment, with values corresponding to the amount of extracellular matrix produced by bacteria in that grid compartment. Macrophages accumulate “apoptotic signal” through exposure to biofilm and internal bacteria. Biofilm is knocked out by removing the biofilms deposited with sessile bacteria, inhibiting bacterial formation of additional biofilm, or both.

RESULTS: Most biofilm is due to deposition, rather than bacterial formation after inhalation. While deposited biofilms are responsible for increased apoptosis and inflammatory signals, there is no significant difference in bacterial loads in biofilm knock-out experiments. Increased inflammatory signals recruit additional macrophages, causing increased inflammation.

CONCLUSIONS: We have developed a multiscale agent-based model that allows us to study the roles of biofilms in the initial colonization and infection in MAC-pulmonary disease on both the cellular- and tissue level. We have found that biofilms are not necessary to establish MAC infection, but do cause increased inflammation. Reducing biofilms in the lung airways may aid the immune system and antibiotic efficacy, but will not prevent infections entirely.

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Estimating the Greenhouse Gas Emissions Payback Period of Planned Offshore Wind Energy Using Multiregional, Environmentally Extended Input-Output Analysis

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Keywords: Offshore Wind, GHG emissions, MRIO, EEIO

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There is a substantial projected increase in energy generation from offshore wind farms in the US over the next three decades due to an increase in legislative commitments and funding from federal and state governments. Achieving ambitious offshore wind targets will be dependent on the expansion of domestic manufacturing and significant transfers of knowledge from world leaders in this technology. Offshore wind energy will provide GHG emissions-free energy during the use phase of the farm, but project construction is associated with significant environmental impacts that are less commonly acknowledged, which offset the touted benefits to a degree. Furthermore, offshore wind energy will be a competing technology for advanced energy materials. Developing offshore wind as a reliable domestic energy source demands a multiregional impact assessment of the economic and environmental spill-over effects of constructing offshore wind farms in major lakefronts and coastal regions. Despite the current lack of commercially operating offshore wind farms in the US, seven states have announced cumulative capacity commitments of over 28 GW by 2035. In this study, the spatial economic impacts of planned projects are estimated by combining the NREL Jobs and Economic Development Impact (JEDI) model for offshore wind energy with a multiregional input-output (MRIO) model of the United States built with the Virtual Industrial Ecology Laboratory (IE Lab). We also use a newly developed multiregional GHG emissions dataset for the US IE Lab to estimate the supply chain emissions of constructing and installing the offshore wind projects. These emissions estimates provide a more complete understanding of the time it will take for proposed cleaner energy projects to offset the environmental impacts of their manufacture and installation compared to those from energy generated from fossil fuel combustion. The multiregional framework will also be used to identify which states may see the largest spill-over effects in terms of emissions generation and economic activity required to support offshore wind projects.

Determining Key Parameters for Heat Sink Design in Pool Boiling

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Keywords: Two-phase cooling, heat sink design, performance predictions

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Two-phase immersion cooling provides a passive, efficient cooling option for high heat flux applications. However, in the case of electronics cooling, the required non-conductive fluids need surface enhancement in order to provide adequate cooling for today's high-power devices. Otherwise, the amount of vapor generated in boiling will envelop the surface and cause temperature increases that could irreparably damage the electronic device. To prevent this failure condition, area enhancement in the form of heat sinks specifically designed for boiling is of particular research interest. Critical length scales, bubble confinement effects, and varying boiling regimes are all key factors in predicting heat sink performance, and experimental evidence of when these become relevant is required. Even in the case of a simple fin array, knowing when and why current performance predictions fail must still be investigated. To examine boiling heat sink design, experiments were conducted on fin arrays to determine the critical length scale for accurate predictions. Using the hypothesis that the bubble departure diameter of the fluid is the key length scale, fins larger, smaller, and on the same order in spacing and height than this value were tested. The experiments were then compared to predictions developed using energy balance through the fin and the heat transfer capability of a flat surface. Results indicate that predictions do in fact only hold for height and spacing larger than the bubble departure diameter. In parallel, novel heat sinks designed for thermal resistance minimization were developed and tested. Even though these surfaces were made with simplifying assumptions such as uniform heat transfer, results show high heat flux capability not yet seen in dielectric fluids. By learning more about boiling performance for heat sink design and novel heat sink possibilities, two-phase cooling can be more widely implemented, saving on cooling energy costs and leading to safer, more efficient high-power devices.

Zero-field spin splitting in high-mobility undoped InSb1-xAsx heterostructures

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Keywords: Semiconductors, Spin-Orbit Coupling, Topological Quantum Computing,

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We report on the electrical properties of a series of undoped InSb1-xAsx quantum wells grown on GaAs substrates. We study three samples with Arsenic concentrations of 5, 13, and 19%. At 5% As concentration the two-dimensional electron gas (2DEG) displays a mobility peak of 24 m^2/Vs at a density of 2.5 Ã— 10^15 m^-2; this value is comparable to previously reported values for binary InSb quantum wells of similar design. High mobility and strong spin-orbit coupling allow us to observe beating in the Shubnikov de Haas oscillations at low magnetic field, facilitating assessment of the Rashba coupling parameter. A gate tunable zero-field spin splitting was observed, increasing with higher As concentration when comparing samples at fixed 2DEG density. The maximum Rashba parameter extracted is ~ 300 meVâ„« for the 19% As sample