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SUMMER UNDERGRADUATE RESEARCH FELLOWSHIPS

2021 SURF SYMPOSIUM
JULY 29 – JULY 30

ABSTRACT BOOKLET

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Day 1 | Morning Presentations

July 29th, 10:00 AM – 11:30 AM EDT

SESSION A: Composites & Structural Materials

Click here to join the session

Nanostructual Characterization of Hydration, Porosity and Mechanical Deformation of Human Bone

SURF ID: 109
10:00 AM – 10:15 AM

*Aaron J. Barker, Elizabeth Montagnino, Caitlin Adams, Thomas Siegmund, and John Howarter**
**PI: School of Materials Engineering*
Purdue University

More than 1.5 million bone fractures occur in elderly Americans every year due to conditions like osteoporosis. Bone can be considered a composite material of the ceramic mineral hydroxyapatite and collagen fibers. At the nanostructual level, bone exhibits variation in porosity and hydration as a result of physiological and environmental factors. The nanostructural and compositional variation can have a direct impact on the fracture toughness of bone. While the mechanical behavior of bones has been investigated in the past, characterizing the mechanical response as a function of hydration and porosity will enable the design of new treatments to mitigate bone deterioration. We will use small-angle x-ray scattering (SAXS), wide angle x-ray diffraction (WAXD), thermogravimetric analysis (TGA), and optical microscopy to characterize the composition of human cortical bone samples. We will also observe nanostructural deformation of bone which has been subjected to controlled mechanical loading. Degree of hydration of the bone will be measured as a potential factor that might affect the structural integrity of the bone under loading. The structure-property relationships established by this work can be used to effectively design next generation therapies to enhance the mechanical integrity of bone to prevent fracture from aging.

Keywords: Hydration, Composite material, Nanostructural characterization, Biological Characterization and Imaging

The Bio-based Future of Carbon Fiber

SURF ID: 113
10:15 AM - 10:30 AM

*Shawn N. Belongia, Bradley McGill, Clayton Westerman, and Jonathan Wilker**
**PI: Department of Chemistry*
Purdue University

In our oceans, marine animals such as mussels and oysters have adapted to their environments by producing natural adhesives. These adhesives exhibit great strength over very little contact area. Through biomimicry of this process, natural adhesives have been synthesized, but much more could be done in its application. Carbon fiber is known in industry for its strength and lightweight properties but its production yields fifteen times the carbon dioxide emissions and requires quadruple the energy as steel. It consists of polyacrylonitrile (PAN) fibers that go through a carbonization process and a nonrenewable bisphenol A (BPA) based epoxy which cannot be recycled or repurposed. With these concerns in mind, new bio-based alternatives are needed. However, not much research has been done. Here we show that modified plant oils with epoxy groups can be used in combination with a curing agent to create an epoxy resin to coat natural plant fibers, forming a bio-based carbon fiber. Through hydrolysis, the oxirane rings can be opened by a nucleophile and bonded to a hydroxyl group. By mixing, coating fibers, and then curing, a hardened semiflexible composite sheet that can withstand significant tension can be made. Results show that modified plant oils can be used to form a fully bio-based material that is both cost effective, low emission, and renewable. This system creates a carbon fiber alternative without negative environmental effects which can be used to replace current petroleum-based systems.

Keywords: Carbon Fiber, epoxy, natural fibers, renewable resources, thermosetting resin

Morphology and Composition of Non-traditional Pozzolans

SURF ID: 130
10:30 AM - 10:45 AM

*Nicholas M. Christ, Raikhan Tokpatayeva, and Jan Olek**
**PI: Lyles School of Civil Engineering*
Purdue University

It is difficult to find a scene in the modern world that does not rely heavily on cement and concrete. Traditional concrete is comprised of several phases: the cement paste, aggregates, pore structure, and pore solution. Many techniques have been developed to create high performance concretes (HPCs), including the addition of water-reducing agents, fillers, and pozzolans. Buildings, bridges, roads,

Keywords: Non-traditional pozzolans, pozzolans, fluidized bed combustion ash, ground bottom ash,

tunnels, and brick mortar all rely on these technologies from the concrete industry, but these technologies must evolve in changing times. In particular, the supply-demand ratio of fly ash, the most prevalent pozzolan in use in the United States, is quickly falling as power plants change rapidly from burning coal (of which fly ash is a byproduct) to burning natural gas. Pozzolans are a key component in HPCs. They undergo pozzolanic reactions by consuming calcium hydroxide (CH), the by-product of cement hydration. Since these materials typically replace between 20-30% of the cement in concrete, they reduce the carbon footprint of cement while increasing the strength and longevity of the concrete. The principal author has performed optical microscopy (OM) and scanning electron microscopy (SEM) tests on eleven samples of non-traditional pozzolans, including fluidized bed combustion ash (FBC), ground bottom ash (GBA), calcined clay (CC), and natural pozzolans (NP). These results will be combined with results of various other tests from the research group to describe the morphology and composition of these non-traditional pozzolans in the context of the development of standards and procedures for their widespread use.

calcined clay, concrete, cement

Effect of Nano-TiO2 on the Hydration Kinetics, Porosity, and Microstructure of Concrete Containing Slag Cement

SURF ID: 132
10:45 AM - 11:00 AM

Elena Cruz, Dan Huang, Miriam Velay-Lizancos and Jan Olek**
**Co-PIs: Lyles School of Civil Engineering*
Purdue University

The use of supplementary cementitious materials (SCMs) as partial replacement of cement is one of the main strategies to reduce the environmental impact of concrete. However, the use of some SCM, such as fly ash or slag cement, often results in the reduced rate of early-age strength development of concrete. When such concrete is placed outdoors late in the construction season at locations experiencing cold climate, it will be more susceptible (compared to concrete without SCM) to damage caused by freeze-thaw cycles and application of deicers. The use of nano-titanium dioxide (nano-TiO2) has been found to accelerate the hydration process and increase the early strength in plain concretes. To better assess the influence of nano-TiO2 on the durability of slag concrete, this research studies its effect on the hydration kinetics, porosity, and microstructure of cementitious composites containing slag cement. Thermogravimetric analysis, isothermal calorimetry, and setting time were used to study the effect of nano-TiO2 on the hydration kinetics of slag pastes. Water absorption test was conducted to investigate the permeability and porosity of nano-TiO2 modified slag concretes. Optical microscope and Air Void Analyzer were used to study the effect of nano-TiO2 on the air void structure of concretes containing slag cement. It was observed that increasing the amount of nano-TiO2 (up to 2%) in the mixtures resulted in acceleration of the hydration process of slag pastes. Addition of nano-TiO2 also reduced porosity and permeability of concrete containing slag cement and modified the characteristics of its air-void system.

Keywords: Nano-TiO2, Slag Cement, SCMs, Hydration Kinetics, Concrete, Porosity

Forensic Investigation of Concrete

SURF ID: 254
11:00 AM - 11:15 AM

*Bibigul Zhaksybay, Carlos Moro, Raikhan Tokpatayeva, and Jan Olek**
**PI: Lyles School of Civil Engineering*
Purdue University

Concrete is the most widely used construction material in the world. Therefore, it is vital to determine the cause of a failure in concrete structures, understand its consequences, and define methods of repair. Many previous studies have shown that forensic investigation can be beneficial when examining failures in concrete installations. Techniques, such as Optical Microscopy (OM) and Scanning-electron Microscopy (SEM), are examples of the semi-quantitative analytical methods that are used to diagnose various symptoms of failure (cracking, discoloration, formation of secondary products, changes in microstructure) related to durability issues. The research seeks to determine whether the specimens studied show symptoms of alkali-silica reaction (ASR), expansion due to the delayed ettringite formations (DEF), freezing and thawing, or carbonation which are some of the most common reasons for cracking or other microstructural changes in concrete elements. This study analyzed cores provided by the Indiana Department of Transportation from different locations throughout Indiana. These samples were then evaluated using SEM and OM techniques. The OM analysis indicated cases of (sometimes intense) cracking and discoloration of concrete and some signs of freezing-thawing deterioration. After further investigation by SEM, it became evident that the evaluated concrete has experienced limited symptoms of both ASR and DEF deterioration. The complexity of ASR and DEF makes it challenging to prevent these deleterious reactions. Thus, thorough and detailed research on alkali-aggregate reactions, ettringite formation, and more ways to

Keywords: Concrete, Alkali-silica reaction, Delayed ettringite formation, Optical Microscope Analysis, Scanning-Electron Microscopy, Microstructure.

prevent them are needed. The results of the analyses would lead to recommendations on ways to mitigate further deterioration.

A Better Bone to Stand On: Microstructural Simulation of Fracture Behavior in Human Bone

SURF ID: 131
11:15 AM - 11:30 AM

*Gregory L. Cook Jr[1], Aaron Barker[2], and John Howarter[2]**
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[1]Oakland University, [2]Purdue University

Keywords: Hydroxyapatite, Bone X-Ray Diffraction, Osteoporosis

Osteoporosis affects the femur bone and lower lumbar region the most. Reduced density in the bone contributes to the production of microscopic voids and creates greater susceptibility to fracture. These voids occur in spongy bone, which include the femur bone head and in joint bone. Bone is hierarchically constructed with the mineral hydroxyapatite which stimulates osteoblast cells to form new bone material. This process directly combats osteoporosis. This unfortunately tends to occur when the bone can't handle impact forces at hand in a given situation. The relationship between mechanical stress, fracture, and bone microstructure may be affected by hydration of the bone and other chemical or pharmaceutical treatments. This research aims to help create a conceptual framework of bone microstructure and mechanical performance, to provide insights to lessen bone fragility and increase fracture toughness. Using SolidWorks, tensile and compression tests were conducted with a simple hydroxyapatite model of bone. The first tests were conducting a tensile and compression test on a simple calcium hydroxyapatite bone model. The tensile test showed the hydroxyapatite bone yielded at 3.8*10^7 MPa. The compression test showed the hydroxyapatite model bone yielded at 6.7*10^5 MPa. This shows that bone fractures easier in response to an abrupt fall that impacts it perpendicularly to a specific joint bone. Microstructural variables were introduced to subsequent simulations to simulate a hydroxyapatite bone matrix with osteoporosis and variation on the size and distribution of porosity in the model bone matrix. The initial tests compared tensile and compressive bone response. The tensile test showed a yield strength of 9*10^7 MPa. The compression test showed a yield strength of 2.7*10^6 MPa. The results show that compressed impact causes fractures more easily with osteoporosis, when compared to tensile impact. Additional simulations which include soft tissue components and degree of hydration will be used to model therapeutic interventions to increase resistance to fracture.

SESSION B: Cellular Biology 1

Click here to join the session

Role of Locus Coeruleus - Norepinephrine System in Novelty Stimulus Recognition

SURF ID: 145
10:00 AM - 10:15 AM

*Catherine Gervais, Mang Gao, Renee Towers, and Alexander Chubykin**
**PI: Department of Biological Sciences-Biology*
Purdue University

The Locus Coeruleus (LC) is a small nucleus in the pons that acts as the major noradrenergic hub, releasing norepinephrine (NE) to many projecting regions of the brain. The LC-NE system is involved in many neurobiological processes, such as response to stress and modulation of the sleep wake cycle. However, the role of the LC-NE system in learning and memory has not been well established. Evidence has shown the role of the LC-NE system in response to salient stimuli helps to form memories, but there are limited studies on the role of LC-NE in novelty perception. In this study, five mice had an adeno associated virus (AAV) expressing channelrhodopsin-2 injected directly into their LC. They were optogenically manipulated while being presented with a novel stimulus while head fixed on a wheel mount. The pupils of the mice were recorded with a camera while being presented with the stimulus and analyzed on DeepLabCut to quantify any pupil dilation changes. This study compares the results from pupillometry and will provide conclusions based on our observation of the change in pupil dilations. A significant increase in pupil dilation when presented with a novel stimulus could indicate that the LC-NE system plays a role in novelty perception. These results will provide a basis for further studies observing familiarity of novel stimuli, and how the LC-NE system plays a crucial role in novelty perception.

Keywords: Locus Coeruleus, Norepinephrine, Pupillometry, Optogenetics, Channelrhodopsin

Simulating Cell Migration in a Mechanical Perspective

SURF ID: 159
10:15 AM - 10:30 AM

*DeVon Young Herr, Jing Li, and Taeyoon Kim**
**PI: Weldon School of Biomedical Engineering*
Purdue University

In development, cells tend towards collective migratory patterns, moving together in large units and groups of cells, which has been recapitulated in numerous live-cell experiments as well as computational models. This collective migration of cells is the driving force for complex important biological processes and systems. Consequently, the ability to modify cell systems and configurations to guide collective migration can better illuminate biological ideas as well as introduce new tools to manipulate biological systems and processes. We use a center-based model, simulating cells as points in space that models cell physics to understand physical principles that underly cellular migration. Our model simulates cell migration through torque, as an extension of previous literature which used force. Hence, we also looked to see if this modelling feature changed migration behavior. We carried out computational cell migration simulations with systematic parameterization. We first varied the modelling assumptions that mathematically described how cells migrate to verify the model against literature. Once accurate parameters were obtained, we then varied parameters relating to laboratory settings, namely cell density and sensitivity of cells to contact. We verified the biphasic relationship between cell density and variation on angular changes in cell migration. Further, we found that cell density and sensitivity to contact affected migratory movement behavior, though with the sensitivity playing a smaller role. The torque results were like force results, but with less variation in behavior. These results indicated general agreement on the force and torque models, with the possibility of exploring the relationship of substrate rigidity.

Keywords: Cell Migration, Biological Simulation and Technology, Material Modeling and Simulation, Cellular Biology.

Mechanisms of Cell Division under Physiological Conditions

SURF ID: 198
10:30 AM - 10:45 AM

*Morgan H. Moses[1], Donghyun Yim[2], and Taeyoon Kim[2]**
**PI: Weldon School of Biomedical Engineering*
[1]University of Alaska Anchorage, [2]Purdue University

Recent studies on the mechanics of cell division in three-dimensional environments showed that cell division occurring under physiologically-relevant conditions is far more complex than that probed in two-dimensional environments in previous studies. Cells are often surrounded by a dense extracellular matrix (ECM). Thus, of critical importance is the ability of dividing cells to generate sufficient pushing forces to adequately deform the ECM and secure sufficient volume to allow the parent cell to divide. However, both the cell itself and the ECM are complex systems showing temporary and permanent time-dependent behaviors. The consequences of varying the properties of the cell and its surroundings are not well explored due to experimental limits. In our study, simulations

Keywords: Computational model, Simulation, Cytokinesis, Cell Division, Extracellular Matrix, Cellular Biology

for cytokinesis were performed with variations in several key parameters over a wide range of values, including i) the pushing and ring contractile forces exerted by a dividing cell, ii) membrane stiffness, iii) volume expansion prior to division, and iv) time delay between two types of cell-generated forces. Using simulation results, we characterized time evolution of membrane shape and elongation, matrix deformation, cell volume change, and forces developed on the matrix. Using the measured data, we identified key governing factors for cell division under physiological conditions. These results will provide guidance to further studies of cell division in three-dimensional environments.

Characterizing the Role of Fungal Cdc14 Phosphatases in Response to Cell Wall Stress

SURF ID: 202
10:45 AM - 11:00 AM

*Noelle Naughton, Andrew DeMarco, and Mark Hall**
**PI: Department of Biochemistry*
Purdue University

Keywords: Cdc14, phosphatase, mitotic exit

Fungal pathogens cause disease within plants and humans, leading to challenges with agricultural productivity and hospital-acquired infections. Fungi can develop resistance to pesticides and antifungal drugs and can bypass plant immune systems and take advantage of compromised human immune systems. There is a constant need for development of new strategies to combat fungal pathogens. The Hall lab has proposed that the Cdc14 phosphatase family may be a useful target for novel antifungal drugs. The primary objective of my project is to characterize the sensitivity of yeast strains lacking the CDC14 gene, including in the human pathogen Candida albicans, to cell wall stress using agar plate spotting assays. Briefly, I will grow cell cultures in liquid media without any drugs to saturation. Agar plates containing the same media with or without different drug concentrations will be poured. The optical density of the cell cultures will be measured using a spectrophotometer and adjusted to ~1.0 by dilution in sterile PBS. Then, serial 8-fold dilutions will be performed to allow single colonies to be visible on the agar plates. Each dilution will be spotted as a 5 μl droplet using a template that is placed under the agar petri plate, proceeding from lowest to the highest cell density. The plates will then be incubated for several days and imaged each day to monitor growth. My results showed that CDC14 deletion strains of C. albicans are hypersensitive to the antifungal drugs micafungin and caspofungin that inhibit cell wall synthesis. Cdc14 thus plays a critical and unexpected role in responding to cell wall stress in Candida albicans and this function may make Cdc14 a useful target for antifungal therapeutics.

Epstein Barr Virus Activation in Stomach Cancer Cells

SURF ID: 227
11:00 AM - 11:15 AM

*Kunming Shao, Srishti Chakravorty, and Majid Kazemian**
**PI: Department of Biochemistry*
Purdue University

Keywords: EBV, EBVaGC, Super enhancer inhibitors, HDACi, Latent, Lytic reactivation

Epstein-Barr Virus (EBV) infects approximately 90% of the world's human population. It is associated with several malignancies including EBV-associated gastric cancer (EBVaGC). This virus typically persists within the host cell in a dormant latent state. However, upon reactivation, the virus can switch from a latent to a lytic state. In the lytic state, several viral proteins or antigens are produced which makes the virus-infected cells visible to the host immune cells. In this project, we investigate the effect of two classes of lytic inducers – Super Enhancer (SE) inhibitors namely THZi and JQ1, and HDAC inhibitors (HDACi) EBV-infected gastric cancer cells. Based on our preliminary experiments, we observed a slight increase in the expression of the EBV lytic genes upon THZi (but not JQ1) treatment compared to control. However, further replicates are necessary to make a correct conclusion. Parallelly, we also explored the role of HDACi such as Entinostat (MS-275) to induce the lytic cycle. To that end, we treated the cells with a specific inhibitor of the PKC-δ pathway - Rottlerin. Induction of this pathway among others is reported to reactivate EBV. Interestingly, we observed that Rottlerin did not abrogate lytic induction suggesting that, the PKC- δ pathway is not the only pathway involved in Entinostat-mediated EBV reactivation. In the future, we will investigate the exact mechanisms of HDACi mediated lytic induction. In summary, we hypothesize that targeting super-enhancers and HDACs may be an effective strategy to treat patients with EBVaGC by inducing a lytic state in the infected tumor cells.

Cdc14 Phosphatase Stimulation by an Intramolecular Substrate-Mimicking Motif

SURF ID: 245
11:15 AM - 11:30 AM

*Benjamin T. Waddey, Kedric Milholland, Andrew DeMarco, and Mark Hall**
**PI: Department of Biochemistry*
Purdue University

Keywords: Cdc14 Phosphatases, Enzymatic Activity, C-terminal Tail, Fungal Pathogens, Regulation

The Cdc14 protein phosphatase family regulates diverse cellular processes, including stimulating mitotic exit and cytokinesis in fungal cells and regulating DNA repair, hearing, and male fertility in mammalian cells. Cdc14 is also required for normal pathogenesis in several plant and human fungal pathogens. The Hall Lab has identified a novel C-terminal sequence motif in S. cerevisiae Cdc14 (ScCdc14) that acts a catalytic enhancer and is widely conserved in fungal Cdc14s. Recent experiments revealed this motif is important for cell wall integrity and pathogenesis in yeasts, but is dispensable for mitotic exit. We recently demonstrated that the human Cdc14A (hCdc14A) C-terminus also contains a similar catalytic enhancer despite lacking sequence homology to the fungal motif, Using site-directed mutagenesis, recombinant protein expression and affinity purification, and steady-state kinetic assays, we show that the ScCdc14 motif accelerates phosphoenzyme hydrolysis by an order of magnitude, and that activity of ScCdc14 lacking the motif is stimulated in-trans by a synthetic peptide containing the motif sequence. Initial experiments with hCdc14A site-directed mutants have failed to pinpoint the sequence responsible for enhancing catalysis, based on Michaelis-Menten kinetic analyses. Next, our investigations will focus on 1) testing the hypothesis that the fungal motif mimics a substrate to bind the Cdc14 active to stimulate hydrolysis of the phosphoenzyme intermediate, 2) understanding how the fungal motif is connected to cell wall integrity and pathogenesis, and 3) searching for the residues within the C-terminal region of hCdc14A that are responsible for strong catalytic stimulation. The presence of sequences outside the core phosphatase domain that impact catalytic rate of diverse Cdc14 orthologs suggests a novel mechanism by which organisms can dynamically control this enzyme activity cell during cell division and in response to stress and other external signals.

SESSION C: Human Factors & Education

Click here to join the session

Understanding and Reducing Major Industrial Plant Disasters

*Ashley R. Bagadiong and Ray Mentzer**
**PI: Davidson School of Chemical Engineering*
Purdue University

SURF ID: 107
10:00 AM - 10:15 AM

Understanding process safety incidents is integral to prevent major industry catastrophes and serious injuries and fatalities (SIFs). A key personnel safety principle, as asserted by Heinrich, is that if lower-level incidents are reduced, then higher-level incidents will be reduced proportionally. However, studies have found that only a small percentage of less serious incidents can lead to major personnel safety incidents. This work seeks to apply these principles to process safety incidents. Major catastrophes can be caused by domino effects, which are large accidents that are escalated by a sequence of smaller events. A literature analysis was conducted to investigate which lower-tier precursors have the potential to lead to higher tier incidents, using the process safety indicator pyramid. This study also explored the factors that may have prevented historic catastrophes that were caused by domino effects. We analyzed the underlying causes of major accidents and reported process safety events (PSEs), namely using reported data from the International Association of Oil & Gas Producers (IOGP). 95 accidents from the U.S. Chemical Safety Board (CSB) database were analyzed to determine the key characteristics and contributing factors to domino effects. This analysis identified that the top contributing factors that led to higher-tier events and domino effects are the same: process hazard analysis (PHA), hazard awareness and identification, and safety culture. These results suggest a deeper focus on such contributing factors to prevent major process safety catastrophes. Additional recommendations were made for further exploration in this area, specifically for the analysis of lower-level events.

Keywords: Process safety, safety triangle, domino effects, contributing factors performance indicators,

Understanding the Influence of Work-Integrated Learning Experiences on Students' Identity Formation in Engineering

*Andrea (Lili) Castillo[1], Brianna Benedict[2], and Allison Godwin[2]**
**PI: School of Engineering Education*
[1]University of California, Irvine, [2]Purdue University

SURF ID: 125
10:15 AM - 10:30 AM

This research paper examined the factors influencing students' access to work-integrated learning experiences (WILs). Several studies have tapped into how WILs enrich students' academic and career development. Yet, there are limited understandings about the factors that impact the accessibility of WILs for engineering students, particularly latently diverse students. Latent diversity refers to students' underlying attitudes, mindsets, and beliefs that provide potential sources for innovation but are not readily visible in the classroom. Building on prior studies that discuss work-integrated learning experiences, this work draws on an adapted framework of identity trajectory theory to examine how latently diverse students' exposure, or lack thereof, influences their identity development in engineering. The data for this paper comes from a larger mixed-method study focused on understanding how latently diverse engineering students experience the culture of engineering and negotiate their identities as engineers. We used analysis of narratives to identify access factors and understand how students' access to internships and co-ops influences their journey to becoming an engineer. This paper highlights how institutional resources and students' networks facilitate their access to work-integrated learning experiences and affects students' performance competence beliefs, career interests, and recognition as engineers. These results have implications for practice and policies in engineering education, particularly enhancing students' access to work-integrated learning experiences and constructing WILs that support students' identity development.

Keywords: Work-Integrated Learning, Accessibility, Identity Trajectory, Latent Diversity, Engineering Education

Developing an Automatic Student Program Analysis Software with American Fuzzy Lop and Django

*Dalilah Vaquera, Shan Huang, and Yung-Hsiang Lu**
**PI: School of Electrical and Computer Engineering*
Purdue University

SURF ID: 242
10:30 AM - 10:45 AM

University computer science courses assess skills through programming assignments, and each assignment typically follows a general outline. Teaching assistants and professors use office hours to debug tedious errors within their students' programs such as memory leaks and incorrect function calls, and thus the time cannot be used to properly advance student's skills. The objective of this

Keywords: Program analysis, American Fuzzy Lop, Automatic grading

research is to develop a software to assess the correctness of programming assignments and provide feedback which will help to teach and improve student's programming skills. Fuzzing software is a method used to test a program by providing invalid, unexpected, or random data as inputs into a program. AFL, American Fuzzy Lop (AFL), is a fuzzing software used to put sample code into and generate test cases to test the correctness of the code. With the use of a fuzzing software, a feedback and program assessing software can be created to provide students with coding guidance. Status received from AFL includes processing time, unique crashes, and paths timed out. By integrating AFL into the automatic grading algorithm, we can use the AFL status to deliver helpful debugging message to students. Students will be able to submit their programming assignment through the terminal command line or via submission on a website, and within seconds will receive feedback on the correctness of functions, outputs, and memory issues. The program will give details on which specific functions or lines the program did not respond as intended, which overall decreases the time, energy, and cost of debugging.

Empowering Secondary School Girls in Rural Senegal: Validation of the Assessment for STEM Self-beliefs.

SURF ID: 187
10:45 AM - 11:00 AM

*Nafissa A Maiga, Dhinesh Radhakrishnan, and Jennifer DeBoer**
**PI: School of Engineering Education*
Purdue University

Keywords: Cognitive Interview, STEM self-beliefs, instrument validation, Senegal, girl education

Lack of female education in the global South is a complex issue with disastrous consequences such as lower wages for women, child labor, early forced marriages, and even female genital mutilation. Education has been shown to improve girls' welfare, their self-image, and even reduce infant mortality. Yet, in Senegal, only a little under 40% of women are literate. Female students are not always encouraged to pursue education due to negative gender stereotypes, especially in rural Senegal. This lack of support causes many girls and women to lose motivation in school which lowers their self-esteem regarding education, and especially their STEM self-beliefs. Perceiving oneself as an engineer remains difficult for numerous women especially in the Global South. In this research we attempt to develop and validate STEM self-beliefs instruments for the female secondary students in rural Senegal who are part of the GirlEngage program. We developed STEM self-belief assessments that include the "draw an engineer" test, and an adapted science and technology self-efficacy questionnaire. These assessments will initially be tested on 3 participants from the Global South. The participants are all familiar with the francophone West African context, and they all have similar education levels as the girls part of GirlEngage in Kédougou. Cognitive interviews using the "think-aloud" protocol as well as verbal probing were used to improve and validate the STEM self-beliefs instruments developed. Participants understood most of the instruments as intended. The results from the cognitive interviews helped us refine the assessment tools that will be deployed in Kédougou.

The Impact of COVID-19 on Traditional and Transformative Transportation in Selected Indiana Cities

SURF ID: 220
11:00 AM - 11:15 AM

*Dale Robbennolt[1], Ricardo Chahine[2], and Konstantina Gkritza[2]**
**PI: Lyles School of Civil Engineering*
[1]University of Illinois at Urbana-Champaign, [2]Purdue University

Keywords: COVID-19, Pandemic, Public Transportation, Mode Choice, Shared Mobility, Travel Behavior

Both traditional forms of public transportation and emerging modes have undergone changes throughout the COVID-19 pandemic. Travel was impacted by fears of infection, changing work and leisure habits, and regulations to control the virus. The objective of this study is twofold: i) to review literature to examine trends in transportation during COVID-19, and ii) to assess travel behavior in selected Indiana cities during the pandemic to compare with pre-pandemic behavior. Data was collected via a survey of Greater Lafayette residents before and during the pandemic. The data includes general travel behavior, sociodemographic information, and use of e-scooters and shared-bikes. The survey results were analyzed using descriptive analysis techniques. Statistical tests (i.e., test of proportions, Mann-Whitney tests) were conducted to compare responses before and during the pandemic. The results are used to understand changes in behavior during the pandemic, including changes in trip purpose and mode choice, which are compared to literature review findings. The statistical test results indicate that COVID-19 caused significant changes to e-scooters and bike-sharing services, with increasing trip length, more frequent use of these services, and a greater likelihood of connecting with other transportation modes. Some variables were unchanged, with no significant difference in the amount that users were willing to pay for service or the time they were willing to search for available vehicles. Understanding changes in behavior at the beginning of the

pandemic is key to understanding how the pandemic continues to impact the transportation sector and influence policymaking in the wake of the pandemic.

The Situational Awareness and Decision-Making Analysis of Experienced Nurses

*Anand Shroff, Nicholas Anton, Guoyang Zhou, Tara Schutter, Passawit Puangseree, and Denny Yu**
**PI: School of Industrial Engineering*
Purdue University

SURF ID: 231
11:15 AM - 11:30 AM

A large part of what makes a nurse effective at what they do is derived from experience. When attempting to properly assess a patient in a time-efficient manner, previous experience can play a large role in determining warning signs of potentially life-threatening medical issues. This study aims to utilize wearable devices to objectively categorize experienced nurse decision making. In order to do this, electro-encephalogram (EEG) and eye-tracking data was collected on simulated patient cases where experienced nurses were expected to identify changes in patient status and alert the physician of the patients' deterioration. There were two types of cases included in these simulations: a stroke patient, which represented a straight-forward case, and a two-patient COVID-19 scenario which is more involved and complex. Eye-tracking data shows what the experienced nurses were looking at when a decision was made and EEG analysis can determine cognitive workload associated with specific tasks. Ultimately our team will use the EEG and eye-tracking data obtained from this study to create a device for nursing students to support their decision making in the simulated clinical environment. The final result will be a wearable device to assist in the training process for nurses.

Keywords: Eye-tracking, EEG, Nurse, COVID-19, Training

SESSION D: Biological Simulation & Technology

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Mathematical Modelling of Various Gut Microbiota in Response to Various Mono- and Disaccharides

SURF ID: 117
10:00 AM - 10:15 AM

*Amanda Blankenberger, Zachary McGuire, Shreya Athalye, and Mohit Verma**
**PI: Department of Agricultural & Biological Engineering*
Purdue University

The gut microbiome is a complex network of interacting bacteria that plays a significant role in the health of human beings. The gut bacteria Lactobacillus acidophilus, Roseburia intestinalis, and Roseburia faecis have not been previously modelled in response to different doses of simple mono- and disaccharides. Growth experiments were conducted on these bacteria with 13 different mono- and disaccharides in three different concentrations in a chemically defined media to measure the optical density (OD). The experiments were conducted in 96-well plates to provide 8 replicates of each test condition. Using a curve fitting code, the data is analyzed for the growth and death rates of each condition. This study provides an understanding of which doses of the mono- and disaccharides the different bacterial strains are able to utilize efficiently. The preliminary results show a lack of growth in the chemically defined media for all strains, possibly due to the lack of a necessary nutrient. The results of this study will provide further information to be used in more complex models for possible analysis of gastrointestinal diseases and treatments.

Keywords: Microbiome, Bacterial Growth Modelling, Biological Simulation and Technology

Optimization of Ultrasound and Photoacoustic Vascular Imaging

SURF ID: 182
10:15 AM - 10:30 AM

*Olivia Loesch, Katie Leyba, and Craig Goergen**
**PI: Weldon School of Biomedical Engineering*
Purdue University

Ultrasound and photoacoustic tomography are widely used noninvasive imaging modalities with the potential to provide vital structural data (i.e. organ, vessel, or tumor size and shape) and physiological data (i.e. hemoglobin levels, lipid content, etc.). Ultrasound imaging utilizes properties of sound, namely echolocation, to display organ and vessel geometry. Photoacoustic imaging is simply ultrasound imaging but includes high wavelength light, which allows us to image functional features such as lipids or collagen. Optimizing both imaging strategies could significantly improve the quality and quantity of data extracted from images, potentially aiding physicians in the diagnosis and treatment of patients. In this study, we enhanced hardware methods and software methods to improve ultrasound and photoacoustic image quality. First, we improved hardware methods by optimizing the tools and equipment used during image acquisition. Specifically, we attempted to enhance photoacoustic imaging by developing a 3D printed holder that could easily adjust the angle of light reaching our sample. We also developed a tissue-mimicking calibration object for photoacoustic imaging in order to test the system. Next, we improved software methods by optimizing image analysis algorithms. We created a simple program in Python to remove noise, any unwanted signal, from images to better visualize the region of interest. This algorithm was tested on images acquired from an already well-developed vessel-mimicking control. Finally, we evaluated the enhanced image quality by measuring the signal to noise ratio, a metric comparing desired signal to undesired signal. After running the algorithm, we found that the signal to noise ratio increased, indicating improved image quality.

Keywords: Biological simulation & technology, imaging, simulation, ultrasound, photoacoustic tomography, imaging phantoms, image processing

Effective and Rapid LAMP Sensor to Detect BRD

SURF ID: 197
10:30 AM - 10:45 AM

*Giuditta Monti[1], Andres Dextre[2], Josiah Levi Davidson[2], Murali K. Maruthamuthu[2], and Mohit Verma[2]**
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[1]Northwestern University, [2]Purdue University

Bovine Respiratory Disease (BRD) is an infectious disease caused by several specific bacteria (i.e. Mannheimia haemolytica, Pasteurella multocida, etc.) and viruses (i.e. Bovine Herpesvirus, Adenovirus, etc.). In the United States, BRD is responsible for economic losses between $800 million and $900 million due to veterinary costs and livestock loss. Moreover, the required antibiotic treatment often induces antibiotic resistance in the treated animals, making the disease increasingly difficult to cure. At its early stages, BRD is difficult to diagnose due to abundant and vague clinical symptoms: depression, lack of appetite, and runny nose. When the disease is diagnosed, a large part of the herd has already been infected. In this project, a Loop-Mediated Isothermal Amplification

Keywords: Bovine Respiratory Disease (BRD), Loop-Mediated Isothermal Amplification (LAMP), Pasteurella multocida, cattle

(LAMP) device is employed to detect the presence of BRD-specific pathogens in bovine nasal swaps. To do so, corresponding primers must be identified. Thus, LAMP screenings are run on different designed primers to determine the most suitable in terms of specificity, timing, and limit of detection. The device is prepared and loaded with all the needed chemicals in the laboratory. Once at the farm, the sample is collected and deposited on the device to be inserted in a heated water bath. If the BRD-specific pathogens are present, the device will change color within one hour. This LAMP device is a cost-effective, rapid, and reliable diagnostic method to determine the presence of bacteria (i.e.Pasteurella multocida), providing farmers and veterinaries with the opportunity to promptly treat the affected animal and stop the spread of BRD to the remaining herd.

Ethanol Effects on Embryonic Zebrafish BMP Signaling as a Model for Fetal Alcohol Spectrum Disorders

SURF ID: 225
10:45 AM - 11:00 AM

*Zoe Elise Schardan, Xiaoguang Zhu, Linlin Li, and David Umulis**
**PI: Department of Agricultural & Biological Engineering*
Purdue University

Approximately one in every 100 babies born in the United States each year is affected by Fetal Alcohol Spectrum Disorders (FASD), which can result in cognitive impairments and growth abnormalities. These growth abnormalities can be modeled in the zebrafish bone morphogenetic protein (BMP)-signaling system, the same signaling system in humans responsible for critical bone and cartilage development. While ethanol (alcohol) has been traced to disruptions in the BMP-signaling pathway, current research has not determined how specific, documented changes in ethanol concentrations play a role in the magnitude of FASD. In this study, we will use the zebrafish system to model how different ethanol concentrations influence downstream BMP-signaling in early embryonic development (3-6 hours post fertilization (hpf)) and explain how our results can be theoretically applied to the human system. To do so, we will expose wild type (WT) embryos to 1%, 1.5%, 2%, and 3% ethanol in a growth medium (E3), along with a growth medium control, and collect them at peak BMP signaling hours. The embryos will be stained using PSmad and Sytox orange and imaged on a confocal microscope, after which the signals in the images will be quantified to determine the BMP signal present. From the results of image quantification, we will be able to compare the BMP signal between the selected genotypes and reach a conclusion as to the role BMP-signaling genetics play in FASD.

Keywords: Biological characterization and imaging, developmental biology, zebrafish, fetal alcohol spectrum disorders

Maturing Chondrocyte Seeded Scaffolds Using a Dynamic Mechanobioreactor System

SURF ID: 259
11:00 AM - 11:15 AM

*Clarisse M. Zigan, Zachary Davis, and Deva Chan**
**PI: Weldon School of Biomedical Engineering*
Purdue University

Millions of people worldwide are affected by osteoarthritis. This progressive condition is characterized by pain and loss of function that can in part be attributed to the loss of articular cartilage, the tissue that covers the ends of bone within the joint. The primary cell type within cartilage, chondrocytes, produce and maintain the complex extracellular matrix that allows for cartilage to withstand loads and minimize friction. One tissue engineering approach to regenerate cartilage has been to grow chondrocytes embedded in biomaterial scaffolds into mature, cartilage-mimicking tissue. The objective of this study is to compare chondrogenic tissue growth within standard monomeric or multimeric collagen gels under varying levels of loading and duration. To do this, we will first design and evaluate a dynamic bioreactor culture system that applies compressive and shear loads to facilitate the maturation of chondrocytes embedded in a collagen gel. A dynamic loading regimen will be directly compared to free-swelling conditions to observe cell growth up to two weeks in sterile culture. Scaffold maturation will be evaluated using biomechanical testing, biochemical assays, and histology. Results of this study will include dynamic loading regimens that best promote chondrogenic maturation of scaffolds and enable comparisons among collagen scaffold types. By improving understanding of how loading factors influence cell behavior and matrix production in in-vitro experiments, we can pave the way to designing new methods to repair cartilage damage before osteoarthritis progresses to later stages.

Keywords: Tissue engineering, Mechanobioreactor, Collagen Hydrogel, Cartilage Repair

SESSION E: Nanotechnology: Fluids & Chemicals 1

Click here to join the session

A Thermal Analysis of Common Pharmaceutical Reagents Using an ARSST Calorimeter

SURF ID: 108
10:00 AM - 10:15 AM

*Michael T. Bai, Boen Cao, and Ray Mentzer**
**PI: Davidson School of Chemical Engineering*
Purdue University

Keywords: Thermal analysis, ARSST, calroimetry, thermal properties

In chemical processes, knowing the properties of a chemical is vital to knowing how to safely handle and use them in an industrial setting. Previous research into specifically the thermal properties of chemicals – their stability, potential for energy release, and at what point that energy is released – has been performed via calorimetry. In this project, we sought to analyze some common reagents used in pharmaceutical manufacturing using an Advanced Reactive System Screening Tool, or ARSST calorimeter. The ARSST was used to measure the heat released by the decomposition reactions of these reagents, and data in the form of temperature vs. time was then analyzed to calculate the thermal properties of these substances. Five chemicals were studied: dicumyl peroxide, 5-amino-3,4-dimethylisoxazole, (2-(1H-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate (HBTU), (2,2,6,6-tetramethylpiperidin-1-yl)-oxidanyl (TEMPO), and T-butylhydrogen Peroxide (TBHP). The samples are heated in the calorimeter until they begin to decompose. Then, the calorimeter matches its own heat rate to the rate at which the decomposition reaction generates heat to achieve an adiabatic process. The data from the calorimeter is used to calculate the thermal properties – namely, the activation energy and heat of reaction of the decomposition. The results indicate ARSST is capable of producing results similar to those produced by other calorimeter types, and that the chemicals tested tended towards exothermic decompositions, and as such require storage and handling methods – such as refrigerated storage – that help to prevent the initiation of these decomposition reactions.

The Effect of Inverse Opal Composition and Pore Size on Photocatalysis

SURF ID: 219
10:15 AM - 10:30 AM

*Paige M. Rich, Yuhang Fang, and David Warsinger**
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Purdue University

Keywords: Inverse Opal, Nanotechnology, Photocatalysis, Photocatalyst

Photocatalysis is a key solution to destroy hazardous compounds related to energy, health, and environmental issues, further augmented by its potential as a solar-powered process. One method to optimize this currently inefficient reaction type is the fabrication of photocatalysts as nanoscale inverse opals. At 1/300 the size of a human hair, the small scale of these structures produces a photonic crystal nature and slow photon effect, an influence much like the natural structural color of bird and butterfly wings. These properties allow the structures to absorb light more effectively, resulting in an increased photocatalytic effect. As pore size and photocatalyst material are fundamental aspects of inverse opal structures, an understanding of their impact on photocatalysis is critical to improve reaction efficiency. This study varied the following three properties of the inverse opals and photocatalysis process: opal diameters of 305 nanometers (nm) and 170 nm, UV light wavelengths of 254 nm and 365 nm, and silica/titania photocatalyst ratios of 0:1, 0.25:0.75, 0.5:0.5, 0.75:0.25, and 1:0. The inverse opal structures were fabricated using a self-assembly sol-gel method. The samples were then placed in methylene blue solutions under UV light for 12 hours to cause a photocatalytic reaction. Comparison of the degradation rates identified which properties corresponded to a greater photocatalytic effect. The results indicate that an opal diameter of 170 nm and silica/titania photocatalyst ratio of 0.25 caused an increased photocatalytic effect. This knowledge can be applied in constructing future photocatalytic systems to increase efficiency.

Tuning Properties of Nanoclusters and Their Mass Spectrometric Analysis

SURF ID: 226
10:30 AM - 10:45 AM

*Lidya Sertse[1], Habib Gholipour-Ranjba[2], Solita Wilson[2], and Julia Laskin[2]**
**PI: Department of Chemistry*
[1]Minnesota State University,[2]Purdue University

Keywords: Nanoclusters, Mass Spectrometry, Cluster Synthesis

Nanoclusters are nanoscale collections of a few atoms that serve as a bridge between atoms and nanoparticles. The synthesis and design of cost-effective nanoclusters have received increased attention over the past few years due to their unique chemical and physical properties for applications in catalysis, energy storage, nanophotonics, sensing, and medical diagnostics. Some of the most effective ways to tune their properties are through surface ligand manipulation and host-guest chemistry. However, identification, purification, and characterization of atomically precise

nanoclusters with conventional methods is challenging resulting in the design of a few types of fine-tuned clusters. This study employs mass spectrometry, which enables the characterization of samples without purification making it a powerful tool in the design of nanomaterials. Synthetic methods were formulated to fine-tune metal chalcogenide and polyoxovanadate nanoclusters through surface ligand manipulation and host-guest chemistry. Mass spectrometry analysis revealed that clusters with different ligands have different stability and the chemical reactivity of their fragments on the surface can be controlled by changing the surface ligands. Similar methods were used to prove that molybdenum-polyoxometalate forms stable complexes with cyclodextrin. This study provides molecular level insight into different nanocluster systems through mass spectrometry and shows how subtle changes to different nanoclusters will affect their electronic, chemical, and structural properties, which paves the way for the design of similar nanoclusters.

Rheological Characterization of Highly Loaded Alumina-Polymer Suspension for Thermal Paste 3D Printing

SURF ID: 212
10:45 AM - 11:00 AM

*Pattiya Pibulchinda, Caitlin Adams, and Kendra Erk**
**PI: School of Materials Engineering*
Purdue University

Keywords: Thermal Interface Materials, Viscoelastic, Paste 3D Printing, Rheology, Materials Processing and Characterization

Demand for smaller electronics requires higher efficiency heat management. Thermal interface material (TIM) pastes are thermally conductive fillers in a polymer matrix that connects heat conductivity pathways. Applying thermal paste by 3D printing technique improves complexity, accuracy and continuity of the material loading process. However, the liquidity of thermal paste causes dripping issues that create tail defects at the end of printed lines. Tailing increases manufacturing machine time, cost, and material waste. This study investigated the influence of rheological factors on 3D printing flow behaviors for TIMs. Highly loaded alumina-polymer suspensions were formulated to model commercial alumina-based TIMs. The suspension properties were adjusted by varying the volume percentage of alumina powder and polyvinylpyrrolidone (PVP) polymer. These model TIMs prove to be practical representatives of the commercial TIM due to similar rheological behaviors. Key properties for characterizing flow are yield stress, viscosity-shear rate dependency, gel point, and cohesive strength. In addition, this project developed rheometric experimental procedures to simulate TIM behavior in the 3D printing process. Printing and dripping issues were identified in several 3D printing protocols as moving and lifting speed changes. The commercial TIM tails more continuously while the model suspension drips discretely in drops. Shear strain and viscosity changes were characterized during cycles of constant applied load and unload. The simulated rheometer data can be related to the tailing effects shown in the 3D printing. This research built a relationship between rheological properties and paste 3D printing, supported by the data comparison between commercial TIM and model TIMs.

Design and Manufacturing of Bio-inspired Nanocomposites for Radiative Cooling

SURF ID: 121
11:00 AM - 11:15 AM

*Jennifer Lynn Cahillane, Andrea Felicelli, and Xiulin Ruan**
**PI: School of Mechanical Engineering*
Purdue University

Keywords: Nanotechnology, bio-inspiration, bio mimicry, radiative cooling, heat transfer, energy saving

Looking at the state of the world, one sees a large issue regarding heating and cooling, from a small residential side, to larger commercial scale, and to global warming. Efforts to cool residences and buildings are responsible for a large portion of the world's energy consumption. These buildings mainly use conventional air conditioning systems to regulate temperature, which transports the heat from the inside to the outside, effectively creating a heat island effect and worsening the global warming issue. In efforts to find solutions to this issue, researchers have begun looking at nature for inspiration, specifically the way many animals have adapted to cooling themselves in treacherous environments. In particular, radiative cooling has gained traction as some animals possess structures that apply this principle to reflect a high percentage of the incident radiation and heat from the sunlight they encounter and push it back into deep space. This both helps provide cooling without great energy consumption and helps global warming. Looking particularly at certain animals and the composition of their shells, one sees a layered structure formation on the micro-scale. This flat layered formation allows for greater reflectance of incident radiation than spherical nano-particles. This concept was put into effect with a variety of different elemental compounds to see what specific nano-particles are most effective. By studying the spectroscopy results and the reflectance of different compounds, the ideal dielectric material was identified. Using this data, recommendations are being made for paints that have an enhanced cooling effect.

Simulation of Nanofluid Flow Through Nozzle of an Inkjet 3D Printer

*Amy Guo[1], Ioanna Katsamba[2], and Xiulin Ruan[2]**
**PI: School of Mechanical Engineering*
[1]California Institute of Technology, [2]Purdue University

SURF ID: 150
11:15 AM - 11:30 AM

Keywords: Additive manufacturing, Inkjet 3D printing, Nanotechnology, Nanofluids, Fluid Mechanics, Finite element method

Nanofluids, nanoparticles suspended in a base fluid, have been gaining popularity in various applications, such as in automotive and electronics manufacturing, due to their superior mechanical, optical and thermal properties. Although prior studies have shown that high nanoparticle concentrations lead to an enhancement of many beneficial properties, it can also result in high nanofluid viscosity values and in aggregation of nanoparticles. This phenomenon can be a challenge regarding the printability of the nanofluid, causing the nozzle, e.g., of an inkjet 3D printer, to clog. This study aimed to simulate nanofluid flow behavior through a nozzle for different material properties and investigate the effect of the viscosity during the additive manufacturing process. The finite element method and COMSOL Multiphysics software were used to successfully characterize the nanofluid flow. The classical conservation of mass and linear momentum equations of a fluid were modified such that a mixture flow of a polymer base with solid nanoparticles was accurately described. Using the created numerical simulation, this study compared the flow behavior for various viscosity values, controlled by the volume fraction of the nanoparticles. The results indicated that viscosity was an important factor for the movement of nanofluid flow. Based on these findings, this study sets the foundation to aid in the improvement of predictive capabilities of nanofluid flow behavior and in the development of more sophisticated AM processes using nanofluids.

SESSION F: Computer Architecture

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Trace-driven Simulation for AMD GPUs Using Accel-Sim

SURF ID: 103
10:00 AM - 10:15 AM

*Weili An, Mahmoud Khairy, and Timothy Rogers**
**PI: School of Electrical and Computer Engineering*
Purdue University

Graphics Processing Units (GPUs) are specialized electronic hardware designed to accelerate graphics computation. Due to the specialized architecture designs, GPUs have also taken significant roles in massive computation workloads like machine learning. To improve GPU design for keeping up the pace of increasing computation requirements, people need accurate simulators to validate their designs. Accel-Sim is a new GPU simulation framework that aims for extensibility via instruction-independent trace-driven functionality, yet it currently only has trace-driven support for the NVIDIA GPU family. This study validates the extensibility of Accel-Sim by adding support for AMD GCN3 GPUs and compared the trace-driven results with those from a reference simulated AMD GPU. Due to the lack of binary instrumentation tools like NVBit from NVIDIA, the traces are generated using a modified version of the MGPUSim simulator which emulates the GCN3 instructions. Additional changes are made to Accel-Sim trace-driven frontend to resolve issues caused by using GPU traces other than those from NVIDIA GPUs. In addition, instruction definition and hardware files are specified according to the AMD GCN3 instruction manual and MGPUSim settings to run the Accel-Sim trace-driven frontend. Data for this study is collected by running GPU benchmarks both in MGPUSim and trace-driven Accel-Sim. This study then compares the simulation result statistics from Accel-Sim and MGPUSim outputs and provides conclusions based on the observation of correlation graphs generated from these two sets of data. The comparison validates the capability of extending Accel-Sim to other GPU microarchitectures besides NVIDIA and enables Accel-Sim to model GCN3-based GPUs.

Keywords: GPGPU, Modeling and Simulation, AMD, Trace-driven

Compression Techniques for Trace Parsing in GPU Simulation

SURF ID: 106
10:15 AM - 10:30 AM

*Emile J. Báez, Mahmoud Khairy, Harikesh Kumar, and Timothy Rogers**
**PI: School of Electrical and Computer Engineering*
Purdue University

In computer architecture, simulating future hardware is essential to the design process of new computer processors. The simulation tools used by leading companies in this industry are not often released to the public. Researchers have taken the task of developing open-source simulators that can accurately model the performance of CPUs and GPUs for different sets of applications. Accel-Sim is a new simulation framework that introduces a frontend to GPU simulators that allows them to simulate the ISA through a trace-driven or execution-driven mode. It provides a great level of flexibility for different machine configurations and a large set of benchmarks to be used for testing of applications. In this project, Accel-Sim is improved upon to allow the trace-driven mode to read and operate from compressed trace files. This trace-driven mode simulates a GPU by converting machine ISA traces into an ISA-independent intermediate representation. Typically, the trace files occupy a considerable amount of disk space and were previously being read directly from the files. With the inclusion of boost C++ libraries, a buffer is created to load in compressed trace files and decompress these when needed. With successful implementation, the disk space used by traces stored is reduced from a total of 3725.76 GB to a compressed size of 159.59 GB which is only 4.28 percent of the original size. Reducing the disk usage for trace-driven mode simulations makes the Accel-Sim more accessible to other researchers and hopefully incentivizes the use of trace parsing for simulations which is typically more accurate.

Keywords: Computer Architecture, Graphics Processing Unit, Instruction Set Architecture

SAFE: Secure Architectural Framework Enhancements

SURF ID: 170
10:30 AM - 10:45 AM

*Frederick J. Kepler[1], John Martinuk[1], David Mayhew[2], and Mark Johnson[1]**
**PI: School of Electrical and Computer Engineering*
[1]Purdue University, [2]Universant Processors, Inc.

Security is a topic of great importance that is applicable to any type of research, especially pertaining to modern computing. In the last couple of years, significant vulnerabilities have been discovered that compromise the security of most modern computer processors. Previous solutions to this problem include software adjustments that only temporarily patch the issue. This study aims to eliminate these vulnerabilities by introducing a slight hardware adjustment to the modern computer processor

Keywords: Security, Computer, Processor, Software, Hardware, Simulation, Secure

architecture. More specifically, we are working together to implement a model in simulation format for a Secure Architectural Framework Enhancements (SAFE) system. This simplified simulation will act as the proof of concept for the SAFE system design. This presentation will showcase my results, being that I have successfully implemented one of the SAFE components and integrated it with others. Also, it will detail the vast security improvements made by our model, and how this model will validate the importance of the SAFE system concept. Based on these improvements we will be able to provide significant conclusions on the current state, and recommendations for the future state of security in computer processing.

Architectural Framework Enhancements (SAFE)

Reducing the Run-Time Memory of Accel-Sim

SURF ID: 174
10:45 AM - 11:00 AM

*Harikesh Kumar, Mahmoud Khairy, and Timothy Rogers**
**PI: School of Electrical and Computer Engineering*
Purdue University

Keywords: GPU, Simulator, run-time memory, workloads, instructions

In modern day computer systems, the GPU is a very important piece of hardware that allows a computer to run heavy and complex programs. Research in the development and improvement of the GPU is constantly underway in the industry by leading technological companies through the usage of GPU simulators. However, these simulators are not open source, or available for use for academic research. The Accelerator Architecture Lab at Purdue have developed an open-source GPU simulator named 'Accel-Sim' to bridge the gap between academia and industry research of GPU architecture. Accel-Sim is one of the more efficient simulators developed in academia. However, it uses a significantly high amount of run-time memory. The goal of this research is to use programming techniques, such as double buffering, to reduce the run-time memory consumption of Accel-Sim. When Accel-Sim simulates a workload, it loads in all the instructions at once and processes them. However, Accel-Sim can only process a certain number of instructions at once while the remaining instructions utilize run-time memory. Therefore, by only loading in a specific number of instructions while keeping track of the remaining instructions, the run-time memory allocation is reduced. This study shows the run-time memory reduction of 6 cutting-edge GPGPU workloads after implementing our double buffering optimization. Several orders of magnitude of memory reduction will certify that our method is an effective way to optimize GPU simulators and allow more complex and larger GPGPU workloads to be supported in Accel-Sim.

Development of Rust Based Low-Level Virtual Machine for AFTx06 chip for development of sample applications

SURF ID: 244
11:00 AM - 11:15 AM

*Nicholas Verastegui, Cole Nelson, John Martinuk, and Mark Johnson**
**PI: School of Electrical and Computer Engineering*
Purdue University

Keywords: LLVM, Machine Learning, ISA, Sparsity,

Microchips are the foundation for a multitude of various electrical devices from smartphones to medical diagnostic devices. These microchips require programs that can translate instructions into machine code to be interpreted by the chip itself. To develop more efficient systems, the programs that translate these instructions need to be able to work faster and run efficiently on their respective chips. Rust is a more reliable and safe programming language compared to other available languages, making it more difficult for programmers to make common mistakes. Rust's memory guarantees such as no buffer overflows or dangling pointers. this makes it an ideal language to be integrated into LLVM systems.

This project aims to develop a Rust-based LLVM that works with the AFTx06 chip developed by Purdue's System-on-Chip team. This LLVM will interface with the chip and bridge the disconnect between hardware and software. This will be accomplished with efficient instruction set architecture (ISA), and software that utilizes sparsity. This research will run sample tests of the LLVM, attempting to demonstrate that it could run basic machine learning tests as well as linear algebra. The successful test runs of sample applications on this chip would indicate the possibility of uploading an operating system onto the chip.

SESSION G: Fluid Modeling & Simulation 1

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Simulations to Better Characterize Ionization Coefficient for Gas Breakdown Calculations

SURF ID: 119
10:00 AM - 10:15 AM

*Cameron Buerke, Haoxuan Wang, Sree Harsha Naropanth Ramamurthy, and Allen Garner**
**PI: School of Nuclear Engineering*
Purdue University

Characterizing gas breakdown for nano- and microscale devices is becoming increasingly important as device sizes continue to shrink its significant contribution to device failure; however, gas breakdown occurs at stronger electric fields for these gap sizes than for macroscale gaps, causing deviations from standard breakdown theories. The standard empirical equation predicting the gas ionization coefficient alpha, which represents the number of ions formed per electron collision with gas per unit length, fails because the breakdown electric fields for these gap sizes fall outside the regime for which alpha was obtained experimentally. This study uses the one-dimensional particle-in-cell code XPDP1 to simulate alpha for numerous pressures and gap distance to extend these empirical equations to include electric fields relevant to microscale and nanoscale experiments. For argon with gap distances above 5 micrometers, alpha is proportional to E/p, where E is electric field and p is pressure, in agreement with standard macroscale scaling laws. For argon with gap distances below 2 micrometers, alpha is proportional to V, where V is the applied voltage. These results demonstrate the importance of appropriately accounting for gap distance and pressure to obtain alpha for these small gaps. Better characterizing alpha is a critical step for developing a comprehensive theory for gas breakdown for any pressure, gap distance, and gas.

Keywords: Ionization Coefficient, Gas Breakdown, Plasma, Dielectric Breakdown

Controlled Ice Nucleation: Effect of Relative Humidity on Nucleation Event

SURF ID: 221
10:15 AM - 10:30 AM

*Josiah L. Rockey, Andrew Strongrichb, and Alina Alexeenko**
**PI: Davidson School of Chemical Engineering*
Purdue University

Lyophilization, or freeze-drying, is used in the pharmaceutical manufacturing process to increase product stability and shelf life. During the freezing step of a typical cycle, the nucleation event is seemingly random among the vials, leading to extensive drying times and vial inconsistency that can significantly decrease production efficiency. To combat this, Controlled Ice Nucleation (CIN) methods have been developed to optimize the lyophilization process. However, scaling these methods up to manufacturing scale is difficult because although the process is known, the cause of the nucleation event in the solution itself is largely unknown for many forms of CIN. This study aimed to determine the effects of relative humidity on the nucleation event during rapid depressurization, a promising form of CIN. Trials of rapid depressurization were performed over a range of chamber pressures. At critical pressures, relative humidity was modulated using a blower attached to a heated water can within the chamber. This study compares the extent of nucleation among the batch of vials at varying humidity levels. Although relative humidity in the chamber was modulated, there was no observed effect on nucleation for most trails and decreased the amount of nucleation for the final trial. Although the goal was to modulate humidity, the hot air blown throughout the chamber could've increased solution temperature, hindering nucleation. Combining these results with slow motion video of the nucleation event, it can be concluded that the key to the nucleation event during rapid depressurization is in the vial's headspace (gas phase).

Keywords: Lyophilization, Controlled Nucleation, Rapid Depressurization, Relative Humidity, Nanotechnology

Development of Continuous Flow Synthesis of Active Pharmaceutical Ingredient in Shortage–Step One

SURF ID: 184
10:30 AM - 10:45 AM

*Corryn Lytle, Shruti Biyani, and David Thompson**
**PI: Department of Chemistry*
Purdue University

Patients on respirators are unable to receive essential medicines because the hospitals are facing a shortage—a situation that has exacerbated during the time of the Coronavirus pandemic. Lorazepam, classified as an essential medicine, is a benzodiazepine used as a relaxant for patients before an operation or medical treatment. The shortage is due to increased need and transfer of the process offshore leading to supply-chain disruption. To address this problem, we are creating a continuous telescoped flow here in the States that will synthesize the active pharmaceutical ingredients (API) with high purity. The synthesis of Lorazepam comprises of five steps, and this summer our research efforts focused on developing the first step of the synthesis in flow. Our strategy incorporated performing

Keywords: Lorazepam, flow chemistry, Chemtrix, flow synthesis, benzodiazepines, sedative shortage, APIs, medical science and technology

solubility tests to identify the most suitable solvents for our starting material and product to prevent the clog in the microchannels while also minimizing the SN2 by-product and maximizing the desired product. We utilized Chemtrix reactor system to perform the flow experiment with a 22 full factorial design strategy with three different solvents (2-methyltetrahydrofuran, toluene, N-methyl-2-pyrrolidone). We used ultra-high performance liquid chromatography (UPLC) to monitor the product profile. Our results indicate that 2-methyltetrahydrofuran produced the highest purity, 74 percent, in comparison to toluene/N-methyl-2-pyrrolidone and pure toluene, 2.83 percent and 0.73 percent respectively. We experimented further with time and temperature, where 10 minutes at 40 degrees Celsius gave 95 percent purity. From these results, we decided to use 2-methyltetrahydrofuran as our solvent at 10 minutes and 40 degrees Celsius.

Vortex Bursting Under Dynamic Adjustment of Angle of Attack

SURF ID: 199
10:45 AM - 11:00 AM

*Chandler James Moy, Tanbo Zhou, Paul Bevilaqua, Alexey Shashurin, Aditya Anilkumar, and Sally Bane**
**PI: School of Aeronautics and Astronautics*
Purdue University

Keywords: Delta wing, Vortex, Bursting, Breakdown, Dynamic, Prevent, Trailing Edge, Water Tunnel, Upstream, Downstream

Delta wings are widely used on supersonic aircraft. However, the lift curve slope of delta wings is low, so delta wing aircraft must approach landing at high angles of attack, limiting pilot visibility of the runway. Although the lift produced by a delta wing is increased by the formation of leading-edge vortices above the wing, the benefit is limited by vortex bursting which occurs when the vortices lose their coherent structure. Preventing bursting will raise the lift curve slope which will allow aircraft to land at lower angles of attack. To investigate the underlying mechanism(s) of vortex bursting, experiments were performed in a water tunnel. We hypothesized that the vortex burst point could be prevented from moving upstream by disturbing the vortex flow. The test article was a 60-degree swept back delta wing. We found that a water jet placed at the trailing edge prevented the vortex burst point from moving upstream. These experiments provide evidence that the vortex bursting is not due to flow instabilities but is analogous to a shock wave. To measure the benefit of arresting the burst point motion, a second set of experiments were performed in a wind tunnel. A 65-degree swept back delta wing model with a 100-psi air jet at the trailing edge was tested. By preventing vortex bursting, the jet of air increased the lift by at least 20% at all angles of attack. The knowledge gained in this experiment will be important for increasing the safety of landing supersonic aircraft.

Mathematical Model Development for Superstructure Optimization of Shale Gas Processing Systems

SURF ID: 223
11:00 AM - 11:15 AM

*Yan M. Saltar[1], Kanishka Ghosh[2], Alexander Dowling[2], Maeve Drummond[3]**
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Keywords: process design, superstructure optimization, techno-economic analysis, shale gas, hydrocarbon conversion

In recent years, there has been a surge in the interest for innovative renewable energy technologies. Even though many advances have been made towards renewable energy generation process development, hydrocarbon-based technology is still expected to play a vital role in global fuel consumption for many years to come. It has been shown in literature that the development of novel modular shale gas transformation processes helps realize the opportunities presented by the shale gas boom. To find the most efficient and economically viable hydrocarbon conversion technologies, many technology alternatives, feedstock, and products need to be evaluated. In this work, we develop mathematical models to describe the proposed natural gas processing systems based on process flowsheet simulations generated by Thrust 4 collaborators. Using the library of mathematical models, we will develop a superstructure optimization framework to rapidly evaluate and rank the design alternatives based on process efficiency, cost-effectiveness, and environmental considerations. Sensitivity analysis shows that changes in process configuration such as extent of separation for specific components significantly affects final product flow rates.

Lyophilization Post-Processing Data Software

SURF ID: 156
11:15 AM - 11:30 AM

*Hallie Renee Harrison, Zachary Mora, Petr Kazarin, Andrew Strongrich, and Alina Alexeenko**
**PI: Davidson School of Chemical Engineering*
Purdue University

Keywords: Modeling and Simulation, Python, Data

Members of the LyoHub lab dedicated significant amounts of their research time to post-processing experimental data using handwritten Python scripts, MATLAB scripts, Excel, and manual interpretation. In addition, the LyoHub group lacked uniformity in these post-processing data

methods. The purpose of this project was to design a Python software that has post-processing data capabilities for large lyophilization data files. To develop the code, existing Python libraries were researched. Feedback was gathered from lab members and then accounted for in the code development process. This allowed the software to include the useful functionalities that lab members agreed to be ideal for data analysis. For example, Pandas is an existing analytical library that is applied in the code because it has a variety of instruments for data analysis and manipulation. Matplotlib was chosen as the plotting library because it outputs high-quality graphics, is compatible with most operating systems, and has an interactive mode. Tkinter is a Python interface that is used to construct graphical user interfaces (GUIs), which is the visual tool that allows users to easily interact with the data and software. The final deliverable will be posted onto the LyoHub members' website allowing users to customize and build plots using data from any lyophilization run. This advanced tool for data post-processing created consistency because all experimental data analysis can be performed utilizing the same software regardless of lyophilizer type.

Analysis, Pandas, Matplotlib, Tkinter, Lyophilization

Day 1 | Afternoon Presentations

July 29th, 2:00 PM – 3:30 PM EDT

SESSION A: Composite Materials & Alloys

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Quantifying the Springback in Polymer Composite Preforms Using a Novel Forming Technique

SURF ID: 136
2:00 PM - 2:15 PM

*Carson M. Denoo, Jessica Lavorata, Teal Dowd, and Jan-Anders Mansson**
**PI: School of Materials Engineering*
Purdue University

Keywords: Springback, Polymer Composites, Hybrid Manufacturing, Thermoplastic Preforms

Hybrid-molded thermoplastic composites introduce local continuous fiber reinforcement to injection molding. By optimizing material properties, these parts are capable of effectively emulating metallic components in a cost-effective manner. The development of repeatable, robust, and high-rate processing methods of continuous preforms is an evolving research area that is essential to progress the applications of this technology. Processing techniques such as tube bending, roll forming, and other variations of metal forming have all been well-established and used throughout industry. However, the transfer of these technologies and methods have yet to be fully adopted in manufacturing polymer composites. One of the largest side effects that composite processing must account for is springback. To determine how springback affects the processing of continuous preforms, testing was done on samples at various temperatures and heating times to create a relationship between the preform's theoretical and actual bend radius and guide production of hybrid molded composites. A computer vision program was used to identify and record the springback during and after forming. Results with this program indicated that springback can be mitigated with certain processing parameters, but the ability to anticipate the result within a degree of the expected is not feasible given the current design of the machine. Rigid samples were consistently produced at 60-degree angles, but quantitatively analyzing this rigidity has yet to be determined. Consolidation around the bend and mitigation in springback correlate with robust samples, which can be used to further this research in the future.

Shear Angle and Other Methods of Analysis for the Fabric Draping Experiment

SURF ID: 160
2:15 PM - 2:30 PM

*Karina Hollis-Brau, Olivia McLaurin, Qingxuan Wei, and Dianyun Zhang**
**PI: School of Aeronautics and Astronautics*
Purdue University

Keywords: Composite Materials, Structural Analysis, Shear Angle Analysis

When composite materials are made to form to complex geometry, individual fibers within the material can deform as their orientation shifts in relation to one another. The fabric draping experiment is often used to study the deformation of fibers, done by taking a sheet of material and conforming it to a mold. In order to make analysis easier, we sought to optimize the fabric draping experiment by determining the best methods to perform it. For the purposes of the experiment, we utilized dry fabric, which mimics the behavior of composite matrix materials. The fabric was conformed to an L-shaped mold as a part of the fabric draping experiment, and a MATLAB code was created that could take an image of woven material as input and output the shear angle between fabric tows. The use of the L-shape mold in the experiment allows for multiple avenues of analysis with flat and curved surfaces and sharp edges. The fabric draping experiment and shear angle analysis can be used in many applications, especially for modeling composite materials. Having a more efficient fabric draping experiment provides an easy tool to comprehend how well a composite material can be implemented in a given situation.

An Automated Approach to Measuring Shear in Composite fabrics

SURF ID: 192
2:30 PM - 2:45 PM

*Olivia McLaurin, Karina Hollis-Brau, Qingxuan Wei, and Dianyun Zhang**
**PI: School of Aeronautics and Astronautics*
Purdue University

Keywords: Local shear angle, composite fabric, optical analysis, automated system, fabric draping

Conforming composite fabrics to 3D molds is becoming more common in industry and there is increased need for a quick way of determining the behavior of deformed fabrics. The behavior that this report focuses on is shear, which can be determined by calculating the shear angle between the intersecting threads (tows) of a fabric. In this report, research was done to create an automated method to calculate the local shear angle of deformed composite fabrics via optical analysis. This method works to specifically make the process of finding the shear angle timely, reliable, and accurate, without the use of complex imaging systems. Through a fabric drape test, a stenciled fabric was deformed and photographed in its deformed state. The pictures were then analyzed using a MATLAB algorithm to plot the intersections of the grid pattern. After the intersections are identified, the grid pattern is recreated digitally by connecting the intersections and the shear angle is found through mathematical calculation. Manual measurements of the shear angles were gathered using ImageJ to validate the accuracy of the results. It has been found that the algorithm can accurately identify the intersections of the grid-pattern on the sample with only two human inputs and minimal mistakes. The shear angle measurements proved to be accurate in relation to their manually gathered counterparts.

Microstructural Characterization of Spark Plasma Sintered Al-SiC-Graphite by 3D X-ray Tomography

SURF ID: 205
2:45 PM - 3:00 PM

*Caitlin A. O'Brien, Hamidreza Torbati-Sarraf, and Nikhilesh Chawla**
**PI: School of Materials Engineering*
Purdue University

Keywords: Materials Processing and Characterization, Segmentation, X-ray Tomography, Composite Materials and Alloys

In today's highly innovative and competitive aerospace and automotive industries, there is a constant demand to develop high performance composite materials and alloys. To maximize efficiency, lightweight materials with high wear and heat resistance are desired. The novel process of spark plasma sintering provides reduced processing times. Little is known about the processing and properties of materials fabricated by this new route. In this study, we examined the microstructure of Al-SiC-Graphite processed through spark plasma sintering, to obtain an understanding of material processing and characterization. X-ray tomography was used to study the microstructure of the material nondestructively and in 3D. Conducting image segmentation in Al-SiC is challenging because the two phases have very similar densities. We developed a novel and robust approach, based on image segmentation algorithms to analyze these data. Once the 3D rendering was obtained, a detailed quantitative study of the microstructure was conducted. The internal structure, including particle size, particle shape, and inclusion amounts of Al-SiC-Graphite were extracted from the analysis. Defects were found in the microstructure, including inclusions and porosity in small amounts. The presence of minimal defects is encouraging for the use of spark plasma sintering for composites. The implications for using our approach to analyze other systems and the understanding obtained from the microstructural analysis for designing new composites will be discussed.

Design and Analysis of Four-Point Bending Fixture for Fatigue Specimen

SURF ID: 209
3:00 PM - 3:15 PM

*Michael R. Pardo, Krzysztof Stopka, and Michael Sangid**
**PI: School of Aeronautics and Astronautics*
Purdue University

Keywords: Alloy, fatigue crack, crack propagation, corrosion

Aluminum alloys that are used in aerospace applications are frequently subject to a combination of corrosion and applied force, both of which can individually cause the material to fail. Currently, there has been little research done on the propagation of a fatigue crack and failure characteristics in aluminum alloys under a combined static tensile load and corrosion. High energy x-ray microscopy and micro-contrast tomography can be used to characterize crack propagation and evolution of microstructure under these conditions. This requires a test fixture that can apply a static tensile load to a specimen while allowing a relatively wide field of view for incoming x-rays to penetrate the material and a corrosion chamber to submerge the gauge section of the specimen in a corrosive medium. In this work, a four-point bending test fixture was designed for use at a synchrotron facility. A finite element analysis (FEA) model was developed to determine the necessary displacement applied in the four-point bend setup to achieve a desired stress and strain in the specimen gauge section. Several constraints of the test fixture are discussed, including the incoming x-ray field of view,

mechanical stability of the four-point bend setup, interference with other equipment at the synchrotron beamline, test fixture manufacturability, flow of the corrosive medium into and out of the corrosion chamber, and seals around the corrosion chamber to prevent leakage. The proposed fixture can be used to elucidate the mechanisms of crack propagation under a combined tensile load and corrosive environment, and may help guide component design guidelines for manufacturers.

Design and Validation of Manufacturing Method for Discontinuous Prepreg Fibers with Controlled Orientation

SURF ID: 230
3:15 PM - 3:30 PM

*Jennifer Short, Teal Dowd, Jessica Lavorata, and Jan-Anders Mansson**
**PI: School of Materials Engineering*
Purdue University

Keywords: Composite Materials and Alloys, Polymer Composites, Long Fiber Thermoplastic, Long Glass Fiber, Fiber Alignment

Long glass fibers (LGF) are a compromise between continuous fibers and short chopped fibers, as they allow complex geometries to be created while still allowing for some fiber alignment. The focus of this paper is the Preform Oriented Fiber Machine (POFM), which utilizes a pellet consisting of 50% (by weight) LGF impregnated with polypropylene (PP) to create layered preforms which were then compression molded into a plate, dog-bone samples waterjet, and tested using a load frame to determine tensile strength and stiffness. It was found that the aligned orientation of the pellets in a unidirectional layup have a significantly higher tensile strength than the randomly oriented pellets. A two-sample T-test confirmed the statistical significance in the increased strength, two-sample t(dt) = 16.14, p = 0.01. A method to create an even distribution of pellets across the plate was devised using a modified plinko set-up, wherein iteratively each layer the stream of pellets is split into two streams, thus creating an even distribution at the bottom. When tested and compared to no distribution apparatus, the standard deviation of mass deposited decreased from 3.52g to 0.65g. The results from these tests suggest that the POFM is capable of improving mechanical properties through controlling orientation, and thus being able to design for strength in the loading direction, allowing for lower weight and cost of parts.

SESSION B: Genetics

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Determining the Role of MicroRNAs in Epithelioid Hemangioendothelioma

SURF ID: 157
2:00 PM - 2:15 PM

*Samuel L. Hartzler, Ant Murphy, Annaleigh Powell-Benton, and Jason Hanna**
**PI: Department of Biological Sciences-Biology*
Purdue University

Keywords: Epithelioid Hemangioendothelioma, MicroRNAs, Cellular Biology

Epithelioid hemangioendothelioma (EHE) is an understudied vascular cancer with a low survival rate. Previous studies have identified the abnormal gene fusions TAZ-CAMTA1 and YAP1-TFE3 as driver mutations of EHE. In addition, YAP1 and TAZ are implicated as regulators of microRNA processing. MicroRNAs are small noncoding RNAs which regulate gene expression and are often involved in cancer-associated pathways. Thus, microRNAs provide important potential therapeutic targets for developing treatments for EHE. This study sought to discover if specific microRNAs are dysregulated in the presence of the fusion proteins. To that end, mouse and human cell lines expressing the fusion constructs were generated. Functional expression of the constructs on the RNA and protein level was validated. The fusion cell lines displayed divergent morphology and cell viability. Based on these results, the project was successful in generating models for EHE that can be used in future research in investigating EHE pathogenesis. These results will be used to identify if microRNA dysregulation is associated with EHE. In addition, specific microRNAs that are dysregulated in EHE will be identified. This will enable further exploration into how the downregulation of these specific microRNAs leads to the generation of the EHE phenotype, leading to the development of better therapeutic treatments for EHE that result in increased patient survival.

Investigating Roles of Fumarase in Response to Double-Stranded DNA Breaks

SURF ID: 166
2:15 PM - 2:30 PM

*Avery Ellen Hurst, Ronard Kwizera, and Ann Kirchamaier**
**PI: Department of Biochemistry*
Purdue University

Keywords: Genetics, Fumarase, Fum1, DNA Damage, Double-Stranded DNA Break Repair

Each day a single eukaryotic cell experiences an average of 1,000 DNA lesions, the worst being Double-Stranded DNA Breaks (DSBs). If unrepaired or repaired incorrectly, DSBs can cause mutations leading to the onset and progression of diseases like cancer. To counteract this problem, cells have developed DSB repair mechanisms, including homologous recombination (HR) which utilizes a template strand to repair the damage, and non-homologous end-joining (NHEJ) which occurs throughout the cell cycle and does not require a template strand and is therefore error-prone. The fumarase enzyme, predominantly detected in the mitochondria and the cytosol, translocates to the nucleus in response to DNA damage and can accumulate at sites of DSBs. Defects in expression of fumarase lead to impaired DSB repair by HR and NHEJ. The role of fumarase in DSB repair is poorly understood; signaling mechanisms and the fumarase-protein interactions that are critical for either translocation of fumarase, recruitment of fumarase, or of DNA repair machinery to the site of DSBs remain largely unknown. This study applies the biotinylation activity of the biotinylase miniTurbo-ID to covalently attach biotin to interacting proteins. To identify the proteins interacting with fumarase, a construct encoding a regulatable fusion protein containing yeast fumarase, Fum1p, and miniTurbo-ID were transformed into a series of yeast strains and immunoblotting experiments were performed to confirm regulatable expression of miniTurbo-ID-based constructs and their biotinylation activity in the developed strains. Our results validate the fumarase miniTurbo-ID fusion protein system to enable identification of fumarase-interacting factors important for responses to DNA damage.

Novel Peptides in Polymer-Mediated Gene Delivery for Targeted Treatment of Cancer Cells

SURF ID: 175
2:30 PM - 2:45 PM

*Zachary E. Lamantia[1], Shreya Kumar[1], Le Zhou[2], Todd Emrick[2], Marxa Figueiredo[1]**
**PI: Department of Basic Medical Sciences*
[1]Purdue University, [2]Massachusetts-Amherst

Keywords: Medical Science and Technology, Gene Therapy, Polymer Engineering, Cellular Biology, Cancer Therapy

Cancer is a disease that leaves options for treatment scarce, and usual treatment options like chemotherapy and radiotherapy are taxing on cancer patients. There exists a need for more effective cancer therapeutics that limit side effects to the patient. One promising method is polymer-mediated gene delivery (PMGD), which delivers genes to cancer cells that cause them to undergo cell death. Polymers with branching peptides are complexed with DNA to form polyplexes, which facilitate cellular uptake of said DNA. It was hypothesized that attaching peptides targeting IL-6R, a receptor that is overexpressed on cancer cells, would increase DNA uptake. Additionally, it was hypothesized that a peptide mimic of relaxin (B7-33) would partially degrade the extracellular matrix (ECM) to allow

for increased distribution of the polyplex. Different cancer cells were exposed to this polyplex which contained a gene for the green fluorescent protein. DNA uptake was measured by counting the number of green cells over time using the Incucyte, a live-cell imaging machine. Toxicity of each treatment was measured by the percentage area occupied by cells. Moreover, B7-33's effect on pro-ECM genes is being investigated. It was determined that SKBR3, a breast cancer line, was optimal for PMGD. However, the targeting peptides did not appear to effectively target IL-6R. Based on the results, modified targeting peptides must be designed to increase DNA uptake. Furthermore, we must optimize concentrations of B7-33 to further test its potential in degrading the ECM. These findings open the door for creative applications of polymer engineering to PMGD.

Characterization of the DNA Cleavage Activity of the Torulaspora Delbrueckii Weird HO Endonuclease

SURF ID: 207
2:45 PM - 3:00 PM

*Tara M. Paarlberg, Sara York, and Frederick Gimble**
**PI: Department of Biochemistry*
Purdue University

Keywords: Homing endonuclease, yeast mating type switching, genetics, protein and DNA interactions

Homing endonucleases are mobile genetic elements that spread themselves throughout a population by a process called homing. In yeast, homing is initiated by a homing endonuclease called VDE that makes specific cuts in DNA. A related yeast endonuclease called HO does not initiate homing, but instead cuts yeast DNA to allow "a" haploids to switch to "alpha" haploids, or vice versa. How did HO endonuclease evolve from VDE? The answer could come from an endonuclease called Weird HO (WHO), recently discovered in the yeast species Torulaspora delbrueckii. The WHO endonuclease also initiates homing, but it is more related to HO than to VDE. To characterize WHO, the protein needed to be purified and the recognition sequence needed to be determined. To create a substrate for the DNA cleavage activity of WHO protein the suspected target sequence of WHO was cloned into pBluescriptII plasmids. WHO protein with an affinity tag was expressed in bacteria and the protein was purified/enriched using immobilized metal affinity chromatography (IMAC). A protein gel showed a protein band corresponding to the expected molecular weight of WHO. Antibodies were used to detect proteins that had affinity tags, and a protein of the expected size was detected in the lysed fraction and in the insoluble fraction, but not in any of the soluble fraction. This suggests the folded protein may not bind antibodies. No activity was observed in DNA cleavage assays using the plasmid substrate. Several different strategies will be used to increase the solubility of the folded protein.

Investigating the Cap Helix of STE14 via Mutagenesis

SURF ID: 218
3:00 PM - 3:15 PM

*Karthik Raja Ravichandran, Akansha Maheshwari, Ariana Cardillo, and Christine Hrycyna**
**PI: Department of Chemistry and Center for Cancer Research*
Purdue University

Keywords: CaaX proteins, hIcmt, Ste14, In-Vitro Methyltransferase Assay

CaaX proteins are proteins which have a CaaX motif located at the end of the C-terminal. This structure consists of amino acids where the "C" is a cysteine residue, "a" are aliphatic residues, and "X" represents one of several amino acids. The modification of CaaX proteins in the body typically involve the addition of either a 15 or 20 carbon functional group followed by endoproteolysis and methylation. The gene STE14 is responsible for this process in Yeast, while hIcmt is responsible in humans. CaaX proteins are involved in many functions including cellular division. RAS is one of the most commonly studied CaaX proteins and is involved in the MAPK signal transduction pathway which causes cell proliferation, and this depends on RAS functioning properly and mutations can result in disorders and carcinomas. A glutamic acid in the cap-helix region of STE14 was mutated to alanine (E227A) to determine if the cap helix plays a role in facilitating the modification of CaaX proteins.

Investigation of Dog Coat Color Variants in Novel Cream Boxers

SURF ID: 229
3:15 PM - 3:30 PM

*Regan E. Sherman, Shawna Cook, and Kari Ekenstedt**
**PI: Department of Basic Medical Sciences*
Purdue University

Keywords: Genetics, Canine, MFSD12, KITLG, Dilution

The Boxer breed standard allows a fawn or brindle base with white markings and/or a black mask. A recent litter of pure-bred Boxer puppies unexpectedly contained three cream-coated dogs, which is a novel color, not seen previously in the breed. Therefore, in this study a candidate gene approach was utilized, under the hypothesis that a new mutation may be present in one of these genes in the cream coated Boxers. Primers were designed to sequence the introns and exons of MFSD12 and the exons of KITLG. DNA from a cream Boxer, the litter sire (brindle coat), and an unrelated, normal-colored control Boxer were subjected to PCR and Sanger sequenced. The cream Boxer showed no notable mutation(s) in either the MFSD12 or KITLG data. This suggests that the cream Boxers may possess a variant in a gene influencing color dilution that has not yet been described in dogs, or that they have a variant in one or a combination of three new candidate loci that have only very recently been associated with coat-color dilution in dogs. Future directions include designing primers to genotype the three newly identified candidate loci, and whole genome sequencing. The latter would allow capture of all mutations across the cream dog('s) entire genome, representing the best method of detecting mutations in new dilution gene(s).

SESSION C: Biomedical Sensing & Imaging

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Adapting a Lambda Phage DNA Calibration Technique for Routine Use with Magnetic Tweezers

SURF ID: 123
2:00 PM - 2:15 PM

*Bianca C. Caminada and Kenneth Ritchie**
**PI: Department of Physics and Astronomy*
Purdue University

Proteins, long chains of amino acids, are a universal example of how the assembly of intricate biological structures is vital to the proper functioning of living systems. Some proteins are involved in gene expression processes, and an accumulation of misfolding processes over time has been shown to be the cause for some neurodegenerative disorders, while others are key for the immune system. Thus, there is a need for understanding such biopolymers and the processes through which they assemble in complex cell environments. In order to understand and map the energy landscape of protein, the biopolymer is held under tension by a magnetic tweezers set-up. The goal of the present work is to verify data previously collected by the Ritchie Lab by executing an independent calibration of the system, utilizing a well-known technique with lambda phage DNA. A flow cell was prepared using biotinylated DNA (48k base pairs), streptavidin-coated glass, and paramagnetic beads, such that one end of of the DNA will be tethered to the glass, while the other will adhere to a bead and be free-flowing. The flow cell will then be put under the same magnet, and the height and transverse movement of the tether will be measured. Then, a force calibration curve will be made to verify the previously collected data. Furthermore, we hope to adopt these techniques to a faster procedure that can be executed routinely before any data collection with the magnetic tweezers.

Keywords: Magnetic tweezers, Lambda DNA, Protein, Energy Landscape, Calibration

Directed Enzyme Deposition with Poly(o-aminophenol) onto Platinum Black Microelectrode Arrays for Multi-Analyte Amperometric Biosensors

SURF ID: 129
2:15 PM - 2:30 PM

*Zein Chehab, James K. Nolan, and Hyowon (Hugh) Lee**
**PI: Weldon School of Biomedical Engineering*
Purdue University

Glucose, lactate, and neurotransmitters, such as glutamate and GABA, are important biomarkers for investigating metabolic and neurological functions with potential drug discovery implications. Biosensors have previously been designed to simultaneously measure the concentrations of glucose, lactate, and neurotransmitters in the body. However, many of these biosensors require laborious and tedious fabrication techniques and are not easily tunable. The majority of the multi-analyte biosensor concepts have not been tested in-vivo, which is required to optimize their performance. Here, we developed a facile fabrication method towards the development of a tunable biosensor for multi-analyte sensing in vivo. To demonstrate this new technique, we designed, fabricated, and tested an electropolymerized biosensor array for measuring glucose and lactate simultaneously. First, we created the biosensors using platinum black microelectrodes, which enhances the sensitivity and adhesion of the electroactive polymer to the electrodes. Second, we used cyclic voltammetry to electropolymerize o-aminophenol and either glucose oxidase or lactate oxidase onto specific electrodes. Polymerization entraps enzymes in the monomer solution near the selected electrode. Therefore, this technique offers spatial control of the functionalization site and the amount of enzyme. Poly(o-aminophenol) also functions as a permselective membrane that reduces interference. Finally, we calibrated the device simultaneously to glucose and lactate. Our results showed that the electrodes had good sensitivity and linear ranges, sub-second response times, and selectivity to glucose or lactate with low crosstalk. This technique is scalable beyond the two analytes prototyped and has a high potential for future in-vivo and lab-on-a-chip applications.

Keywords: Medical science and technology, Biosensors, Multi-analyte sensing, Glucose, Lactate

Studying the role of Transcription Factors Clock and Cycle in Fruit Fly Photoreceptor Neurons

SURF ID: 188
2:30 PM - 2:45 PM

*Makayla N. Marlin, Juan Jauregui, and Vikki Weake**
**PI: Department of Biochemistry*
Purdue University

Daily rhythms, from mammals to fruit flies, are controlled by molecular mechanisms known as the circadian clock. The circadian clock is a feedback loop that consists of transcription factors, two of these are Clock and Cycle, which form a heterodimer to regulate gene expression. Interestingly, disruption of the circadian clock has been associated with aging and neurodegeneration. Preliminary data from the Weake lab shows that disruption of the Clock-Cycle heterodimer in Drosophila

Keywords: Drosophila melanogaster, transcription factors (TF), Clock (Clk), Cycle (Cyc), photoreceptors, circadian clock

melanogaster photoreceptor neurons leads to progressive light-dependent retinal degeneration. These previous studies used the expression of the dominant-negative (DN) versions of Clock and Cycle to study transcription in adult fly photoreceptors. Dominant-negative versions lack the DNA binding domains so they form the heterocomplex but do not activate transcription. When we expressed the dominant-negative transgenes we observed photoreceptor degeneration at days 5 and 10, but not day 2. My study aims to establish if the DN versions are being transcribed at a timepoint that precedes retinal degeneration (day 2). To test this, we extracted RNA from 2-day old flies that express the DN and performed quantitative PCR to determine the transcript levels. A negative control used was flies that do not express the DN transgene. We detected expression of the Clock dominant-negative transgene from qPCR data. Therefore, we conclude that expression of the DN precedes retinal degeneration. These studies suggest that regulation of circadian clock transcription factors contribute to age-related retinal degeneration in fruit flies.

Designing Folate-Targeted Conjugates to Accelerate Kidney Clearance

SURF ID: 164
2:45 PM - 3:00 PM

*Roxanne Huff, Spencer Lindeman, Da Sol Jung, and Philip Low**
**PI: Department of Chemistry*
Purdue University

Folate-targeted drug therapies have been shown to successfully deliver payloads to diseased cells like cancer while avoiding nearby healthy cells. These payloads can be tailored for specific purposes such as imaging or therapy, making them a valuable research tool. The reason why folate-targeted drug therapies have not made it to human clinical trials is from high retention of folate molecules in the kidneys. This affects the ability to see how much of the compound internalizes into diseased cells and increase the risk for kidney toxicity. Previous studies show that a specific sequence of amino acids will be cleaved by brush border membrane enzymes in the intestines. By attaching them to the drug molecule, the folate component will be flushed from the body while the drug internalizes into the cell and reduces the amount of folate signaling in the kidneys. Several versions of folate-targeted drug imaging compounds were tested in tumor-bearing mice through injection via tail-vein and imaged at various time points of the course of a week. Over the course of a full week, the full body scans show a significant reduction of signaling in the kidneys with an increase of signaling in the tumors. The addition of the brush border membrane enzyme-cleavable linker sequence proves to be a valuable addition to the structure of folate-targeted drug compounds. Future studies are planned to test other variations of amino acid sequences and protein binders to further increase the effectiveness of the folate-targeted drug therapies.

Keywords: Medical Science and Technology, Cellular Biology, Targeted-Drug Therapy, Folate, Brush Border Membrane-Enzyme Cleavable Linkers.

A Semi-Automatic Pipeline for the Characterization of Synapses

SURF ID: 235
3:00 PM - 3:15 PM

*Hailey M. Szadowski, Junkai Xie, and Chongli Yuan**
**PI: Davidson School of Chemical Engineering*
Purdue University

The connectivity, morphology, and protein composition of a synapse are closely related to their ability to transmit, process, and store information. Abnormal synaptic characteristics are commonly observed in instances of neurological and neurodevelopmental diseases, implying that synaptic characteristics are correlated with their onset. Therefore, studying the diversity of synapse structures and arrangement is highly applicable to the study of neurological diseases, such as Alzheimer's and Parkinson's disease. Studies of synaptic diversity are restricted by the small size, large number, and complex arrangement of synapses within a neuronal circuit, which makes the quantification and characterization of synaptic puncta difficult. This research focused on using existing methods of synaptic analysis to develop a pipeline that can be applied to characterize the morphology of synapses within neuronal networks. We tested several synapse quantification programs using fluorescent images of neuronal culture derived from human induced pluripotent stem cells (iPSC) and mice brain slices. A pipeline consisting of immunostaining, fluorescence microscopy, and the use of an unsupervised synapse quantification program was found to be the most optimal in characterizing synapses both within culture and tissue slices. By determining the optimal threshold, we established a robust approach to efficiently quantify and characterize synapses.

Keywords: Synapse, Image Analysis, Immunofluorescence, Neuron, Synapse Quantification, Synapse Morphology

Glycosylation Reactions Utilizing Tetrafluoropyridyl Donors

*Dalton D. Polley, Zhongdong Sun, and Abram Axelrod**
**PI: Department of Chemistry*
Purdue University

SURF ID: 214
3:15 PM - 3:30 PM

Carbohydrates play significant roles in the fields of oncology and immunology and have become an intense area of recent research. Oligosaccharides are involved in innumerable biological processes, can modulate the immune system, and are found in cancer antigens. Currently, the only way to prepare homogenous oligosaccharides is through chemical synthesis, which has the ability to prepare various cancer antigens for biological study and vaccine development. Although carbohydrate synthesis has matured significantly over the last 50 years, there is need for the development of new, selective glycosylation reactions to enable practical access to important glycans. This study aimed to build upon previous research of pyridyl glycosyl donors using newly synthesized tetrafluoropyridyl donors in glycosylation reactions. Small, predetermined amounts of tetrafluoropyridyl donor, alongside a protected methyl-glucopyranoside acceptor, is prepared for the glycosylation reactions. Tested reaction conditions include the solvent used, catalyst and temperature. Reaction progress is tracked and analyzed using thin-layer chromatography (TLC). Reactions are allowed to run for up to twenty-four hours. Crude reaction mixtures are purified using flash chromatography and analyzed using proton NMR spectroscopy. This study compares results from previous research and draws conclusions based on their stereoselective and glycosyl donor abilities.

Keywords: Glycosylation, carbohydrates, donors, substitution, stereoselectivity

SESSION D: Fluid Modeling & Simulation 2

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Permeability Characterization and Machine Learning

SURF ID: 190
2:00 PM - 2:15 PM

*Noah D. Martin, Ryan Enos, and Dianyun Zhang**
**PI: School of Aeronautics and Astronautics*
Purdue University

The fluid permeability of fiber preforms is a vital material characterization parameter required to model resin infusion in Liquid Composite Molding (LCM) processes. More specifically, permeability is required to determine the time necessary to force a liquid resin through a fibrous preform which, if not given the proper time, can affect the composite material's quality and properties. A significant amount of research involving permeability prediction of porous media through experimentation has found that human error largely contributes to high amounts of inaccuracy and variability. In addition, the current prevailing experimental methods for determining permeability involve complex procedures and are very time consuming and costly. Further research has found that Computational Fluid Dynamics (CFD) simulations can more accurately predict the permeability of materials numerically, however this also comes at a cost of large computational expense. Thus, the purpose of this study is to experimentally obtain fabric permeabilities for process modeling and to investigate the application of machine-learning based models as a faster and more cost-effective approach to predicting the permeability of materials for LCM processes. In addition, methods are discussed for obtaining the experimental data for use in the training of machine-learning models. Finally, recommendations are made for experiment methods and data collection as well as for the basic architecture of a machine-learning model.

Keywords: Machine Learning, Permeability, Material Characterization, Liquid Composite Moulding (LCM), Computational Fluid Dynamics (CFD).

Stable Static Liquid Positions in Toroidal Propellant Tanks

SURF ID: 243
2:15 PM - 2:30 PM

*Don-Terry Veal, Jr.[1] and Steven Collicott[2]**
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[1]Morgan State University, [2]Purdue University

Without the influence of gravity, trivial phenomena can become immensely complex. A grand oversight in the study of space travel is rocket fuel's static positioning while experiencing microgravity. Precision is sacrificed when overlooking such a factor and can offset a spacecraft's guidance, navigation, and control. Tank designs, and frankly spacecrafts, cannot be optimized until total comprehension of all variables is accounted for. Using the Surface Evolver software to model the fuel and its tank provides a deeper understanding of how the stable state of the fuel will sit while in orbit. Numerically modelling a tank and its fuel grants a precise and accurate measurement of surface energy for applications in spacecraft design. The essential variables to investigate are the liquid fuel's volume and contact angle to then conclude which tank topology yields the lowest energy state, allowing the selection of the most optimal solution. Results highlight potential problems and solutions of toroidal propellant tanks to be addressed in tank design. Future propellant management devices need to incorporate static fuel positioning to deviate risk, guarantee safety, and eliminate assumptions. Although the irregular movement of fuel in weightless motion (slosh) is an expanding topic, the stable state of fuel is equally as important, if not more.

Keywords: Toroidal tank, propellant management device, surface evolver

Identifying and Resolving Issues with the Hollow Cathode Emitter and SPT-100 Hall Effect Thruster

SURF ID: 137
2:30 PM - 2:45 PM

*Aditya H. Desai, Andrew Myers, Adam Patel, and Alexey Shashurin**
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Purdue University

Electric propulsion could hold the key to long range space travel, and devices like the SPT-100 Hall Effect Thruster provide researchers with the ability to test the capabilities of electric propulsion from here on Earth. However, the hollow cathode emitter that provides electrons to this thruster had not been functioning properly for some time, halting any potential research. This project aimed to diagnose and correct the issues with the thruster so experiments can be conducted using it again. Initial testing focused on potential problems in the vacuum chamber, including gas purity, diffusion pump oil, and system gas leakages. The tank of Krypton gas was replaced with ultra-pure Argon and the flow rate of the inert gas was varied and pulsed to try to create conditions under which the cathode could ignite. Eventually, the cathode was even brought to a different vacuum chamber at another site for testing. This study evaluated every component of the thruster's setup, beginning with the cathode

Keywords: Electric Propulsion, Hollow Cathode Emitter, Hall Effect Thruster

and its corresponding subsystems. Every component was verified to work independent of the system, but further testing revealed that a short had been created between two connections on the cathode itself, rendering it unusable. These results meant a new cathode would have to be built or purchased, but in the interim, a temporary cathode of thoriated tungsten wire was installed while designs for the new permanent cathode were drafted.

Experimental Investigation of Optimal Winglets Design on Wake and Efficient Performance of Horizontal Axis Model Wind Turbines

SURF ID: 153
2:45 PM - 3:00 PM

*Maison Hackett[1], Diego Siguenza Alvaradoon[2], Rita Appiah[2], and Luciano Castillo[2]**
**PI: School of Mechanical Engineering*
[1]Morgan State University, [2]Purdue University

Wind energy is one of the most vastly available and quickest growing renewable energy sources in the United States. Horizontal Axis Wind Turbines (HAWT) are used to generated wind energy. Studies have been shown by adding a winglet to the end of the blade tip will improve the turbine efficiency. Winglets can efficiently control spanwise velocity, minimize generated drag in the tip area, diminish wingtip vortices, and therefore contribute to more favorable aerodynamics with a minimum expansion of the blade tip. A challenge that will occur is the unpredictability of incoming wind flows is one of the most notable problems for wind energy, resulting in variable-power production and aerodynamic loads for wind turbines. In addition, induced drag generated by wingtip vortices has a significant impact on wind turbine performance. Attaching a winglet to the tip of the blade of a HAWT is a recent approach to improving these turbines' performance. The objective of the research is to analyze several winglet designs to find the best one for efficient performance by designing four different CAD models. The four intake conditions tested improved turbine power and thrust coefficients: turbulent boundary layer, negative shear, positive shear, and LLJ peak velocity. In a wind tunnel, test four horizontal-axis model wind turbines with equal rotor diameter by using 3D design software. Three of the turbines have downwind-facing winglets, while one has a conventional rotor design. The expected outcome will hopefully show the Reynolds stress distribution in the four different rotors. The wind tunnel testing and data analysis will be conducted by graduate students Diego Andres Siguenza Alvaradoon and Rita Appiah at later date in August of 2021.

Keywords: HAWT, winglets, wind energy, wind tunnel, winglet on a wind turbine, turbine efficiency

Systematic Study of the Viscosity of Room Temperature Ionic Liquids on the Electrochemical Performance of Redox Active Species

SURF ID: 162
3:00 PM - 3:15 PM

*Danny M. Hristov[1], Hugo Samayoa-Oviedo[1], Sekhon Jagdeep-Kaur[2], Edward Quitevis[2], and Julia Laskin[1]**
**PI: Department of Chemistry*
[1]Purdue University, [2]Texas Tech University

Studying the electrochemical behavior of ion species has led to significant discoveries of new and more efficient ways to run electrical systems, such as lithium batteries, that support society and everyday life. Present studies have focused on including solvents with low environmental toxicity, high conductivity, and stability to improve the performance of batteries. Room temperature ionic liquids (RTIL's) satisfy those conditions, given that they are stable over a wide electrochemical window. We characterized RTIL's of increasing length of the side alkyl chain, which increases their viscosity, and related that to the electrochemical performance of select redox-active species. Such performance was evaluated by calculating the electron transfer rate, diffusion, and reversibility of three redox active species of different initial charge states. Cyclic voltammetry (CV) is an electroanalytical technique in which the current produced by an electrochemical system is monitored as a function of the applied potential. The different RTILs were scanned via CV to measure their potential window of stability. When the redox active species are present, the cyclic voltammogram shows distinct peak currents that can be used to calculate their diffusion coefficient and electron transfer rate constant to assess the overall reversibility of a system. Experimental data shows that the complexity of the alkyl chain of each RTIL affects both the diffusion and the electron transfer kinetics of analytes. The results from this experiment can be utilized to find an efficient and sustainable solvent/analyte alternative to modern electrochemical systems.

Keywords: Room Temperature Ionic Liquids, Diffusion Coefficient, Electron Transfer Rate Constant, Viscosity, Cyclic Voltammetry

Membrane Heat Exchanger for Air Cooling and Dehumidification

*Songhao Wu, Andrew Fix, David Warsinger, and Jim Braun**
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Purdue University

SURF ID: 252
3:15 PM - 3:30 PM

Keywords: HVAC, Dehumidification, Membranes, Parametric study

Heating, ventilation and air conditioning (HVAC) equipment consumes 35% of total building energy use in the US, among which a large share is used for cooling and dehumidification. The majority of air dehumidification systems take the conventional approach of moisture condensation removal. It requires air to be cooled below its dew point temperature and is an energy-intensive process, especially for areas with hot and humid climates. Vapor selective membrane systems are promising alternatives for air dehumidification as they do not require cooling energy for latent (humidity) heat removal. It allows water vapor transport through the membrane while blocking air. Previous thermodynamic modeling of a membrane-based HVAC device developed by our group, referred to as the Membrane Heat Exchanger (MHX), has shown great potential for energy savings. High air/water selectivity membranes were fabricated and tested. A prototype of MHX with the outdoor air simulation (OAS) system was designed and assembled to test the real system performance against modeled performance. Temperature and humidity supplied to the prototype were varied across a broad range to simulate different climate conditions. 30%-%50% humidity removal was achieved along with notable cooling capacity. The results compliment the previous modeling studies of MXH that investigated the potential improvement in air conditioning energy consumption. The prototype design demonstrates the constructability of the proposed MHX system and serves as a pivotal step towards system scale-up for energy savings at the building level.

SESSION E: Engineering the Built Environment

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Design and Modeling of a Dome Structure for Extra-Terrestrial Habitat Testbed

SURF ID: 126
2:00 PM - 2:15 PM

*Guillermo Castro Martinez[1], Jaewon Park[2], Yuguang Fu[2], Amin Maghareh[2], Shirley Dyke[2], and Davide Ziviani[2]**
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[1]Pennsylvania State University, [2]Purdue University

Keywords: Cyber-Physical Testbed, Inflatable Bladder, Pressurization, Extra-Terrestrial Habitat

Establishing long-term extra-terrestrial colonies is among the greatest engineering challenges humanity is facing. A potential multi-planetary human presence is extremely attractive from a scientific and economic point of view and can potentially secure the future of humanity in the centuries to come. Therefore, it is imperative to develop resilient and sustainable human habitats capable of withstanding the hazardous environments of outer space. The Resilient Extra-Terrestrial Habitat Institute (RETHi) is designing a cyber-physical testbed capable of applying the conditions present in deep space environments on a habitat system, making it possible to perform complex tests for a scaled space. A key component in the testbed is a physical structural dome, which emulates both pressure and temperature variation and distribution in deep space. A challenge that comes with designing a dome structure is choosing an appropriate inner layer with reasonable dimensions to hold inner pressure without causing any damage to the dome. This study proposes a design of an inflatable bladder capable of applying the pressure load to the structure by inflating it to the desired pressure. Modeling software (SolidWorks and Abaqus) was used to simulate the pressurization of the bladder and analyze the stresses and deformations of both the bladder and structural dome. Variables such as bladder dimensions, material characteristics, and desired pressure loads were tested to optimize the design. A material selection of Nylon 66 in conjunction with a bladder thickness of 0.1 inches provided the most optimal design without causing yielding in either the structural dome or bladder.

Mobile Air Quality Sensors and the Internet of Things

SURF ID: 127
2:15 PM - 2:30 PM

*Daniel J Ceglio, Pankaj Meghani, and Greg Michalski**
**PI: Department of Earth, Atmospheric, and Planetary Sciences*
Purdue University

Keywords: Environmental characterization, Engineering the built environment, Internet of Things, Air quality, Low-cost sensors

With the ever-growing problem of climate change and more and more fossil fuels being burned, air quality is becoming an issue that people will need to start paying attention to; as seen in multiple cities across Asia. And although monitoring air quality is becoming more and more relevant in daily life, there is currently no way for the general public to view air quality data on a street-to-street basis. In this study, we combined different microcontrollers, sensors, and visualization methods, and then attempted to determine what combination of those three things would result in the cheapest, yet most accurate sensor possible that could provide precise air quality data. After testing combinations, we found that using a Raspberry Pi 3 Model B+ as the microcontroller, along with the Alphasense OPC-N3 as the sensor and Thingsboard as the visualizer, offered the best results. These results suggest that visualization of air quality on a street-to-street basis is not only possible, but can be done for a relatively small amount of money.

Development of a Cost Model for the Evaluation of Extra-Terrestrial Habitats

SURF ID: 191
2:30 PM - 2:45 PM

*Kathleen Martinus, Ali Lenjani, Dawn Whitaker, Ilina Adhikari, and Shirley Dyke**
**PI: School of Mechanical Engineering*
Purdue University

Keywords: Cost Model, Equivalent System Mass, Deep Space Habitats, Habitat Systems, Space Exploration, Engineering Built Environment

The desire to explore space and celestial objects has existed long before humanity's first steps on the moon. Including people on long-duration, deep-space missions require resilient extra-terrestrial habitat systems that can withstand the most extreme environments. Such a habitat consists of multiple subsystems and components that must interact seamlessly with each other. In the Resilient Extra-Terrestrial Habitats institute (RETHi), we developed a simulation environment to investigate different configurations of potential habitats. A cost model was needed to compare these configurations and subsystems, along with estimating cost needs. This model looks at establishing the habitat and its operations over its lifecycle. We used an Equivalent System Mass (ESM) method which looks at four parts of a habitat: Power, Structures, Environmental Control and Life Support (ECLSS), and Intelligent Health Management (IHM) subsystems. ESM is used to create a sum of a subsystem's cost, represented as mass (kg). This is done to eliminate the need to analyze many quantities with varying units; one sum of mass can instead be evaluated. A Python interface was then developed to provide a dashboard of

the mass requirements, along with providing a display for analysis of ESM values. This allows users to utilize the cost model for evaluating habitat designs and technologies, along with being a catalyst for decision making and future trade studies. The results of the cost model will be a crucial tool for evaluating deep space habitats and an important mechanism for the future of space exploration.

Mobile Air Quality Sensing and Internet of Things

SURF ID: 193
2:45 PM - 3:00 PM

*Pankaj Meghani, Daniel Ceglio, and Greg Michalski**
**PI: Department of Earth, Atmospheric, and Planetary Sciences*
Purdue University

Keywords: Internet of Things, Air Quality Measurement, Data Visualization, Environmental Characterization, Engineering the Built Environment

Recent research has shown that more than 10.2 million deaths in 2018 can be attributed to inhaling particulate matter with diameters smaller than 2.5 micrometers (PM 2.5) making it imperative have PM 2.5 data as a baseline for improving air quality around us. This study aims to measure PM 2.5 levels in our cities using cheap and portable sensors. The city that we would like to deploy these sensors is Arequipa, Peru, but we will be testing them in West Lafayette for the duration of the program. Multiple combinations of sensors, IoT devices, and visualization options were evaluated to find one that would not only be the most accurate but also the most cost-effective.
The approach that we found worked best was using Thingsboard as a visualizer, Raspberry Pi for hardware interfacing, SHT-21 for temperature and humidity measurement, Alphasense OPC-N3 for particulate matter measurements, and Adafruit FONA 3G for cellular communication. This approach allows us to service our hardware without bringing it back to the lab. These results suggest that it is possible to monitor street-by-street pollution levels for a relatively low cost (<$500) per module.

Characterizing Combustion of Solid Rocket Propellants using Laser Absorption Spectroscopy

SURF ID: 213
3:00 PM - 3:15 PM

*Raghav Poddar, Austin McDonald, and Christopher Goldenstein**
**PI: School of Mechanical Engineering*
Purdue University

Keywords: Hybrid Rocket Motors, Laser Absorption Spectroscopy, Combustion and Propulsion, HTPB

The necessity of squeezing out more from less is paramount for all rocket powered vehicles, be they space faring or defense related. Understanding the combustion characteristics of novel solid propellants like Ammonia Borane (AB) in Hybrid Rocket Motors is imperative to determine their efficiency and consequently their use cases. These characteristics include but are not limited to, temperature, regression rate, and mole fraction of product compounds across the height of the flame, that can all be simulated using chemical kinetic models. However, like all theoretical models, physical validations in replicable environments need to be carried out. The goal of this study is to conduct Laser Absorption Spectroscopy experiments with well documented propellants such as Hydroxyl Terminated Polybutadiene (HTPB) to ratify the legitimacy of our test setup, so that results from newer propellants such as AB can be trusted. In specific Direct Absorption Spectroscopy (DAS) is used using mid infrared Quantum Cascade Lasers in an opposed flow burner setup. This allows us to study the flames in the form of a sheet while varying the amount of oxidizer (99.5% O2) provided. DAS works by directing a laser beam of varying wavelength through a flame to a detector. Temperature of the flame and mole fraction of Carbon monoxide are found by comparing how laser light transmitted differs to that incident. Initial results with HTPB are positive in the trends of how temperature and mole fraction of CO change across height match its well documented combustion characteristics. This helps build confidence in our setup, to further pave the way to study more exciting propellants like AB.

Simulation of Hazardous Scenarios of a Deep-Space Habitat with a Cyber-Physical System

SURF ID: 247
3:15 PM - 3:30 PM

*Linzhe Wang, Jaewon Park, Yuguang Fu, Davide Ziviani, and Amin Maghareh**
**PI: School of Mechanical Engineering*
Purdue University

Keywords: Deep-Space habitats, Cyber-Physical System, Finite-Difference Method, Heat Transfer

Designing resilient deep-space habitats and developing permanent human settlement technologies beyond earth is a critical step of spacefaring civilizations. This study aims to advance the fundamental knowledge of designing resilient space habitats by developing a framework for simulating hazardous scenarios such as meteorite impacts and testing the habitat's dynamic thermal response to a harsh environment similar to the Moon. A Cyber-Physical System is developed to emulate the extreme temperature fluctuations caused by the Moon's rotation as external disturbances, and meteorite impacts are modeled as a heat transfer problem involving multiple layers. The numerical model includes two components: 1) the structural protective layer, 2) the structural habitat. The structural habitat is physically constructed in the Ray W. Herrick laboratories, and the structural protective layer functions as a cyber environment. A numerical reference model is developed to simulate the temperature fluctuations of the layers by utilizing the explicit finite-difference method. The reference model is partitioned into cyber and virtual components, and the feedback loop is placed to ensure proper communication between the systems. This study investigates the solutions from numerical simulations, conducts in-depth analyses of the results, and provides recommendations and frameworks for the physical testbed.

SESSION F: Machine Learning: Applications in Health & Safety

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Examining Human Safety Technology Interactions in a High-Risk Work Environment: Assessment of Neuro-Psychophysiological Responses in a Mixed Reality.

SURF ID: 101
2:00 PM - 2:15 PM

*Wahab W. Akanbi, Shiva Pooladvand, and Sogand Hasanzadeh**
**PI: Lyles School of Civil Engineering*
Purdue University

The construction industry is one of the hazardous industries worldwide. Many studies indicate that time pressure and mental load negatively influence workers' safety performance. However, it is unclear how this increased stress under time pressure signals workers to work out of sequence, generate work defects, and even cut corners regarding safety to meet the schedule and production demands. The fundamental research questions addressed by this objective relate to determining new concepts for latent changes in worker behavioral and decision frameworks when the physical condition becomes moderately safe at the jobsite. We combined a multi-modal mixed-reality environment with wearable neuro-psychophysiological sensors to examine changes in 33 workers' decision dynamics under different experimental conditions. The use of multiple sensors allows us to measure changes in hazard identification, risk perception, and risk-taking behavior by various qualitative and quantitative measures, thus better capturing the changes in the decision dynamics of workers. Specifically, a wireless, non-invasive neuroimaging device – Functional Near-Infrared Spectroscopy (fNIRS) collected worker's brain activities by measuring hemodynamic responses associated with mental workload, fatigue, and stress. Real-time recognition of at-risk behavior is still challenging in construction environments, and fNIRS can be reliable for studying individual affective and experiential risk perception in risky and stressful construction jobsites. This multidisciplinary research contributes to the body of knowledge by affecting safety training approaches and the controls needed when providing workers with safety protection and new technological advances.

Keywords: Human and Technology Interaction, construction safety, cognitive demand, risk-taking behavior, decision-making, fNIRS, Virtual/mixed reality,

A Demographic Networked SIHRVD Model for COVID-19 Spread in the U.S.

SURF ID: 146
2:15 PM - 2:30 PM

*María E. Gibbs[1], Chi Ho Leung[2], and Philip E. Paré[2]**
**PI: School of Electrical and Computer Engineering*
[1]The University of Texas at Austin, [2]Purdue University

The COVID-19 pandemic has devastated the world in an unprecedented way, causing enormous loss of life. Mathematically modeling the dynamics of the pandemic is imperative to understand the disease's behavior and to mitigate its spread. This study proposes an SIHRVD networked compartmental model to describe and forecast the current spread of COVID-19 in the United States. We build on the classic SIR (Susceptible-Infected-Recovered) model, existing literature, and knowledge of the disease's dynamics to add compartments for hospitalized (H), vaccinated (V), and deceased (D). Within each compartment there are two demographic nodes: one for the population under the age of 65, the other for those aged 65 and older. We analyze the model and investigate stability conditions. Leveraging insights from the theoretical results, we explore the causality between vaccination levels and hospitalizations in the pandemic spread via simulations in order to encourage Americans to become vaccinated.

Keywords: Machine Learning: Big Data, COVID-19, Epidemic Modeling, Mathematical Modeling, Data Science

Predicting Mental Workload during Semi-Autonomous Driving using Physiological and Driving Performance Measures

SURF ID: 178
2:30 PM - 2:45 PM

*Justin S Lee, Nade Liang, Gaojian Huang, and Brandon Pitts**
**PI: School of Industrial Engineering*
Purdue University

Vehicle automation is developing at a rapid rate worldwide. Some SAE Level-1 automated driving systems (ADS), or semi-autonomous driving systems, are becoming widely available. Examples include Adaptive Cruise Control (ACC) and Lane Keeping System (LKS). There are new challenges to road safety when using these types of ADS as continuous driver input is still needed. Some of these challenges are associated with suboptimal driver mental workload (MWL). Predicting a driver's MWL can help mitigate these challenges and improve road safety. The goal of this study is to investigate the capabilities of a selection of supervised Machine Learning (ML) classification techniques to produce driver behavior-driven prediction models of driver's MWL. Subjective measurements of MWL using the NASA Task Load Index was used as comparison to determine the effectiveness of the ML classification techniques. Data used in this study was collected on a medium fidelity driving simulator.

Keywords: Human Factors, Mental Workload, Semi-Autonomous Driving, Eye Tracking, Machine Learning, Random Forest

Driver behavior was monitored using a combination of physiological and driving performance measures. Findings show that the random forest classification models performed the best in predicting MWL compared to other models such as decision tree or support vector machine. Heart rate and heart rate variability data, followed by eye tracking data, were the most significant features for the classification models. The result of this study provides key insights into the importance of measuring heart rate and eye tracking data when designing future systems that predict MWL of drivers in real-time.

Predicting Lifting Risks From Pressure Exerted By Various Hand Regions

*Jiachen Jiang, Guoyang Zhou, Deyuan Sun, and Denny Yu**
**PI: School of Industrial Engineering*
Purdue University

SURF ID: 167
2:45 PM - 3:00 PM

Lifting due to overexertion has been one of the leading causes of injury at workplace. It is difficult to estimate the degree of overexertion directly from the weight of the object being lifted. Our research aims to build a model to predict lifting risks based on the pressure exerted on various hand regions. Lifting risk is measured by Lifting Index (LI), a calculated number based on several factors of the lifting task, such as object weight and height. In general, a LI value of 1.0 or less indicates a nominal risk to employees. A LI value greater than 1.0 denotes that the task is at high risk for some population. In the study, participants were asked to complete lifting tasks with different risk levels quantified by LI. Low-risk is defined as LI < 1. Medium-risk is defined as 1 < LI < 2. High-risk is defined as LI > 2. Several machine learning models, including logistic regression, random forest, and support vector machine, were trained and evaluated. A mixed-effects ordinal multinomial logistic regression model was also fitted to examine the statistical significance of various hand regions. The results suggest that the pressure exerted on certain hand regions, such as right index and middle finger, can reflect lifting risks.

Keywords: Lifting Risk, Pressure, Machine Learning, Logistic Regression

Epidemic Mitigation with Limited Resources

*Avik Wadhwa, Ciyuan Zhang, and Philip Paré**
**PI: School of Electrical and Computer Engineering*
Purdue University

SURF ID: 246
3:00 PM - 3:15 PM

Various COVID-19 mitigation strategies have been employed in different parts of the world, including quarantine, redeployment of healthcare workers, social distancing, contact tracing, etc. Not only does an accurate and precise model help track the spread and develop non-pharmaceutical intervention (NPI) strategies to mitigate the disease, but it also could be used to develop optimal methods for vaccine delivery. Using a discrete time susceptible-infected-recovered (SIR) model, we capture the spread of SARS-CoV-2 virus over the system of a sub-population network. Then, we construct an observation model to estimate the system states from testing data. We examine optimized resource distribution strategies to minimize the spread of infection with limited cost. We propose an optimization problem for the mitigation of the spread of infectious diseases and simulate it with well-defined parameters over a network model. Our results will provide insights for policymakers as they choose between various mitigation strategies.

Keywords: Epidemic Process, Optimization, Mitigation Strategies, Non-pharmaceutical Intervention, Learning and Evaluation

SESSION G: Nanotechnology: Fluids & Chemicals 2

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Mussel-Inspired Underwater Hot Melt Adhesives: Introducing Catechol Chemistry to Thermoplastic Polymer Systems

SURF ID: 158
2:00 PM - 2:15 PM

*Morgan R. Heidingsfelder, Bradley McGill, Clayton Westerman, and Jonathan Wilker**
**PI: Department of Chemistry*
Purdue University

Underwater adhesion is a natural phenomenon that exists in several marine species, such as mussels, oysters, and other sea organisms. Some of these creatures can secrete adhesive proteins with high catechol content that enable adhesion in wet conditions. Comparatively, commercial glues are intended for dry applications. Thermoplastic polymer-based adhesives, such as hot melts, are applied molten and harden upon cooling but function inadequately underwater. Adhesive failure in wet environments has led researchers to design synthetic biomimetic polymers including hot-curing adhesives and hydrogels. Biomimicry has been a successful approach for synthetic underwater adhesives; however, little is known regarding the ability to replicate this success for hot melts. This study aims to adapt current hot melt formulations using a thermoplastic polymer combined with catechol and additional nonpolar additives. The adhesives were synthesized by melting polymer or via solvent casting, followed by the addition of other components. Results from testing the hot melts in various conditions indicate that incorporating crosslinkers and amino acids demonstrate initial signs of underwater adhesion. The addition of catechol compounds with a tackifier and thermoplastic polymer created adhesives that fully adhere underwater, suggesting that catechol content assisted by hydrophobic and tacky materials impacts the wet adhesion capabilities of hot melts. This study offers a basis for developing underwater hot melt adhesives with future potential applications in fields such as packaging, construction, and maintenance.

Keywords: Underwater adhesion, hot melt adhesive, biomimicry, catechol, thermoplastic polymer, mussels

Capillary Based Microfluidics for Droplet Generation

SURF ID: 186
2:15 PM - 2:30 PM

*Jack J. Maher, Andres Barrio-Zhang, and Arezoo Ardekani**
**PI: School of Mechanical Engineering*
Purdue University

Droplet microfluidics has become an increasingly popular tool to create complex emulsions. The high controllability of flow parameters, including the droplet size and quantity produced, allows for various applications of the droplets such as creating mini bioreactors or capturing cells to mimic a variety of important biological processes. We wanted to find whether it was possible to generate an emulsion containing monodisperse soybean oil droplets of a controllable size within aqueous solutions. Devices were created consisting of differently sized capillaries tapered to diameters of approximately 40, 90, and 100 micrometers, which were aligned within outer square capillaries. The device setups allow for either two or three separate coflowing fluid flows, soybean oil and aqueous solutions of varying viscosities, to be controlled using syringe pumps. It was found that generally, for single layer droplets, as the continuous flow rate decreased the droplet size increased. The dispersed flow rate had less of an effect on droplet size at a single continuous flow rate, but it was found that dispersed flow rates of 10 and 40 microliters per minute produced the largest droplets. As the continuous flow rate increased, the number of droplets produced also increased. These results can be applied to processes where droplets need to be produced within a continuous flow, of viscosity like the fluids presently studied. More broadly, this research can be easily applied to processes that require a continuous change in droplet size, since there is no need for an exchange of parts to alter the droplet size.

Keywords: Microfluidics, Droplet, Capillary, Soybean Oil

Characterization of Concentrated Surfactant Solutions through Rheological Response

SURF ID: 201
2:30 PM - 2:45 PM

*Bradley K. Nance, Caitlin Adams, and Kendra Erk**
**PI: School of Materials Engineering*
Purdue University

Synthetic surfactants are used in household personal care products worldwide. With increased consumer desire for more ecofriendly products, there is growing demand for more sustainable processing in industry applications. A comprehensive understanding of concentrated surfactant solutions, which are known to self-assemble into a fluid lamellar phase, did not exist prior and is needed to conduct a thorough investigation into industrial-scale implementation. Basic rheological measurements of concentrated sodium lauryl ether sulfate surfactant solutions and concentrated solutions containing sodium chloride were conducted across a range of shear rates, shear strains,

Keywords: Materials Processing and Characterization, Concentrated Surfactant, Sodium Lauryl Ether Sulfate, Lamellar Self-Assembly

angular frequencies, and axial forces to generate complete relationships between the surfactant microstructure and rheological response of the bulk material. A unique hysteresis effect is noticeable within the range of 0.008 to 0.2 reciprocal seconds upon initial shearing of the concentrated surfactant solution. Addition of sodium chloride to the concentrated surfactant solutions increased deformation energy from values of 0.03 joules in the control samples to 0.54 joules in the solution containing 5 weight percent sodium chloride. This study sought to characterize the flow behavior found in highly concentrated surfactant solutions, providing a basis for later formulation of prediction methods to use when analyzing processability and performance.

Effect of Chemistry on Surface Mechanical Properties of Polymer Lung Surfactants

*Sungwan Park, Daniel Fesenmeier, Seyoung Kim, and You-Yeon Won**
**PI: Davidson School of Chemical Engineering*
Purdue University

SURF ID: 210
2:45 PM - 3:00 PM

Keywords: Polymer Chemistry, Lung Surfactant, Pulmonary Surfactant, Acute Respiratory Distress Syndrome, Block Copolymer Micelle

Every year, around 200,000 new cases of acute respiratory distress syndrome (ARDS) with the mortality rate of 25~40% are being reported in the United States. To treat these ARDS patients, new lung surfactants should be injected into their alveoli to reduce the alveolar surface tension. Our group has previously discovered that micellized poly(styrene)-b-poly(ethylene glycol) (PS-PEG) can become one of the promising candidates to replace traditional protein or lipid-based lung surfactants, which are mostly costly. The nanomicelles stay at the air-water interface and reduce the interfacial tension close to 0 mN/m under high compression. Nevertheless, it has been schematically assumed that the strong affinity of the micelles to the air-water interface without getting submerged into the water subphase even under high compression is due to their high hydrophobicity. To confirm the hydrophobicity, physical properties and interfacial behavior of assorted amphiphilic block copolymer micelles with different chemical characteristics have been analyzed. It has been found that micellized PS-PEG with methoxy (OCH_3) PEG end group is more hydrophobic than other block copolymer micelles via surface pressure-area isotherms and contact angle measurement experiments. PS-PEG micelles, which have high hydrophobicity, high glass transition temperature of hydrophobic core, and nonpolar PEG end group yielded higher surface pressure under high compression, so the surface tension was dramatically reduced. Understanding the chemical parameters which affect surface mechanical properties will later enable us to design more biocompatible and biodegradable synthetic polymer-based lung surfactants.

Investigation of Epoxy Curing Dynamics in a Laminar Flow

*Gabriella Schalm, Yanbin Wang, Zijan He, and Tian Li**
**PI: School of Mechanical Engineering*
Purdue University

SURF ID: 224
3:00 PM - 3:15 PM

Keywords: Fluid Dynamics, Phase Transition of Organic Materials, Microtechnology, Thermal Management

Ranging from biomedical applications to micro-scale chip sealing, the need for epoxy to produce robust and flexible insulation coating layers in a reasonable timeframe has increased drastically in recent years. However, the curing dynamics of epoxy are seldom studied when it is flowing through confinements. This paper discusses epoxy curing in a laminar flow under various conditions, where the epoxy recipe, curing condition, and flow profile are the most critical factors affecting the final product's shape. This process is aimed at producing high resolution results with a low curing time. Several rounds of testing were performed for this study, including development of the epoxy recipe, evaluation of this epoxy's properties such as viscosity and curing time, and testing of the material in flow. The formula's time and location dependent temperature was noted throughout the process using an infrared camera and thermocouple, and the group found the optimized epoxy curing temperature to be approximately 150 degrees Celsius. Lastly, implementation of a temperature control system for experiments is discussed. This testing led the team to finalize a reliable epoxy recipe, as well as refine the specifics of curing temperature and time. The epoxy recipe's flow through a restricted environment was monitored with an infrared camera, capturing temperature distribution as a function of location and time. The research team's primary findings included the final recipe and optimized applied temperature to cure the epoxy, with a curing time falling in the 10-20 minute range, as well as proposed processes for further testing and validation.

Virtual Reality Animations of Blood Flow in a Vessel Network

SURF ID: 258
3:15 PM - 3:30 PM

*Jiahao Zhu, Yu Leng, and Hector Gomez**
**PI: School of Mechanical Engineering*
Purdue University

Large scale computation used in fluid analysis is becoming ubiquitous these days, especially in the field of biomedical research. Computational analysis of blood flow in tumor-induced capillaries is important in a well-rounded understanding of cancerous diagnosis and treatment. However, in clinic, it is inconvenient or even elusive to comprehend simulation results from intricate computational models. Virtual Reality (VR) helps to visualize simulation results of fluid analysis and convey convoluted characteristics of the results in a simple immersive three-dimensional (3D) model. In this work, we utilize the software ParaView and the VR device Oculus Rift S to visualize the simulation results based on prior studies. We illustrate this with a large dataset including blood flow in microvessels and the growth of a cancerous tumor. From the VR visualization, we can condense the large dataset into a comprehensible VR model and advance our knowledge of the cancerous diseases. We present the elaborate procedures to set up the immersive environment combined with modeling analysis software. Our work focuses on converting simulation results of blood flow in tumor-induced microvascular network from ParaView to VR headset. From our work in the figurative expression of vascular structure and blood fluid, we envision that this VR imaging method could be used in the clinic when computational analysis becomes routine in the future.

Keywords: 3D Visualization, Virtual Reality, Computational Modeling, Vascular Analysis

Day 2 | Morning Presentations

July 30th, 10:00 AM – 11:30 AM EDT

SESSION A: Material Modeling & Simulation 1

Click here to join the session

Multiphysics Simulation Guided Optimization of Acoustically Tensioned Metastable Fluid Detectors

SURF ID: 111
10:00 AM - 10:15 AM

*Troy M. Barlow, Stepan Ozerov, Nathan Boyle, and Rusi Taleyarkhan**
**PI: School of Nuclear Engineering*
Purdue University

Keywords: Neutron, Detector, Acoustics, Optimization, Simulation

High efficiency fast and thermal neutron detection is a difficult task due to the highly penetrating nature of these particles, with key applications in the nuclear, medical, and public safety sectors. The novel Acoustically Tensioned Metastable Detector (ATMFD) has previously been developed and optimized for neutron detection. ATMFDs use acoustic waves to place the detecting fluid into a tensioned (metastable) state (negative, yes – subvacuum pressures), similar to a laser resonant cavity, which allows for the detection of incident neutrons inside the ATMFD sensitive volume. Knowledge of the magnitude and profile of the negative pressure states in the ATMFD is integral for future development and optimization of ATMFD sensitivity. Multiphysics simulations and experimental methods were used to evaluate and guide the optimization of the sensitive volume. The ATMFD was modeled and simulated via the COMSOL Multiphysics platform (accounting for electromagnetics, piezoelectrics, acoustics, structural dynamics as well as fluid-structure interactions) and a parametric study was performed. Additionally, a figure of merit was developed to compare and determine optimal configurations resulting from the parametric study. The results of this optimization study show that changing the height by small amounts of the ATMFD acoustic reflector cavity dramatically affects the acoustic pressure profile and magnitude. Overall, the simulation-guided experimental methods offered considerable insight into the pressure profile of the current ATMFD system, as well as opportunity for further optimization of ATMFD configuration to maximize sensitivity.

Laser-Based Profilometry of the Centrifugally Tensioned Metastable Fluid Detector

SURF ID: 168
10:15 AM - 10:30 AM

*William T. Kelley, Catalin Harabagiu, Stepan Ozerov, Nathan Boyle, and Rusi Taleyarkhan**
**PI: School of Nuclear Engineering*
Purdue University

Keywords: Tensioned Metastable Fluid Detector, Laser-Based Profilometry, Neutron Detector

Neutron radiation detection and measurement has applications in a variety of industries including the nuclear, medical, and public safety sectors. Purdue's Metastable Fluids and Advanced Research Laboratory have developed Tensioned Metastable Fluid Detectors (TMFDs), that boast high intrinsic detection efficiency (~99% for alpha) and ~80% for fast and thermal neutrons. One architecture of TMFDs that has been extensively developed is the centrifugally tensioned fluid detector (CTMFD). The CTMFD uses centrifugal forces to place the fluid inside the detector under a negative (sub-vacuum) pressure state. In these negative pressure states, the CTMFD is sensitive to neutron/alpha/fission events while remaining 100% blind to gamma-beta background radiation. The CTMFD negative pressure states can be easily tailored by altering the rotation frequency, and it is possible to calibrate these pressure profile states inside of the CTMFD with an nanosecond pulsed N2 laser. To do so, the focal point of the laser was focused throughout the sensitive volume of the CTMFD, and thin strips of attenuating material were added or removed from the beam line in order to raise or lower the intensity of the laser resulting in laser induced cavitations at various negative pressure thresholds. Using multiple strip thicknesses, the negative pressure profile throughout the sensitive volume of the CTMFD was mapped, providing valuable insight to the radial negative pressure drop-off within the detector. The known negative pressure thresholds required for laser induced cavitations is planned to be combined with COMSOL Multiphysics (nuclear, electromagnetics, piezo-electrics, acoustics and fluid-structure interaction) modeling of the acoustically tensioned metastable fluid detector (ATMFD) to accurately determine the profile and intensity of the sensitive volume within the ATMFD.

Verification of a Deterministic Solver to the Full Boltzmann Equation

SURF ID: 237
10:30 AM - 10:45 AM

*Allison Taylor[1], Brian Morton[2], Nirajan Adhikari[2], Jingwei Hu[2], and Alina Alexeenko[2]**
**PI: School of Aeronautics and Astronautics*
[1]University of Notre Dame, [2]Purdue University

The Boltzmann equation is an integro-differential equation that governs the behavior of gaseous flow. Solving this equation is of particular interest as it provides solutions to rarefied flow cases that are unobtainable through continuum models like the Navier-Stokes-Fourier equations. The most popular method of doing so is the Direct Simulation Monte Carlo (DSMC) method which utilizes stochastic algorithms to approximate molecular collisions. While this method has been integral to the understanding of rarefied gas dynamics, the solver is computationally expensive at low Knudsen numbers and its stochastic nature introduces inherent noise in the solution. For this reason, our research examined methods of solving the Boltzmann equation in a deterministic manner, particularly, the discontinuous Galerkin fast Fourier spectral (DGFS) method. We ran two test cases: a one-dimensional normal shock wave with Mach number 1.59 and one-dimensional Couette flow with plate velocity ±50 m/s. The results of the DGFS method were compared to that of the benchmark DSMC method for the same cases with the same operating conditions. These results showed clear agreement between the macroscopic property distributions of the two methods. Furthermore, the DGFS method obtained such accuracy with over 90% less grid cells for each test case. Our findings also indicate the DGFS method reduces computational time for low-speed flows as shown in the Couette flow case. Considering its higher order accuracy, reduced computational requirements, and increased applicability to general collision kernels, we verify the DGFS solver as a highly accurate, deterministic solver to the full Boltzmann equation.

Keywords: Discontinuous Galerkin Method, Fast Fourier Spectral Method, Deterministic Solver, Full Boltzmann Equation, Rarefied Gas Dynamics

INCORPORATING A SERIES RESISTOR INTO MICROSCALE BREAKDOWN THEORY

SURF ID: 249
10:45 AM - 11:00 AM

*James C. Welch III, Adam Darr, Amanda Loveless, and Allen Garner**
**PI: School of Nuclear Engineering*
Purdue University

Gas breakdown occurs when sufficiently strong electric fields create current across the gas filled gap between electrodes. This phenomenon, called Townsend avalanche, is modeled by Paschen's law and caused by electrons colliding with gas molecules, creating more electrons via ionization; this multiplies charge exponentially across the gap. Normally, breakdown voltage – the minimum voltage across the gap above which Townsend avalanche can occur – is a U-shaped curve with a minimum at a specific gap distance for a given gas and pressure. For microscale gaps, breakdown voltage instead continues to decrease linearly due to field emission, where the electric field strips electrons from the negative electrode.

Experimental field emission and microplasma devices use resistors to limit current into the emitter to protect them, causing the applied and gap voltages to diverge. This becomes problematic because theories predict breakdown using gap voltage, meaning that the experimentalist may not necessarily know the relationship between applied and breakdown voltage a priori. In this investigation, we alter microscale gas breakdown theory to determine applied voltage at breakdown as a function of resistance and gap parameters. We perform simulations incorporating field emission, Townsend avalanche, and circuit equations, numerically comparing with theory. We determine the series resistance for various gap distances where contributions from modified Paschen's law and Ohm's law match to determine when resistance drives breakdown behavior. At high resistances and smaller gap distances, applied breakdown voltage varies linearly with resistance according to Ohm's law, demonstrating the necessity to modify microscale gas breakdown predictions under these conditions.

Keywords: Breakdown, Paschen's Law, Townsend Avalanche, Field Emission, Nanotechnology

Statistics of Dislocation Line Orientation Distributions as Tests for CDD Plasticity Theories

SURF ID: 239
11:00 AM - 11:15 AM

*Jose M. Torres López[1], Joseph Pierre Anderson[2], and Anter El-Azab[2]**
**PI: School of Materials Engineering*
[1]University of Rochester, [2]Purdue University

Line defects known as dislocations are the carriers of plastic deformation in crystalline materials. Because of the computational limitations associated with simulating large numbers of individual dislocations, dislocation-based plasticity is often studied through continuum dynamics models based on average dislocation density quantities. In this presentation, we focus on the underlying assumption of the vector-density theory (line-bundle assumption), namely that dislocation lines are locally parallel to the direction of their mean direction. Given the importance of this postulate, we evaluate numerically its accuracy by means of local distribution functions for dislocation orientations. To carry

Keywords: Discrete Dislocation Dynamics, Continuous Dislocation Dynamics, Line-bundle, Dislocation Vector Density, Dislocation Orientation Statistics.

out this analysis, we analyze discrete dislocation data by introducing a partition of the material sample into voxels and examining statistical measures of the angular distribution of dislocations within each voxel.

The resulting distributions show a sharp concentration of dislocations around their local mean orientation, especially for smaller voxel scales and independently of other variables. More concretely, they can be fitted by an exponential function decreasing with angular distance (root mean squared error ≤ 0.03). This provides a quantitative test of the line-bundle assumption, suggesting that the vector-density approach is accurate at the scales studied.

SESSION B: Environmental Characterization 1

Click here to join the session

Effects of Plant Characteristics and Hydrological Gradients on the Soil Environment in Agricultural Wetlands

SURF ID: 118
10:00 AM - 10:15 AM

*Jackson T Brady, Jacob Hosen, Danielle Winter, and Sara McMillan**
**PI: Department of Agricultural & Biological Engineering*
Purdue University

Keywords: Environmental Characterization, Wetlands, Biogeochemistry, Emergent Macrophyte, Greenhouse Gases, Organic Carbon

Wetlands are excellent at cycling excess nitrogen which is deleterious to aquatic ecosystems. Wetlands also produce the greenhouse gases nitrous oxide and methane. Wetland restoration and creation should balance water quality enhancement and climate impacts. It's unknown whether the type of plant or the hydrology of the soil is influential in promoting nutrient cycling and reducing greenhouse gas release. The objective of this research is to understand how plant characteristics/hydrology impact the soil environment to better control the tradeoff between water quality and greenhouse gas release. We collected aboveground and belowground biomass from 7 emergent macrophytes and surrounding soil to investigate plant characteristics. To investigate hydrology soil samples were taken along a hydrological gradient. We analyzed soil samples for gravimetric moisture content, organic matter quantity, calcium carbonate concentrations, and pH. We characterized the quality of water-extractable soil organic carbon with catalytic oxidation combustion and spectroscopy. We will characterize the same soil metrics along a hydrologic gradient. PCA analysis from the plant characteristics experiment shows grouping of between sampling sites, possibly due to changes in hydrology. The hydrology experiment showed that some soil characteristics were significant at different hydrological zones. These experiments will provide insight on how to impact the soil environment to control denitrification and greenhouse gas release. Promoting denitrification and mitigating greenhouse gas release are essential for making wetlands a viable option to process nitrogen pollution. Understanding the impact of plant type and hydrology on soil will allow wetlands to be better optimized.

Toxicity of a "Forever Chemical" in an Estuarine Fish: Does Salinity Mediate the Toxicity of Perfluorooctanesulfonic Acid (PFOS)?

SURF ID: 120
10:15 AM - 10:30 AM

*Lucy E. Burcham, Tyler Hoskins, Grace Coogan, Elizabeth Allmon, and Maria Sepulvida**
**PI: Department of Forestry and Natural Resources*
Purdue University

Keywords: PFOS, salinity, estuaries, sheepshead minnows, toxicology, ecology

Per- and polyfluorinated alkyl substances (PFAS) pose risks to human and environmental health. PFAS are widespread due to use in products like food packaging and makeup, among others. Toxicity of PFAS to estuarine species is understudied and little is known about how fluctuating salinities, typical of estuaries, might mediate toxicity. Our central objective was to evaluate the toxicity of PFOS, a ubiquitous contaminant of estuaries, and whether salinity mediates toxicity in sheepshead minnows (Cyprinodon Varietgatus). We hypothesized that 1) PFOS reduces survival, growth, and developmental rate in a dose-dependent manner and 2) salinity and PFOS interact non-additively on these same responses. Embryos were exposed through hatching to 0, 1, 10, 100, 1000, or 10,000 parts per billion (ppb) at 10 or 30 parts per thousand salinities in a factorial design with 15 replicates per treatment. We assessed 96-hour survival, time-to-hatch, and standard length at hatching. PFOS was not acutely toxic to sheepshead minnow embryos. Survival was unaffected, indicating that mortality is unlikely in the environment. Both 1000 and 10,000 ppb PFOS delayed hatching by 4.7%. Hatchlings were 1.7% longer at 10 ppt salinity relative to 30 ppt. There were no salinity by PFOS interactions observed. Overall, our study suggests that PFOS is not particularly toxic to sheepshead minnow embryos, as the lowest observable effect concentration (LOEC) in our study was 1000 ppb for time-to-hatch. Future studies should focus on toxicity of PFOS across salinity gradients in recently hatched larvae, which are generally more sensitive to contaminants than embryos.

Chlorine Decay in a New Home Water Softener

*Katharine R. Del Real, Caroline Jankowski, Christian Ley, Caitlin Proctor, and Andrew Whelton**
**PI: Lyles School of Civil Engineering*
Purdue University

SURF ID: 135
10:30 AM - 10:45 AM

Keywords: Stagnation, Water Quality, Chlorine Decay, Softener, Plastic

There are more than 10 million water softeners in residential buildings across the U.S. These devices remove dissolved minerals from water to prevent mineral build up in plumbing, shortened appliance life, and a greater dose of detergents for bathing and laundry purposes. When softeners are new, such as in newly constructed buildings, water can stagnate, or not move, in plumbing. Because water softeners contain polymer (plastic) resin beads, this resin may leach chemicals into the water. Chlorine is the most popular drinking water disinfectant chemical that is used to prevent microbiological growth. This study's goal was to better understand water softener resin and its interaction with chlorine disinfectant. A four-person household water softener typically contains 15 to 20 gallons of water and 1 ft3 of resin. This device was estimated to contain more than 83 million resin beads (0.4 mm < Φ < 0.7 mm). Total resin bead surface area ranged from 43 m2 to 132 m2. This is approximately 30 times the surface area of all the cold-water piping in a single home. Free available chlorine decay was examined for two new softener resins over a five-day period (Ci 3.3 mg/L as Cl2, pH 7.5, 23˚C). Because drinking water delivered to buildings often has 0.2 mg/L as Cl2, the resin examined would reduce chlorine to nondetectable levels in approximately 1.5 days. Additional work is needed to understand how disinfectant reactivity varies based on pH, disinfectant type, the presence of biofilm, scale, and resin service life.

Microbiological Water Quality During Commissioning of a New Plumbing System

*Catherine Fleming, Christian Ley, Katharine Del Real, Caitlin Proctor, and Andrew Whelton**
**PI: Lyles School of Civil Engineering*
Purdue University

SURF ID: 144
10:45 AM - 11:00 AM

Keywords: Water Quality, Stagnation, Cell Counts, Chlorine, Plumbing System

Building water systems sometimes see periods of highly reduced use. During this time, stagnation can cause an increase in microbial growth and therefore changed water quality. This microbial growth is of public concern as it can be harmful to human health and the water distribution system (e.g., microbial corrosion or biofilm issues). In this study, a pilot rig was constructed to include hardware found in a typical residential building, including copper and PVC. To investigate the relationship between chlorine and potential growth, water entering the system was stagnated in glass bottles and monitored over a period of 72 hours. Testing focused on total cell count and intact cell count to determine how different periods of stagnation and chlorine levels affect the microbiological water quality. While free chlorine concentrations of 0.1 and 0.15 mg/L (amounts frequently seen in the plumbing rig) caused almost complete cell death within the first 2 hours, intact cell count increased after 48 hours in both concentrations. In the pilot plumbing rig, an increase in microbiological growth is expected whenever stagnation exceeds 24 hours, and growth may also occur when chlorine levels are particularly low. Since water in buildings also experiences stagnation, growth is very likely, even if all cells are thought to be previously killed.

Quantification of Recent Shoreline Movement Along Lake Michigan's Southern Coast

*Hannah R. Tomkins and Cary Troy**
**PI: Lyles School of Civil Engineering*
Purdue University

SURF ID: 238
11:00 AM - 11:15 AM

Keywords: Lake Michigan, Indiana Shoreline, GIS Analysis, Shoreline Change

Lake Michigan has experienced large fluctuations in water level over the past two decades, and the shoreline has changed dramatically in response to these fluctuations. Quantifying how the shoreline changes in response to these varying water levels will help in the development of models capable of predicting future shoreline responses, ultimately guiding the design and maintenance of more resilient shorelines. This study hypothesizes that in spite of recent rapid and large shoreline changes observed for Lake Michigan, this recent behavior is consistent with previous shoreline responses in times of high water level. It is anticipated that the period of low water levels of 1998-2013 provided the opportunity for beach growth not commonly experienced between past periods of high water level. To quantify how the shoreline has changed along the southern coast of Lake Michigan, orthorectified aerial images were compiled and the shoreline (water-land intersection) was isolated. Digital Shoreline Analysis System (DSAS), a plugin for ArcGIS, was then used to compare the shorelines at regular cross-shore transects and calculate shoreline movement. Imagery was used for 1998, 2003, 2008, 2013, and 2020. These years represent the decline in water level beginning around 1998, the consistent low water level from 2002-2013, and the high water point that occurred in 2020.

While results vary along the diverse coast of the Indiana, it was observed that beaches experienced an average 52 meters of growth during the low water level period, with most of this shoreline advancement occurring during the 1998-2002 period when the water level was falling. During the water level resurgence of 2013-2020, it was observed that the shoreline progressed landwards on average 57 meters, with the exception of historical accretion zones updrift of large coastal barriers. Due to the beach rebuilding period of 1998-2013, the widespread erosion of 2013-2020 did not result in the majority of locations experiencing severe net beach loss. Additionally, it was found that the shoreline advancement and recession slopes during these changing water level periods are approximately 50:1 and 35:1, respectively. These results indicate that the shoreline position does correlate to Lake Michigan's water level, but there are other factors that impact the resulting shoreline. Additional variables for investigation include storms, anthropogenic actions such as beach nourishment and dredging, natural cross-shore and long shore sediment transfer, and the presence of coastal structures.

SESSION C: Cellular Biology 2

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Discovery of New Targets on Tumor Infiltrating Immune Cells by Single-Cell Sequencing

SURF ID: 105
10:00 AM - 10:15 AM

*Maansi Asthana, Bo Huang, Weichuan Luo, and Philip Low**
**PI: Department of Chemistry*
Purdue University

The immune cell population within the tumor microenvironment can impact the outcome and progression of lung cancer. Understanding key biomarkers leads to targeted immune therapies. By characterizing T cells at an individual level, through single-cell RNA sequencing (scRNA-seq) analysis, we can identify key biomarkers in the tumor microenvironment which can guide novel targets for immune therapies. This study comparatively analyzed T cell features and biomarkers of non-small cell lung cancer (NSCLC) and normal tissues at an individual cellular level. scRNA-seq data from three NSCLC samples and three healthy lung samples were used from the Gene Expression Omnibus. After data quality control and normalization, the R package Seurat was used to perform cell clustering, or the identification of cells expressing similar markers. The cell types were then characterized through the CellMarker database and gene expression analysis was conducted through differential expression and functional enrichment methods. Through a comparative analysis of tumor and normal samples, up-regulated genes of T-cell in NSCLC samples will be identified. These genes can then be confirmed through in vitro and in vivo experimentation to further classify cell infiltration in solid tumors. By characterizing T cell expression markers in the tumor microenvironment, the unique biomarkers can be targeted when developing novel immune therapies.

Keywords: Lung cancer, single cell RNA sequencing, immune therapy, immune oncology, gene markers

Development of an Elastin-Like Polypeptide Fusion Protein for Enhanced Detection and Imaging of Non-Muscle Invasive Bladder Cancer

SURF ID: 112
10:15 AM - 10:30 AM

*Brooke D. Barnett, Saloni Darji, Aayush Aayush, and David Thompson**
**PI: Department of Chemistry*
Purdue University

The most common type of bladder tumor, non-muscle invasive bladder cancer (NMIBC), has extremely high recurrence rates with majority of patients having a minimum of one relapse. The standard method for detecting and diagnosing bladder cancer has been white light cystoscopy (WLC), which is an invasive technique that has low sensitivity. Blue light cystoscopy is an alternative that relies on fluorescence, but cannot distinguish between bladder inflammation and tumor, which leads to false positive diagnoses. To decrease the high rate of recurrence, specific detection methods are necessary. The goal of this project was to develop a fluorescently-tagged elastin-like polypeptide (ELP) fusion protein that can participate in targeted receptor-mediated binding to bladder cancer cells. By developing a fusion protein that is targeted, both overall systemic effects to the patient and incorrect diagnoses would be reduced due to its specificity in detection. We have previously developed a rapid organic extraction purification method coupled to acetonitrile precipitation to successfully purify this ELP fusion protein, allowing for its use in further experimentation. After purification, we tested the activity of the fusion protein by both western blots and dot blots. Knowing the activity allowed us to create a toxicity profile of the compound by cell-based assays with MB49, K9TCC-SH, and K9TCC-original cell lines, and furthermore test the binding in vitro. This study focuses on the binding efficiency and activity of our targeted ELP-Dye fusion protein, and provides conclusions based on our observation of the fluorescently-tagged cancer cells when incubated with our compound.

Keywords: Bladder Cancer, Targeted Delivery, Elastin-Like Polypeptide, Detection, Cellular Biology

Application of Machine Learning to Identify Mechanobiologic Parameters for a Computational Breast-Conserving Surgery Model

SURF ID: 155
10:30 AM - 10:45 AM

*Zachary J. Harbin, David Sohutskay, Carly Mendenhall, Sherry Voytik-Harbin, Muira Fontaine, and Adrian Buganza-Tepole**
**PI: School of Mechanical Engineering*
Purdue University

Breast cancer is the most diagnosed cancer in women, with over 2 million cases each year worldwide. The preferred standard of care for these patients is breast-conserving surgery (BCS; otherwise known as lumpectomy), allowing for tumor removal while preserving healthy breast tissue. The surgery creates a tissue cavity, which heals by contraction and scar formation, making oncologic and cosmetic outcomes for individual patients difficult for surgeons to predict. To overcome these challenges, we

Keywords: Computational modeling, Mechanobiology, Breast cancer, Wound healing, Machine learning,

are developing a predictive computational mechanobiology model that simulates patient-specific breast healing following BCS and informs design parameters for new therapeutic approaches (e.g., soft tissue fillers). A mechanobiological skin wound model was adapted to a reference breast geometry with a specified lumpectomy void domain. Model parameters were identified and calibrated based on available preclinical and human clinical data. A machine learning method, the Gaussian process (GP), was used to define parameter values and relationships unavailable in the literature. Model simulations trained the GP, outputting predictive wound contraction results that were compared to available clinical data. Four model parameters, specifically the contractile force of fibroblasts and myofibroblasts, rate of plastic tissue deformation, and the saturation of mechanical force by collagen, were analyzed through the GP, resulting in the identification of parameter relationships and desired ranges of parameter values. These results provided definition of key model parameters, allowing for proper calibration of breast cavity contraction following BCS. This work represents the first step towards the development of a new tool to assist surgeons and patients with personalized treatment planning.

Biological simulation and technology

Antitumor Ability of Engineered Neutrophils Against Solid Breast Cancer

SURF ID: 165
10:45 AM - 11:00 AM

*Sydney N. Hummel, Yun Chang, and Xiaoping Bao**
**PI: Davidson School of Chemical Engineering*
Purdue University

Chimeric antigen receptor (CAR) tumor targeting immunotherapies derived from human pluripotent stem cells (hPSCs) present promising technology for targeting cancer tumors. hPSCs can be genetically edited to present chimeric antigen receptors on their surface as an off-the-shelf source of immune cells. CAR technology has successfully been shown to target various hematological, or blood-related, malignancies using immune cells such as T cells, NK cells, and macrophages. However, these mentioned immune cells have yet to effectively target solid tumors, such as breast cancer. Neutrophils are the most prevalent leukocyte, or white blood cell, in the body and have been presented as an alternative immune cell to be used for its tumor killing abilities. This project investigates the use of CAR technology in neutrophils to eradicate solid breast cancer cells in vitro. In this project, genetically engineered hPSCs with anti-fluorescein (FITC) CAR structure were successfully differentiated into functional neutrophils through an innovative robust serum- and xeno-free differentiation protocol. Bridged with FITC-folate, these CAR hPSC-derived neutrophils conjunct with breast tumor cells by immunological synapse and then effectively kill these target cells. This development in cancer immunotherapy could complement current strategies and be used to more effectively eradicate in vivo solid tumors.

Keywords: Medical Science and Technology, Tumor Immunotherapy, Neutrophils, Human Pluripotent Stem Cells

Development of a Breast Surgical Computational Model: Evaluation of Tumor-to-breast Volume Ratio on Surgical Outcomes

SURF ID: 195
11:00 AM - 11:15 AM

*Carly Mendenhall, Zachary Harbin, Adrian Buganza Tepole, David Sohutskay, and Sherry Voytik-Harbin**
**PI: Weldon School of Biomedical Engineering*
Purdue University

Breast-conserving surgery (BCS; otherwise known as lumpectomy) is an available treatment for breast cancer, where the goal is removal of cancerous tissue while preserving, as much as possible, normal breast appearance and sensation. The healing of the tissue cavity varies with patient and treatment characteristics, including tumor-to-breast volume ratio (TBVR), tumor location, radiation therapy, and breast composition. Consequently, surgical outcomes and adjunct radiation targeting are difficult to predict. To better predict BCS outcomes and improve patient-specific therapeutic planning, we aim to develop and adapt a computational mechanobiology model simulating breast void healing post-lumpectomy. We adapted a mechanobiological skin wound model to a breast geometry with parameters identified from available clinical studies. A tumor-to-breast volume ratio analysis was conducted, with clinically relevant TBVR ranging from 0.54 to 14.61 percent, and the observed time-variant cell and cytokine density within the cavity, relative cavity contraction, permanent deformation of the cavity, and whole breast contraction were measured. The results showed that the TBVR trends concerning the model's whole breast contraction and visible surface deformation are consistent with clinical data: as cavity volume increases, total deformation increases. Next steps involve further calibration of the model with available patient-specific data to improve and validate its predictability. These findings contribute to the prognostic capability of the model, ideally lending to a more informed prediction tool which will ultimately better apprise surgeons and patients of surgical treatment outcomes.

Keywords: Computational modeling, Tumor-to-breast volume ratio, Breast cancer, Wound healing, Biological simulation and technology

SESSION D: Additive Manufacturing & Energetic Materials

Click here to join the session

Studying the Effect of Reactive Component Orientation Using Multi-View Dynamic X-Ray Imaging

SURF ID: 115
10:00 AM - 10:15 AM

*Hayden Bilbo[1], Diane Collard[2], and Steven Son[2]**
**PI: School of Mechanical Engineering*
[1]University of Texas at San Antonio, [2]Purdue University

Keywords: Energetic Materials, Solid Propellant, Additive Manufacturing, Reactive Materials

The performance of solid propellants has been enhanced using a variety of different methods including altering propellant chemistry, using catalytic nanorods, embedding inert wires, and changing ammonium perchlorate (AP) oxidizer particle size. The advent of additively manufactured (AM) reactive components in propellant systems has more recently been shown to increase overall burning rate by locally increasing the effective surface area. This study incorporated multiple view X-ray radiography in determining the effect of the orientation of nano-aluminum (nAl) and polyvinylidene fluoride (PVDF) reactive fiber on propellant burn rate. Reactive fibers were made from stoichiometric nAl/PVDF filament extruded into strips 0.85mm in diameter and cut at a 5:1 (length to diameter) aspect ratio. The fibers were mixed in an AP and hydroxyl-terminated polybutadiene (HTPB) propellant and extruded in a prescribed direction, resulting in fibers with vertical, horizontal, and 45-degree orientations within the propellant. A dual-view X-ray source and intensified camera imaging system was used to capture data during testing. Matlab preprocessing coupled with a tomographic reconstruction of the images was performed to create a 3D representation of the propellant burning profile. The reconstructions were used to find and compare the volumetric consumption rates and surface profile evolution. Preliminary results demonstrate this as a viable mechanism for further enhancing the solid propellant burning rate using embedded reactive fibers.

Artificial Aging and Microstructural Characterization of an Additively Manufactured Aerospace Aluminum Alloy with Ceramic Additions

SURF ID: 152
10:15 AM - 10:30 AM

*Krish N. Gupta, Daniel Sinclair, and Nikhilesh Chawla**
**PI: School of Materials Engineering*
Purdue University

Keywords: Selective Laser Melting, Aluminum Alloys, Materials Processing and Characterization, Composite Materials and Alloys

Selective laser melting (SLM) is a method of additive manufacturing that uses lasers to fuse together a bed of metallic powders. SLM of aluminum alloys is advantageous for aerospace applications as this combination allows for rapid prototyping and weight reduction in typical lightweight alloys. Post-processing heat treatments are frequently employed to obtain precipitation strengthening in aluminum alloys. In this project, we explored AA7050 processed by Reactive Additive Manufacturing (RAM). The RAM process introduces ceramic particles for grain refinement and strengthening during SLM. Effects of artificial aging on mechanical properties were characterized through Vickers hardness testing. Microstructure was characterized through optical and electron microscopy for rods of two diameters (3mm and 12mm). An aging curve showed that a peak Vickers hardness value (HV) was reached for both rod dimensions after 24 hours of artificial aging at 120°C, matching behaviors of similar wrought alloys. The peak-aged condition was harder than a T74 overaged condition. The interior region was compared to the contour region generated during SLM. The contour was softer overall and did not reach a peak hardness by 24 hours. Optical and electron microscopy of etched samples revealed several microstructural differences between the contour and interior that may contribute to the hardness differences. The contour step during SLM manufacturing has been shown to affect the microstructure and aging behavior as compared to the interior region. This difference could result in important property variations based on part size and should be considered in the design of SLM materials that are artificially aged.

N-Amination and Oxidation: 1-amino-3,5-dinitro-1,2,4-triazole and 1-methoxy-5-nitrotetrazole

SURF ID: 177

10:30 AM - 10:45 AM

*Janine Lee, Shannon Creegan, and Davin Piercey**
**PI: School of Materials Engineering*
Purdue University

Keywords: Materials Characterization, Energetic Materials, Triazoles,

Energetic materials is a growing field within materials engineering, and it has numerous applications in both the public and private sectors. Current research is focused on developing novel compounds with increased stability and insensitivity, as well as minimizing the environmental impact. For my research on high-nitrogen heterocyclic compounds, I attempted to synthesize multiple precursors,

which includes the ammonium salt of 3,5-dinitro-1,2,4-triazole (DNT), 1-amino-3,5-dinitro-1,2,4-triazole (ADNT), 1-methoxy-5-aminotetrazole (1M5AT), and 1-methoxy-5-nitrotetrazole (1M5NT). I utilized the previously synthesized compound 3,5-diamino-1,2,4-triazole, with several different procedures, to create an ammonium salt of DNT, which I then aminated using tosylhydroxylamine compound to make ADNT. For my second project, I cyclized cyanogen bromide and sodium azide to create 1M5AT. From that point, I applied various oxidizing agents, such as potassium superoxide, sodium nitrite, and titanium superoxide, to synthesize 1M5NT. I tested different batches of each compound, including the intermediate stages, by mass spectrometry and nuclear magnetic resonance (NMR) for purity and structure. The ADNT was successfully synthesized; however, there were numerous purity issues that need to be addressed before it can be used as a future precursor to other compounds. The 1M5AT was successfully synthesized and obtained in a pure state. The oxidation reactions to create 1M5NT were so far unsuccessful, but the work will be continued.

Tetrazoles, Nitrogen Heterocycles

Dynamic Mechanical Characterization of Additive Manufactured Mock Gun Propellants

*Jalen R. Macatangay, Andrew Roginski, and Weinong Chen**
**PI: School of Aeronautics and Astronautics*
Purdue University

SURF ID: 185
10:45 AM - 11:00 AM

The mechanical response of energetic materials is important to characterize so that one may better understand and design viable explosives and propellants. Energetic materials primarily function under high strain rate applications, which cause their mechanical properties to deviate from their quasi-static counterpart. Therefore, optimizing the design and manufacturing of these materials to mitigate premature detonations has received much attention. Recent developments in 3D printing technology have led to widespread interest in implementing additive manufacturing to produce certain energetic materials. While additive manufacturing provides an alternate method with lower production costs and time relative to traditional cast approaches, quantification of their dynamic mechanical properties remains unclear. Consequently, the performance of additive manufactured energetic materials subject to high strain rates is not well understood. In this work, printed and cast mock specimens were formulated based on a polymer-bonded explosive binder used in a common gun propellant. Compression tests were conducted dynamically with a Split Hopkinson Pressure Bar and quasi-statically with an 810 Materials Test System. These tests revealed that higher strength levels and lower elongations were achieved with increasing strain rates. Furthermore, the printed specimens demonstrated enhanced mechanical performance relative to cast specimens. Therefore, the results suggest a strain rate and manufacturing method dependency of the material's mechanical behavior.

Keywords: Additive manufacturing, Split Hopkinson Pressure Bar, Dynamic Loading, Gun Propellants

Electrochemical Synthesis of 1,2,3-triazoles

*Natthakan Welaha[1], Joseph Yount[2], and Davin Piercey[2]**
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[1]University of South Florida, [2]Purdue University

SURF ID: 248
11:00 AM - 11:15 AM

Modern trends in energetic material development have focused on incorporating a high nitrogen content (more than 60% nitrogen by mass), high enthalpy of formation, and high ring strain into new energetic formulations. These attributes enhance energetic performance by allowing for the rapid decomposition to environmentally friendly N2 gas. However, traditional syntheses of heterocyclic energetic backbones, such as 1,2,3-triazoles, are often plagued by toxic heavy reagents and poor atom economy (conversion efficiency of a chemical process). Herein we attempt the electrochemical synthesis of 1-amino-1,2,3 triazole via electrochemical oxidation of bishydrazone glyoxal (BHG) without the need for additional heavy metal oxidants. Starting materials were synthesized and analyzed by cyclic voltammetry (CV) to discern electrochemical reactivity. All materials synthesized were identified using multi-nuclear Nuclear Magnetic Resonance (NMR) spectroscopy, and Electrospray Ionization Mass Spectrometry (ESI-MS). From these results we verified our initial hypothesis that we were in fact able to electrochemically cyclize BHG to 1-amino-1,2,3-triazole without the need for toxic heavy metal reagents.

Keywords: Electrochemistry, Energetic material, Green Chemistry, 1,2,3-triazoles

SESSION E: Medical Science & Technology

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Towards Osteoarthritis Special Translation

SURF ID: 141
10:00 AM - 10:15 AM

*Stephen R. Douglas, Doug Brubaker, and Deva Chan**
**PI: Weldon School of Biomedical Engineering*
Purdue University

Post-traumatic osteoarthritis (PTOA) is a chronic joint disease characterized by joint pain, stiffness, and decreased range of motion. It develops in response to joint injury, affecting the knee in 50% of the cases of a torn ACL within 10-20 years. Due in part to the shortened timeline of disease progression, lower cost, and availability of genetically modified strains, mouse models have become instrumental to studying the progression of the disease and evaluating the effectiveness of potential treatments and interventions. A great variety of mouse models are used to mimic certain aspects of osteoarthritis progression, including surgical models, injection models, and non-invasive models. Destabilization of the medial meniscus (DMM) is a widely used surgical model that is well established in literature. ACL rupture via single tibial compression (ACLR) is a recently characterized non-invasive model, developed to eliminate the confounding effects of surgery, especially at early time points. Understanding the clinical significance of each model has become increasingly important in order to best direct research efforts. In this study, I analyzed gene expression data from the DMM and ACLR models to look for differentially regulated genes during PTOA progression common to and differentiating both models. We expect to highlight significant genes and signaling pathways in each model to use for further comparison against clinical data obtained from patients with late-stage osteoarthritis.

Keywords: Medical Science and Technology, Mouse Model, ALCR, DMM, Gene Expression

Analyzing Objective and Subjective Metrics of Surgeon Ergonomics

SURF ID: 147
10:15 AM - 10:30 AM

*Alexis A. Gies[1], Nicholas Anton[1], Hamed Asadi[1], Dimitrios Stefanidis[2], and Denny Yu[1]**
**PI: School of Industrial Engineering*
[1]Purdue University, [2]Indiana University

Musculoskeletal symptoms highly impact surgeons as part of the nature of their job. Laparoscopic surgeries present significant benefits for patients in that they decrease recovery time and damage to surrounding tissues. However, these surgeries may increase a surgeon's risk of developing musculoskeletal symptoms and injuries. This pilot study aims to observe the levels of muscular and mental discomfort in experienced and training surgeons during traditional and robot-assisted laparoscopic surgeries in the operating room as a whole case and during critical phases of a surgery. Objective and subjective metrics were applied to assess musculoskeletal discomfort. Participants were given validated questionnaires assessing their perceived levels of discomfort immediately before and after each procedure. Electromyography (EMG) and inertial measurement unit (IMU) sensors were worn by participants during each procedure to collect objective data on the muscle activity of their deltoids and trapezii and record their postural changes. Video data was collected to verify the sensor data. There were no differences between the two surgery methods with respect to muscular activity and postural changes for the entirety of the surgery and during critical phases of the procedures. Further, no significant differences were present between muscular activity and postural changes between experienced and resident surgeons for either surgery type. Surgeons reported increased irritability and more difficulty concentrating after robotic procedures than after traditional laparoscopies. Additional research on how muscular fatigue develops during specific steps of select procedures should be investigated.

Keywords: Ergonomics, medical science and technology, laparoscopic surgeries, robot-assisted laparoscopic surgeries, musculoskeletal symptoms

Evaluation of the Novel Automated Segmentation Algorithm of Trabecular and Cortical Region

SURF ID: 176
10:30 AM - 10:45 AM

*Hyunseo Lee, Zachary Davis, and Deva Chan**
**PI: Weldon School of Biomedical Engineering*
Purdue University

Micro-Computed Tomography (μCT) has become an important tool to quantify the trabecular and cortical bone microstructure in human and animal studies. However, it is difficult to obtain structural and composition information because the intersection between the trabecular and cortical bone in μCT is hard to determine and there is no contrast between the two regions. Commonly, segmentation of trabecular region is done manually on a slice-by-slice basis but is time-intensive and subjective, providing motivation for automated segmentation. This study tests the sensitivity of the parameters of the novel centroid-based algorithm and evaluates the segmentation algorithm against the manually

Keywords: Automated Segmentation, Trabecular, Cortical, thresholding, micro-CT, 3D Mask, Image Segmentation, Dice

segmented reference. Parameters tested are the number of spokes, smoothing parameters (kernel size), binarization parameters, max curvature parameters and the size of the sphere for erosion and dilation coupling that affects the smoothness and delineation of the segmented 3D mask. After the modification of the parameters, the results were evaluated against manually segmented reference from the same six Hindlimb Unloaded Proximal femur head sample µCT images. Initially, spatial overlap-based index - Dice Similarity Coefficient (DSC), True Positive Rate (TPR), and spatially distance-based index - Hausdorff Distance (HD), Mahalanobis Distance (MHD) were analyzed to validate comparable parameter values. Then, the success of the automated algorithm was determined based on the Dice Similarity Coefficient (DSC) calculated against the reference which was considered acceptable if DSC ranged between the recommended number of 0.7 ~ 1. Efficient automated segmentation of cortical and trabecular sections will enable researchers to perform user-specific microstructural analysis of long bones.

An Adaptable Prosthetic Limb: Discovery of Product-Application Fit, Conceptualization, and Design Inception

SURF ID: 216
10:45 AM - 11:00 AM

*Shivani Pranatharthi Haran, Soumya Bandyopadhyay, and Justin Weibel**
**PI: School of Mechanical Engineering*
Purdue University

Tunable products are ubiquitous in modern-day application ranging from miniaturized electronic devices to automobiles. Tunable products refer to devices that have multiple operating modes depending on some external stimulus or controlled input. In this project, an iterative product-application discovery process was implemented, and three main application areas were investigated. Performance enhancement of portable electronics was first explored, where the adaptable product would have multiple thermal conductance states for maintaining the chip and display/cover temperatures within thresholds; however, the extreme geometric and other constraints in the electronic devices pose significant challenges in the design space. Next, a different application of tunable technologies in controlling the actuation of valves, thereby modulating the flow of refrigerant, in HVAC systems was evaluated. Finally, the application of adaptable prosthetic hands for enabling human to perform daily tasks were explored. Using an unbiased weighted decision matrix, this prosthetics application out-ranked the others, primarily on the basis of impact. Existing technologies for robotic hands were surveyed, as a benchmark in different industrial applications. The needs and requirements for designing an anthropomorphic robotic hand for children aged between 7 and 14, that would enable them to use touch-screen-based portable electronic devices were subsequently identified and outlined. The engineering design and the conceptualization of different components of the design of a prosthetic human hand are presented. Finally, a representative design of an anthropomorphic human finger was presented, which would be subsequently modified to incorporate the required engineering systems to enable complete functionality and end-user satisfaction.

Keywords: Product, application, adaptability, tunability, human dexterity, maneuverability, prosthetics, robotics, machine learning

Evaluating Finger Flexor Tendon Fatigue Using High-Frequency Ultrasound Based Strain Algorithms

SURF ID: 134
11:00 AM - 11:15 AM

*Andrew J. Darling, Conner Earl, Fredrick Damen, Nan Chen, Guoyang Zhou, Denny Yu, and Craig Goergen**
**PI: Weldon School of Biomedical Engineering*
Purdue University

Ultrasound speckle tracking can be used to study the movement of the flexor digitorum superficialis, which is a tendon responsible for finger contraction. Under cyclical loading, this tendon is known to demonstrate fatigue and injury; however, there is no standard method for measuring the mechanical properties. This study aimed to investigate the differences in strain estimations over a predetermined contraction and relaxation cycle where the flexor digitorum superficialis tendon undergoes stress. We hope to provide a novel, reliable, and noninvasive method for estimating strain. Participants were asked to perform 5 variations of a contraction and relaxation cycle in which the flexor digitorum superficialis tendon performed grip strength exercises. A high-frequency ultrasound imaging system was used to collect ultrasound videos of the tendon. The images were then exported to a custom-built image analysis script allowing us to estimate strain using speckle tracking. Subjects demonstrated a constant strain during relaxation and hold periods. Horizontal strain estimates varied in magnitude from 6% to 25% during the contraction period (n=1). While results have been observed for short term contraction and relaxations, long term analysis of strain may be needed to be able to quantify fatigue. Initial results indicate that strain in the FDS tendon recovers quickly after the contraction period

Keywords: Strain, High-frequency Ultrasound, Tendon, Medical Science and Technology, Biological Characterization and Imaging

concludes. Overall, we also showed that we can estimate tendon strain using an in vivo, non-invasive imaging approach. In vivo strain estimation provides a quick and safe method of measuring tendon strain that has the potential to improve workplace safety and recovery from injury.

RF Reader for Battery-less RFID Tag in Implanted Neural Recorder

SURF ID: 256
11:15 AM - 11:30 AM

*Ruichao Zhang, Zhize Ma, and Saeed Mohammadi**
**PI: School of Electrical and Computer Engineering*
Purdue University

Keywords: RFID, RFID Reader, Neural Recorder, Active Reader Passive tag

Radio-frequency identification (RFID) readers are used in wirelessly communication with a central system and a remote RFID tag. The neural recorder developed in our group is similar to an RFID tag and is expected to be implanted in free moving organisms sensing and collecting neural signals. In this project, an RFID reader will be developed for transmitting and receiving signals from and to the integrated neural recorder (tag). In other words, the neural recorder will behave as the tag in this RFID system and it receives commands and transmits collected neural data from and to a computer directly connected to the reader. To work properly with the neural recorder, the device needs to handle carrier frequency from 900MHz to 1500MHz. The transmitter leakage signal to the receiving path is the main problem for the active reader with passive tags pair. The analog front end of the reader consists of three main parts: a receiver, a transmitter, and a cancellation chain, to establish solid bidirectional communication with the tag. The perturbation and observation method of maximum power point tracking (MPPT) algorithm is implemented in the cancellation chain to solve the problem. From the measurements on an oscilloscope, the receiver shows that the two resulting waves, in-phase and quadrature images, are clear and expected with good transmitter leakage cancellation; the transmitter also gives power-amplified, solid, and stable signals. After implementing the link between the antenna, and the on-chip battery-less tag, the RF system should work properly, which facilitate testing of the world's smallest neural recorder.

SESSION F: IOT for Agriculture

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Analyzing Efficacy of Nitrogen-Fixing Biological Amendments in Maize Using Agronomic Metrics and Experimental IoT LiDAR

SURF ID: 122
10:00 AM - 10:15 AM

*Rebecca E.H. Caldbeck[1], Garrett Verhagen[2], Brendan Hanson[2], David Cappelleri[2], Brian Huang[2], and Tony Vyn[2]**
**PI: Department of Agronomy*
[1]University of Kentucky, [2]Purdue University

Though nitrogen (N) comprises 78% of the atmosphere as N2, the essential compound cannot be harnessed by plants without modification. Unlike their leguminous counterparts, commercially grown maize (Zea mays L.) is incapable of symbiotically interacting with N-fixing rhizobium bacteria. Proven, a product of Pivot Bio, is the first commercially available N-fixing biological to associate with maize. Centered on a genetically altered γ-proteobacterium, Proven claims to fix between 20-30 pounds of N per acre and to boost maize yields at low-to-moderate N rates. Proven could provide an economic advantage to farmers via a net reduction of the expenditures associated with synthetic N application. Proven, and its biological successors could positively impact the environment via mitigating deleterious impacts of excess synthetic N, such as waterway eutrophication, reactive-N greenhouse gas emissions, nutritional imbalances, and soil acidification. This study examines phenotypic responses of maize to a prototype biological applied at planting and fertilized at various N rates. For quantitative data collection, direct and novel imaging approaches were applied at multiple development stages to analyze plant morphology during late vegetative and early reproductive growth. Measurements included lower stalk diameter, plant height, whole-plant above-ground biomass, and relative leaf greenness. The efficacy of N-fixing biological amendments was analyzed in maize using traditional quantitative metrics, in addition to an IoT (Internet of Things) LiDAR (Light Detection and Ranging) proof-of-concept approach, collected via a ground robot. Tentative conclusions are provided, based primarily on lower canopy observations, to illustrate how the biological amendment impacts maize development.

Keywords: LiDAR, Nitrogen Fixation, Biologicals, Maize, Ecology and Sustainability, Environmental Characterization, Machine Learning: Big Data, Biological Simulation and Technology

Precision Agriculture: Autonomous Corn Leaf Sampling

SURF ID: 163
10:15 AM - 10:30 AM

*Brian B. Huang, Juncheng Li, Kuvarjit Sagar, Wendy Kim, and David Cappelleri**
**PI: School of Mechanical Engineering*
Purdue University

The world population is estimated to reach 9.7 billion by the year 2050, and current agricultural practices are inefficient in terms of water, energy, and agrochemical usage. Along with inefficient practices, farmers lose 400-500 acres of land every year due to a variety of diseases, such as fungi and bacteria. One crop that is particularly susceptible to this is corn. This project aims to create an autonomous mobile robot that will be able to collect corn leaves throughout the growing season. The collected samples will be used for current state assessment and prognostics for the corn and allow for appropriate interventions to be implemented if indications of disease are identified that threaten the plants. A Jackal mobile robot platform has been customized for this project. The robot was equipped with a custom sensor suite mounting system that was able to hold a visual-inertial tracking camera, an RGB camera, and a light detection and ranging sensor. On the other end of the robot, there is a robotic arm fitted with a custom vision-guided nichrome wire end-effector used to cut the corn leaves. Machine learning algorithms were used to train the Jackal to identify corn leaves and corresponding collars at the exact location to cut. The sensor suite mounting system and end-effector system were both successfully fabricated and integrated into the Jackal mobile robot platform. Field tests utilizing each subsystem have been performed. The machine learning algorithms have been tested and were successful at identifying corn leaves of interest and their collars. This project demonstrated how computer vision can be adapted to agricultural vehicles and how mechanical systems can help save time and money for farmers, increasing crop production, and feeding people around the world.

Keywords: Precision agriculture, leaf sampling, machine learning, autonomous agriculture vehicle

Atmospheric Correction: Comparison of the Empirical Line Method with Radiative Transfer Models on Hyperspectral Data

SURF ID: 171
10:30 AM - 10:45 AM

*Nicole M. Kozel, Karoll Quijano, and Melba Crawford**
**PI: Lyles School of Civil Engineering*
Purdue University

Images collected through remote sensing, whether gathered from satellites or unmanned aerial vehicles, require correction for both the sun angle and atmospheric distortion. Multiple methods exist to correct images, including the empirical line method (ELM) and radiative transfer models. We want to understand the differences between ELM, QUick Atmospheric Correction (QUAC), and Fast Line-of-sight Atmospheric Analysis of Hypercubes (FLAASH), a radiative transfer model. Additionally, we want to know if we can improve the results from FLAASH if the parameters used are more precise. Hyperspectral crop data was gathered from experimental fields of corn and sorghum at Purdue's Agronomy Center for Research and Education (ACRE). The data was brought to the lab to be processed with ELM, QUAC, and FLAASH to get reflectance data. This process was repeated for each set of data. The reflectance data from each method was compared over five targets including soil, vegetation, a panel with eleven percent reflectance, a panel with thirty percent reflectance, and a panel with fifty-six percent reflectance. Additionally, the data was corrected with FLAASH multiple times with changes made to different parameters. From these results, we can determine what can be done to improve results using FLAASH if we have more precise parameters. The results obtained provide new insights into atmospheric impacts on remote sensing data, improving current operations for atmospheric correction.

Keywords: Remote Sensing, Unmanned Aerial Vehicles, Empirical Line Method, Radiative Transfer Models, Hyperspectral Imagery, Atmospheric Correction

ISOBlue Lite: Collecting Data from Agricultural Vehicles Using a Raspberry Pi

SURF ID: 204
10:45 AM - 11:00 AM

*Zachary T. Neel, Fabio Castiblanco, Andrew Balmos, Dennis Buckmaster, and James Krogmeier**
**PI: School of Electrical and Computer Engineering*
Purdue University

The internal communications of agricultural machinery has become an important source of data for precision agriculture. By analyzing this data, researchers and farmers can better understand equipment performance and operator behavior. The ISOBlue project was started so researchers would be able to collect and analyze this data, but the computer hardware required was not ideal for all use cases. Specifically, the Toradex Apalis boards used on the previous ISOBlues were expensive, and therefore, not easy to deploy on a large fleet of agricultural vehicles. This research project used a Raspberry Pi 4, a low-cost, single-board computer, as an alternative embedded computer to collect the vehicle's internal CAN-bus (Controller Area Network) data and GPS data. This was accomplished by porting the ISOBlue project's latest software stack, Avena, to the Raspberry Pi. Finally, the ISOBlue Lite was field tested on a tractor and sprayer to determine whether the Raspberry Pi could be used in place of other embedded computers. Our team found that, with the essential features available on the ISOBlue lite, the Raspberry Pi is a viable low-cost alternative to the other, more expensive embedded computers used in other ISOBlues. In conclusion, by integrating ISOBlue Avena onto the Raspberry Pi platform, our team was able to create a low cost device which can provide information on the performance of agricultural vehicles.

Keywords: Raspberry Pi, ISOBUS, Precision Agriculture, Open-Source, Controller Area Network, Internet of Things

Path Loss Using Low-Power Wireless Communication Techniques in Digital Agriculture Applications

SURF ID: 222
11:00 AM - 11:15 AM

*Chris Alejandro Rodriguez, Yaguang Zhang, Andrew Balmos, Fabio A Castiblanco, Dennis Buckmaster, and James Krogmeier**
**PI: School of Electrical and Computer Engineering*
Purdue University

The ability to have an efficient and reliable communication protocol especially in areas where good communication connectivity is scarce, such as agricultural areas is a problem that is constant, specifically in digital agriculture applications where sensor networking and the acquisition of data with agricultural machinery is essential. To improve connectivity in rural areas such as in farms, evaluating and analyzing the performance of LoRa (long range) which is a technique for long-range low power wireless communications, will be important in determining whether the implementation of LoRaWAN (LoRa Wide Area Network) in ISOBlue, an open-source data telematic device for agricultural machinery, would be useful in GPS data collection for a vehicle of interest in real time when LoRa connection is available. To determine whether it would be a good solution to our problem, path loss analysis was performed using python on data sets that were acquired around ACRE (Agronomy Center

Keywords: ISOBlue, ISOBUS, Open-Source, LoRa, LoRaWAN, SNR (Signal-Noise-Ratio), RSSI (Received Signal Strength Indication), ACRE (Agronomy Center for Research and Education), Internet of Things, Path Loss

for Research and Education). Calculating the SNR (Signal-Noise-Ratio) at random points, in a 5 miles radius around the cell tower, gave us more insight in how LoRa would perform. The bigger the SNR at further distances, the better, along with bigger RSSI (Received Signal Strength Indication) numbers. This means that LoRaWAN will be effective as a radio on agricultural machinery/equipment. In conclusion, adding LoRaWAN to ISOBlue would mean a better alternative in GPS data collection for agricultural machinery.

Single- and Multi-UAV Trajectory Optimization and Simulation

*Jiecheng Zhang, Vinayak Suresh, and David Love**
**PI: School of Mechanical Engineering*
Purdue University

SURF ID: 255
11:15 AM - 11:30 AM

Keywords: UAV, telecommunication, energy efficiency, convex optimization, fractional programming, trajectory optimization, agricultural sensing

Recently, unmanned aerial vehicles (UAVs) have attracted significant interest in wireless communication systems and agricultural uses due to their high versatility, functionality, and portability. Applications include the use of UAV(s) to collect sensor data from fields and machineries, relaying data from different ground terminals, etc. While UAVs are a promising technology, they can be quite energy consuming to operate. The energy expended by a UAV is a function of its flight profile. In this paper, we study ways to optimize the trajectory of one or more UAVs communicating with moving ground terminals (GTs), to achieve maximum energy efficiency. Here, energy efficiency is defined as the ratio of the total data rate to the total energy expenditure, and GTs represent either sensors or moving farm machinery. Using models of signal transmission and UAV mechanics documented in previous works, we derive a nonconvex maximization problem with general constraints on velocity, acceleration, and kinematic laws. Then, we reformulate the constraints to obtain a fractional programming problem that can be solved iteratively to obtain the optimal trajectory. The study is then extended to include scenarios of multiple UAVs with the consideration of collision prevention. Our numerical results demonstrate that trajectory optimization increases energy efficiency both for the single- and multi-UAV cases, compared to the other benchmarks.

SESSION G: Sensors & Microsystems

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Near-infrared Sensor Model Development

SURF ID: 183
10:00 AM - 10:15 AM

*Derek Lynn, Rexonni Lagare, Yan-Shu Huang, and Gintaras Reklaitis**
**PI: Davidson School of Chemical Engineering*
Purdue University

Keywords: Near-infrared Sensor, Composition, Density, Model Development, Pharmaceutical Manufacturing

Near-infrared (NIR) sensors are useful in pharmaceutical manufacturing because they are non-destructive and can be used to characterize flowing powders in real time. They have been demonstrated to be effective in monitoring the composition and density of flowing powders, which are attributes that are critical to the quality of pharmaceutical products. In literature, the monitoring of these critical-to-quality attributes were conducted separately. The goal of this study is to develop a model that can use the NIR measurements to infer the powder composition and density altogether. This requires the use of multivariate statistical methods and concepts that are suitable for handling NIR spectra, which typically results in large amounts of data. Samples of known composition and density were used to collect data. Different amounts of microcrystalline cellulose powder (MCC) and acetaminophen powder (APAP) were hand mixed to create the different composition samples. The density of a sample was changed by tapping it on a benchtop at different amounts of taps. The developed models were tested by applying them to a real time continuous measurement where they predicted the different attributes of the samples. Based on the predictions from the model, more than one attribute can be monitored from a single NIR probe.

Membrane Mechanical Parameter Extraction from Laser-Induced Vibrations

SURF ID: 169
10:15 AM - 10:30 AM

*Scott E. Kenning, Adam Behnke, Thomas Pollei, and Kevin Webb**
**PI: School of Electrical and Computer Engineering*
Purdue University

Keywords: optical force, resonance, membrane, parameters, silicon nitride

Silicon nitride (SiN) membranes are of use in many fields, particularly optomechanics, sensing, and MEMS. Precise estimations of their mechanical parameters are often required to deduce information such as resonance frequencies. To do this, the membrane must be excited in some way, which is currently limited to mechanical excitation strategies. For membranes with high resonance frequencies, mechanical excitation is difficult. It is much simpler to utilize a laser which has a high modulation frequency typically spanning into the hundreds of megahertz. A method to excite membranes using optical force is proposed along with two methods to extract parameters depending on the experimental setup. A comprehensive optical force model on bare SiN membranes is developed to model deflection from impinging laser light. With experimental data, it is possible to employ an optimization algorithm to fit the forward model to the experimental data, thus estimating the parameters of interest. This work may be useful in new mechanical parameter measurement devices to provide precision measurements of micrometer and nanometer scale mechanical resonators. Optical-force-induced vibrations as vehicle for parameter extraction may be extended to other mechanical structures to provide a novel and comprehensive strategy for understanding small scale mechanical devices.

Stretchable, Functional, and Biocompatible Cellulose-based Fibrous Composite Fabrication and Characterization

SURF ID: 180
10:30 AM - 10:45 AM

*Yuwei Katherine Liu, Wenhui Xu, Yanbin Wang, and Tian Li**
**PI: School of Mechanical Engineering*
Purdue University

Keywords: Nanotechnology, Cellulose Composite, Hierarchical Scaffold, Functional Fibers

To better cooperate with flexible, self-powered, and direct-current generating wearable devices, the stretchable, biocompatible, and conductive materials that replace the traditional inflexible ones are needed. In this work, natural cotton fibers are used as a hierarchical scaffold incorporating other materials into the spacing among the cellulose microstructures and nanofibers. Therefore, composite fibers can be made towards functional devices. Different cellulose-based fibrous composites are fabricated by infiltrating conductive or biocompatible materials to the multiscale structures, thus sharing the properties of each phase. Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT: PSS), Carbon Nanotube (CNT), and hydrogel are utilized to tune the structures and properties of cellulose-based fibrous composites. In addition, different intertwining and fabrication processes are explored to see the changes in electrical, mechanical, and other properties. Conductive particles are entrapped in the cellulose scaffold by infiltrating cotton fibers with pre-prepared PEDOT:

PSS and CNT solutions. A crosslinked-hydrophilic polymer is attached to the cellulose scaffold by incorporating cotton fibers in the hydrogel synthesis process. The cellulose-based fibrous composites are successfully fabricated, having scalability, mechanical strength, and uniformity. This study suggests potential in introducing other materials to the cellulose hierarchical structure, further applications, and room for performance improvements of cellulose-based fibrous composites.

Automated Measurement of Acoustoelectric RF MEMS for Wireless Communication Applications

SURF ID: 133
10:45 AM - 11:00 AM

*Jaideep Damle, Jackson Anderson, Matthew Storey, and Dana Weinstein**
**PI: School of Electrical and Computer Engineering*
Purdue University

Keywords: RF MEMS, Acoustoelectric Effect, Beamforming, Antennas

Many of the technologies required in the modern 5G era of wireless communication, including beamforming and multiple-input, multiple-output (MIMO), require larger arrays of antennas. As a result, it is desired to replicate radio front end circuitry on the micro/nano scale and integrate numerous devices on to a single chip, including amplifiers, circulators, and phase shifters - all of which can be created in acoustoelectric radio frequency microelectromechanical systems (RF MEMS). Utilizing dual DC biasing for the acoustoelectric interactions allows for control over both amplification and phase shift of the input RF signal. Characterizing these devices by manually applying these two voltages over a large range is very time-consuming and inefficient. Automation code was developed to synchronize a network analyzer and two DC pulse sources that were applied to the device simultaneously. This code allows for characterization of the devices with increased resolution of over 1600 bias combinations that would not be feasible with manual instrument control. RF performance was collected with bias voltages ranging from -20 to 20 V in 1 V increments, collected over approximately eight hours, demonstrating an acoustoelectric gain of -20.7 to 23.8 dB and phase shift of -3.3 to 40.3 degrees. This data aligned well with manual measurements taken over an extended period with 5V resolution, thereby proving that the automation code can apply voltages and output data as accurately and more efficiently than manual measurements.

Optimizing Conjugated Ligand Incorporated Two-Dimensional Lead-Free Perovskites for Field Effect Transistors

SURF ID: 143
11:00 AM - 11:15 AM

*Joseph Farrell, Yao Gao, and Letian Dou**
**PI: Davidson School of Chemical Engineering*
Purdue University

Keywords: Molecular Engineering, Crystal Structure, 2D Halide Perovskite

Halide perovskite is a promising alternative to silicon in field effect transistors, but it suffers from environmental instability, particularly in tin-based perovskite field effect transistors. This project investigated a series of conjugated ligands and the effect they had on the crystallization process of two-dimensional (2D) Sn-based perovskites, to find an ideal thin film morphology while maintaining high crystallinity and environmental stability. To achieve perovskite crystallization, precursor solutions were deposited onto silicon substrates as a thin film using a combination of spin coating and thermal annealing. Additionally, additives were mixed into some precursors and direct antisolvent dripping while spin coating was employed. The polycrystalline perovskite thin films were characterized using a combination of the materials' innate photoluminescence and X-ray diffraction measurements. This project analyzes X-ray diffraction measurements and optical microscope pictures to show how the 2T, and 3T ligands behaved while varying conditions such as annealing temperature, precursor additives, and antisolvents dripped onto the thin films.

Investigating the Feasibility of On-line Particle Size Distribution for Real-Time Condition Monitoring of a Continuous Dry Granulation Process

SURF ID: 104
11:15 AM - 11:30 AM

*Mariana Araujo da Conceicao, Rexonni Lagare, Zoltan Nagy, Marcial Gonzalez, Yan-Shu Huang, Ariana Acevedo, and Gintaras Reklaitis**
**PI: Davidson School of Chemical Engineering*
Purdue University

Keywords: Material Processing and Characterization, Chemical Unit Operations, Particle Size Distribution, Particle Flowability.

Real-time condition monitoring is the key to achieving greater process control and economic viability for continuous pharmaceutical manufacturing process. The ability to obtain real-time information allows the early detection of process faults, which helps prevent costly and unnecessary shutdowns and enables greater control over product quality. To achieve this, data collected through the use of sensors should be converted into information about the process conditions to further establish a control system for quality assurance. The Eyecon2TM sensor is a direct imaging particle analyzer that can collect particle size distributions (PSD) and shape measurements in real-time. Particle size and

shape are two strong indicators of powder properties given their effects on other properties such as powder flowability, compressibility, and dissolution time. This research aims to establish the feasibility of the Eyecon2TM sensor in monitoring particle characterization by using polystyrene and sieved granulated sugar samples. Two strategies were employed: comparing the sensor measurements to the established PSD measurement tool Morphologi G3, and exploring the potential of the measurements to predict the condition of powder flowability. The studies revealed that the Eyecon2TM produced similar reading trends to the Morphologi G3, confirming the reliability of its measurements. Furthermore, the Eyecon2TM was not demonstrated to be capable of predicting flowability properties of granules that are directly relevant to the condition of the process. This was likely due to composition variability, which needs to be controlled in future research work.

Day 2 | Afternoon Presentations

July 30th, 2:00 PM – 3:30 PM EDT

SESSION A: Material Modeling & Simulation 2

Click here to join the session

Development of Predictive Radiation Hardening By Design Tools

SURF ID: 124
2:00 PM - 2:15 PM

*Landon Carre, John Martinuk, David Kortge, and Mark Johnson**
**PI: School of Electrical and Computer Engineering*
Purdue University

As the limits of human exploration are expanded to increasingly extreme, radiation-filled environments, so is the necessity for the implementation of radiation hardened integrated circuit designs. The inaccessibility and rigidity of the fabrication process makes it necessary for IC designers to be able to predict radiation hardness of a design prior to fabrication. We sought to gather information and create a radiation effects simulation tool to test designs to lend the SoCET team and affiliated programs the ability to pursue radiation hardening by design using a predictive tool before chip fabrication. We initially focused efforts on developing a 2-D simulation of single event effects. The simulation program was written in Cadence Virtuoso using the SKILL language. The methodology we followed for the 2-D simulation involves injecting charges at multiple nodes where a simulated particle would collide with the layout causing a change in voltage. Once this is done, we will then be able to plot the waveforms of outputs nodes and calculate the area of voltage glitches to determine the sensitivity of a particular region on the design. We have used the 2-D simulation to learn the basics of a radiation effects simulation, but all sources have indicated that a 3-D design is needed for predictive results. The 2-D design can be useful for quick design testing and guidance, but we have begun research into tools such as TCAD to give us the capability of developing a predicative 3-D simulation and have developed a plan of learning/implementation.

Keywords: Radiation hardening, Radiation Simulation, Cadence Virtuoso, Skill Scripting, TCAD, predictive designing, Space technology

Application of Space Radiation Environments Software and Models on Magnetoresistive RAM Technologies

SURF ID: 149
2:15 PM - 2:30 PM

*Aaron H. Guo and Peter Bermel**
**PI: School of Electrical and Computer Engineering*
Purdue University

Space radiation poses a significant risk to electronics, particularly in memory devices. While specialized radiation-hardening fabrication processes exist, they are not generally utilized in commercial electronics. The objective of this research is to evaluate the efficacy of existing space radiation environments software (e.g., CRÈME, SPENVIS) to quantify total ionizing dose (TID) and single event upsets (SEUs) in magnetoresistive random-access memory (MRAM), an emerging non-volatile memory that uses nanoscale ferromagnets to store information. The SPENVIS software was first used to evaluate the anticipated dose of ionizing radiation for common satellite orbits in low Earth and geosynchronous environments. A combination of the AP8/AE8 trapped proton and electron models, in addition to empirical data on galactic cosmic rays (GCR), was used to evaluate TID. Although effective at determining dose levels in space environments, device-level analysis is lacking in SPENVIS. As such, further physical experimentation or alternative simulation solutions (such as TCAD) are warranted to draw conclusions on MRAM susceptibility to TID. To evaluate SEUs, the CRÈME suite, using the Monte Carlo transport model, was implemented to evaluate physics-based phenomena in an MRAM stack structure. Upon defining a sensitive volume within the device, the software allows for the calculation of energy deposition in various space environments, in addition to a prediction for the SEU rate. Although an improvement from previous SEU models, results from CRÈME-MC were found to overemphasize the effects of trapped protons within the MRAM device, leading to higher-than-expected upset rate calculations for orbits within the Earth's magnetic field.

Keywords: TID, SEU, galactic cosmic rays, trapped radiation, solar particle events, MRAM

Initial Evaluation of a Perovskite Semiconductor for a Betavoltaic Application

SURF ID: 200
2:30 PM - 2:45 PM

*Andrew J. Mulrenin, Darrell Cheu, Thomas Adams, and Shripad Revankar**
**PI: School of Nuclear Engineering*
Purdue University

Keywords: lead halide perovskite, MAPbI3, betavoltaic, tritium, MCNP, Material Modeling and Simulation

Betavoltaic cells convert the kinetic energy from a beta-emitting source into electrical current, similar to how solar cells utilize photons from the sun. Organic-inorganic lead halide perovskites are a certain category of semiconductors that have been successfully applied in solar cells, due to high power conversion efficiencies and low manufacturing costs but have only recently been explored in the context of betavoltaic cells. The perovskite MAPbI3 was evaluated as a potential semiconductor for betavoltaic devices in terms of power output performance. MCNP6.2 was used to simulate electron transport in an MAPbI3 device under electron beam irradiation from an SEM ranging from 2 to 19 keV, mimicking a tritium source's emission spectrum. Absorption depths were determined with the F6 tally measuring energy deposition and were used to compute I-V curves with the Shockley-Diode model. At an activity of 90 mCi, theoretical power output was estimated to be 37.68 nW, which is slightly lower than measured NanoTritiumTM cells of similar activity at 39.11 nW. At an activity of 253 mCi, power output was estimated to be 102.35 nA, which is significantly lower than other comparable perovskite-betavoltaic designs at 534 nW. These results suggest that MAPbI3 is not likely suitable for betavoltaic applications, especially considering it has been reported to rapidly degrade from electron radiation under 10 keV.

Space Environment Radiation Effects on Commercial Magneto-resistive Random Access Memory (MRAM)

SURF ID: 217
2:45 PM - 3:00 PM

*Matthew J. Rahfaldt and Peter Bermel**
**PI: School of Electrical and Computer Engineering*
Purdue University

Keywords: Magneto-resistive RAM, MRAM, Random Access Memory, Space environment, Radiation, Commercial, Off-the-Shelf, Cobalt-60, Spin-Transfer Torque MRAM, Gamma radiation

With increasingly ambitious activities taking place in outer space, more advanced electronics suitable for this environment are needed. While cutting-edge commercial electronics offer attractive capabilities, they are often not designed for the higher ionizing radiation levels of space. Magneto-resistive Random Access Memory (MRAM) is an emerging commercial memory technology relying on permanent magnets rather than electrostatic charge used in other types of RAM. While MRAM may be less susceptible to radiation effects than conventional RAM, further investigation is needed to quantify the sign and magnitude of this effect, and to develop appropriate shielding designs for various space missions. This project investigated how a commercial off-the-shelf MRAM device behaves under radiation doses like those experienced by satellites in low Earth orbit. Using a 1.62 Krad per hour cobalt-60 gamma emitter, we will expose a 16 Mbit Renesas Spin-Transfer Torque MRAM device to an accelerated dose of radiation that would normally be experienced after approximately 3 years in low Earth orbit. Before and after exposure, the device properties, write/read operations, and the number of errors were observed and measured. In this study, we compare the measurements of the experiment with other devices used in space to evaluate the use of the Renesas MRAM device in space applications, and discuss the generally observed and expected effects of radiation on MRAM devices.

IoT Based Sensing Platform for Real-Time Compressive Concrete Strength Monitoring

SURF ID: 257
3:00 PM - 3:15 PM

*Bowen Zheng, Nithin Raghunathan, Thirawat Bureetes, Enrique Silva, Na Lu, Vishal Saravade, Zhihao Kong, and Luna Lu**
**PI: Lyles School of Civil Engineering*
Purdue University

Keywords: Concrete, Strength of materials, Internet of Things, Materials Processing and Characterization, Material Modeling & Simulation

The concrete compressive strength variation with time at the early age of poured concrete is an integral component of quality control and durability of concrete used in the construction industry. The present research aims to develop an automated, field deployable, and cost-effective Internet of Things (IoT)-enabled system for the real-time monitoring of compressive concrete strength with the least human interactions. The proposed system has an automated cloud-based platform interconnecting several nodes without the delay of shifting among tasks. The data acquisition utilized lead zirconate titanate (PZT) sensors and temperature sensors. Then the wireless data transmissions are realized through Bluetooth Low Energy (BLE) and Long Range communication (LoRa) among devices. Finally, data are uploaded to the server and processed to visualize on the website. The five prototypes are developed to test the proposed system. Besides, the power consumption test, resistive temperature sensor measurement test, BLE functionality and signal strength test are conducted to validate the

developed prototypes. Moreover, the feedback resistor and gain factor resistors are also optimized for various sensors. The results from prototypes are found to match the relationship of concrete compressive strength variation with time, which are measured using other established equipment and predicted based on maturity relationships for concrete mixes developed filling standard specifications. The results demonstrated the effectiveness of the proposed automated process of the real-time monitoring of the early age compressive concrete strength based on maturity methods.

SESSION B: Environmental Characterization 2

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Industrial Water Consumption Coefficients and the Effect on Regional Water Availability

*Annalynne P. Doll[1], Hua Cai[1], Ting Liu[2], and Inez Hua[1]**
**PI: Lyles School of Civil Engineering*
[1]Purdue University, [2]Arizona State University

SURF ID: 139
2:00 PM - 2:15 PM

Gaps within water use data are common due to a lack of regulations and the requirements on reported information differing between the state and federal levels. This study aimed to increase the accuracy of consumptive water coefficients and their respective environmental impacts in Indiana by finding commonalities between state and federal data sets. Understanding water consumption and the associated environmental impacts will allow for gaps within the current data to be filled and then used to inform industrial water use based on regional water availability. For each state, three datasets were used to match the state-level facility water use registration number to a federal National Pollutant Discharge Elimination System (NPDES) permit. Using the criteria of facility name, county, city, standard industrial classification (SIC) code, and location across the three datasets, facility matches were found. Available withdrawal and discharge data were then matched with a unique facility, leading to the computation of consumptive coefficients. Through geographic information systems (GIS), matched facilities were mapped and overlayed with water stress and watershed layers to determine the environmental impacts of current water consumption as well as locations of concern. Conclusions and recommendations based on GIS mapping will provide a guide for the mitigation of environmental impacts and sustainable use of available water. These results suggest that the methodology for data matching and GIS mapping are not unique to Indiana and can be used to bridge data gaps across the United States.

Keywords: Ecology and sustainability, Environmental characterization, Industrial water use, Industrial water consumption

Workflow Design and Visualization of Water Quality Data

*Anushka Gupta, Benjamin Hancock, and Dharmendra Saraswat**
**PI: Department of Agricultural & Biological Engineering*
Purdue University

SURF ID: 151
2:15 PM - 2:30 PM

LOAD ESTimator (LOADEST) is a software program that uses multiple regression models to predict instantaneous constituent loads for irregularly recorded water quality data from streams and rivers. Water quality data processing with LOADEST is faced with a complicated workflow for the creation of input files. To simplify the input data creation, the current study focused on designing a detailed workflow for a guided generation of input files before running them through the LOADEST software. As a proof of concept, nutrient samples (comprising of inorganic nitrate and phosphorus) from one water quality monitoring station in Indiana with at least fifteen years of record, was downloaded from the United States Environmental Protection Agency's (EPA) Water Quality Portal (WQP). For the same station, the United States Geological Survey (USGS) acquired daily streamflow data that was available and downloaded for further use. Both the retrieved datasets were used to initialize input files and then processed through LOADEST using load estimation methods. Last step involved transforming the processed data from the sample station to be visualized on a web map. The web application was designed using map pop-ups that enabled interactive querying of time-series graphs of the LOADEST results to allow better interpretability of changes in daily, monthly or annual nutrient loads.

Keywords: Water Quality, LOADEST software, Process Workflow, Workflow Design, Data Processing Tools, Environment Modelling, Web-based Application, Web-mapping

3-Dimensional Analysis of Two Fluid Model Developments

*James Howard, Raghav Ram, and Martin Lopez-de-Bertodano**
**PI: School of Nuclear Engineering*
Purdue University

SURF ID: 161
2:30 PM - 2:45 PM

The study of two-phase flow (TPF) undergoing heat transfer is important to the design and operation of many cooling systems. A general mathematical model of TPF called the Two Fluid Model demonstrates that the fluid's properties are unsteady. Additional terms to the momentum equations in the model have been proposed in the Transient Two-Fluid Model Development Report to allow for better convergence of the instability. This study simulates the Two Fluid Model with the recently proposed modifications to the momentum equations by using the computation fluid dynamics software ANSYS CFX. The simulation consists of a straight vertical pipe with an upward flow. The additional momentum terms are added into the equation solver and the , and the simulation is run. Graphing the fluid properties, namely the liquid velocity and void fraction, show a wave of vapor propagating up the tube. The graphs are compared to the results of the source report, which has

Keywords: Thermal Technology, Material Modelling and Simulation, Energy and Environment

tested the equations in 1 and 2 dimensions. Conclusions on the accuracy and applications of the new momentum terms are drawn from the comparisons.

Developing a Low-Cost and Low-Power Device for Community Water-Based Ecological Research

SURF ID: 189
2:45 PM - 3:00 PM

*Shayne Stephen Marques[1], Ken Chong[1], Zaven Arra[2], and Jacob Hosen[1]**
**PI: Department of Forestry and Natural Resources*
[1]Purdue University, [2]DeployIO

Keywords: Water-based research, environmental sensors, firmware development, design choices, data collection, sensor deployment

Human activity has been increasing atmospheric greenhouse gas levels, driving broad-reaching environmental change, and impacting wildlife, forests, and water bodies. Existing devices that quantify these changes are expensive, power-inefficient, high maintenance, difficult to use, and have other fundamental issues. This study continues the development of a microcontroller, WaterBear, that improves on these areas. Its development was motivated by the notion of supporting independent and public environmental research through community science projects that monitor water quality and other aspects of environmental health. Design decisions were made to ensure an easily customizable and understandable setup process by creating extensive documentation and instructions, and by being coded to allow for user changes and adaptations. We simplified the process of connecting new and prototype sensors by developing a system of hardware drivers for WaterBear and a command-line interface (CLI) to facilitate device configuration. Additionally, we prototyped hardware and optimized firmware to reduce costs and power consumption, which makes having multiple devices deployed for long periods practical. Sensor performance was tested in laboratory conditions to evaluate data quality, battery life, and ease of use. As a case study, WaterBear microcontrollers with analog embedded methane sensors were configured and then installed in depressional wetlands in Indiana. Data collected from these sensors was analyzed and evaluated for consistency and accuracy compared to Li-Cor Trace Gas Analyzers. By comparing the data with that of previous sensor deployments and other studies, we found that WaterBear successfully captured accurate data while maintaining low cost and power consumption.

Indoor Aerosol Dynamics in Residential Buildings

SURF ID: 208
3:00 PM - 3:15 PM

*Sarah May Palmer, Jinglin Jiang, Chunxu Huang, Nusrat Jung, and Brandon Boor**
**PI: Lyles School of Civil Engineering*
Purdue University

Keywords: Air Pollution, Indoor Air Quality, Particulate Matter, Environmental Characterization, Engineering the Built Environment

In the United States, most particulate matter exposure occurs indoors due to decreasing air pollution outdoors and increasing time individuals spend inside. However, indoor particulate matter sources and dynamics are not well understood. The 2021 zEDGE iRACE (zero Energy Design Guidance for Engineers – indoor Radical and Aerosol Chemistry Experiment) study sought to characterize particle size distributions and indoor air chemistry under different household conditions. The zEDGE iRACE study took place in the zEDGE Tiny House at Purdue University, in collaboration with Indiana University. Instruments measuring particulate matter from 1 nm to 10 μm and gas analyzers were used to characterize indoor emissions in zEDGE to clarify the link between oxidants, volatile organic compounds, new particle formation, and indoor air chemistry. Gas- and particle-phase emissions were investigated during common indoor activities (e.g., cooking, cleaning, applying personal care products) to explore how these activities impact indoor air. Over 100 single emission events were completed along with two full day experiments. One full day experiment focused on gas combustion emission events, and the second focused on electrical appliance use. The particle concentration data from the gas and electric full day experiments was compared to evaluate the indoor activities completed. Preliminary analysis showed that particle concentrations were substantially higher during the combustion day. Additionally, the terpene concentration from one cleaning event during each full day experiment was analyzed. Understanding emissions from common indoor activities will facilitate creating indoor air quality standards and will improve understanding of indoor particulate matter exposure.

SLIC Segmentation and Deep Learning for Plant Disease Area Identification from Handheld Images

SURF ID: 211
3:15 PM - 3:30 PM

*Hieu Phan[1], Aanis Ahmad[2], and Dharmendra Saraswat[2]**
**PI: Department of Agricultural & Biological Engineering*
[1]Miami University, [2]Purdue University

Plant diseases pose a threat to crops yield worldwide. Traditional approach to track the spread of diseases rely on manual scouting. Recent advances in deep learning for image classification has provided motivation for its use in recognizing plant diseases using imagery data. Although image classification is popularly used in analyzing agricultural data, it lacks the ability to accurately identify diseased regions on plant leaves. This study uses simple linear iterative clustering (SLIC) segmentation to create super-pixels, a cluster of pixels representingcommon characteristics, by using PlantVillage dataset. Five different pre-trained models, namely VGG16, ResNet50, DenseNet121, Xception, and InceptionV3, were used to identify five different super-pixel classes (healthy, northern leaf blight, gray leaf spot, common rust, and background) on a single corn leaf. Each model was trained by varying the number of segments, spatial value (sigma) and training:testing split ratio when applying SLIC segmentation. The highest testing accuracy of 94.52% was achieved when the ResNet50 model was trained using a 90:10 split ratio, with five SLIC segments per image and a sigma value of five. Training:testing split ratios of 90:10, 80:20 and 70:30 generally yielded higher results than 50:50 and 60:40 strategies. Common rust and northern leaf blight diseases are sometimes misclassified because super-pixels might have both diseases, while healthy, gray leaf spot and background were classified almost correctly. The overall performance results of deep learning-based image classification models have shown promising results to suggest that researcher will be able to train models capable of generalizing to different conditions and datasets.

Keywords: SLIC Segmentation, Image Classification, Super-pixel, Corn Leaf Disease Classification

SESSION C: Machine Learning: Applications in Science & Engineering

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Data-Driven Model for Electrode Property Prediction

SURF ID: 116
2:00 PM - 2:15 PM

*Brennan S. Birn, Venkatesh Kabra, and Partha Mukherjee**
**PI: School of Mechanical Engineering*
Purdue University

Lithium-ion batteries are present in everything from vertical take-off aircraft to mobile devices. A LIB enables the shuttling of lithium ions between its porous electrodes, which are divided by a porous separator. These porous electrodes provide a high-reaction area and enable low resistance to ion shuttling, quantified with tortuosity, and facilitate electron movement, measured with conductivity. These kinetic and transport properties influence battery performance. Although empirical relations exist for electrode structures made up of non-overlapping particles, the structure-property relations of electrode structures with overlapping particles have yet to be fully quantified. Physics-based Direct Numerical simulations on a computer-generated electrode structure are used for calculating effective properties such as tortuosity, conductivity, and interfacial area that serve as outputs. The model takes the physical descriptors of the electrode structure such as composition (volume fractions), particle radius, etc., as inputs. Several machine learning (ML) algorithms are then trained on the input and output data to determine structure-property relationships. Data cleaning strategies such as removing highly correlated input features and outlier removal mitigate overfitting and instability. Accuracy of the ML model improves when increasing the number of input descriptors, whereas too many feature functions lead to issues such as overfitting, when the model performs well on training data but poorly on testing data. The best regression model achieves a mean accuracy of 99.8% for interfacial area, 99.9% for conductivity, and 96.7% for tortuosity. Using single feature analysis reveals simple relations for all outputs, enabling transport and kinetic properties to be predicted with physical descriptors.

Keywords: Li-ion Batteries, Battery Electrodes, Machine Learning: Big Data, Energy and Environment, Supervised Learning

Analysis of Multiple Large-Scale Reaction Classification Methodologies Employing Support Vector Machine

SURF ID: 138
2:15 PM - 2:30 PM

*Calleb J. Diaz Acevedo[1], Ryan Brown[2], Trevor Teague[2], Pushkar Ghanekar[2], and Allison Godwin[2]**
**PI: Davidson School of Chemical Engineering-Center for Innovative and Strategic Transformation of Alkane Resources (CISTAR)*
[1]University of Puerto Rico, Mayagüez Campus, [2]Purdue University

Reaction classification is crucial to the acceleration of large scale data analysis, to the modeling of chemical reactions, and to the discovery of new drugs. Modern techniques for classification employ machine learning based approaches to extract chemically relevant relationships from large reaction databases. Reaction fingerprints are often generated for machine learning based approaches to represent the chemical characteristics of each reaction. In this study, various methods for reaction fingerprint generation were evaluated to determine the optimal parameters for the classification model. A dataset consisting of 50,000 reactions was employed for training and validating multiple support vector machine models using reaction fingerprints. Model performance was assessed by using classification metrics, such as the F1-score and accuracy. The most efficient fingerprint generated was the differential reaction fingerprint, with agents included as reactants, and a concatenated agent feature array. The optimal support vector machine model successfully predicted 97.9 percent of the labeled reactions on the validation test sample. This model was then used to predict the reaction class of 50,000 unlabeled reactions from a U.S. patent database. Through this analysis we demonstrate how machine learning techniques like support vector machines will be essential to the future of data classification.

Keywords: Machine Learning, Classification, Support Vector Machine, Reaction Fingerprint, Data-Driven

Classification of Chemical Reactions Using Molecular Fingerprints and Logistic Regression

SURF ID: 172
2:30 PM - 2:45 PM

*Amel J. Ksaibati[1], Pushkar Ghanekar[2], Ryan Brown[2], Trevor Teague[2], Shiyan Wang[2], and Allison Godwin[2]**
**PI: Davidson School of Chemical Engineering-Center for Innovative and Strategic Transformation of Alkane Resources (CISTAR)*
[1]University of Wyoming, [2]Purdue University

Chemical reactions classification can be utilized for a variety of applications such as drug design or chemical synthesis planning. However, the process of hand-coding reaction data and subsequent reaction type prediction, can be tedious. To that end, machine learning (ML) algorithms can be used to automate this process. Before any ML modeling and predictions can be developed, chemical

Keywords: Machine Learning, Logistic Regression, Molecular Fingerprint, Chemical

reactions are to be encoded as 1-D vectors called molecular fingerprints. This study looks into different types of molecular fingerprints encoding schemes on a Logistic Regression (LR) model to classify a 50-class patent dataset of unclassified chemical reactions. This was done by combining two previously studied successful techniques, a LR model and a mixture of different chemical fingerprinting protocols. A patent dataset of 100,000 chemical reactions was split into a training and validation dataset of classified reactions, as well as a set consisting only of unlabeled reactions. The labeled training and validation datasets were used to train and evaluate the ML model. Next, the trained model was used predict reaction classes of the unlabeled dataset and the corresponding confidence in the subsequent predictions. The LR classification model with appropriate choice of molecular fingerprints, was able to improve on the results from the previous work. This model correctly predicted 98% of reactions in the validation set. In summary, this study successfully proposed an improvement in the reaction classification task as seen by the increase in the prediction accuracy from previous studies.

Reactions, Classification Analysis, Data Science

Evaluation of Different Fingerprinting Techniques for Classification of Large-Set Organic Reaction Data Using the Random Forest Algorithm

SURF ID: 206
2:45 PM - 3:00 PM

*Lainey J. Orr[1], Pushkar Ghanekar[2], Shiyan Wang[2], Ryan Brown, Trevor Teague, and Allison Godwin[2]**
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[1]Rochester Institute of Technology, [2]Purdue University

Reaction classification is important for expanding the knowledge of reactive processes as well as chemical discovery and synthesis planning. Due to the extensive amount of chemicals and possible reactions, there is an increasing demand to develop machine learning classifiers which can make efficient use of large reaction datasets. An established method for algorithmic reaction classification involves the generation of molecular fingerprints: boolean arrays which encode information about a molecule's chemical and geometric properties. In this study, we examine the application of various available fingerprinting methods in order to determine the most appropriate methods for building a classification model. Using a large set of labeled reactions from public US patent data, fingerprints were generated and used to train a random forest classifier to categorize the reactions into 50 classes. Model performance and robustness was analyzed using cross validation and different scoring metrics: F1-score, precision, and recall. The most effective method was found to be difference reaction fingerprints with concatenated agent feature arrays; the most successful models achieved a macro-averaged F1-score of 0.979 on the hold-out test data. Variation of molecular fingerprint type did not result in significant change to model performance. The results suggest that Topological Torsions, Morgan, Pattern, or the RDKit fingerprinting techniques are all suitable for this type of modeling. Additionally, we explore the use of our model on a set of unlabeled reaction data to develop insight into possible classification of these reactions.

Keywords: machine learning, big data, cheminformatics, reaction fingerprints, organic reactions, random forest classification

Geometric Sensitive Loss Function for X-ray Micro-Tomography Segmentation

SURF ID: 240
3:00 PM - 3:15 PM

*Christopher Trombley[1], Hamid Torbati-Sarraf[2], and Nikhilesh Chawla[2]**
**PI: School of Materials Engineering*
[1]University of Louisville, [2]Purdue University

Microscopic feature segmentation is important for X-ray Microtomography in 3D Materials characterization. In recent years, deep learning based segmentation has demonstrated impressive state of the art performance across different disciplines. There have been recent attempts to segment microscopic features using deep learning; however, the majority of current approaches suffer from over-segmentation. To mitigate the over-segmentation issue, we hypothesize that segmentation accuracy will improve by using a geometry-sensitive custom loss function. A weighted geometry-sensitive loss function combined with the classical cross-entropy loss function was implemented and used with the U-Net architecture to segment X-ray tomograph of Al-SiC-Gr microscopic composite. It was found that by using a geometric loss function performance can increase up to 3.4%. This work demonstrates the potential to use geometric information to improve micro-tomography image segmentation.

Keywords: Deep learning, X-Ray Microtomography, Segmentation, Loss Function, Microstructure

Leveraging Recurrent Neural Networks with Bidirectional Long Short-Term Memory for Top Quark Reconstruction

SURF ID: 241
3:15 PM - 3:30 PM

*Nischay Uppal, Amandeep Bakshi, Eric Reinhardt, and Andreas Jung**
**PI: Department of Physics*
Purdue University

When protons collide at the Large Hadron Collider (LHC), they emit gluons, which initiate a decaying process in which only the initial and final state particles are detected by particle detectors. The undetected intermediary particle states decay immediately, and so, scientists have limited knowledge on the characteristics of these intermediary particles in the search for new physics: top quarks and anti-top quarks. A proposed solution to reconstruct the top and anti-top quarks is to utilize Recurrent Neural Networks (RNNs). RNNs are a class of artificial neural networks that efficiently process and compute sequential data; thus, the temporal nature of the decay processes' can be processed appropriately. The scope of our research is to demonstrate that an RNN can process the information of the final state particles and the system's missing transverse energy to reconstruct the top anti-top quark intermediary particles more accurately. We will be using a variation of RNNs called the RNN Bidirectional Long Short-Term Memory Model (RNN-BLSTM) to address the short-term memory restriction of RNNs and prevent vanishing gradients. The reconstruction data produced by the RNN-BLSTM will be compared to generator level data by current Monte Carlo methods to evaluate the network's performance. The main implication of our research is the recent suggestion by theorists who suggest the bound state of the top and anti-top quark, which form a topomium. Topomium is an intermediary particle that momentarily exists before it decays. If such a particle state is discovered, its characteristics can aid in the search for new physics.

Keywords: Keywords: Machine Learning Algorithms: Recurrent Neural Networks, Bidirectional Long Short-Term Memory, Top Quark Reconstruction, Toponium Intermediary Particle State, High Energy Particle Physics

SESSION D: Biological Signaling

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Development of a Co-Culturing Method for Understanding Astrocyte's Role in Autism Spectrum Disorder

SURF ID: 140
2:00 PM - 2:15 PM

*Aksana Doss, Eugene Kim, Karin Ejendal, and Tamara Kinzer-Ursem**
**PI: Weldon School of Biomedical Engineering*
Purdue University

According to CDC, in 2020, approximately 1 in 54 children are affected by autism spectrum disorder (ASD), usually diagnosed in early childhood. Most of the mutations that cause this neurodevelopmental disorder are strongly associated with protein-encoding genes, like SYNGAP 1. However, besides the SYNGAP 1 gene, the researchers suggest that astrocytes play an important role during the period of brain development too. Neuronal cells were collected from the embryonic wild-type mice, and astrocytes were collected from 2-day old mice pups. Both neurons and astrocytes were co-cultured for two weeks and compared to neuronal culture without astrocytes. Cell cultures were fixed and imaged by confocal microscope at days 3, 5, 7, and 14 to track cell development and neuronal outgrowth. Understanding the role of astrocytes in neuronal cell development can help design a better pharmaceutical solution to neurodevelopmental disorders. The findings may change the view on the mechanism of disorder progressions.

Keywords: Autism spectrum disorder, Astrocytes, a neurodevelopmental disorder

cArgo: an Argonaute Mediated COVID-19 Detection Device

SURF ID: 154
2:15 PM - 2:30 PM

*Manuela Haddad Correa, Lauren Novak, Grace (Jieun) Lee, Victor Pacheco, Grace Cook, and Kari Clase**
**PI: Department of Agricultural & Biological Engineering*
Purdue University

The COVID-19 global pandemic has hastily demanded the emergence of medicinal technology to rapidly and accurately test this highly contagious virus. In the rush to produce mass testing, companies have occasionally forgone accuracy and designed diagnostic procedures that have high false-negative rates. In order to mitigate these errors from the antibody test, molecular-biology based PCR saliva, and nasal SWAB tests, cARGO was designed. The cARGO is an argonaute mediated microfluidic diagnostic device that can rapidly and easily detect the virus in the saliva of individuals. This process begins with the patient's saliva being inputted into the microfluidic chip. RNA is then extracted from the saliva by an embedded chitosan capillary and converted to DNA and amplified, producing double stranded DNA (dsDNA) via recombinase polymerase amplification (RT-RPA), an alternative to PCR. Argonautes that have been incubated with DNA guides cut the dsDNA to generate single stranded DNA (ssDNA) which will bind to the molecular beacon. Fluorescence is then emitted and quantified via spectrophotometer and the result is outputted on a smartphone compatible app. The results in this study will not only be implemented in the COVID-19 pandemic but other possible incoming pandemics and already present viruses, such as the Zika virus. cArgo will provide point-of-care testing at an accessible cost and lead to safer and rapid practices regarding virus testing.

Keywords: Medicinal Science and Technology, Argonaute, ttAgo, h2Ago, COVID-19, Microfluidic Chip, Chitosan

Differential Tractography as a Patient-Specific Tool to Monitor Alzheimer's Disease Biomarkers

SURF ID: 194
2:30 PM - 2:45 PM

*Noah J. Mehringer, Tyler Diorio, and Vitaliy Rayz**
**PI: Weldon School of Biomedical Engineering*
Purdue University

Early identification of Alzheimer's disease (AD) patients would expand their treatment options, so recent research has investigated how diffusion-tensor magnetic resonance imaging (DTI) can identify AD biomarkers in the brain earlier than conventional methods. Particularly, DTI studies have generated maps of white matter (WM) tracts called tractograms which indicate that WM degrades differently in AD compared to healthy and mild cognitive impairment (MCI) subjects. However, the clinical utility of tractography is limited because it relies on comparing patients to cohort averages. Differential tractography is a novel DTI-based methodology positioned to address this issue by measuring patient-specific changes in WM degradation over time. This study assessed differential tractography as a tool for identifying and monitoring AD biomarkers. Baseline and follow-up DTI images were collected from the Alzheimer's Disease Neuroimaging Initiative database. Subjects represented 2 each of healthy and MCI, and one AD. The images were processed through a differential tractography pipeline to produce patient-specific maps of only the WM tracts which

Keywords: Differential tractography, Alzheimer's disease, biomarker, white matter tracts

showed >15% decrease in structural integrity. The resulting differential tractograms were analyzed for tract-based patterns that could classify disease states. The subjects in healthy and MCI groups were not easily distinguishable from each other, but the AD patient uniquely demonstrated >15% degradation in the posterior corpus callosum – a finding similar to AD patients in other studies. Although this demonstrates the potential for differential tractography as a tool to identify and monitor AD, more investigation should be conducted with increased sample size and higher quality DTI images.

Temperature Dependence of Ion Channels in Neurons with Demyelination

SURF ID: 253
2:45 PM - 3:00 PM

*Kayla M. Yates, Tyler VanDyk, and Tamara Kinzer-Ursem**
**PI: Weldon School of Biomedical Engineering*
Purdue University

The fatty myelin sheath which insulates axons in the central nervous system (CNS) is critical for efficient signal propagation, allowing for rapid neuronal communication necessary to support life. In axons with demyelinated lesions, such as might be observed in spinal cord injury (SCI) or Multiple Sclerosis (MS), signal propagation is impaired or even blocked, disrupting many bodily functions. Additionally, symptoms associated with MS are heightened when body temperature rises – a phenomenon clinically known as Uhthoff's sign – although the exact pathophysiology of this phenomenon remains uncertain. This study aims to characterize the molecular mechanisms by which bioelectric propagation is dysregulated in response to core temperature changes using computational modeling. We hypothesize that the slowing of signal propagation is due to the increased temperature dependence of constituent potassium and adaptive sodium channels that results from the deterioration of myelin. Using the Python implementation of the NEURON simulation environment, we developed a model of a healthy myelinated neuron, including physiological geometries and ion distributions at each node of Ranvier, modeled as four distinct compartments: the center node, paranode, juxtaparanode, and internode. We stimulated this model with a current clamp at the axon hillock to generate action potentials, and studied the influence of demyelination and core temperature on nerve conduction velocity and efficiency. Fully understanding and characterizing the temperature dependence of ion channels in demyelinated neurons is crucial in developing effective and specialized treatments of neurological diseases.

Keywords: Double Cable Model, Demyelination, NEURON Simulation, Medical Science and Technology, Biological Simulation and Technology

PLA-PCL Polymer Microsphere Formulation for the Deterrence of Prescription Opioid Abuse by Smoking

SURF ID: 250
3:00 PM - 3:15 PM

*Elyssia N. Wellington, Anastasiia Vasiukhina, and Luis Solorio**
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Opioids are increasingly prescribed across the country for pain treatment. However, these pharmaceuticals are widely abused. Patients given a ten-day supply of opioids have a twenty percent chance of becoming a long-term user. Additionally, it takes three days of ingesting prescription opioids to become addicted. Abuse deterrent formulations (ADFs) for prescription opioids have shown up to a sixty percent decrease in normal abuse according to the FDA. Although ADFs have been developed for the common abuse methods, there is currently no ADF for the smoking abuse route. In this study, we show a new approach to deter smoking of a model prescription opioid drug, thebaine, by using microspheres prepared from polylactic acid (PLA) and polycaprolactone (PCL) that function as a sink for the active drug and its degradation products. We utilized thermogravimetric analysis (TGA) and high-performance liquid chromatography (HPLC) to test the ability of PLA-PCL microspheres to deter smoking of thebaine. Additionally, we compared the abuse-deterring performance of PLA-PCL microspheres to that of activated carbon and mesoporous silica, two materials with excellent and well-established drug-adsorbing properties. We found that our proposed microsphere formulation was effective at entrapping the vaporizing active drug, as well as the volatile degradation products from thebaine. We also determined that, while the abuse-deterrent performance of our microspheres was inferior to that of activated carbon, it was comparable to mesoporous silica. In conclusion, our data indicate that PLA-PCL blend microspheres can potentially be used to create a deterrent formulation for common prescription opioids against abuse via smoking.

Keywords: Keywords: Smoking, Opioids, Abuse deterrent formulation, Microspheres, Medical Science and Technology

SESSION E: Fabrication & Robotics

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Wing Kinematics of Insect Robot

*Saw Yan Naung, Linmeng Liu, and Xinyan Deng**
**PI: School of Mechanical Engineering*
Purdue University

SURF ID: 203
2:00 PM - 2:15 PM

Flying insects with the ability to hover and traverse in the air have intrigued researchers with their stability and control. Previous bio-inspired insect robot has the ability to hover and to navigate in a given aerial space, however, it lacks the freedom to navigate autonomously due to the tethered wires and lack of sensory devices. In this study, force analysis is performed on the wings of an autonomous bio-inspired insect robot that is being built based on the previous robot designed and a single-wing test platform is designed. The purpose is to determine how a previous robot design can be scaled up to a size that can house and carry sensory devices. A single wing test platform is desgined to measure the instantaneous wing kinematics and aerodynamic forces generated on the wings. Simulations are performed through a quasi-steady aerodynamic model on the wings to estimate the generated forces. This study present the predicted lift and drag with the data from simulations and provides a conceptual design for a testing platform.

Keywords: Bio-inspiration, Micro air vehicle, Autonomous Robot, Flexible Wings, Flapping Flight, Aerodynamics

Form + Function 4D Printing: Surface Preparation

*John W. LePage, Raymond G. Godjali, Sara A. Swanlund, Datta M. Sheregar, and Richard Voyles**
**PI: School of Engineering Technology*
Purdue University

SURF ID: 179
2:15 PM - 2:30 PM

3D Printing has been growing rapidly over the last decade, however it has been largely limited to only printing the mechanical form of an object. Form + Function 4D Printing introduces the addition of function to 3D Printing and attempts to take the difficulty of printing with multiple materials away from the user. This is done using a 3d printer with modular printer heads. The printer utilizes a Fused Deposition Molding (FDM) head alongside a liquid extrusion head. With these, it can print any traditional 3D printed substrate as well as plastic parts with silver ink printed onto them, which allow for electricity passage. It also allows for the printing of other materials such as dielectric (used for transistors and capacitors) and PEDOT:PSS (used for resistors). Liquid extrusion on the 3D substrate was difficult as it required the surface to be extremely flat. This was solved using selective ironing, where the FDM head melts the plastic and creates paths for silver to be printed. This is used alongside friction stir-welding, a technique in which a spindle tool with a boring bar is dragged along the surface where it melts the plastic to create a smoother surface for the silver ink. Utilizing these two techniques together, the printed substrate is proven to become much smoother, which greatly improves the quality of silver ink and dielectric printing. This increase in smoothness allows the printer to print a fully functional circuit through the printing of components such as resistors, capacitors, and eventually transistors.

Keywords: Additive Manufacturing, 3D Printing, Material Modeling and Simulation, Materials Modeling and Simulation, Printed Electronics

Detailed Design of a Laser-Driven Flyer System

*Kristen Stava, Kerry Ann Stirrup, and Weinong Chen**
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Purdue University

SURF ID: 233
2:30 PM - 2:45 PM

A laser-driven flyer system is a highly modular tool used to study the reactions of materials during high strain deformation. This system is operationally dependent, so using previous papers as reference, a new design must be made for our specific purposes. We have researched designs for the primary purpose of evaluating the deformation of polymer bonded explosives. There are many sources that compare the mono and multi-layer assembly of the flyer plate which will be used to aid in flyer plate design. The flyer will impact the sample within a vacuum chamber, whose design must accommodate the laser, a replaceable flyer plate, and detachable sample plate. Further, the chamber must allow space for externally mounted characterization equipment, including a high-speed camera to document the sample reactions. Special considerations, such as in-house manufacturability and its ability to withstand multiple trials, are large influences on the final design. This paper outlines the process and final conclusions for the design of a laser-driven flyer chamber. Costs, a list of materials, and steps required to construct the chamber are outlined.

Keywords: Laser-driven flyer, design, vacuum chamber, impact, deformation

Investigation of the Implementation of 4D Printed Strain Gauges

SURF ID: 234
2:45 PM - 3:00 PM

*Sara Swanlund[1], Thomas Guthrie[2], Mohamed Ayad[3], Jack LePage[1], Raymond Godjali[1], Datta Sheregar[1], and Richard Voyles[1]**
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[1]Purdue University, [2]Berea College, [3]Oswego College

Keywords: 4D printing, strain gauges, liquid extrusion

Additive manufacturing has been instrumental in the popularization of rapid prototyping and the fabrication of complex geometries. Specifically, the widespread accessibility of personally owned 3D printers has made it possible for anyone to easily make both simple and complex shaped parts for a variety of purposes. Much in the same way a 3D printer simplified the task of manufacturing mechanical parts, a 4D printer has the ability to vastly simplify and streamline the prototyping and manufacturing process of mechatronic systems, which have mechanical, electrical, and computational components, by adding an extra layer of function to a 3D printed form. By utilizing this concept, this work attempts to develop a novel approach to 4D printing by embedding sensory input onto a 3D printed substrate. The goal is to achieve signal routing through a strain sensor. The printing method for these circuits utilizes a liquid extrusion head to deposit a silver-based ink onto a given substrate, then utilizing the surface tension of the ink to spread it around in specific geometries, similar to how a calligrapher's pen functions. The experiment successfully yielded functional strain sensors that were able to vary resistance in response to deflection of the 3D printed substrate.

4D Printer Project

SURF ID: 148
3:00 PM - 3:15 PM

*Raymond Gregory Godjali, Datta Sheregar, Jack Lepage, Sara Swanlund, and Richard Voyles**
**PI: School of Engineering Technology*
Purdue University

Keywords: Smart materials. 3d printing, printing electronics, 4d printing, form + function

With the rapid innovation of electronics and the rise of areas where it is required, the need for the ability to rapidly create electronic prototypes with special abilities are increasing. Mainstream uses of 3D printing have helped designers and manufacturers in rapid prototyping and creating unique parts. In 4D printing, we add an extra dimension to the 3D form by implementing multiple materials to create electrical functions within the form created. With 4D printing, the aim is to use a printer to print an object with both electrical and mechanical function without any specific fabrication skills. In this paper we are exploring a design process that removes the level of expertise needed in multi-material printing, and in this paper we are using a cement working analogy to form pads into conformity. The cement working analogy involves using the needle tip to push down the bigger silver particles into the cavities of a 3d printed plastic surface. In theory, this will allow us to print a smoother surface and with smooth silver pads we will be able to create electrical components more consistently. By creating a method that allows us to print silver ink more consistently, we will open a new gate of possibilities to integrate form and function through the means of printing.

SESSION F: Deep Learning & Cyber Security

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Purposefully Public, Yet Vulnerably Exposed: Probing Web Services for Regex Denial of Service Vulnerabilities

SURF ID: 110
2:00 PM - 2:15 PM

*Efe Barlas, Xin Du, and James Davis**
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Purdue University

Keywords: Cybersecurity, regular expressions, denial of service attacks, empirical software engineering

In the last decade, many web services have adopted the practice of using formal specifications to provide documentation for developers. These specifications support regular expressions (regex) which are a textual syntax for describing valid input and checking the validity of user input. Concerningly, some regexes are much slower at matching specially crafted input; hence they could slow down the entire web service and can cause regex denial-of-service (ReDoS) vulnerabilities. Such regexes are prevalent in open-source software. We measure to what extent formal specifications expose web services to ReDoS attacks, to show the degree of necessity of ReDoS mitigations in regex-executing software. We parsed and obtained regexes from specifications found in an online database. We analyzed these regexes for attack vectors triggering slow behavior. With these vectors, we ethically probed web services. If the resultant response times had deviations, we concluded that the web service is potentially vulnerable. Out of 2231 specifications, 23.6% contained regex-validated input parameters. 8% of the latter pool contained a potentially vulnerable regex. In total, we found 63 probe surfaces. We probed eight surfaces containing the slowest regexes and observed response time deviations in two. We reported these deviations to affected web services; one of them responded that our results did not present a security concern. These results suggest that further investigation of the untested probe surfaces and other specification corpora may find additional potential ReDoS vulnerabilities. As a reference for sound mitigation, we have proposed a proof-of-concept modification to Ajv, a popular input validator.

Hidden in Plain Sight: Suborning Client-side Sanitization of HTML Forms to Launch Regex Denial of Service (ReDoS)

SURF ID: 142
2:15 PM - 2:30 PM

*Xin Du, Efe Barlas, and James Davis**
**PI: School of Electrical and Computer Engineering*
Purdue University

Keywords: Regular Expression Denial-of-Service, Web Measurement Study, Crawling the Web

Web services play a major role in modern society. To ask for what we need, we often inform web services by filling out forms, such as the login form of any social media. When web services receive your input, they implement rules to sanitize input to prevent malicious attacks. Regular expression (regex) is commonly used to describe these rules. However, some regexes could be computationally expensive and slow down servers, which is called regex Denial-of-Service (ReDoS) when exploited by attackers. Previous research has studied ReDoS vulnerabilities in both software libraries and JavaScript-based services, but we still know relatively little about the extent to which general web services are vulnerable to ReDoS. This paper aims to understand to what extent general web services are vulnerable to ReDoS. We infer the existence of ReDoS vulnerability through the examination of regexes used in forms. We crawl the top 1000 web services. For each webpage that has forms, we find regexes being used by JavaScript instrumentation and browser automation. For those that have vulnerable regexes, we probe the web services and determine whether ReDoS vulnerabilities exist by measuring change in response latency. So far, we have crawled 96015 webpages and found 5577 client-side regexes. 279 of them are vulnerable. We have started probing web services, and no potential vulnerability has been found. Nonetheless, we do expect to find more vulnerabilities once we probe more web services. Our finding provides useful information to people who want to improve the safety of regexes in web services.

Counterfactual Multi-Agent Reinforcement Learning

SURF ID: 215
2:30 PM - 2:45 PM

*Rohan Potdar, Tong Yao, and Shreyas Sundaram**
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Keywords: Reinforcement Learning, Machine Learning, Multi-Agent

Reinforcement Learning is the application of Machine Learning to Optimal Control problems. Deep Reinforcement Learning uses neural networks as function approximators in reinforcement learning. While Deep Reinforcement Learning has had many breakthroughs in recent years, it is insufficient for control of multi-agent systems. A key problem in Multi-Agent Deep Reinforcement Learning is the

credit assignment problem, where agents must learn the effect of their individual actions on a shared reward function. The Counterfactual Multi-Agent Policy Gradients (COMA) algorithm introduced a counterfactual baseline that performs credit assignment by taking the policy-weighted sum of expected rewards over all actions for each agent. However, COMA is only applicable to discrete action spaces, and is sample inefficient due to its on-policy nature. We extend COMA to off-policy methods in continuous action spaces using Soft Actor Critic with importance sampling. We then compare COMA to Independent Actor-Critics, Parameter Sharing, and Multi-Agent Deep Deterministic Policy Gradient (MADDPG) on the cooperative, competitive, and mixed-sum environments present in OpenAI's Multi-Agent Particle Environments. We demonstrate that COMA performs comparably to MADDPG while being less computationally expensive than MADDPG due to its single shared critic.

Are Two Identically Trained Models Equally Fair? Variance in the Fairness of Models.

SURF ID: 236
2:45 PM - 3:00 PM

*Prithviraj Praveen Tarale[1], Shangshu Qian[2], Hung Pham[2], and Lin Tan[2]**
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[1]University of Washington, [2]Purdue University

Keywords: Fairness, deep learning, variance, empirical study

Recent research has shown that the underlying implementation of the mainstream deep learning libraries (e.g., PyTorch and Tensorflow) introduces non-determinism in the training process. Consequently, two instances of training under the same hyperparameters and fixed seeds may result in different models. The issue of fairness in deep learning models remains an imminent and important problem. This variance has been established on popular metrics such as accuracy. However, we study how much variance this non-determinism introduces in the fairness of models. We demonstrate this on the task of software-defect prediction on two popular software projects – QT and OpenStack. We first predict buggy/clean labels with seven instances of trained models. We then use genderComputer, an off-the-shelf tool, to resolve the genders of the projects' contributors. We evaluate a popular bias metric – equality of opportunity - for the seven training instances with the true labels, predicted labels, and the protected labels. With the model bias scores across seven identical rounds of training with fixed hyperparameters and seeds, we found a variance of 2.4e-6 and a difference of up to 0.00476. We hope that this work emphasizes the need for better research and development practices while comparing the fairness of deep learning models.

A New Approach for Program-by-Example Program Synthesis

SURF ID: 251
3:00 PM - 3:15 PM

*Siyu Wu, Yanjun Wang, and Xiaokang Qiu**
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Keywords: Program Synthesis, Divide-and-Conquer, Program-by-Example, Syntax-Guided Synthesis

Syntax-Guided Synthesis (SyGuS) aims to generate programs automatically from both semantic specifications and syntactic constraints provided by users. A special class of SyGuS problems, called program-by-example (PBE) problems, which takes a set of input-output examples as semantic specification, is to find programs satisfying all the input-output example pairs. Existing approaches to SyGuS PBE problems either are not able to generate programs efficiently, or the generated programs are too lengthy and unreadable to be adopted by users. In order to push the performance limit of SyGuS solvers further, in this paper, we propose a novel approach for PBE SyGuS problems with bit-vector background theory. Our approach adopts a divide-and-conquer technique to break down original SyGuS problems into subproblems and solve each subproblem using an enumerative synthesis technique. We implemented our approach into a SyGuS synthesizer DryadSynth and evaluated on a wide range of benchmarks from the annual SyGuS Competition. Experimental results show that DryadSynth has comparable running time to another state-of-the-art SyGuS solver CVC4 and generates smaller-size solutions than CVC4. DryadSynth also outperforms another state-of-the-art SyGuS solver EUSolver in terms of running time.

SESSION G: Chemical Catalysis & Synthesis

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Understanding the Speciation of Chloropalladate Ions for the Viral Synthesis of Palladium Nanomaterials through an Original Python Algorithm

SURF ID: 102
2:00 PM - 2:15 PM

*David F. Amelemah[1], Jeanette Hill[2], Anuradha Bhat[2], and Michael Harris[2]**
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[1]Princeton University, [2]Purdue University

Palladium is a rare, silvery-white metal that is more expensive than gold in the current market. Synthesizing palladium nanomaterials using plant viruses, like the Tobacco Mosaic Virus (TMV), is the overarching focus of this research. Palladium is valuable for its broad applicability, as evidenced by its usage in nanoelectronics, battery anodes, sensors, and catalytic converters. This study chose palladium for its ability to readily bind to the surface of TMV. For decades, plant viruses have been used as biotemplates for the synthesis of nanomaterials. Previous studies have examined the adsorption of palladium on TMV, but the current literature does not display a thorough quantitative understanding of chloropalladate speciation under different experimental conditions. Understanding the speciation is important, because only certain chloropalladate ions can adsorb onto the surface of TMV. Thus, this study aims to address this problem by developing an original algorithm in Python. This algorithm solves multi-reaction equilibria using the Newton-Raphson method and graphically displays the speciation of chloropalladate under different starting concentrations of Chlorine ions and different pH levels. The quantitative results will lead to a better understanding and manipulation of palladium nanoparticle synthesis. The conclusion will suggest ideal experimental conditions for the viral synthesis of palladium nanomaterials.

Keywords: Chloropalladate speciation, Nanomaterial synthesis, Tobacco Mosaic Virus, Barley Stripe Mosaic Virus, Biotemplating

Defining and Mitigating Deactivation of Pt-based Dehydrogenation Catalysts

SURF ID: 128
2:15 PM - 2:30 PM

*Isha Chavan, David Dean, and Jeffrey Miller**
**PI: Davidson School of Chemical Engineering*
Purdue University

The dehydrogenation reaction is used to convert light alkanes, such as ethane and propane, to alkenes used as a feedstock for oligomer and polymer production. Pt-based catalysts are used to decrease the required energy input for dehydrogenation. The biggest challenge with Pt-based catalysts at high temperatures (~550 to 800 °C) is the deactivation via numerous mechanisms, such as coke formation, sintering, or phase changes. The deactivation necessitates frequent regeneration of catalysts via complex, expensive processes and also results in a relatively short catalyst lifespan. This study looks at oxidation-reduction catalyst regeneration for PtSn, Pt, and PtZn catalysts supported on silica to minimize sintering and phase changes while maximizing coke removal. Additionally, this study investigates the role of co-feeding hydrogen during propane dehydrogenation (PDH) reactions in minimizing the deactivation rate by preventing the formation of carbonaceous precursors. Propane dehydrogenation is performed with and without co-feeding H2 and dilute propane at 550 °C. The results indicate that co-feeding of hydrogen significantly decreases the catalyst deactivation rate. The regeneration cycle, at 400 °C in air for one hour, restores the catalyst activity to close to that of the fresh catalyst. Dilute H2 regeneration at 550 °C does not play a role in regenerating the catalyst, while dilute H2 regeneration at 800 °C can negatively impact the activity of the catalyst due to sintering. Overall, we have devised an industrially relevant dehydrogenation system that merits further investigation via industrial scale-up.

Keywords: Propane dehydrogenation, Pt-Sn, Pt-based catalysts, Regeneration cycles, Coke formation, Sintering, Co-Feeding Hydrogen, Energy and the Environment

Automatic Process Synthesis using a Global Optimization Approach

SURF ID: 114
2:30 PM - 2:45 PM

*Arsh Bhatia, Zewei Chen, and Rakesh Agrawal**
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Purdue University

As the world pushes for more sustainable and cost-effective methods of chemical production, there is a greater need for a computational method to generate the best process flowsheet to achieve a required process. Previous work has been done either in creating such models for specific examples, like distillation separation, or in constructing superstructure based on heuristics, but few works have systematically synthesized all possible flowsheets for a general chemical process, which includes reactions, separations, etc. In this project we have created a holistic globally optimiz mathematical algorithm that can generate all the possible flowsheets based on their corresponding separation-reaction networks. We developed constraints based on physical and mathematical insights to ensure

Keywords: Process Synthesis, Superstructure, Optimization, MILP, GAMS

the feasibility of our solutions. The algorithm is implemented in GAMS with a representative shale gas model case study.

Synthetic Approaches to Independently Vary Al Distribution and Density in MEL Zeolites

SURF ID: 232
2:45 PM - 3:00 PM

*Hannah Elizabeth Snider[1], Elizabeth Bickel[2], Songhyun Lee[2], and Rajamani Gounder[2]**
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Keywords: Catalysis, zeolites, crystallization

Zeolites are a class of solid, microporous, crystalline catalysts composed of silicon atoms tetrahedrally coordinated to oxygen. Substitution of silicon (Si4+) with aluminum (Al3+) generates a negative charge that is compensated by a proton (H+), which serves as a catalytic Brønsted acid active site. The proximity of H+ sites in zeolites influences the rates of hydrocarbon upgrading reactions such as propene oligomerization to heavier alkenes. Zeolite synthesis approaches that influence Al proximity often concomitantly affect other important catalyst properties such Al density (Si/Al) and crystal size. Here, we discuss efforts to synthesize MEL zeolites with independently varied Al density and proximity using combinations of structure directing agents (SDAs), cations that assist zeolite crystallization and charge compensate AlO4- in the zeolite lattice during crystallization. MEL synthesis gels were prepared with fixed Al content (Si/Al 50) and different ratios of two SDAs: tetrabutylammonium (TBA+) and sodium (Na+) (Na+/TBA+(gel) 0-5). X-ray diffraction patterns were characteristic of MEL for syntheses using Na+/TBA+ (gel) of 0.0-1.5, while peaks characteristic of MEL and another zeolite topology (MFI) were observed for MEL synthesized with Na+/TBA+(gel) ≥ 3.0, indicating that higher Na+ contents led to MFI impurities. Quantities of TBA+ occluded in the solid product (TBA+/u.c.) decreased (4.0-1.5) while Na+/u.c. increased (0.0-2.4) with increasing Na+/TBA+ (gel), suggesting Na+ displaces TBA+ as an SDA in MEL. Differences in proximal Al sites were assessed by titration with Co2+ and will also be discussed. Overall, this work demonstrates the use of multiple SDAs in MEL synthesis to independently influence Si/Al and Al proximity.

Computational assessment of Brønsted acid site proximity in chabazite and its effect on protolytic propane cracking and dehydrogenation kinetics

SURF ID: 181
3:00 PM - 3:15 PM

*Huston Locht[1], Bereket Bekele[2], Ricem Diaz Arroyo[2], Alexander Hoffman[2], David Hibbitts[2], and Rajamani Gounder[2]**
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Keywords: Material modeling and simulation, Protolytic alkane cracking, Proton proximity, Chabazite, Propane

Brønsted acid zeolite-catalyzed conversion of light alkanes to alkenes is of industrial interest because alkene products can be converted to larger hydrocarbons (e.g., through oligomerization), which can be used as transportation fuels. H-SSZ-13 zeolites with the chabazite (CHA) framework can be selectively synthesized with fixed Brønsted acid site (H+) content and varying fractions of H+ sites in paired configurations—where two Al share a six-member ring (6-MR) and can exchange divalent Co2+—and isolated configurations that cannot exchange Co2+. Increasing the fraction of paired H+ sites within H-SSZ-13 increases measured reaction rates of monomolecular propane cracking and dehydrogenation, with measured apparent activation entropies becoming less negative as the fraction of paired sites increases while apparent activation energies remain nearly constant. Prior theoretical studies of these reactions, however, have only examined isolated acid sites. Here, we study monomolecular propane cracking and dehydrogenation reactions on both isolated and paired acid sites using periodic density functional theory (DFT) calculations. These DFT calculations indicate that monomolecular alkane cracking proceeds via a pentavalent carbonium-ion in which the C–C bond breaks and decomposes into one of three products, with apparent activation energies of ~130 kJ mol−1 relative to gas-phase propane for all site configurations. However, these calculations do not accurately capture entropic effects during catalysis. Additional DFT calculations combined with ab initio molecular dynamics (AIMD) simulations would enable exhaustive searches for the lowest potential energy and most accurate free energy of all reaction states, which may provide more insight into experimental observations.