

MISSOURI UNIVERSITY OF SCIENCE AND TECHNOLOGY 2023 GRADUATE RESEARCH SHOWCASE



Wednesday, April 12, 2023

Havener Center



Graduate
Education

A warm welcome to the **2023 Graduate Research Showcase** at Missouri S&T. We are a Carnegie R2 doctoral university, that is, a university with *high* research activity. It is one of the North Star Goals (<https://chancellor.mst.edu/initiatives/north-star/>) of Chancellor Dehghani and his leadership team to attain Carnegie R1 classification, to become a university with *very high* research activity. The 2023 Graduate Research Showcase highlights some of the tremendous research achievements across the three colleges and demonstrates outstanding examples of graduate student success and passionate guidance by our highly talented faculty advisors and mentors. *We are well on track to moving up!* This year's event features many more posters than in previous years and includes an inaugural oral presentation session. Graduate students, this is your event! Enjoy presenting, enjoy the presentations by your peers, inspire visiting undergraduate students, and engage and impress faculty and employer judges. *Graduate Education* is rooting for all of you!

For the *Graduate Education* team,

A handwritten signature in black ink that reads "Rainer Glaser". The signature is written in a cursive, flowing style.

Rainer E. Glaser, Ph.D., M.S., Dipl.-Chem.
FRSC, FAAAS, FACS, FAIC
Interim Vice Provost of Graduate Education

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Poster Session

Session Details:

Location: Second Floor Atrium, Havener Center

Time: 10 a.m. to 12 p.m.

Campus Judges:

Dr. Hanli Wu, Civil, Architectural and Environmental Engineering

Dr. Sanjay Madria, Computer Science

Dr. Sanaz Vajedian, Geosciences and Geological and Petroleum Engineering

Dr. Daoru Han, Mechanical and Aerospace Engineering

Dr. Viraj Ashok Athavale, Materials Science and Engineering

Dr. Fateme Fayyazbakhsh, Mechanical and Aerospace Engineering

Dr. Vadym Mochalin, Chemistry

Dr. Michel Gueldry, Arts, Languages and Philosophy

Dr. Rachel Kohman, Kummer Student Programs

Guest Judges:

Brandi Suhre, Thermo Fisher Scientific

Chris Coffman, Ocelot Consulting

Christy Truluck, Liberty Energy and Water

Megan Russom, Sonoco Products Company

Dillynn Cook, U.S. Army Corps of Engineers

Wes Safarik, U.S. Army Corps of Engineers

Session Abstracts:

Toward Soliton Splitting via Compact Repulsive Potentials for the Nonlinear Schrödinger Equation

Christopher Hogan¹, Jason Murphy¹

¹ *Mathematics and Statistics*

We study the soliton scattering behavior of the focusing nonlinear Schrödinger equation with a compactly supported repulsive potential and high-velocity soliton initial data. This analysis is motivated by hypothetical applications in fiber optics as well as empirical and numerical results from physics and mathematics, so we first establish a goal for our analysis consistent with these results. As our analysis is

a natural extension of a related 2007 result of Holmer, Marzuola, and Zworski to more general repulsive potentials, we leverage the structure of their argument as a strategy for our problem and address the challenges inherent to our scenario which require adaptation of their strategy. Finally, we present the most recent technical result from our analysis together with our additional progress toward our goal and outline the remaining work necessary to complete our analysis of this scattering behavior.

Poster #1

Characterization of the Structure of Amorphous Oxide Semiconductors and Connection to Properties

Corey Burris¹, Julia E. Medvedeva¹

¹ *Physics*

Amorphous oxide semiconductors (AOS) possess many unique properties, including high carrier mobility (\gg a-Si:H) and optical transparency, making them attractive materials for a wide range of optoelectronic applications. A microscopic understanding of the structure and the development of structure-property relationships is vital for the creation of next-generation materials with tunable properties for improved performance in applications. The use of ab-initio molecular dynamics simulations, combined with accurate density-functional calculations and computational analysis tools allow for a comprehensive study of the structural complexity in AOS and its role in the resulting electrical and optical properties. This work presents new computational tools developed to characterize and analyze the structure and electronic properties of AOS and demonstrates their use in revealing the breadth of complexity in the structure of AOS. Many of the computational tools use standard output files of the widely used Vienna Ab initio Simulation Package (VASP) to generate data files and visuals which characterize and analyze structure and electronic properties of materials simulated. Some examples of these tools are the ability to calculate the displacement of a metal atom from the center of mass of nearest-neighbor oxygen atoms which can serve as a directional measure of polyhedra distortion and a tool to integrate the charge density in the region between two neighboring metal atoms which has been used to investigate the effects of structural parameters on charge localization due to metal-metal bonds. Specifically, our results for indium oxide with variable oxygen stoichiometry have shown that there is a broad distribution in the local polyhedral characteristics, the medium-range structure linking nearest-neighbor polyhedra, and the long-range structure involving large numbers of polyhedra that form the metal oxygen network that leads to co-existence of the delocalized, weakly localized and deep electron trap states that govern the carrier generation and carrier transport in AOS. Furthermore, the structural dynamics in AOS have shown that as much variety exists for the degree of structural reorganization, revealing the time scales at which it occurs and the specific time-dependent behaviors in room-temperature molecular dynamics. Using machine learning approaches that involve a large number of structural parameters and the insights gleaned from analysis using the new computational tools, predictive structure-property relationships are being developed for next-generation AOS materials.

Poster #2

Cationic Metal Sites Exhibiting Dual Behavior Towards Synthesis of Three- and Five-Membered N-Heterocycles

Suraj Sahoo¹, Pericles Stavropoulos¹, Brent Harfmann¹, Lin Ai¹, Quiwen Wang¹, Sudip Mohapatra¹, Amitava Choudhury¹

¹ Chemistry

Aziridines are important synthetic targets with immense possibilities towards structural expansion and rearrangement. This arises due to a high strain contained in the three-membered ring. The nature of nitrogen substituent controls the type of aziridine-ring expansion methodology. The most predominant among which is the formal (3+2) cycloaddition of aziridines with an array of dipolarophiles (olefins, ketones, aldehydes, imines, nitriles etc.) leading to generation of a range of five-membered N-heterocycles such as pyrrolidines, imidazolines, oxazolidines, imidazolidines etc.

In this work, a family of cationic divalent metal complexes (M = MnII, FeII, CoII) using tris[(tetramethylguanidino)phenyl]amine and corresponding bipodal congener (N-methyl-bis[(tetramethylguanidino)phenyl]amine) were generated. An extensive comparative study was then carried out in terms of nitrene transfer chemistry towards aziridination of olefins with certain metal complexes showing additional activity towards formation of five membered heterocycles (pyrrolidines and imidazolines) in presence of excess olefins or acetonitrile. Notably, styrene with electron-donating para substituents such as 4-Me- and 4-tBu-styrene are significantly more productive in the synthesis of pyrrolidines at the expense of aziridines with yields up to 60% and 73%, respectively. In the presence of carbonyl substrates, styrene can undergo nitrene transfer (NTs) which can undergo subsequent incorporation of the carbonyl component to generate the corresponding 1,3-oxazolidine in situ via (2+1+2) cycloaddition. Cycloaddition of styrene, PhINTs and acetone (2+1+2) provides practicable yields (70%) of the 1,3-oxazolidine as the sole product. As anticipated, a small increase in the yields of the corresponding oxazolidines is observed with the electron-rich 4-Me- and 4-tBu-styrene (71% and 75%).

The catalytic reactions were then judiciously optimized with a range of substrates using the most productive iron reagents, and mechanistic studies uncovered the dual role of the metal as a nitrene-transfer agent and a Lewis acid in the synthesis of high value 5-membered hetero-cyclic compounds.

Poster #3

Long-Range-Fit: A Program to Fit Long-Range Interactions

Adrian L. Batista-Planas¹, Ernesto Quintas-Sánchez¹, Richard Dawes¹

¹ Chemistry

Long-range molecular interactions play an essential role in atmospheric and environmental chemistry, astrochemistry, and many other relevant fields; as well as in the automobile and aircraft industries, with the development of exciting new technologies like low-temperature combustion. For modeling purposes, these interactions can be better understood by constructing a potential energy surface (PES) for the system of interest: a relationship between the energy and the geometrical system configuration. However, the construction of a PES, being a science in and of itself, constitutes a very demanding time- and resource-consuming computational effort, typically requiring the resource-expensive calculation of numerous ab initio energy points, which will later be fit to an analytical expression. Furthermore, although the theoretical description of physical interactions in the long-range of a PES (namely electrostatic, induction, dispersion, etc.) is a well-known subject, the implementation of its mathematical

formulation can be extremely challenging, considering that the analytical expressions (which constitute a sum of terms for each of the different interactions) could be in some cases tens-of-pages long just for a single term, and changes from system to system. Our program, "Long-Range-Fit" (LRF), is an interactive, user-friendly interface designed to assist in fitting the long-range region of a PES for systems composed of (any) two molecules. Once the symmetry of each of the two fragments is specified, LRF is programmed to automatically generate and fit the corresponding analytical expressions describing the long-range interactions (up to the desired order of accuracy, also specified by the user) for the most common symmetry groups, including from simple molecules like an atom or a linear chain of atoms to much more complex ones such as proteins. The software has already been successfully employed in more than ten systems of atmospheric and astrophysical interest.

Poster #4

Carbon Aerogels Derived from Polybenzoxazine and Polybenzodiazine Aerogels as High-Capacity Desiccants

Vaibhav Edlabadkar¹, Chariklia Sotiriou-Leventis¹

¹ Chemistry

Structurally analogous polybenzodiazine (PBDAZ) and polybenzoxazine aerogels (PBO) were prepared from suitable monomers via HCl-catalyzed ring opening polymerization. Both types of aerogels undergo complete ring-fusion aromatization at 200-240 °C under O₂ or air. The fully aromatized versions of those aerogels were subjected to pyrolytic carbonization at 800 °C under Ar yielding carbon aerogels, which were further etched at 1000 °C under flowing CO₂ to increase porosities, open-micropore volumes, and surface areas. The polymer aerogels were characterized with 15N NMR, CHN elemental analysis, XPS, SEM, and gas (N₂ and CO₂) sorption porosimetry. Carbon and etched-carbon aerogels were investigated as desiccants at 273 K, 298 K, and 313 K. Long-term performance and cycling stability was studied by switching the atmosphere around the carbon aerogel samples between humid and dry, staying for 24 hours in each environment. No performance deterioration was detected after 50 cycles. Carbon aerogels from both PBDAZ and PBO showed significantly higher water adsorption capacities from the high humidity (99%) atmosphere (43% and 42% w/w, respectively) than typical commercial desiccants like silica or Drierite, which were used as benchmarks. (The latter two absorbed just 20% and 15% w/w of water at 298 K, respectively) CO₂-etched PBDAZ- and PBO-derived carbon aerogels showed even higher water uptake capacities, reaching 117% w/w and 140% w/w at 298 K, respectively. Most importantly though, adsorbed water was released quantitatively just by reducing the relative humidity of the environment to 10%. These properties render these carbon aerogels ideal materials for water collection from desert environments. High uptake of water was traced to preferential pore filling of micropores, and multilayer adsorption of water on already adsorbed water inside the mesopores along with H-bonding.

Poster #5

Correlation of the Nanomorphology of Aerogels to Their Drug Uptake and Release Profiles

Stephen Owusu¹, Lia Sotiriou-Leventis¹

¹ Chemistry

The effects of carrier morphology on the drug delivery potentials of aerogels have been explored using polyurea aerogels as the model system. Polyurea aerogels were used in this study, because they can be formulated into different morphologies, described by the so-called K-index, by varying the monomer,

catalyst concentration and the solvent. The K-index is defined as the Q-to-P ratio, where Q is the contact angle of water droplets resting on the material and P is the porosity.

A physical adsorption method was employed to load a hydrophilic drug (5-FU) onto selected aerogels within each K-index group, and the correlation of their drug loading capacities with several material properties of interest was investigated. The drug loading capacity was generally found to increase proportionally with porosity for aerogels within the same K-index group. Highly porous aerogels with K-index 1.5 (random 3D assemblies of fused nano particles) showed the highest drug loading capacity of ~30% w/w.

Drug release profiles of the selected aerogels were analyzed, and the data were fitted with several mathematical models. Samples with K-index equal to 1.5 released 5-FU quickly (~0.15 mg/mL/30 min) whilst those with K-indexes equal to 1.2 and 1.6 released the same drug more slowly (~0.03 mg/mL/30 min). The drug release profiles of the aerogels were also found to be affected by changes in physiological conditions such as pH and temperature. Overall, aerogels with K-indexes equal to 1.2, 1.3 and 1.6 released 5-FU slowly over an extended period in correlation with concentration, whilst those with K indexes equal to 1.6-1.9 generally released equivalent amount of 5-FU at regular time intervals independent of concentration of drug.

Poster #6

Molybdenum Phosphate-Based Frameworks as Cathode Materials for Rechargeable Batteries

Sutapa Bhattacharya¹, Amitava Choudhury¹

¹ Chemistry

Polyanion based cathode materials for Li-ion batteries have received a lot of attention due to their electrochemical stability during cycling because of the strong covalent bond between oxygen and the central atom of the polyanion. The redox potential of the transition metal couple can be tuned by using different polyanion with central atom of different electronegativity. Phosphate (PO₄³⁻) based polyanion cathode materials containing various transition metals such as Fe, Co, Ni, Mn, V has been explored for the increase in working voltage owing to the inductive effect of PO₄³⁻ group. Olivine type LiFePO₄ was first demonstrated by Goodenough to show high capacity and electrochemical stability. In this regard, we synthesized molybdenum-based phosphate materials to explore the possibility of accessing the Mo⁴⁺/Mo⁵⁺ redox. Molybdenum phosphate-based materials have also been studied earlier by Mundi et. al. and Peascoe et. al. for their reversible absorption properties.

In this work, we have synthesized lithium ion containing molybdenum phosphate framework by hydrothermal method. It crystallizes in non-centrosymmetric C2 space group [LiMo₂O₂(PO₄)₂(H₂PO₄)] and centrosymmetric C2/c space group [Li₃Mo₂O₂(PO₄)₂(H₂PO₄)] depending on the reaction time. The phase transformation has been confirmed by ex-situ powder X-ray diffraction study. The structure of both phases was determined by single crystal X-ray diffraction studies. The anhydrous phase of both compound is structurally same and ~ 3 Li ions could be intercalated and deintercalated in initial charge-discharge cycles when studied as Li-ion cathode. In summary, the molybdenum phosphate-based materials show potential to act as alkali ion battery cathodes due to presence of large channels in their structure.

Poster #7

Internal Rotation Analysis and Structure Determination of R-Carvone*Nicole Moon¹, Garry S. Grubbs¹*¹ *Chemistry*

When the rotational spectrum of R-carvone was collected at Missouri University of Science and Technology in preparation for a three-wave mixing experiment, splittings within the rotational transitions were observed that were unassigned in both the original study of S-carvone by Moreno et al. and the monoterpene study by Loru et al. It was discovered that these splittings were due to internal rotations caused by two non-equivalent methyl rotors. This prompted a reinvestigation into the pure rotational spectrum of R-carvone using chirped-pulse, Fourier transform microwave (CP-FTMW) spectroscopy within the 5-18 GHz region of the electromagnetic spectrum. Since initially reporting this finding, all parent species and singly substituted isotopologues for the six conformers of carvone have been analyzed using XIAM. Within this presentation, the results of the reinvestigation will be reported, including the experimentally derived molecular structures for the six conformers as well as the experimentally determined potential barrier heights to internal rotation.

Poster #8

Single Particle ICP-MS Reveals the Fate and Uptake of Engineered Metallic Nanoparticles in Lettuce Tissues*Lei Xu¹, Hu Yang¹, Honglan Shi²*¹ *Chemical and Biochemical Engineering*² *Chemistry*

Engineering metallic nanoparticles (NPs) have been increasingly used in agriculture as nano-based pesticides and fertilizers. It is imperative to quantitatively detect the NPs in plant tissues for food safety. In this study, macerozyme R-10 enzyme digestion followed by single particle inductively coupled plasma-mass spectrometry (SP-ICP-MS) method was advanced and used to analyze silver nanoparticles (AgNPs) and cerium oxide nanoparticles (CeO₂NPs) in dried shoot and root tissues of lettuce grown in soil treated by AgNPs (0–200 mg/kg) and AgNPs-CeO₂NPs (100 mg/kg). Sodium citrate (2 mM, pH 7.2) was applied to stabilize AgNP and CeO₂NP stock suspensions. The SP-ICP-MS method showed the low particle concentration detection limits (2,631 AgNPs/mL and 4,586 CeO₂NPs/mL) and reduced particle size detection limits (19 nm for AgNP and 16 nm for CeO₂NP), with a good reproducibility and particle concentration spike recovery. Lettuce tissue analysis indicated that the concentrations of AgNPs and CeO₂NPs increased substantially by the NP treatment. The presence of CeO₂NPs in soil elevated the AgNPs concentration in shoots, but significantly reduced AgNPs content in roots. Data demonstrated that this SP-ICP-MS method would advance the NP detection in plant tissues and provide a powerful tool to elucidate the complex plant-NPs interactions in soil ecosystems. This research is funded by the US National Science Foundation (Award no. 1900022).

Poster #9

Head and Neck Cancer Treatment by Poly I:C Loaded Lipid Nanoparticles

Vidit Singh¹, Hu Yang¹

¹ Chemical and Biochemical Engineering

The incidence of head and neck squamous cell carcinoma (HNSCC) ranks as the sixth most common human cancer globally, and over 600,000 cases are newly diagnosed annually. Cancer immunotherapy is looked into to prove that it is a viable strategy for cancer therapy. Immunotherapy brings new hope to the fight against cancer. Immunotherapy stimulates the host immune system to recognize tumor cells as non-self and eliminate them. We observed the antitumor efficacy of TLR agonists (Poly I:C) in cancer cells by encapsulating them in liposomes. The hypothesis was that liposome encapsulation of TLR3 agonists could protect them from rapid degradation extracellularly and increase their uptake by HN12 cells. Lipids DOTAP, Egg PC, cholesterol, and DSPE-PEG 2000 were used to make liposomes. High molecular weight polyinosinic-polycytidylyl acid (Poly I:C) (1.5-8 kb) was used as the TLR3 agonist. The lipids were mixed in a 3:2:2:0.3 molar ratio of DOTAP, Egg PC: cholesterol, and DSPE-PEG 2000.

Multiple methods to make liposomes were used, among which the hydrodynamic focusing method using microfluidics gave the best results: small size (<150 nm), low PDI (0.21), high zeta potential (48 mV), and high encapsulation efficiency (98%). Gel electrophoresis and TEM analysis showed the high binding efficiency and spherical morphology of the liposomal nanoparticles. Cellular uptake studies by flow cytometry showed 100% uptake in HN12 cells. The cytotoxicity study in HN12 cells shows that liposomes loaded with Poly I:C have higher cytotoxicity than the controls for HN12 cells and have an IC 50 value between 3-5 µg/mL concentration of Poly I:C.

Biodistribution studies in NU/J outbred mice via intra-tumoral (IT) and intravenous (IV) injections showed IV as the preferred method of injection as there was increased accumulation in tumor and decreased accumulation in the liver. 24 hours after IV injection of DiR-labeled liposomes, there was increased circulation in the body as compared to IT injection. Therapeutic studies with a 5 mg/kg dosage of Poly IC in liposomes) indicated a significant difference in the tumor size of Poly I:C liposomes as compared to the controls (blank liposomes, Poly I:C, and PBS).

It was concluded that the liposome encapsulating TLR3 agonist (Poly I:C) is an effective immunotherapy strategy for head and neck cancer therapy. Future studies would focus on the reduction of tumor size by using targeted lipid nanoparticles (sugars and antigens) and combination therapy with TLR3 agonists and other drugs.

Poster #10

Dendrimer-Based Nanoparticles for Atherosclerosis Diagnosis and Therapy

Huari Kou¹, Hu Yang¹

¹ Chemical and Biochemical Engineering

Statement of Purpose: Cardiovascular disease has been one of the leading causes of death worldwide. Early detection and targeted therapy play an essential role in halting or reversing atherosclerosis progress. Multifunctional nanoparticles possessing diagnostic and therapeutic capabilities are desired for diagnosing and treating atherosclerosis. In this work, we designed and synthesized dendrimer-based nanoparticles with combined modalities for both PET imaging and drug delivery.

Methods and Characterization: Synthesis: 1) G5 and $\text{Cu}(\text{NO}_3)_2$ solutions were mixed under stirring and reduced with excessive NaBH_4 . To obtain G5-Cu-PEG-mannose, PEG-Mannose with NHS Ester was reacted with the G5-Cu solution for 2 h. 2) Four solutions were mixed to synthesize nanoparticles using multi-inlet vortex mixer device including: NHS Ester cross-linker in acetone, G5-Cu-PEG-mannose in DI water and two DI water. 3) ATO methanol solution was mixed with G5-Cu-PEG-mannose overnight. Then it reacted with a cross-linker via the multi-inlet vortex mixer device.

Particle characterization: Zeta sizer and TEM were applied to characterize the size distribution and morphology of nanoparticles.

Cellular uptake kinetics study: RAW 264.7 cells were incubated with FITC labelled nanoparticles for 24 h. Then FITC fluorescence of cells was tested via flow cytometry. Intracellular drug release: RAW 264.7 cells were incubated with ATO loaded nanoparticles and harvested at different time points. ATO concentrations were tested by LCMS.

Results: The sizes increased from 8 nm to 25 nm after PEG-Mannose linked to G5, and increase to 125 nm after cross linking reaction (Fig. 1a). TEM element mapping also showed the uniform distribution of copper in nanoparticles (Figure 1b). Flow cytometry results in Figure 1c indicate a stronger intensity was obtained by the cells incubated with mannose-labelled nanoparticles, suggesting mannose receptor-mediated endocytosis. Drug release profiles are shown in Figure 1d. Compared with free ATO, ATO-loaded nanoparticles can help maintain a higher drug level in cells in initial 10 hours.

Conclusions: This well-designed nanoparticle complex can be readily used in PET imaging by substituting copper with its radioactive counterpart. This nanoparticle can be further functionalized with different groups and metals for targeted atherosclerosis diagnosis via MRI, CT, and PET imaging. Future work also includes testing the developed nanoparticles in an animal model of atherosclerosis.

Poster #11

Synthesis and Characterization of Dendrimer-Based Nanogels with ROS-Scavenging Activity

Lin Qi¹, Hu Yang¹

¹ Chemical and Biochemical Engineering

Statement of Purpose: It's well documented that excess reactive oxygen species (ROS) underline the pathogenesis and progress of various eye diseases such as age-related cataracts, dry eyes, and open-angle glaucoma (POAG). Therefore, ROS scavenging is a promising strategy for the prevention and treatment of these diseases. The successful application of common ROS scavengers such as natural polyphenol and glutathione (GSH) in the treatment of eye diseases, however, is limited by their poor cornea permeation. Our previous study reported that polyamidoamine (PAMAM) dendrimer-based nanogels can pass through the cornea efficiently. Herein, we report the development of PAMAM dendrimer-based nanogels with broad-spectrum ROS scavenging activity by crosslinking of polyamidoamine (PAMAM dendrimer with ROS-responsive linker (TK-NHS). We tested whether or not this nanogel can serve as a novel ROS-scavenger with excellent cornea permeation for the treatment of eye diseases.

Method: Synthesis of nanogel: Synthesis of NGs (G5-TKNHS): PAMAM (G5) in water was conjugation with -TKNH dissolved in acetone to form nanogel particles by using a multi-inlet vortex mixer (MIVM). Then condensation instrument was used to remove the acetone; the nanogels were dialyzed for 48h in

water and then dried under a vacuum to yield a white powder. Characterization: 1) TEM was applied to characterize the morphology of nanoparticles. 2) Zeta sizer was applied to detect the size distribution of nanoparticles. Functional Assays: 1) Determination of ROS-Scavenging capability with DPPH (200 μ M in ethanol), H₂O₂, and hydroxyl radical incubate in different concentrations of nanogel (37 °C 0.5). 2) ROS-Scavenging in Raw264.7 cells.

Results and Discussion: The nanogel has a uniform size distribution. DLS results are also in agreement with the TEM image. Nanogel shows a scavenging capacity of DPPH, hydroxyl radicals, and H₂O₂ in a dose-dependent profile after incubation. In the cell experiment, Raw264.7 cells were treated with LPS alone as a model group, and another group was treated with LPS and nanogel. The group shows a low-level signal in the nanogel treatment group. From the study result, Nanogel shows a scavenging capacity to LPS-introduced in Raw264.7 cells.

Conclusion: A broad-spectrum ROS scavenger of NGs was successfully synthesized. The ROS-responsive linker exhibited effective scavenging of DPPH hydroxyl radicals and H₂O₂. Meanwhile, NGs effectively scavenged ROS generated in RAW264.7 cells induced by LPS. This nanogel held great potential in developing efficient antioxidant eyedrops. Meanwhile, it can also act as a carrier for drug delivery to improve cornea permeation.

Poster #12

Fungal Communities in Streams Under a Gradient of Streamflow

Syeda Tasfia Imam¹, Dev Niyogi¹, David Duvernell¹

¹ *Biological Sciences*

Aquatic fungi play a key role in ecosystem functioning and nutrient cycling. Leaves submerged in streams are important habitats for fungal colonisation and growth, and the impact of the amount of stream water on the diversity of fungal communities on submerged leaves is not well understood. In this study, we aim to compare the diversity and functioning of fungal communities from streams with varying amounts of streamflow as a model for future impacts of climate change.

We will collect leaves from streams with varying streamflow, from ephemeral to perennial flow regimes. DNA will be extracted from the leaves, and fungal communities will be sequenced using Illumina MiSeq sequencing technology. The resulting data will be analysed to compare the diversity and composition of fungal communities on leaves submerged in different amounts of stream water. We hypothesise that leaves submerged in perennial streams will have a higher diversity of fungi, as they may provide more stable microhabitats for fungal colonisation.

We will use bioinformatics tools to process the sequencing data, including quality control, filtering, and assembly. Taxonomic classification of the sequences will be performed using a reference database such as UNITE or NCBI. We will also analyse the diversity and richness of the fungal communities using alpha and beta diversity metrics such as Shannon, Simpson, and Bray-Curtis indices.

In addition, we will explore the functional diversity of the fungal communities using predictive metagenomic analysis. This will involve predicting the functional genes present in the fungal communities using tools such as PICRUSt or HUMAnN2. The resulting functional profiles will be compared between the different flow regimes, providing insights into the potential role of fungal communities in ecosystem functioning.

This study will provide valuable insights into the impact of streamflow on fungal diversity and composition and will contribute to our understanding of the role of fungi in stream ecosystems. The results will have important implications for the management and conservation of these ecosystems, as changes in flow from climate change or human activities can alter the diversity and composition of fungal communities on leaves and other substrates in streams. Overall, this study has the potential to contribute to our understanding of the diversity and function of fungal communities in freshwater ecosystems and inform management and conservation strategies for these important ecosystems.

Poster #13

Environmental DNA Metabarcoding as a Tool for Fish Community Assessment in Wetlands

Eric Ludwig¹, David Duvernell¹

¹ *Biological Sciences*

Environmental DNA (eDNA) metabarcoding is a novel method of assessing biodiversity in aquatic environments. While the efficacy of eDNA surveys has been well documented in riverine and marine systems, it has been relatively underemployed in freshwater wetland environments. In this study, we conducted an eDNA metabarcoding survey of fish diversity and its seasonal variation in a wetland along the Mississippi River in the Missouri Bootheel. Samples were collected from both permanent and seasonal water bodies including oxbow lakes, a shallow lake, a ditch, and a slough. For each of the 28 sites in this study, 3 water samples were collected in late May. The area was revisited in early October and sites that still held water were resampled. A combination of two, universal fish primer sets were used to amplify fragments of the mitochondrial 12s and 16s rRNA genes and Illumina sequencing was used to generate DNA sequences. A total of 57 species representing 37 genera and 17 families were detected between both markers from the spring samples. Our results indicated that the detected fish communities among different water bodies were distinct from one another despite interconnectivity between them. Our study adds to the evidence that eDNA metabarcoding is an effective method of assessing species diversity and contributes to our understanding of fish community structure in complex wetland environments.

Poster #14

Investigating New Methods for Evaluating Soil Characteristics by Geophysics, Drones (UAV), Remote Sensing Data, and Machine Learning

Effat Eskandari¹, Katherine R. Grote¹

¹ *Geosciences and Geological and Petroleum Engineering*

The integration of geophysical methods, drones (UAV), remote sensing data, and machine learning algorithms has the potential to revolutionize the evaluation of soil characteristics. Conventional methods of soil characterization, such as collecting soil samples, can be time-consuming, expensive, and not representative of the entire area. Geophysical methods, such as GPR and electromagnetic methods, can provide high-resolution data but require more expertise and are costly.

Using a combination of innovative methods, such as using drones equipped with multispectral and thermal cameras, can provide non-destructive and cost-effective measurements with very dense data sets.

On the other hand, Machine learning algorithms can be trained using large datasets of soil properties and their corresponding remote sensing and geophysical data to predict soil characteristics.

To be more specific, for example, a construction engineer utilizes soil characteristics to estimate soil strength, assess landslide hazards, design foundations, and select appropriate building and road materials. Soil characteristics also play a crucial role in climate change models, where they affect water-holding capacity, electrical conductivity, soil salinity, and volumetric water content. Soil salinity, for example, is used to map salt accumulation in soils, while volumetric water content influences the timing and amount of irrigation to satisfy crop needs while conserving water resources and reducing the negative environmental impacts of agriculture.

The main goal of current study is to use collected UAV multispectral and thermal data for training of a machine learning algorithm to predict soil characteristics, such as soil permeability, soil texture, volumetric water content, and electrical conductivity can have a positive effect on agriculture, construction, environmental protection issues, water resource management, and climate change studies.

Poster #15

High Resolution Characterization and Stratigraphic Variability of the Tuscaloosa Marine Shale: Implication on Fine-Grained Sedimentation Dynamics on the Continental Shelf

Chukwuma Mgbenu¹, Wan Yang¹

¹ Geosciences and Geological and Petroleum Engineering

This study characterizes the spatial and temporal, multi-order variabilities in composition and stratigraphy of the Upper Cretaceous shelf marine Tuscaloosa Marine Shale (TMS) from the Gulf of Mexico, USA. This is used to develop high-resolution macro- and micro-stratigraphy to understand the origin of this deposit and establish the major controlling processes and factors of clastic and biogenic fine-grained sedimentation. The research combines core study, spectral analysis, and petrographic analysis. Preliminary logging of five cores shows six lithofacies, interpreted as tractional, mixed, pelagic, and microbial deposits. Cyclicity in parasequences is observed in the core, represented by bipartite and tripartite repetition of lithofacies. Regularity in stratigraphic variability at the mm-sub-mm scale is being tested using grayscale and scratch curves of unconfined compressive strength. Petrographic analysis reveals several structures that control the accumulation of muddy sediments. This study deepens our understanding of the macro- and micro-stratigraphy and processes controlling fine-grained sedimentation. It sheds light on a broader question of the controls and magnitude of variability of fine-grained sedimentary rocks. Understanding fine-grained sediments is crucial to advancement in the paleogeographic reconstruction of the northern Gulf of Mexico and Western Interior Sea and enhancing resource exploration within the basin.

Poster #16

The End-Triassic Hyperthermal Event: An Analog for the Recent Hunga Tonga – Hunga Ha’apai Volcanic Eruption

Ahmed El Manharawy¹, Francisca Oboh-Ikuenobe¹

¹ Geosciences and Geological and Petroleum Engineering

Hyperthermal events (HTEs), episodes of rapid climate warming, have substantially affected the composition, structure and functioning of marine ecosystems in the past. Extinction selectivity based on

specific clade and/or trait can be considered as a fingerprint of the main trigger for extinctions during such events. The end-Triassic (ET) mass extinction was driven by euxinia, and this is supported by extinction selectivity of infaunal bivalves and solitary cnidarians, which are euxinia intolerant traits. The ET hyperthermal event can be used as an analog for the recent Hunga Tonga – Hunga Ha’apai (HTHH) igneous eruption which resulted in euxinia. Thus, the outcomes of this research are applicable to other similar locations worldwide that have experienced euxinia.

Poster #17

Investigation of the Relationships between Hydraulic, Physical, and Biological Soil Parameters at a Vineyard in Saint James, Missouri

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Soil is a living, dynamic system that performs vital functions such as crop production, organic matter decomposition, and the flow and transport of water. Given the pressures of food and in some locales water security, climate change, and sustainability, farmers, scientists, and other related specialists and stakeholders must have access to understandable soil health indicators as well as the soil hydraulic function parameters to maximize crop growth while maintaining soil health. Although biological and physical soil parameters are different, we aim to evaluate their relationship at the field scale. Hydraulic conductivity in the vadose zone may be especially important, as it affects the flow of air and water that control many biological and chemical processes. This study makes use of recent advancements in mapping hydraulic conductivity using ground-penetrating radar techniques in a vineyard in St. James, Missouri. These maps were used to select sample locations of varying hydraulic conductivity, which was used in turn to acquire other soil parameters that are indicative of the biotic system, specifically the microbial activity and carbon cycle. This study observed that the soil health parameters strongly positively correlated with the hydraulic parameters, but neither correlated with the particle size analysis of the soil. This suggests that hydraulic conductivity is tied to the carbon cycle. We also investigated the potential for estimating soil parameters that are more difficult or expensive to measure, such as the field saturated hydraulic conductivity and soil respiration, using soil parameters that are easier or cheaper to measure, such as aggregate stability, soil organic carbon content, and bulk density. Adjusted bulk density and soil organic carbon were strong predictors of hydraulic conductivity.

Poster #18

Characterization of Tellurium, Gold, and Silver from Copper Porphyry Processing Streams

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The U.S. Department of Energy (DOE) classified tellurium (Te) as a “critical mineral” for its importance to clean solar energy. A substantial increase in Te demand is projected to de-carbonize the electric energy systems. Therefore, the mining and metallurgical industries must increase Te production from existing and inefficient supply chains. For example, most of Te associated with copper sulfide ores is lost to tailings during the froth flotation process. Thus, increased Te production can be achieved by improving Te recovery in flotation concentrates and/or reprocessing the tailings.

This research provided an improved understanding of the distribution of Te, Au, and Ag minerals in the processing streams during the flotation process of copper sulfide ores to identify potential streams from which these minerals can be recovered. The samples used in this research were flotation feed, concentrates, and tailings provided by a copper mine in the U.S. The analytical techniques used for quantitative and qualitative characterization included reflected light microscopy, scanning electron microscopy (SEM-EDS), electron-microprobe analysis (EMPA), and TESCAN's Integrated Mineralogical Analysis (TIMA). Characterization studies of the feed and tailings showed that Te was mainly associated with Au and Ag tellurides and Te sulfosalts. These minerals were hosted primarily in pyrite as small inclusions of $< 10 \mu\text{m}$. Analyses of concentrates showed a strong association of Te with Ag in pyrite, whereas Au was mainly hosted in chalcopyrite. Results affirmed that Te was deported to the tailings; therefore, reprocessing sulfides in the tailings stream from the copper flotation process is a feasible strategy to enhance Te, Au, and Ag recoveries.

Poster #19

Securing Smart Water Metering Infrastructures: A Scalable Approach to Detecting False Data Injection

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¹ *Computer Science*

Smart water metering (SWM) infrastructure collects real-time water usage data used for automated billing, leak detection, and forecasting of peak periods. Cyber/physical exploits on smart water meters can lead to data falsification attacks on water usage data.

This paper proposes a learning approach that converts city scale smart water meter data into a Pythagorean mean-based invariant that is highly stable under normal conditions but deviates under attacks. We show how adversaries can launch deductive or camouflage attacks in the SWM infrastructure to gain benefits and impact on the water distribution utility. Then, we describe what causes the bad data and how it can be handled. Next to detect anomalies in large-scale SWM infrastructure, we first propose a clustering algorithm that is able to identify houses with similar water usage to maximize the covariance by combining information theory and graph theory. Within these clusters, we apply a two-tier approach of stateless and stateful detection, reducing false alarms without significantly sacrificing the attack detection rate. We validate our approach using real-world water usage data of 92 households and 1,099 households in Alicante, Spain for varying attack scales and strengths and prove the our method limits impact of undetected attacks and expected time between consecutive false alarms.

Poster #20

Using Geographic Location-Based Public Health Features in Survival Analysis

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Time elapsed till an event of interest is often modeled using the survival analysis methodology, which estimates a survival score based on the input features. There is a resurgence of interest in developing more accurate prediction models for time-to-event prediction in personalized healthcare using modern tools such as neural networks. Higher quality features and more frequent observations improve the predictions for a patient, however, the impact of including a patient's geographic location-based public health statistics on individual predictions has not been studied.

This paper proposes a complementary improvement to survival analysis models by incorporating public health statistics in the input features. We show that including geographic location-based public health information results in a statistically significant improvement in the concordance index evaluated on the Surveillance, Epidemiology, and End Results (SEER) dataset containing nationwide cancer incidence data. The improvement holds for both the standard Cox proportional hazards model and the state-of-the-art Deep Survival Machines model. Our results indicate the utility of geographic location-based public health features in survival analysis.

Poster #21

Secure and Efficient Federated Learning in LEO Constellations Using Decentralized Key Generation and On-Orbit Model Aggregation

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In recent years, satellite technologies have advanced drastically, leading to a heated interest in launching small satellites into low Earth orbits (LEOs) to collect high-resolution images for various applications. However, the high speeds of LEO satellites, limited bandwidth, and the high communication costs associated with transmitting these images to a ground station (GS) present significant challenges to both downloading the images and preserving data privacy. Although introducing federated learning (FL) into LEO constellations is a promising solution, the sporadic and irregular connectivity of LEO satellites with GS leads to large convergence delays, and the required transmission of FL model parameters poses a potential risk of inferring the raw data and hence compromises privacy. To address these issues, we propose FedSecure, a secure FL approach designed for LEO constellations. FedSecure consists of two novel components: (1) decentralized key generation which protects the privacy of satellites' data using a functional encryption scheme, and (2) on-orbit model aggregation which generates a partial global model per orbit to minimize the idle waiting periods between invisible satellites and the aggregation server (the GS in the context of FL). Our extensive evaluation demonstrates that FedSecure significantly reduces convergence time from days to only a few hours, yet achieves even higher accuracy up to 91.6%. FedSecure also has lightweight communication overhead, making it more efficient than existing privacy-preserving aggregation algorithms.

Poster #22

HatEmoTweet: Low Level Emotion Classifications and Spatio-Temporal Trends of Hate and Offensive COVID-19 Tweets

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Social media platforms (like Twitter) positively and negatively impact users in diverse societies; one of Twitter's negative effects is the usage of hateful and offensive language. Hate speech fosters prejudice; it also harms the vulnerable. There are always emotions associated with hateful and offensive actions. This work addressed hate and offensive tweet detection and low-level emotional classifications using 28 labels to train transformer models in three ways (model 1 - BERTG28, model 2 - BERTG27 and model 3 - RoBERTaG27) before predicting the hateful and offensive tweet emotions. Model 1 was trained on low-level labels, and model 2 and 3 were trained on 27 labels, excluding the neutral label. This study also performed topic modeling to extract the discussed theme, spatiotemporal trends to determine where and

when these tweets occurred, and event summarization for identified hate and offensive tweets. GoEmotions and Ekman were used for direct and indirect assessment, respectively, to evaluate the model's precision, recall, and F1-score. In terms of precision evaluation, the model 1 outperformed Google Research on GoEmotions. Furthermore, this study's model 2 and 3 outperformed the Google research on both the GoEmotions and Ekman's evaluation in terms of precision and F1-score. Generally, model 2 was the best model in the analysis for both recall and F1-score while model 3 performed better for precision. Due to the training on samples without the neutral label, model 2 obtained 27% and model 3 achieved 29% label prediction out of the 30% neutral sample that was predicted in model 1 for hate and offensive tweets. This study has made a noteworthy advancement in optimizing the classification of emotions by reclassifying the false neutral class, thereby enhancing the accuracy of the results. Additionally, it has successfully identified topics and events that are associated with hate and offensive tweets over a period of seven months, and has also established the relationship between users based on tweet propagation, engagement, and visibility.

Poster #23

A Parallel Framework for Efficiently Updating Graph Properties in Large Dynamic Networks

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Graph queries on large networks leverage the stored graph properties to provide faster results. Since real-world graphs are mostly dynamic, i.e., the graph topology changes over time, the corresponding graph attributes also change over time. In certain situations, recompiling or updating earlier properties is necessary to maintain the accuracy of a response to a graph query.

Here, we first propose a generic framework for developing parallel algorithms to update graph properties on large dynamic networks. We use our framework to develop algorithms for updating Single Source Shortest Path (SSSP) and Vertex Color. Then we propose applications of the developed algorithms in Unmanned Aerial Vehicle (UAV) based delivery systems under time-varying dynamics. Finally, we implement our SSSP and vertex color update algorithms for Nvidia GPU architecture and show empirically that the developed algorithms can update properties in large dynamic networks faster than the state-of-the-art techniques.

Poster #24

Localized Residual Stress Evaluation in Cubic Titanium Manufactured via Powder Bed Fusion

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High magnitude residual stresses are problematic to components produced via Additive Manufacturing (AM). Caused by high thermal gradients, they can negatively impact the mechanical performance of the material as well as deform the net shape. Methods to evaluate these stresses at the micro scale are limited. A novel method developed by MS&T faculty and students will be used to evaluate stresses in a cubic titanium alloy designed for AM to develop a greater understanding of how these stresses interact within the unique microstructural features of AM. The AM process imparts a structure of intertwined melt tracks and pools similar to welding beads and experience a complex thermal history. Stress patterns are observed and analyzed in the context of the meltpool/track structure.

Poster #25

Additive Manufacturing of a Precipitation-Strengthened HEA

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Additive manufacturing (AM) is a novel manufacturing technique which can produce near-net shapes and complex internal geometries. AM will be essential to the construction of certain parts in advanced nuclear reactors, but the rapid cooling rate and repeated passes inherent in the AM process can result in microstructures vastly different from traditional casting and processing. A Co-free precipitation-strengthened high entropy alloy (HEA), (Fe_{0.3}Ni_{0.3}Mn_{0.3}Cr_{0.1})₈₈Ti₄Al₈, has been previously found to have high strength but poor ductility after aging at 650 °C for 120 hours. This alloy composition was fabricated using direct energy deposition (DED), an AM technique which injects elemental powders into a laser and deposits a pattern onto a 316 substrate. After printing, the HEA shows an impressive combination of 1300 MPa strength and 15% ductility. To further improve the strength, aging was conducted at 600 °C and 650 °C for varying times up to 72 hours, resulting in hardness higher than that produced by casting and aging. The microstructure was evaluated using scanning electron microscopy (SEM), electron backscatter diffraction (EBSD), transmission electron microscopy (TEM), and atom probe tomography (APT). Using these techniques, it was determined that the as-printed condition possessed fine grains (3 μm) with small B2 precipitates but no nanoscale L12 precipitates. Aging resulted in nanoscale (<10 nm) L12 precipitates and the formation of B2 and χ on grain boundaries. The study of the differences in microstructure after AM will help design HEA compositions which produce optimal properties when printed.

Poster #26

Studying the Effects of Fly Ash Chemistry on Properties of Calcium Aluminate Binders

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Calcium aluminate cement (CAC) is widely considered to be an energy- and carbon-efficient alternative to Portland cement (PC). Due to its excellent early strength and thermal resistance, CAC has been used for the construction of physical infrastructure, especially those for extreme environments. Though CAC is an alternative to PC binders a lot of research focuses on the replacement of CAC with supplementary cementitious materials (SCMs) to lower the cost of concrete and reducing the environmental impact of CAC, and still be able to achieve better mechanical properties. Fly ash (FA) – an industrial byproduct – is used to partially substitute CAC in concrete or completely replace CAC to mitigate concrete's environmental impact. The chemical composition and structure of FAs significantly impact hydration kinetics and compressive strength of concrete. Due to the heterogeneity in the composition of FAs, it has been difficult to develop an analytical model to predict the reactivities of FA. To address this concern, a singular parameter called “number of constraints” derived from the topological constraint theory (TCT) is used to determine the reactivity of FAs. Quantitative analyses are employed to reveal the relationship between cumulative heat release and compressive strength; and to describe the influence of reactivity (i.e., number of constraints) and content (replacement level) of FAs on compressive strength and hydration kinetics of the binders. Based on these analyses, two simple, closed-formed analytical models are developed to predict cumulative heat and compressive strength of [CAC + FA] binders in relation to replacement level and number of constraints of FA.

Poster #27

Spatial Thermal Mapping of the Water-Cooled Upper Shell of an Electric Arc Furnace Using Fiber Optic Sensors

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Modern Electric Arc Furnaces (EAF) employ ultra-high-power electrical input to minimize the scrap melting time. Increasing the operating voltage increases arc length and enhances the active power, but radiation energy losses also increase if the arc is exposed to the furnace, resulting in a drop in thermal efficiency and causing hot spots in the furnace. The present work shows how fiber optic sensors may be used to create a real-time spatially distributed thermal map of the EAF's water-cooled upper shell, which can be helpful in detecting operational anomalies and improving EAF energy efficiency. To achieve this goal, a lab-scale setup consisting of tubular water panels was developed, employing copper coil tubing (with a uniform water flow rate) and instrumented with fiber-optic sensors. These sensors are able to perform measurements with a spatial resolution of 2 mm and a 1 Hz acquisition rate. We conclude that the preliminary setup is a promising tool to perform spatial thermal mappings of an EAF water cooling panel.

Poster #28

Design and Detection of False Data Injection Attacks in Power System State Estimation

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In this work we developed a technique to design false data injection attacks (FDIA) that falsify the state estimate information as observed by the system operator. The FDIA attacks designed here consider the nonlinear alternating current power flow (ACPF) equations, and factors such as sparseness of the attack vector, minimal change in the measurement residual post attack, and an attack goal are considered. A novel detection technique based on statistical metrics that relies on the system level measurement residuals is developed while to localize and obtain the magnitude of the FDIA attack vector the low rank of a measurement data matrix is considered. Particularly, the Chi square distance is utilized for FDIA detection, Go Decomposition (GoDec), and the dual problem (DP) are utilized for locating and obtaining the magnitude of attack vector. Simulation results on an IEEE 14 bus system shows the efficacy of the proposed approach in detecting and locating the FDIA attacks in AC static state estimation.

Poster #29

Active Microwave Thermography

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Active Microwave Thermography (AMT) is a coupled electromagnetic-thermal nondestructive testing (NDT) technique that utilizes an electromagnetic source to induce heat with subsequent thermal investigation by an infrared camera. This type of induced heat is accomplished through dielectric and magnetic heating. Dielectric and magnetic heating is dependent upon a material's dielectric and magnetic properties. These properties are complex (i.e., real and imaginary components) and are often referenced to free-space as $\epsilon_r = \epsilon_r' + j\epsilon_r''$ (dielectric) and $\mu_r = \mu_r' + j\mu_r''$ (magnetic). The imaginary portion,

$\epsilon r''$ and $\mu r''$ (i.e., electric and magnetic loss factors, respectively), are of particular interest to AMT as this is the component that dictates the ability for a material to absorb electromagnetic energy (i.e., generate heat). This heat then propagates through the material to an inspection surface and is observed by an infrared camera. The data from the infrared camera can be analyzed raw or post-processed through the following: edge detection, Fast Fourier Transform, thermographic signal reconstruction, etc. While much of the future for AMT will be in the post-processing spectrum, there is still work to be done in creating a uniform heating pattern to resemble that of traditional thermography. This uniformity is currently accomplished by a randomly phased antenna array. Recent work utilizing such an array consists of a 2-D planar array where the phase of each antenna element (within the array) is randomized in such a way that each element never has an identical phase, and the phase is not repeated until all phases (within -180 to 180 degrees) have been utilized. In addition to the NDT aspect, AMT has found success in thermal materials characterization as well (specifically for thermal diffusivity). For in-plane (inspection surface) thermal diffusivity a spatial resolve approach was utilized with successful comparison to the known thermal diffusivity. Additionally, out-of-plane (i.e., through a material as opposed to the inspection plane) thermal diffusivity has recently been calculated by AMT measurements. The electromagnetic energy penetrates the superstrate, allowing for the substrate to absorb the incident electromagnetic energy and diffuse the heat to the surface, where thermal diffusivity can be calculated from the results. The future for AMT materials characterization is in calculating additional thermal material properties such as thermal conductivity and specific heat.

Poster #30

Corrosion Damage Detection in Aircraft Data Transmission Lines Using Vector Network Analyzer

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Maintaining performance-capability of aging aircrafts persist to be a challenge in aircraft industry. This is due to increasing fleet of aging aircrafts flying beyond their design life, or use of refurbished aircrafts sold to third world countries. Aging aircrafts are more prone to operational damages, such as corrosion in aging aircraft structures and systems. Corrosion affects not only Aircraft structures but also all the wiring systems including data transmission lines at the points of mechanical damages and connections. The reliability of data transmission is essential for maintaining performance-capability of aircraft and safety of flights. Unfortunately, there are no current methods to detect corrosion existence and predict its effect for any wiring system including aircraft data transmission lines (ADTLs). Detecting corrosion and predicting its effect would prevent unexpected system failures and catastrophes. This paper presents the result of investigation of the effect of corrosion on ADTLs-aircraft coaxial cables. The effect of corrosion was investigated in damaged aircraft coaxial cable TCA311201 used in navigation, communications, and other aircraft systems. Damaged coaxial cables were corroded in Q-Fog accelerated corrosion chamber (Model#CCT600) according to standard ASTM G85-A5 Prohesion test, that resembles aircraft environment, for up to 14 weeks (2352 hours). After every week (168 hours) of exposure to corrosive environment, damaged coaxial cables were taken out of the corrosion chamber and investigated using a Vector Network Analyzer (VNA). Signals with frequencies from 0 to 6GHz were swept into the cable. Computed power of reflected and transmitted signals acquired in time domain and compared with power signals obtained from measurement in the pristine condition of the cable. Tracking of signal change in width and peak prominence of all the measurements from all hours of exposure in the corrosion chamber with measurements obtained in pristine condition was performed

for determining the effect of corrosion on signal reflection and transmission. By alteration of the signal, level of corrosion was determined. Analysis of results show that corrosion effect is not arbitrary and can be tracked over time and predicted. Reflected signal peak width also changes with time of ADTLs exposure in the corrosive environment and is proportional to the real corrosion width propagation inside the ADTLs. The progress in the research will be presented.

KEYWORDS: Aging aircraft, Corrosion, Aircraft data transmission line, Coaxial cable, Signal reflection and transmission, Vector Network Analyzer, Accelerated corrosion testing, Damage detection.

Poster #31

Optimization of the System of Systems (SoS) Meta-Architecture of Algae Systems for Cost-Effective Pollution Remediation

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To help safeguard the environment and its inhabitant organisms, it is essential to incorporate algal systems into the remediation of nutrient pollution at the initial nutrient or pollution source by using the systems to grow algae and cyanobacteria. To maximize output and cut costs, it is crucial to understand the algal System of Systems with a focus on the meta-architecture of the photobioreactor while comparing system attributes to an open algal system.

Algal systems are complex systems, and for qualitative reasons, it is important to comprehend how the pieces behave and, how they interact to produce the behavior of the whole. For a photobioreactor focusing on the interactions of the parts together rather than their performance accessed separately can help to manage the system efficiently and optimally. These interfaces are collectively monitored by a cyber-physical system (CPS) in which the mechanism is controlled by computer algorithms called the System of Systems (SoS) explorer.

In this paper, using the Engineering Management and Systems Engineering's SoS Explorer tool the systems and characteristics of the algal system were accessed, noting the characteristics, capability, and key performance attributes. These factors further aided in achieving the optimal performance using the genetic algorithm coherently with the fuzzy assessor as a fitness function to obtain the best fit of the system to recognize improvements for future performances.

The application of algorithmic techniques to the system resulted in an optimized design with key performance attributes (KPA) values of affordability at 71.6%, availability at 100%, characterizability at 80.74%, robustness at 59.81%, and sustainability at 68.86%. The outcomes obtained from the Flexible and Intelligent Learning Architecture System of Systems FILA-SoS revealed that more attention should be devoted to enhancing the sustainability and robustness of the algal system.

The developed meta-architecture for the algal system provides valuable insights into the essential systems, capabilities, characteristics, and interfaces that need to be considered and showed that sustainability, robustness, and cost control are critical factors that should not be compromised. The findings also suggest further investigations, including the use of exact mathematical modeling to better

understand the discussion and determine the meta-architecture model's applicability in comparison to actual system designs.

Poster #32

Human-Robot Collaboration in Manufacturing

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This research focuses on the integration of drones and multi-modal sensing techniques to enhance the collaboration between humans and robots in the manufacturing industry. One of the key aspects of this research is the use of multi-modal sensing to capture implicit communication cues and predict human intentions and actions. Two primary techniques for intention prediction are explored: eye gaze tracking analysis and brainwave signal monitoring. These techniques provide insights into the focus of attention, decision-making, and action planning processes of humans. By interpreting these signals, robots can respond more accurately and efficiently to human needs, resulting in improved collaboration. In addition, drones are integrated into human-Robot Collaboration (HRC) systems as they offer several benefits, including accessing hard-to-reach areas, providing aerial views, and transporting tools and parts to human teams. Computer vision techniques is employed to analyze visual data from Red-Green-Blue-Depth (RGB-D) cameras mounted on drones, enabling them to autonomously detect and transport tools and parts to desired locations, improving the efficiency and safety of manufacturing processes. Overall, the research contributes to the advancement of HRC in the manufacturing industry by leveraging multi-modal sensing and drone integration. By predicting human intentions and enabling autonomous tool and part transportation, the collaboration between humans and robots becomes more effective and efficient, enhancing the overall productivity and safety of manufacturing processes.

Poster #33

Spatially Informed Thermal Feedback Control of Glass Filament Additive Manufacturing

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The additive deposition of optically transparent glass affords unique opportunities to quickly produce optical components, such as functionally graded optics, which cannot be realized via subtractive methods. While the inherent porosity of traditional powder-based additive processes typically inhibits optical clarity, directed energy methods utilizing fully-dense filament feedstocks can uniquely achieve transparent glass deposition.

However, precise process control of the deposition geometry is challenging due to glass material properties and requisite process temperatures. Notably, minor variations in either material or process can produce large variations in output part quality.

Here, we investigate the use of a thermal camera to provide in-situ feedback on the material thermal distribution during deposition. With the aim of rejecting undesirable variations in the thermal profile, several methods are considered for producing a spatially-weighted feedback control metric.

Laser power is adjusted through feedback to maximize thermal profile consistency, as evaluated in both rastered (in-layer) and layer-to-layer paths. This presentation will report on both the performance results of the regulated process as well as avenues for future research.

Poster #34

Development of a Coaxial Wire-Feed Deposition Process

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The robotic wire-feed deposition cell in the Laser Aided Manufacturing Processes (LAMP) lab is a research cell primarily for titanium 3D printing. The project goal is to develop a fully operational deposition cell integrated with the deposition head loaned by GKN Aerospace so that it may be used for future research and investigation. The main challenges for this project include the mechanical design of an end effector, designing and implementing a fully integrated control system, performing deposition for analysis, developing mechanical testing techniques, and creating demonstration parts. Current progress to date includes fully integrating the equipment, process benchmarking, implementing process monitoring and control methods, and creating deposited demonstration parts. A delta robot has been fully integrated with a Miller Autocontinuum Hot Wire system, Fraunhofer COAX Wire deposition head and 4kW Laserline diode laser. The system is controlled through LinuxCNC with a module for using delta style kinematics. Mechanical testing methods that are currently being investigated include mini-tensile and mini-fatigue testing, micro-CT scanning, and microstructure analysis using SEM imaging. Miniature tensile testing is executed using the LAMP designed MT2 tensile test specimen. Work is also being performed on developing a miniature axial fatigue specimen to allow thin-walled AM depositions to be characterized by location. Micro-CT scanning uses the ZEISS Xradia 620 Versa to non-destructively image samples to inspect internal geometries and defects. Based on the types of defects present in the specimen, deposition parameters can be altered to reduce harmful defects in the deposits. SEM imaging of a chemically etched specimen provides information on a deposit's microstructure. The microstructure can be used to predict mechanical properties for the deposited material. By tuning the microstructure of the deposit, optimal mechanical properties can be achieved. Laser power control (LPC) is being developed to control heat buildup in a deposit. The task of determining optimal sensors and system parameters to track in the creation of a digital twin is underway. The deposition cell already has some of the necessary sensors needed for a digital twin but additional sensors will be needed to account for further system parameters. The work will focus on the development of the abovementioned mechanical testing techniques and of laser power control. With a unified control system and a solid understanding of the mechanical properties of the deposits, the wire-feed cell will be capable of depositing material that is up to aerospace manufacturing material standards.

Poster #35

Shock Wave Boundary Layer Interaction in a Double-Bend Duct

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The complex flow interaction of a shock wave transmitted through a double-bend two-dimensional duct geometry is studied numerically. OpenFOAM is used to simulate the shock propagation using the Euler equations and $k-\omega$ SST turbulence model. The results are compared against existing experimental and numerical work on the double-bend duct geometry. The incident Mach number is varied to determine the impact the Mach number has on tertiary shock and shock wave boundary layer interaction formation. Turbulent simulations show shock wave boundary layer interaction, not observed

in other numerical simulation studies, supporting experiments by other investigators. Locally supersonic structures merge to form the triple point between the primary vortex and SWBLI vortex. Inlet duct height was varied to explain why the triple point has never been examined. A larger double-bend geometry is simulated to study the natural interaction and evolution of the primary and SWBLI vortices.

Poster #36

Using Vibration to Insert Rebar Reinforcement into 3D Printed Concrete

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Concrete is a widely used structural material. In order to be useful and able to survive tensile loading, however, it must be reinforced, typically with steel rebar reinforcement. It would be very useful to 3D print concrete structures, but a current limitation of concrete 3D printing is placement of reinforcement. This research project uses a granular, friction-based concrete mix design. Such a mixture enables creation of a local, vibration-induced fluidization zone to insert rebar reinforcement into unhardened 3D printed concrete layers. Large aggregates create force chains that transfer stress through direct contact, leading to high unhardened yield strength which is good for printing multiple layers. The yield strength can be lowered by vibrating the mixture, and turning on vibration causes the material to flow. Preliminary results achieved an order of magnitude reduction in yield strength of the material due to mixture vibration. Similarly, a local, focused vibration can be used to insert rebar into the standing, unhardened concrete. The primary concern is collapse of the concrete during rebar insertion. Preliminary results using a slump cone test showed very low slump (1/4" - 3/4") before and after rebar insertion. In the lower portion of the cone, the concrete stuck to the rebar after insertion, indicating the vibration did not leave a hole around the reinforcement, which would negatively impact bond strength.

Poster #37

Reinforced Masonry Shear Walls in High Rise Buildings

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Reinforced masonry shear walls are widely used as one of the seismic forces resisting system for low-rise structures in North America. With increased building code safety requirements for structures subjected to severe seismic action, much research is currently being conducted to evaluate the behavior and performance of reinforced masonry shear walls (RMSWs). The current seismic design philosophy for RMSWs assumes that adequate seismic performance is achieved through increased ductility, which allows for greater energy dissipation. However, TMS 402 (Building Code Requirements and Specification for Masonry Structures) ensures ductile behavior of the reinforced shear walls with limitations on axial load and maximum reinforcement. This means RMSWs cannot be used in high-rise structures. This research tested and evaluated seismic performance and behavior of 33 large scale reinforced masonry shear walls subjected to high axial load while being seismically loaded in-plane and out-of-plane. State-of-the-art testing setups were built to simulate real-world scenarios of heavily axially loaded shear walls subjected to seismic loading. Force-displacement behavior, masonry and steel reinforcement strain profiles, curvature, ductility, extent of plasticity and energy dissipation were studied. Moreover, parametric study was done with finite element analysis and modeling using LS-DYNA to predict the behavior of such shear walls in an event of an earthquake. The study aims to propose verified limits on

axial loading on reinforced masonry shear walls thus allowing this cost-effective and viable construction method to be used in high-rise structures.

Poster #38

Numerical Modelling Investigation of Precast Concrete Girders under Vehicle Collisions

Haitham AbdelMalek¹, Mohamed A. ElGawady¹

¹ *Civil, Architectural and Environmental Engineering*

Precast concrete girders are susceptible to failure when exposed to extreme loading conditions, such as vehicle collisions. Ensuring resilient bridges, adequate design is required to safeguard the bridge members against such hazards and mitigate the probability of collapse. However, the lack of experimental data and reliable finite element models is one of the main reasons why the current code lacks clear design procedures for such loads. To address this issue, high-fidelity finite element models were developed using LS-DYNA and validated against experimental data. The calibrated models were then implemented to perform a parametric study to investigate the key factors affecting the dynamic response of precast girders under vehicle collisions. Several parameters, including vehicle speed, mass, girder span, and girder type, were analyzed in terms of demand intensity and mode of failures. The study revealed that the most critical factor affecting the dynamic response of precast girders was impact impulse. In addition, a full bridge model was developed and compared against individual girders with a composite deck slab to study the effect of reducing the number of girders. The reduced model exhibited similar behavior to the full bridge when the deck was restrained against lateral and rotational translation. The study provides valuable insights into the behavior of precast concrete girders under extreme identifies key parameters that should be considered in the design of precast bridges. The results of this study can assist the quantification of the dynamic demand and the development of design guidelines that will enhance the safety and resilience of precast bridge structures.

Poster #39

Circular Economy Strategies for Curbing Embodied Emissions of the US Commercial Built Environment: A System Dynamics Modeling Approach

Radwa Eissa¹, Islam El-adaway¹

¹ *Civil, Architectural and Environmental Engineering*

As efforts to decarbonize operations of the built environment become more prevalent, concerns over the amount of embodied carbon generated during the extraction, transportation, manufacturing, construction, and disposal of building materials are growing steadily. Commercial building stocks, which are a major source of embodied carbon, can contribute significantly to national climate goals by transitioning to a circular economy (CE). However, research on embodied carbon reduction is limited, and there is sparse data on the impact of different CE strategies and their scalability for nationwide commercial building stocks. To address this knowledge gap, this research aims to provide policymakers with a conceptual model that illustrates the potential of CE strategy portfolios to reduce embodied carbon in commercial building stocks. Using US commercial buildings data from the Energy Information Administration, a system dynamics model was developed to derive a baseline value for existing embodied emissions and evaluate the influence of various policy packages over a planning horizon between 2022 and 2050. Results highlighted that early design and construction CE interventions were more effective than end-of-life strategies such as recycling, as well as traditional and business-as-usual approaches. Ultimately, the established system can support decision-makers in analyzing multiple

"what-if" scenarios for their policies. In addition to that, the model can also serve as a building block to a scalable decision-support tool to identify the most effective strategies for narrowing material loops and curbing embodied emissions.

Poster #40

Oral Session A: Advancing Equations, Algorithms & Models

Session Details:

Location: Turner Room, 204A

Time: 1 p.m. to 3 p.m.

Campus Judges:

Dr. Hanli Wu, Civil, Architectural and Environmental Engineering (session chair)

Dr. Sanaz Vajedian, Geosciences and Geological and Petroleum Engineering

Guest Judge:

Megan Russom, Sonoco Products Company

Session Timeline:

- 1:00 p.m. Phases and Phase Transitions in q-State Quantum Clock Model, **Gaurav Khairnar**
- 1:20 p.m. Ensemble Methods for the Magnetohydrodynamics Equations, **John Carter**
- 1:40 p.m. Characterization of Chemically Reacting Hypersonic Flows, **Kyle Worden**
- 2:00 p.m. Combining Stakeholder Input and Literature Review Focusing on Effective Human-AI Team Performance, **Harishankar Vasudevanallur Subramanian**
- 2:20 p.m. MinerFinder: A GAE-LSTM Method for Predicting Location of Miners in Underground Mines, **Abhay Goyal**
- 2:40 p.m. From Phenotyping Electronic Health Records to Generating an Explanation Space, **Raghu Yelugam**

Session Abstracts:

Phases and Phase Transitions in q-State Quantum Clock Model

Gaurav Khairnar¹, Thomas Vojta¹

¹ *Physics*

Recently, buckling transition in planer crystals of strongly interacting ultra-cold atoms was explained using q-state clock model. In this work, we study the phases and phase transitions in q-state quantum clock model using large-scale Monte Carlo simulations. The clean case of this system shows the emergence of intermediate quasi-ordered phase between paramagnetic and ferromagnetic phases. While earlier studies have provided detailed understanding of the clean case, the effect of the disorder on the phases is vastly unknown. By varying the disorder strength, we study the phase transitions and

the associated critical behavior. We find the intermediate phase shrinks and eventually vanishes as we increase the disorder strength. The system shows a non-trivial crossover from disorder independent weak to disorder dependent strong regime in the critical behavior. In the strong disorder limit, we show the evidence of previously predicted infinite-randomness physics. As a result of this work, we provide the understanding of the effects of disorder and verify earlier predictions.

Ensemble Methods for the Magnetohydrodynamics Equations

John Carter¹, Daozhi Han¹, Nan Jiang¹

¹ *Mathematics and Statistics*

In this oral presentation, we investigate second-order ensemble methods for fast computation of an ensemble of MHD flows. Computing an ensemble of flow equations with different input parameters is a common procedure for uncertainty quantification in many engineering applications, for which the computational cost can be prohibitively expensive for nonlinear complex systems. We propose multiple ensemble algorithms that reduce the computational cost and simulation time by requiring only solving a single linear system with multiple right-hand sides instead of solving multiple different linear systems. Specifically, we define an ensemble mean for the velocity and electric potential of the reduced MHD equations at small magnetic Reynold's number and present the corresponding algorithm. Next, we extend this approach to the viscosity and magnetic resistivity of the full MHD equations and combine it with a generalized positive auxiliary variable technique (GPAV) to achieve an algorithm that's unconditionally stable with respect to a modified energy. We also present numerical tests that illustrate the theoretical results and demonstrate the efficiency of the resulting algorithms.

Characterization of Chemically Reacting Hypersonic Flows

Kyle Worden¹, Serhat Hosder¹

¹ *Mechanical and Aerospace Engineering*

Hypersonic vehicles, such as spacecraft reentering the Earth's atmosphere like Apollo or the more recent Orion, experience extreme conditions that make survivability difficult including vibrational excitation of molecules, chemical reactions and, ionization. Due to these challenges, flight testing of hypersonic reentry vehicles is limited, and so computational models and ground test facilities provide the best insight into the performance of these vehicles, however the test conditions must be well characterized, and the physics understood because flight conditions can never be perfectly reproduced. This work expands on previous tools to characterize the chemical behavior of the flow by using a novel approach to characterize the chemical kinetics for a hypersonic vehicle by expanding on the concept of the Damköhler number.

The Damköhler number, which relates the chemical time scale to the flow time scale, has previously only been applied to chemical kinetics with a strong directional bias such as combustion. This is due to the ratio being defined in part by the net mass production of a species. By instead defining a reaction rate based Damköhler number, which encompasses the gross mass exchange due to a reaction, the behavior of individual chemical reactions can be well characterized. Results for a spherical body experiencing reentry conditions are investigated, showing the regions of chemical equilibrium, non-equilibrium, and frozen flow as you move away from the stagnation point.

This methodology provides a way to design ground test experiments to match the chemical behavior of a hypersonic vehicle in flight by using a reaction rate Damköhler number, much like how Reynolds number matching does for viscous forces. The characterization of chemical non-equilibrium is vital to reduce uncertainties regarding surface-gas interaction for thermal protection system materials, and for predicting radiative heating values experienced by the vehicle. Previously only chemical composition could be matched for hypersonic flows, not the chemical kinetics.

Combining Stakeholder Input and Literature Review Focusing on Effective Human-AI Team Performance

Harishankar Vasudevanallur Subramanian¹, Casey Canfield¹, Daniel B. Shank²

¹ *Engineering Management and Systems Engineering*

² *Psychological Science*

Over the past years, the use of AI recommender systems has increased significantly in sectors such as healthcare, legal, and defense. With this rise of use, users are now wanting to understand how an AI system makes a decision. Explainable AI is a growing field of research that aims to open the inner workings of an AI recommender system, so that users can understand and interpret its decisions. In an ongoing project focused on developing an AI recommender system to reduce the number of kidney discards, we collaborated with kidney transplant stakeholders to understand their needs and constraints in the current workflow. The kidney transplant stakeholders comprise of three major groups – (1) Transplant Centers in charge of placing a donor kidney in a Recipient, (2) Organ Procurement Organization in charge of procuring deceased donor kidneys and matching it with a Transplant Center and, (3) Recipients who choose to receive the deceased donor kidney. The kidney transplant stakeholders participated in multiple personal interviews and group workshops to identify system requirements and provide Explainable AI feature preferences. Consequently, we conducted a literature review of Explainable AI methods used in the human-AI collaboration context. The paper begins by briefly summarizing the findings from the stakeholder engagement contextualized within the literature reviewed. The major findings include, user preference only sometimes match performance, the level of information required for decision making depends on domain expertise and individual case complexity, and measures like trust and perceived usefulness are improved with Explainable AI methods. The improvement in user trust, however, does not always correlate to improvement in Human-AI team's overall task accuracy. The findings also highlight the importance of providing global level AI information as well rather than local level AI information alone, so that the users develop appropriate mental model of the AI. Additionally, a critical challenge in XAI is the lack of proper method to signify outlier use cases which ultimately affects user's accuracy and reliance in the system. The work also discusses steps for future work in human-subject experiments involving explainable AI.

MinerFinder: A GAE-LSTM Method for Predicting Location of Miners in Underground Mines

Abhay Goyal¹, Sanjay Madria¹, Samuel Frimpong²

¹ *Computer Science*

² *Mining and Explosives Engineering*

Recent reports by the Mine Safety and Health Administration suggest that several injuries and fatalities could be attributed to the inability to accurately locate miners in case of disasters. Since underground mines have a complicated geometrical landscape and technological constraints such as no GPS information available, it is difficult to predict the location of a miner and hence may cause delays and

inefficiencies in rescue operations during a disaster. A significant amount of research has been done to capture complex spatio-temporal relationships of movement of the nodes/people/things with time, spatial and temporal features to separately extract these relationships for location prediction. Although Markov Chains (MC) and Recurrent Neural Network (RNN) based methods have been used to predict locations, not all of them specifically mention the spatial locations, their connections and the aggregation techniques which would allow for the actual representations of the trajectory of miners. Addressing these concerns, we develop a first-of-its-kind end-to-end system entitled MinerFinder to predict the future location of the miners by incorporating Long Short Term Memory (LSTM) for trajectory information with Graph Autoencoder (GAE) for spatial environmental information representing the node connectivity. In addition, our approach will combine the miners' previous trajectories and daily repetitive patterns enhancing the prediction robustness. We evaluated MinerFinder over synthetic dataset to analyze the structure and location topology of an underground mine compared with foreground locations. Our model outperforms state of the art models and achieves an AP score ranging from (0.62 - 0.68) and Receiver Operating Characteristics (ROC) ranging from (0.63--0.68) with increasing percentage of prominent locations (most visited) to 50%.

From Phenotyping Electronic Health Records to Generating an Explanation Space

Raghu Yelugam¹, Donald C. Wunsch II¹

¹Electrical and Computer Engineering

Serving as the medical journal, electronic health records register the information of the patient's disease presentation, course, response to medication, and prognosis. Inherently, journaled information in medical records can be used to improve the quality of patient care, thus, leading to several methods to identify phenotypic information and classify patient groups. However, much must be done to bring phenotyping and classification into a single pipeline. To this end, a series of studies were conducted on phenotype lists extracted using the factory standard UMLS MetaMap on neurological disease medical records. The phenotype lists were reduced to superclasses using ontological subsumption to produce phenotype vectors to study the classification accuracies. Further, members from neurological disease classes represented as subsumption phenotype vectors were clustered using naive and subspace clustering methods. A visual explanation space was generated using heatmaps and word clouds for the clustering results to verify the biological plausibility. In studies on phenotyping, MetaMap showed a recall of 61-89%, a precision of 84-93%, and an accuracy of 56-84% for identifying phenotype concepts. The biological plausibility of classification made by subspace clustering methods was judged better than naive clustering by a domain expert using the visual explanation space.

Oral Session B: Powering Innovation

Session Details:

Location: Carver Room, 204B

Time: 1 p.m. to 3 p.m.

Campus Judges:

Dr. Irina Ivliyeva, Arts, Languages and Philosophy (session chair)

Dr. Karen Head, English and Technical Communication

Guest Judge:

Dillynn Cook, U.S. Army Corps of Engineers

Session Timeline:

- 1:00 p.m. Investigating the Potential of Blended Feedstocks for Biofuel Production via Pyrolysis process: Thermogravimetric and kinetic analysis, **Hasan J. Al-Abedi**
- 1:20 p.m. Walking through High Temperatures (Up to 1600°C) Unscathed, **Ogbole Inalegwu**
- 1:40 p.m. Building Block Approach of Designing New Materials for Li-Ion Battery Application, **Santhoshkumar Sundaramoorthy**
- 2:00 p.m. Inter-Bonded Carbon Nanofibers for Lithium-Ion Batteries, **Tazdik Patwary Plateau**
- 2:20 p.m. TM-Mode Resonator for Accurate Dk Extraction of PCB Material, **Chaofeng Li**
- 2:40 p.m. The Role of LIDAR Sensors in Future 6G Networks, **Omar Rinchi**

Session Abstracts:

Investigating the Potential of Blended Feedstocks for Biofuel Production via Pyrolysis Process: Thermogravimetric and Kinetic Analysis

Hasan J. Al-Abedi¹, Haider Al-Rubaye¹, Joseph Smith¹

¹ Chemical and Biochemical Engineering

As concerns about climate change and energy security continue to grow, the search for sustainable and renewable energy sources has become increasingly urgent. Biofuels, produced from organic feedstocks using the pyrolysis process, which is decomposition by heat without oxygen, offer a promising alternative to fossil fuels.

In this study, Thermogravimetric analysis (TGA) and kinetic analysis using two-parallel reaction model have been utilized to evaluate the pyrolysis performance of the co-pyrolysis process for the blended

feedstock. The feedstocks that have been used in this research are Corn Stover (CS), refused derived fuel (RDF), Sub bituminous Coal (SBC), and Oil Shale (OS). Furthermore, the combination of (CS-RDF), (CS-SBC), (CS-OS), (RDF-SBC), and (RDF-OS) with a weight ratio of (50% each) were studied. The kinetic parameters, including activation energy (E_a) and frequency factor (A), were obtained from the TGA data with temperature range of (200 °C-700 °C) and a heating rate of 10 °C/min and under Nitrogen gas atmosphere. The average activation energy for the CS, RDF, SBC, and OS were (87.91, 85.73, 46.88, and 115.24) kJ/mol, respectively. On the other hand, the average activation energy values for the blended feedstock combinations were (70.17, 53.38, 68.09, 88.55, and 53.36) kJ/mol, respectively, and had a high correlation coefficient (R^2) of above 0.97. The results showed a positive synergy effect for all the binary combinations, indicating that the interactions between the molecules had a beneficial impact. It is worth noting that there are two more analysis tools that were utilized to further investigate the pyrolysis process are differential thermal analysis (DTG) and differential scanning calorimetry (DSC), both of which provided valuable information on the feedstock decomposition as pure and blended materials.

Walking through High Temperatures (Up to 1600°C) Unscathed

Ogbole Inalegwu¹, Jie Huang¹, Rex E. Gerald¹

¹ *Electrical and Computer Engineering*

This work presents a distributed Fiber Bragg Grating (FBG) sensor for high temperature steelmaking applications (up to 1600°C). The FBGs were fabricated in-house using the femtosecond laser located in the Lightwave Technology Lab, EECH G23, Missouri S&T. We were able to instrument the bottom anode of a steel mill with multiple optical fiber sensors (each with five FBGs). The FBGs for the reported application (Steel Mill Bottom Anode Instrumentation) were fabricated on a single-mode fiber (SMF) for distributed high temperature measurements up to 900°C. The results demonstrate a novel and distributed approach to sensing for steel production that outperforms the current single point sensing using a thermocouple. In addition, the sensor can measure temperatures close to the tip of the bottom anode (approximately 1.15 m high), whereas the single-point thermocouple temperature measurement can only measure to a height of 0.28 m. In summary, using optical fibers, we are able to provide complete knowledge of the temperature profile along the length of the bottom anode pin. Works are ongoing to instrument the Burner, Rocker Arm, Spray Cool Panel and Tundish lining in the Steel Mill. This research will make a tremendous contribution to improving the efficiency and cost of steel production.

Building Block Approach of Designing New Materials for Li-Ion Battery Application

Santhoshkumar Sundaramoorthy¹, Amitava Choudhury¹

¹ *Chemistry*

Ever since the commercialization of the rechargeable Li-ion Batteries (LIBs) in 1991, portable electronics and electric vehicle applications were dominated by LIBs. Electrodes (cathode) capacity in LIBs are limited by the transition metal redox and the corresponding amount of moles of Li-(de)insertion, which restricts the energy density of the material. Owing to the surge in demand for high energy density materials and uneven geographical distribution of raw materials, researchers are placing more emphasis on designing new cathodes to meet current demands. In this regard, for the first time, a solid solution between Li⁺ and Cu⁺ was formed Li_{5-x}Cu_xGaS₄ through a facile solid-state metathesis reaction and its potential application in LIB's were evaluated. The cathode material showed reversible capacity of 200mAh/g at a current density of 10mA/g. The spectroscopy studies showed that the redox contribution for such huge capacity was provided by cation triggered anion redox process. In-situ

diffraction shows excellent structural stability through the electrochemical cycle. Further, the material was tested for fast charging applications and the results showed 75% of its initial capacity retention at a current density of 200mA/g. Hence, this idea opened the door to explore new class of cathodes for LIB applications with higher capacity with low cost.

Inter-Bonded Carbon Nanofibers for Lithium-Ion Batteries

Tazdik Patwary Plateau¹, Jonghyun Park¹

¹ *Mechanical and Aerospace Engineering*

Binder-free electrodes offer advantages such as improved performance, enhanced durability, and reduced cost. However, challenges include poor adhesion and electrode fragmentation due to the lack of a binder, as well as increased manufacturing complexity and costs. This study presents a high-quality CNFs anode that exhibits improved inter-bonding in both planar and thickness directions. This design enables the anode to achieve high areal capacity by enhancing the pathways for species movement through improved joints between the fibers. In this study, a semi-interpenetrating (IPN) polymer, polyvinylpyrrolidone (PVP), was electrospun with a polyacrylonitrile (PAN) precursor to create intermolecular bonding between the nanofibers in the thickness direction. The semi-IPN assisted inter-bonded morphologies in the thickness direction build robust connections between the fibers after carbonization. The addition of a small amount of nickel in the fiber precursor resulted in enhanced conductivity, increased capacity, and improved stability of the fiber anode. The synergistic effect of adding nickel and vertically inter-connected CNFs yields a favorable anode composite material with an areal capacity as high as 1.85 mAh/cm² after 500 cycles at a current density of 1.16 mA/cm² and excellent cycling stability. The study also comprehensively reports the electrical and mechanical properties of the inter-bonded CNFs, as well as the effects of Ni doping in CNFs. Superior mechanical flexibility has been achieved by enhancing the inter-bonding network in the CNFs. Though addition of nickel results in a reduction in the flexibility. The combination of IPN with PAN greatly improves the overall mechanical strength and bendability even after repeated cycles of bending. The stiffness and hardness (1 GPa) of the CNFs film increased after increasing the nickel content in the precursors.

TM-Mode Resonator for Accurate Dk Extraction of PCB Material

Chaofeng Li¹, DongHyun Kim¹

¹ *Electrical and Computer Engineering*

Accurate extraction of effective dielectric constant (Dk) and loss tangent (Df) of multi-layer dielectric medium is essential for signal integrity analysis in high-speed printed circuit board (PCB) application in modern electronics such as data center servers and high-end personal computers. Most PCB designers relay on the Dk and Df values obtained from transverse electric (TE) mode split post dielectric resonator (SPDR) to secure signal integrity for high-speed channels. In this research, we validated the inaccuracy of Dk and Df values obtained from TM SPDR for inhomogeneous dielectric layers (IDLs) in PCB. To overcome the inaccuracy of Dk and Df values, a transverse magnetic (TM) mode dielectric resonator design is proposed and simulated using full-wave simulation tools to extract the effective Dk and Df of IDLs in PCB with higher accuracy. The electric fields in the TM mode dielectric resonator are vertical to the multiple layers in PCBs, which is similar to the electric field distribution in strip-line with IDLs. The accuracy of Dk and Df results using the proposed method is verified by comparing stripline-based

method and the TE mode SPDR method. The simulated Dk values are validated with measurement of fabricated TM mode dielectric resonator.

The Role of LIDAR Sensors in Future 6G Networks

Omar Rinchi¹, Ahmad Alsharoo¹

¹ Electrical and Computer Engineering

With the increasing demand on quality of services (QoSs), future sixth-generation cellular networks (6G) are expected to exceed the typical communication services to enable integrated sensing, localization, and communication (ISLAC) capabilities. However, future wireless networks will be subjected to set of common wireless challenges such as the blockage of line-of-sight, communication over large distances, and the required overhead to conduct channel estimation. A protentional solution to these limitations relies on sensor integration with wireless equipment. The utilization of light detection and ranging (LiDAR) in particular has shown a great potential. As a result, we propose a two-stages solution to improve the performance of a challenging 6G channel scenario with dynamic targets moving in a multipath channel model. Firstly, we utilize the LiDAR to scan the environment to predict future beamforming vectors based on a deep learning solution. Further, we exploit the LiDAR to improve wireless localization by supporting sparse recovery algorithm with partial given support of the surrounding environment. Our numerical results suggest that the proposed LiDAR/6G integration can outperform the current existing solutions found in literature.

Oral Session C: Improving Health & Wellness

Session Details:

Location: Missouri Room, 207A

Time: 1 p.m. to 3 p.m.

Campus Judges:

Dr. Daoru Han, Mechanical and Aerospace Engineering (session chair)

Dr. Fateme Fayyazbakhsh, Mechanical and Aerospace Engineering

Guest Judge:

Wes Safarik, U.S. Army Corps of Engineers

Session Timeline:

- 1:00 p.m. Development of Novel 3D Printed Metallic Materials for Human Bone Replacement, **Saeid Alipour Masoumabad**
- 1:20 p.m. Prospects in Biomarkers and Treatment for Traumatic Brain Injury Associated Neurotrauma, **Olajide Adetunji**
- 1:40 p.m. uPA-Mediated Polyamidoamine Dendrimer-Based Targeted Drug Delivery System for Triple Negative Breast Cancer, **Hsin-Yin Chuang**
- 2:00 p.m. Metal Free Self-Healing Hydrogels, **Yugandhara Eriyagama**
- 2:20 p.m. Protein Concentration Differences in Predicted Long-Lived and Predicted Short-Lived Flies Based on Sleep Characteristics, **Jennifer Harrell**
- 2:40 p.m. Mind Your Reality: Enhancing AR Interaction with SSVEP-Based BCI, **Yasmine Attia**

Session Abstracts:

Development of Novel 3D Printed Metallic Materials for Human Bone Replacement

Saeid Alipour Masoumabad¹, Arezoo Emdadi¹

¹ Materials Science and Engineering

Bones in the human body consider as one of the most important parts which not only protect the internal organs but enable us to move and do our daily works. However, sometimes individuals with untreatable bone-related diseases may need to have affected bones removed from their body. Bone replacement can be remained as the only promising solution in such circumstances. The present research aims to develop novel 3D printed metallic materials that resembles natural human bone structures with exceptional

combination of mechanical performance and biocompatibility. Hence, in this research, based on the thermodynamic and phase calculations we have developed novel β -Ti-Nb-Ta-Zr-Mo alloy containing minor Copper (Cu) alloying element with minimum elastic modulus near the natural body bone to reduce the stress shielding which is one of the main reasons for premature fracture and revision surgeries. Our previous study showed that addition of Copper (Cu) to Ti bone implant can inhibit the biofilm formation on the surface of implant and gives intrinsic antibacterial property to the implant through contact sterilization and $\text{Cu}^{2+}/\text{Cu}^+$ ion releasing mechanisms. To mimic the natural human bones, we designed a novel triply periodic minimal surface (TPMS) geometry for the proposed bone replacements. These designed structures offer sufficient surfaces for bone formation inside them and presence of interconnected in designed geometry led to vascularization, which is the process of growing blood vessels into a tissue to improve oxygen and nutrient supply. Cylindrical samples with TPMS structures printed through selective laser melting (SLM) as a 3D printing technique. After printing the samples, post-processing techniques including stress relieving have been done to reduce the thermal stresses. Then, a novel layer-by-layer coating applied to prevent implant-associated infections and stimulate bone tissue regeneration through enhanced osteogenic differentiation of mesenchymal stem cells (MSCs). Since the biocorrosion resistance is of paramount importance, the potentiodynamic corrosion test performed in simulated body fluid (SBF) as a standard tool to test the bioactivity of bone implants. The mechanical properties of the implants measured through compression tests and compared with natural human bones. Finally, in-vivo biological assessments and histotomography examined on rabbits to monitor the real performance of the proposed approach for novel β -Ti bone replacement implants. The outcomes of this interdisciplinary research between materials science, biomedical engineering, and mechanical engineering opens a new avenue to develop high-quality patient-specific implants with exceptional combination of microstructural, biocorrosion, antibacterial, and mechanical properties with engineered architectures.

Prospects in Biomarkers and Treatment for Traumatic Brain Injury Associated Neurotrauma

Olajide Adetunji¹, Paul Ki-souk Nam¹

¹ Chemistry

A major neuro-consequence of traumatic brain injury (TBI) involved in both inception and aftermath of trauma is oxidative stress which can lead to the generation and/or proliferation of reactive oxygen and nitrogen species. The depletion of antioxidant defenses and alteration in concentrations of certain small molecules also occur chronologically with the disease progression. Conventional TBI diagnosis is partly insensitive to milder forms of TBI, which is the most common injury affecting the military population. Furthermore, currently available treatment options for this disease are non-specific and majority are focused on symptom management. The TBI diagnosis can be potentially performed by investigating the already identified TBI biomarkers related to the oxidative stress, neurotransmission, and brain homeostasis. Direct treatment approach using N-acetylcysteine amide (NACA) which is an antioxidant prodrug and amide derivative of FDA approved N-acetylcysteine (NAC), can be helpful in potentially limiting the oxidative stress characteristic of TBI and consequently improving overall health of the TBI patient. NACA trumps over NAC due to the hydrophobic moiety present on it, leading it pose better bioavailability of crossing the blood-brain barrier more efficiently than NAC. The levels of potential TBI biomarkers in the brain tissue, plasma and urine of rats induced with TBI through explosives (mimicking real-life situation) were determined using LC-MS/MS. This investigation can provide valuable information regarding the TBI disease progression, treatment efficacy and spot-on diagnosis. NACA treatments of the test rats were conferred by sub-cutaneous injection of specified dose for multiple days.

The test rats were euthanized and biomatrices (urine, blood, brain) were collected, stabilized, and processed for LC-MS/MS analysis of TBI biomarkers using electrospray ionization in both positive and negative modes with two different LC-MS/MS methods. Sample preparation protocol was carefully tailored for accurate determination of the selected biomarker levels. This research was supported by the Army Research Laboratory and the Leonard Wood Institute.

uPA-Mediated Polyamidoamine Dendrimer-Based Targeted Drug Delivery System for Triple Negative Breast Cancer

Hsin-Yin Chuang¹, Yue-wern Huang¹, Hu Yang²

¹ *Biological Sciences*

² *Chemical and Biochemical Engineering*

Around 15% of breast cancers are triple negative breast cancer (TNBC), which is characterized by the absence of three common receptors—estrogen receptor, progesterone receptor, and human epidermal growth factor receptor 2, and therefore do not respond to hormonal or anti-HER2 therapies. It is urgent to explore targeting therapeutic strategies for TNBC due to its poor prognosis and rare effective targeting therapy. In this study, we developed a polyamidoamine (PAMAM) dendrimer-based targeted drug delivery system to utilize urokinase-type plasminogen activator (uPA) to target uPA receptor (uPAR), which is highly expressed in both TNBC cells and cancer-associated stromal cells. The constructed system was tested for its ability to target cancer and its microenvironment and improve the transfection efficiency of anticancer nucleic acid. Results of ¹H NMR spectrum, dynamic light scattering, and MTT assay showed characterization of functionalized dendrimers (13.43 nm) and their high biocompatibility (25 ug/ml) in MDA-MB-231 TNBC cell line. Results of flow cytometry and confocal microscopy showed that uPA-dendrimer improved the transfection efficiency of GTI-2040, an anticancer oligonucleotide, in MDA-MB-231 cell line and HCC2218 fibroblast cell line up to 6-fold compared to the GTI-2040 only group. GTI-2040 delivered by dendrimers killed cells by ~30% through knock-downing human ribonucleotide reductase component (R2) by 35%. In addition, biodistribution studies showed uPA-dendrimer's targeting capacity and retention in tumors; therapeutic studies showed a significant inhibition of tumor growth in the TNBC orthotopic xenograft mice model with uPA/GTI administration for 14 days. Collectively, uPA-dendrimers improved the transfection efficiency of anticancer nucleic acids in both breast cancer cells and cancer-associated stromal cells, showed the targeting capacity, and attenuated tumor growth in mice model. This uPA-dendrimer has great potential in developing efficient targeted delivery systems to treat TNBC in clinical.

Metal Free Self-Healing Hydrogels

Yugandhara Eriyagama¹, Thomas Schuman¹

¹ *Chemistry*

Self-healing hydrogels are a promising class of materials with unique properties that make them suitable for a range of applications, from drug delivery to tissue engineering. Unlike traditional hydrogels, which remain broken after damage or deformation, self-healing hydrogels can autoadhere to a bulk form, regenerating bulk mechanical properties. In many occasions, self-healing may be achieved by either reversible chemical bond formations or by hydrophobic interactions that occur in physically crosslinked hydrogels formed through hydrophobic interactions, between the ruptured interfaces. Other classes of self-healing hydrogels rely on metal ions like Cr³⁺, Zr⁴⁺ to provide chain entanglement between polymer chains to attain this property, which are environmentally persistent and may be toxic in nature.

To tackle the issue of inherent metal ions we have developed a new technology to achieve self-healing in a hydrogel with a new class of monomers, which neither require reversible chemical (vitriimer) bonds nor metal ions. This new class of monomers which contains a polar head group and a non-polar tail group to provide increased chain mobility to produce chain entanglement which lead to self-healing. To test our hypothesis, bulk gels were formulated with varying concentrations of new monomer and were transformed into dried, preformed particle gels (PPGs). PPGs rehydrated in 2% KCl brine were visually observed for any reassociation into bulk gels.

By altering the tail group of the monomer and changing comonomer ratio in a simple acrylamide gel system, we were able to achieve self-healing in traditional hydrogels of low crosslinker concentration. The elastic modulus of the novel self-healing gel is near that of metal-incorporated gels. The new PPG provides an alternative, greener method to achieve self-healing in a traditional hydrogel without the use of metal ions. Furthermore, this technology can reduce the cost of production of self-reassociating PPGs.

Protein Concentration Differences in Predicted Long-Lived and Predicted Short-Lived Flies Based on Sleep Characteristics

Jennifer Harrell¹, Matthew S. Thimgan¹, Robin Verble¹

¹ *Biological Sciences*

Background: Longitudinal studies have shown inadequate sleep is associated with diseases such as cardiovascular, type 2 diabetes, depression, and obesity – all affecting lifespan and systems driven by proper protein function. The need to track sleep patterns in a quantitative, noninvasive manner for experimentation led us to choose *Drosophila melanogaster*, the fruit fly, as the model organism because it sleeps and has molecules homologous to humans; making it useful for examining the molecular mechanisms, such as protein concentration, associated with disease to elucidate a difference at a molecular level. Categorizing the flies by predicted lifespan allowed for exploration of molecular differences between groups.

Methods: Sleep patterns were tracked over 30 days. Multiple Linear Regression (MLR) and Functional Principal Component Analysis (FPCA) were both used to make lifespan predictions, allowing for more accuracy by accounting for as much variation as possible. We then binned the flies into two groups – those predicted to have long lifespans and those predicted to have short lifespans. Based on those predictions, a Bicinchoninic Acid (BCA) Assay was used to determine overall protein concentration in each category of flies. Western Blot Assays were used to examine proteins of interest. Brightfield microscopy, with stage micrometer, was used to compare the size of flies between groups.

Results: Death rates of flies from prediction time to pulling them for experimentation were significantly higher in the predicted short life flies ($p=0.05$). There was a 1.5-fold increase in protein concentration in the predicted long-life group ($p<0.001$). Preliminary results from Western Blot Assays have indicated a higher level of superoxide dismutase 2 (SOD2) – a protein protecting cells from damage - in predicted long lived flies than was found in predicted short lived flies. Examination of flies from predicted long-lived group and predicted short-lived groups yielded no significant difference in size ($p>0.49$).

Conclusion: We have obtained significant data indicating that the predicted short-lived flies contain less protein than the predicted long-lived flies, leading us to hypothesize that there is a problem with protein synthesis in predicted short life flies. Ruling out size as a contributing factor in the protein concentration difference – we attribute this variation to the sleep characteristics of the fly. Our statistical models are

able to bin flies into categories based on sleep characteristics with significant success, indicating that we can use this noninvasive method to reliably separate flies for further investigation of molecular mechanisms associated with disease.

Mind Your Reality: Enhancing AR Interaction with SSVEP-Based BCI

Yasmine Attia¹, Tony Luo¹

¹ *Computer Science*

Brain-Computer Interface (BCI) has been primarily used to create assistive tools for physically impaired individuals, but recent developments have integrated BCI with Augmented Reality (AR) to create mainstream applications for healthy users. This integration allows for a more seamless interaction with the AR environment using brain signals, specifically the Steady-state Visually-evoked Potential (SSVEP) pattern.

The proposed approach in this work introduces SSVEP-BCI as an additional communication channel to control the AR environment. This method allows users to choose AR commands by simply looking at them, while also allowing for head rotations up to 45° to explore the AR environment. The proposed approach utilizes a machine learning-based approach to recognize the frequency of the recorded SSVEP patterns.

The results of the study showed that the ensemble classification technique outperformed other approaches in subject-dependent testing, reaching a mean accuracy of 96.73% and 93.45% for 5 sec and 2.5 sec stimulation times, respectively. In subject-independent testing, the ensemble classification technique achieved a mean accuracy of 92.18% and 76.91% for 5 sec and 2.5 sec stimulation times, respectively.

The proposed ensemble classification approach improved performance by an average of 7% per subject. These results indicate the feasibility of using BCI as an additional input modality to AR, while also demonstrating the utility of the proposed ensemble classification approach in enhancing the performance of SSVEP-based BCIs. Overall, this study represents a significant step towards utilizing BCI for mainstream AR applications, with the potential to enhance the quality of life for both physically impaired and healthy individuals. Further research can be done to improve the accuracy and usability of BCI-AR applications, potentially leading to a more seamless and intuitive interaction with the AR environment.

Oral Session D: Building Sustainability & Resilience

Session Details:

Location: Ozark Room, 207B

Time: 1 p.m. to 3 p.m.

Campus Judge:

Dr. Chang-Soo Kim, Electrical and Computer Engineering (session chair)

Guest Judges:

Brandi Suhre, Thermo Fisher Scientific

Chris Coffman, Ocelot Consulting

Session Timeline:

- 1:00 p.m. Zoom Fatigue and Virtual Interviewing: The Effects of Interpersonal Distance, **Lillian Schell**
- 1:20 p.m. Investigating Strain Partitioning in Hispaniola through Geodetic Analysis, **Yi-Chieh Lee**
- 1:40 p.m. Detection of Potential Failure Zones in Levees Using the New Towed Transient Electromagnetic Method (tTEM) System, **Kolawole Arowoogun**
- 2:00 p.m. Fe³O₄-Coated Activated Carbon Catalysts for Drinking Water Disinfection and Toxic Disinfection Byproduct Control, **Sargun Kaur**
- 2:20 p.m. Delineation of Isotopic and Hydrochemical Evolution of Karstic Aquifers with Different Cluster-Based (HCA, KM, FCM, and GKM) Methods, **Effat Eskandari**
- 2:40 p.m. A 9500-Year Record of Climate and Floristic Dynamics in the Lake Izabal Basin, Eastern Lowland Guatemala, **Erdoo Mongol**

Session Abstracts:

Zoom Fatigue and Virtual Interviewing: The Effects of Interpersonal Distance

Lillian Schell¹, Clair Ann Reynolds Kueny¹

¹ *Psychological Science*

Virtual communication platforms have become essential tools in the workplace, requiring many workers to attend and participate in multiple video conferences a day. This has led many to experience what is now known as “Zoom Fatigue.” Zoom fatigue can be defined as the exhaustion and burnout caused by

the difficult nature and overuse of virtual communication platforms. Many causes of Zoom fatigue have been proposed. Some examples include the increased effort to send as well as decode nonverbal cues, increased self-evaluation due to seeing live footage of oneself, and reduced mobility during and between meetings.

Another proposed cause is breached interpersonal distance. Interpersonal distance describes how close two people are comfortable being from one another and is often determined by how familiar the individuals are with one another. When a person is closer than we are comfortable, and breach interpersonal distance, psychological arousal increases.

In a virtual meeting, our perception of how close other meeting participants are varies greatly depending on monitor size, how close one is sitting from the monitor, and the number of participants. If we perceive others to be too close and breach interpersonal distance, our psychological arousal may increase. The increase in psychological arousal over long periods of time during virtual conferences may lead to Zoom fatigue.

This research examines breaches of interpersonal distance within the context of a job interview. Participants of the study are assigned to one of three conditions: 3ft, 8ft, and 13ft. Participants watch an asynchronous video interview in which the size of the job applicant's face varies between conditions to stimulate the three different levels of interpersonal distance. After watching the video, participants rate the job applicant's likability and hireability. To measure Zoom fatigue, participants complete a Zoom Exhaustion and Fatigue scale at least one hour before watching the video and right after rating the applicant.

It is proposed that when an interviewer perceives a job applicant to be close to them, Zoom fatigue increases and ratings of the applicant decrease. After data collection is concluded, data analysis will be conducted using multiple regression and a mediation analysis. Significant results would suggest that breaches of interpersonal distance are related to Zoom fatigue. These findings could be used to guide virtual conferencing best practices and thus reduce negative effects of Zoom fatigue such as depression, anxiety, stress, and decreased levels of well-being and life satisfaction.

Investigating Strain Partitioning in Hispaniola through Geodetic Analysis

Yi-Chieh Lee¹, Jeremy Maurer¹

¹ Geosciences and Geological and Petroleum Engineering

Earthquake is one of the most devastating natural disasters, causing significant damage and loss of life. To mitigate their impact, it is crucial to accurately predict when and where they will occur. Traditional methods of earthquake prediction rely on historical data and seismographs, but these methods are limited in their ability to predict earthquakes. In contrast, advanced geodetic measurements, such as GPS and InSAR, provide a new and innovative approach to predicting earthquakes by tracking the Earth's surface movement and understanding strain accumulation and distribution. In this study, we utilized a combination of GPS and InSAR to estimate the surface velocity of Hispaniola with horizontal and vertical components. By merging data from multiple sources, we achieved a higher spatial resolution velocity field than GPS datasets alone, providing a more comprehensive understanding of the strain accumulation and deformation patterns across the island.

Our innovative approach revealed new insights into the dynamics of the North American and Caribbean plate boundary in Hispaniola. Our preliminary results show that the maximum shear strain rate is somewhat uniformly distributed across the whole island, with a significant compression in eastern Hispaniola and extension in middle and western Hispaniola. We hope to apply these findings to provide a more accurate representation of subduction north of Hispaniola, which is critical for better understanding seismic activity and the geometry of subduction. Our method has the potential to improve earthquake forecasts, enabling improved disaster planning. By incorporating advanced geodetic measurements into our models, we can gain a more comprehensive understanding of strain accumulation and deformation patterns in subduction zones, improving our ability to mitigate the impact of earthquakes in high-risk areas.

Detection of Potential Failure Zones in Levees Using the New Towed Transient Electromagnetic Method (tTEM) System

Kolawole Arowoogun¹, Katherine R. Grote¹, Jeremy Maurer¹

¹ *Geosciences and Geological and Petroleum Engineering*

Levees serve as barriers constructed to protect the surrounding environment from flooding. Thus, it is essential to evaluate the structural stability of levee foundations to avoid catastrophic failures which have been observed in the past. However, assessing levee foundation is challenging due to its heterogenous geology and extensive lengths covering several miles. Traditional methods like drilling are expensive and destructive to the environment. Hence, there is a need for faster and non-destructive techniques for assessing levees' foundation. This study proposes the use of a new towed transient electromagnetic imaging system (tTEM) to map the electrical resistivity of soils near the levees quickly and more efficiently compared to the traditional methods. The resistivity maps from the tTEM will be interpreted to identify areas where the subsurface stratigraphy is likely to fail. To prepare for fieldwork, the study modeled various geologic scenarios that frequently lead to foundation failures in levees using the AarhusInv code. According to the forward modeling results, the tTEM can map the sediments near the levees and detect fine-grained surficial materials if the top layer is over 2 m thick. However, imaging fine grained layers that are less than 2 m thick is challenging. The study plans to conduct fieldwork in the future, and the field results will be compared the forward modelling results. The study will demonstrate the effectiveness and limitations of the new tTEM system in identifying potential failure zones beneath levees.

Fe³O₄-Coated Activated Carbon Catalysts for Drinking Water Disinfection and Toxic Disinfection Byproduct Control

Sargun Kaur¹, Paul Nam¹, Honglan Shi¹, John Yang², Bin Hua²

¹ *Chemistry*

² *College of Agriculture, Environmental and Human Sciences, Lincoln University*

Traditional drinking water disinfectants such as chlorine not only deactivate pathogenic microorganisms in raw source water but also react with dissolved organic matter or dissolved organic carbon (DOC) from natural and anthropogenic sources, leading to the formation of numerous toxic disinfection byproducts (DBPs). Most DBPs are potentially toxic or carcinogenic to human and pose a significant risk to public health.

The strong oxidants generated through catalytic decomposition of hydrogen peroxide (H₂O₂) by iron oxide (Fe₃O₄) are proposed to simultaneously remove DOC, mitigate the formation of toxic halogenated DBPs (such as trihalomethanes (THMs) and haloacetic acids (HAAs)), as well as disinfect harmful pathogens in drinking water treatment. Our experiments confirmed that Fe₃O₄ is able to catalyze the decomposition reaction of H₂O₂.

Magnetic Fe₃O₄ catalyst can be recovered and reused at pH values relevant to drinking water treatment. Granular Activated Carbon (GAC) are used to disperse Fe₃O₄ and thus increase the number of active catalytic sites. Large GAC surface area can enhance the adsorption of DBP precursors and microorganisms, thereby, facilitating the reactions between the reactants (hydroxyl and superoxide radicals) and the targets (DBP precursors and microorganisms). Recovery of solid Fe₃O₄ catalysts from the product water is readily achieved with an applied magnetic field.

A headspace-SPME-GC/MS method for THM analysis and an IC-MS/MS method for HAA analysis are developed to study the disinfection efficiency of the Fe₃O₄-GAC catalyst on drinking water. This study is financially supported by U.S. Department of Agriculture, Grant No. 2021-38821-34705.

Delineation of Isotopic and Hydrochemical Evolution of Karstic Aquifers with Different Cluster-Based (HCA, KM, FCM, and GKM) Methods

Effat Eskandari¹, Katherine R. Grote¹

¹ *Geosciences and Geological and Petroleum Engineering*

Environmental protection, sustainability, and water resource management in vulnerable and complex karstic regions, especially in border areas, are important topics when it comes to water resources. Understanding of groundwater evolution could reveal valuable characteristics of the aquifer system and increase the understanding of the complexity of the aquifers. Amongst the available methods being exercised in statistical hydrogeology, the isotopic and hydrochemical evolution of karstic aquifers could be distinguished and categorized by using advanced clustering analysis methods.

This work is one of the first efforts to assess and address groundwater evolution in a complex region using the CA method. The study utilized multi-tracer exploration, including water chemistry and stable environmental isotopes of $\delta^{13}\text{C-DIC}$, $\delta^{18}\text{O}$, and $\delta^2\text{H}$, to achieve its objectives. Four clustering analysis (CA) methods were used, including hierarchical cluster analysis (HCA), K-means (KM), CA Fuzzy logic fuzzy C-mean (FCM), and genetic K-means (GKM).

The performance of each method was evaluated, and FCM and GKM were found to have the best performance and provided meaningful results. Based on the results, five distinct clusters of water resources in the region were identified, with two clusters showed to have mixing, two having solo origination with no sign of mixing, and a seasonal spring categorized as a separate cluster.

The study demonstrated that CA methods combined with isotope hydrology could be a strong tool to study water resources in vulnerable and complex regions and could be used as the basis for future scientific attempts involving isotopic-hydrogeochemical studies with advanced statistical analysis. The study was published in the Journal of Hydrology in 2022.

A 9500-Year Record of Climate and Floristic Dynamics in the Lake Izabal Basin, Eastern Lowland Guatemala

Erdoog Mongol¹, Francisca E. Oboh-Ikuenobe¹, Alex Correa-Metrio²

¹ *Geosciences and Geological and Petroleum Engineering*

² *Instituto de Geología, Universidad Nacional Autónoma de México*

Aim: The Holocene has been characterized by multiple changes in precipitation on different time scales from annual to millennial, modulating the composition and structure of vegetation. The palynological study of lacustrine sedimentary records offer an opportunity to study the temporal relationship between climate and vegetation. For this purpose, we analyzed a sedimentary sequence from Lake Izabal, lowland Guatemala, to reconstruct regional vegetation dynamics during the last 9500 years, aiming to identify patterns of climatic variability based on the pollen record.

Location: Lake Izabal, Eastern Guatemala, Central America. Data: Pollen, elemental geochemistry, and charcoal Methods: A sediment core was analyzed for pollen, element geochemistry, and charcoal concentrations to reconstruct vegetation variability and environmental dynamics during the last 9500 years BP. Modern occurrences of the taxa found in the sedimentary record were used to model the environmental distribution of flora, which was in turn used to estimate temperature and precipitation seasonality changes of the past. The accumulation of elements in the sediments was linked to erosion and precipitation regimes, while the charcoal distribution was associated with regional and local fires.

Results: Reconstructed regional vegetation trends coupled with Holocene insolation patterns of the Northern Hemisphere at millennial scale. Centennial scale variability observed was probably associated with more regional phenomena such as changes in the spatial configuration of the North Atlantic Subtropical High (NASH) and other regional and local factors. According to our findings, conditions were warm and wet during the early Holocene and characterized by high seasonality through mid and late Holocene. Quantitative estimations suggest that vegetation patterns may have been amplified and modulated by human disturbances and other local factors. Precipitation seasonality was substantially variable across early, mid, and late Holocene.

Main conclusions: The sedimentary record from Lake Izabal show a variable precipitation seasonality through the Holocene that follows the solar insolation pattern on millennial timescales. Fire regimes as defined by charcoal concentrations also appear to be driven by insolation rather than anthropic activities or randomness. However, other factors such as anthropic impacts, microclimate of the Lake Izabal Basin, etc., apparently defined the vegetation cover on centennial to lower timescales.