AIChE 2026

MID-AMERICAN REGIONAL CONFERENCE

WHERE REACTIONS GROW

The University of Iowa

April 10 & 11 2026

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WELCOME

On behalf of the University of Iowa American Institute of Chemical Engineers Student Chapter, we want to thank you for attending the 2026 Mid-America Regional Conference. We sincerely hope this conference provides you with opportunities to build meaningful professional relationships, develop new technical skills, connect with employers, showcase your research, and gain recognition for your hard work. This guide includes general conference information such as campus maps, a schedule of events, and various amenities available to you. For more information, please contact aiche-regional-conf@uiowa.edu or our Conference Co-Chairs, Ria Patel and Don Roberts, at ria-a-patel@uiowa.edu or donald-k-roberts@uiowa.edu.

AIChE
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IOWA

CONFERENCE RESOURCES

Conference GroupMe

Join our GroupMe for any schedule updates or to ask questions!

Campus Resources

University of Iowa Police Department
Non-Emergencies
Phone: (319)-335-5022

UI Health Care Medical Center
Phone: (319)-356-1616

UI Campus Bus Routes and Schedules
https://transportation.uiowa.edu/cambus/routes

CONFERENCE RESOURCES

Wi-Fi

UI Guest is a wireless network intended to be used by guests and visitors to the University. To connect to UI Guest, you need to:

- Click on the wireless icon located in the system tray in the lower right corner close to the clock.
- Click on UI Guest to expand the menu.
- Click Connect
- On the webpage pop-up, accept the Terms of Use.

DOWNTOWN IOWA CITY

Food & Drink

Pullman Bar & Diner
Vine Tavern & Eatery
Bluebird Diner
Bo James
St. Burch Tavern
Baroncini Ristorante Italiano
Basta Pizzeria Ristorante
Oasis Falafel
Hamburg Inn No. 2
Wilder
Get Fresh Cafe
Hyper Energy Bar
Java House
Pointdexter
Midnight Coffee
Daydrink
Bread Garden Market & Bakery

PARKING & MAPS

Parking

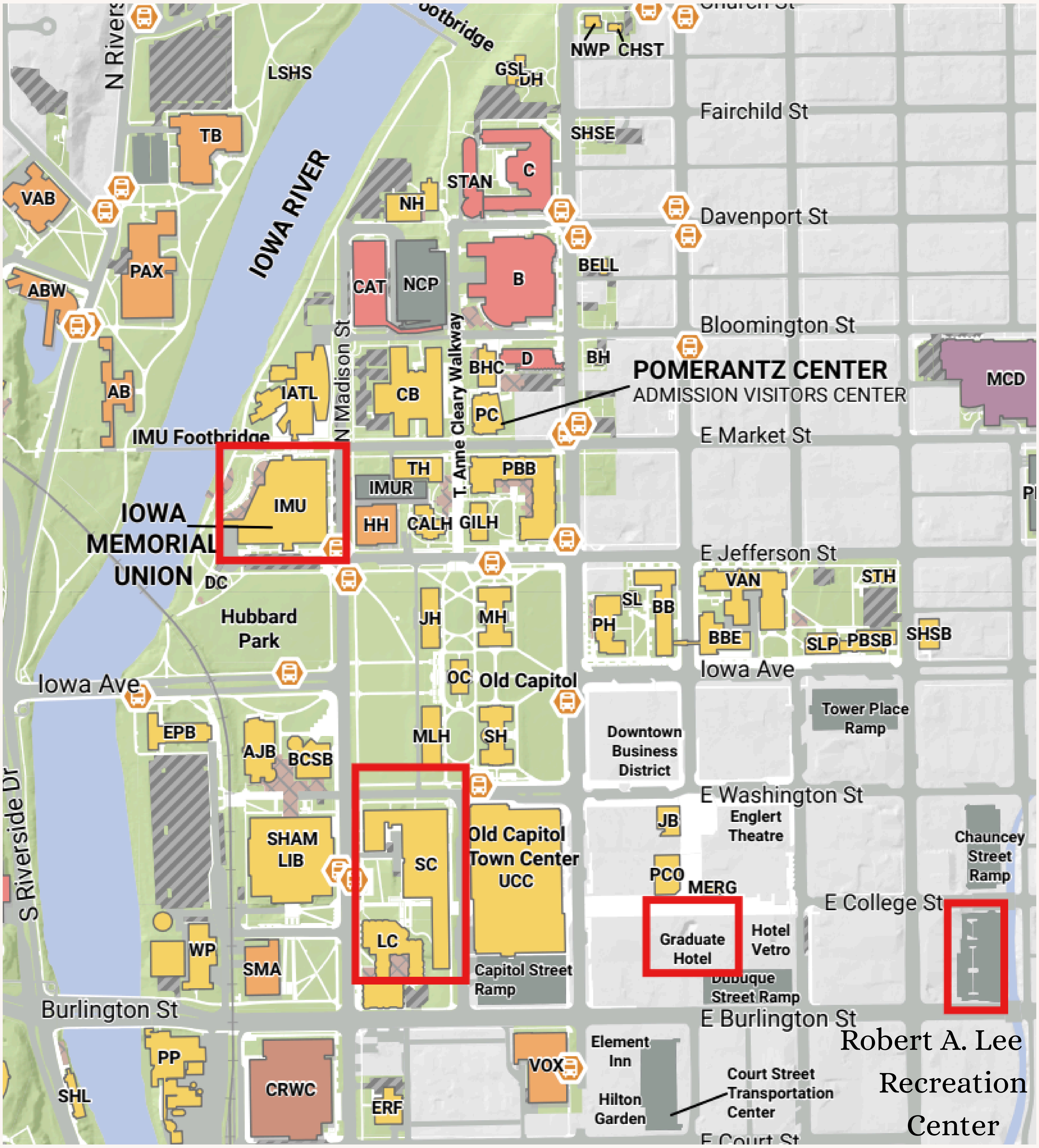
There are numerous parking garages available around campus.

- The **IMU Parking Ramp**, located across from the Iowa Memorial Union, is free for the first 30 minutes, then is an additional $1.75 an hour
- The **Capitol Street Ramp**, located across from the Seamans Center, is free for the first hour, then is an additional $2 an hour

There are also metered parking spots located around campus and downtown Iowa City. These accept payment through coins, credit cards, and the mobile parking app ParkMobile.

If you are staying at **the Graduate Hotel**, the adjacent parking ramp is included in your stay.

PARKING & MAPS



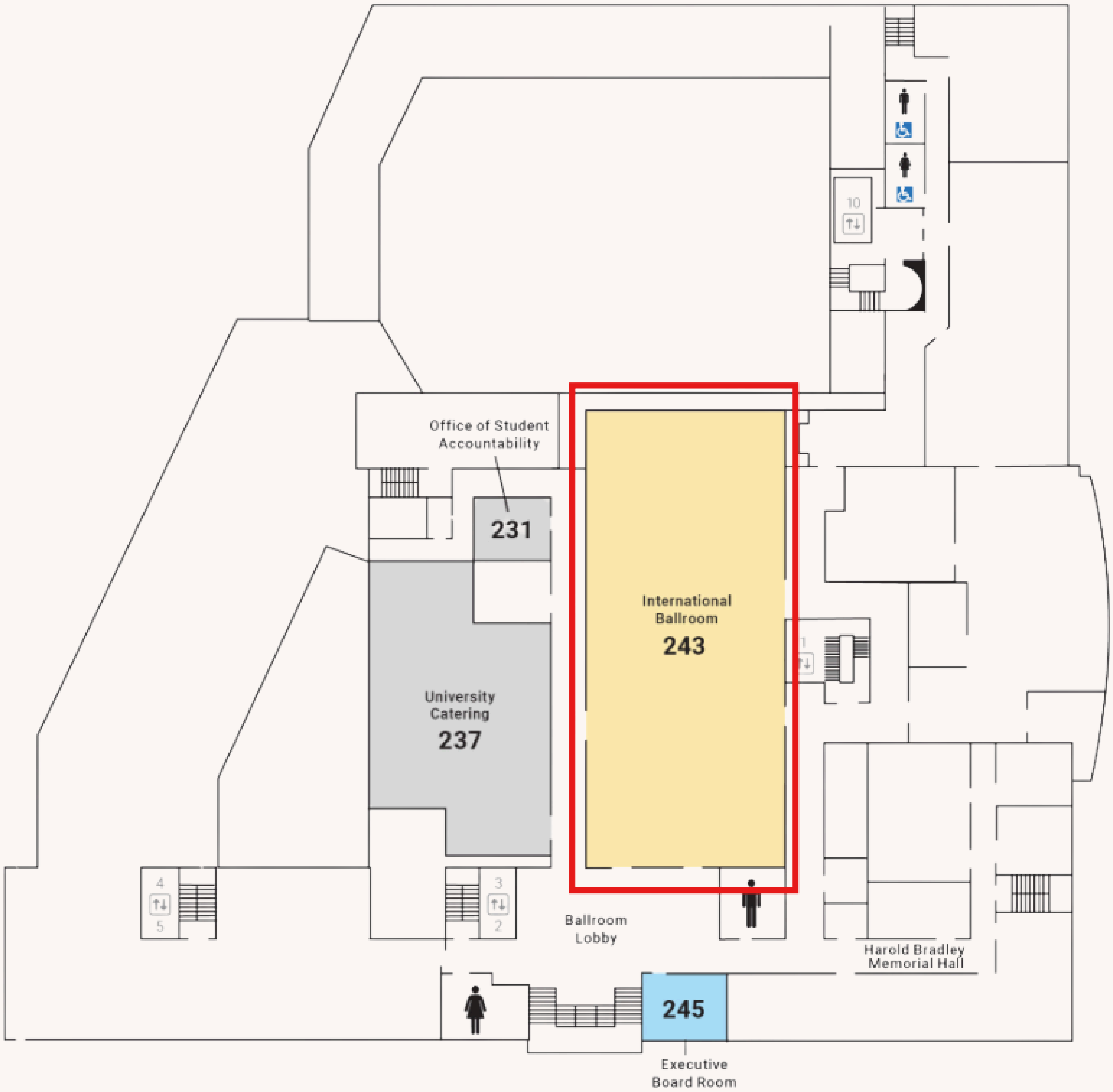
There is a direct route to the Seamans Center from the Graduate by going through the Old Capitol Town Center, which opens at 10 AM.

PARKING & MAPS

Iowa Memorial Union (First Floor)

PARKING & MAPS

Iowa Memorial Union (Second Floor)



SCHEDULE OF EVENTS

Friday, April 10

Check-In and Registration: 4-10 PM
The Graduate Hotel

ChemE Car Safety Inspection and Poster Registration: 6-8 PM
Second-Floor Common Area - Seamans Center

Social Mixer: 6-8 PM
Robert A. Lee Recreation Center

SCHEDULE OF EVENTS

Saturday, April 11

ChemE Car: 7-10:30 AM
International Ballroom - Iowa Memorial Union
Prep: 7-9 AM
Competition: 9-10:30 AM

Regional Student Technical Presentation Competition Session 1: 10:45 AM-12:00 PM
Rooms 2217 and 2229 - Seamans Center

Lunch Break: 12:00-1:00 PM
Second-Floor Common Area - Seamans Center

Advisors/Presidents Lunch: 12:00-1:00 PM
Room 4511 - Seamans Center

Networking Fair: 1:00-4:00 PM
Room 2040 - Seamans Center

Regional Student Technical Presentation Competition Session 2: 1:00-2:30 PM
Rooms 2217 and 2229 - Seamans Center

Regional Poster Competition: 2:30-4:00 PM
Second-Floor Common Area - Seamans Center

ChemE Jeopardy: 3:30-6:00 PM
Rooms 2229, 3505, 3630, and 3655 - Seamans Center

Awards Banquet: 6:00-9:00 PM
Wayne Ballroom - The Graduate Hotel

COMPETITION INFORMATION

ChemE Car Teams

ISU Cardinal - Iowa State University

ISU Gold - Iowa State University

Methylene Mobile - Missouri University of Science and Technology

Robo Copper - University of Tulsa

Hoggenheimer - University of Arkansas

The Jay Wagon - University of Kansas

The Shelldon - University of Missouri

COMPETITION INFORMATION

Technical Presentation Schedule

Session 1: 10:45 AM-12:00 PM

Room 2217
10:50 AM: Nour Bou Alwan
11:15 AM: Sage Paschall
11:40 AM: Andrea Carbonell

Room 2229
10:50 AM: Ellie Albertoni
11:15 AM: Rhea Fisch
11:40 AM: Bailey Butler

Session 2: 1:00-2:30 PM

Room 2217
1:00 PM: Sarah Bakarat
1:25 PM: Kiersten Harris
1:50 PM: Brooke Ruff
2:15 PM: Olivia Reid

Room 2229
1:00 PM: Lilly Hutchinson
1:25 PM: Jacob McCormick
1:50 PM: Lali Nozadze
2:15 PM: Basmala Aldamak

COMPETITION INFORMATION

Research Posters

Dayton Hartsell (University of Arkansas) - Silver Electrolysis with a Twist

Ian Popp (University of Arkansas) - Next Generation C2C12 Models: Leveraging dCas9 Gene Editing to Accelerate Discovery of Neuromuscular Disease Modifiers

Natalie Erickson (University of Arkansas) - A Baseline Study of Artificial Intelligence Use among Chemical Engineering Undergraduates at the University of Arkansas.

Sage Paschall (University of Arkansas) - Constructing a Probabilistic Approach to Multiscale Simulation: Evaluating Machine-Learned Backmapping Models of Diphenylalanine

Alex Quast (University of Iowa) - Lithium Uptake by Hydrogen Manganese Oxide: Influence of Particle Size and Solution Properties on Performance

Arthur Benson (University of Kansas) - Interfacial Behavior of Anti-Reductive Electrolytes in Lithium-Sulfur Batteries

Corey Van Oosbree (University of Kansas) - Genetic Algorithms for Decision Dependent Batch Scheduling Under Yield Uncertainty

Madison Jones (University of Kansas) - Deep Eutectic Solvents and Ionic Liquids for the Separation of Azeotropic Refrigerant Mixtures Thrust 1, Project 1.1

Nora Jennings (University of Kansas) - Synthesizing Organic Semiconductors from Y6:PM6 Nanoparticles

Edward Stone (University of Nebraska Lincoln) - Exploring Metabolic Adaptations in Treponema pallidum through Genome-Scale Metabolic Modeling

COMPETITION INFORMATION

Research Posters

Bruce Baker (University of Nebraska-Lincoln) - Fighting Freezing Rain: Surface Texturing for Improved Hydrophobicity

Kate Wattenbarger (University of Oklahoma) - Understanding the Effects of Acid Electrolyte Anions on Pt, Pd, and IrO_2 Surfaces for Oxygen Electrocatalysis

Nour Bou Alwan (University of Oklahoma) - PFAS Capture Using Zr-MOFs: A Computational Study

Mandisa Masonya (University of Oklahoma) - Computational Investigation of Short-Chain PFAS Capture by Zirconium-Based Metal-Organic Frameworks

Alseny Boiro (University of Oklahoma) - Title: Controlling Hydrogel Properties with Polymer Additives

Shomoy Kamal (University of Tulsa) - Removal of Chromium Metal Using One-Step and Two-Step Activated Biochar-Based Adsorbents

Sungwon Lee (University of Tulsa) - Parametric Study of Renewable Methanol Production via CO2 Hydrogenation: Process Simulation and Sensitivity Analysis

Alexa Wienhoff (Washington University in St. Louis) - Developing Analytical Methods for Iowa's Emerging Aqueous Contaminants

Andrea Carbonell (Washington University in St. Louis) - Lithium Battery Recycling: Highly Selective Critical Mineral Recovery from NMC Cathodes via Pulsed Electrodeposition in Deep Eutectic Solvents

COMPETITION INFORMATION

ChemE Jeopardy Bracket

Preliminary Round
3:30 p.m.

1

Room 3505
(Emcee: Gabi Fiedor)
(Judge: Eric Nuxoll)

- ISU Gold (Iowa State University)
- FC and the Gang (The University of Tulsa)
- The Tiger Turbines (University of Missouri)

2

Room 3630
(Emcee: Shourya Singh)
(Judge: Tom Mansell)

- OK-State (Oklahoma State University)
- Nu Tang Clan (University of Iowa)
- Distillation Nation (University of Missouri)

3

Room 3655
(Emcee: Natalie Schlichte)
(Judge: David Murhammer)

- The Juicy Wiggles (Iowa State University)
- Fugacity Fighters (University of Iowa)
- Team Flodman (University of Nebraska)

4

Room 2229
(Emcee: Evelyn Moorhouse)
(Judge: David Rethwisch)

- KSU ChemE (Kansas State University)
- Competitively Inhibited (University of Iowa)
- Sooner Than U (University of Oklahoma)

Semi-Final Round
~4:30 p.m.

5

Room 3505
(Emcee: Gabi Fiedor)
(Judge: Eric Nuxoll)

- ISU Cardinal (Iowa State University)
- 1st Place from 1
- highest non-winning score

6

Room 3630
(Emcee: Shourya Singh)
(Judge: Tom Mansell)

- The Fluid Mechanics (University of Missouri)
- 1st Place from 2
- 2nd highest non-winning score

7

Room 3655
(Emcee: Natalie Schlichte)
(Judge: David Murhammer)

- 1st Place from 3
- 1st Place from 4
- 3rd highest non-winning score

Final Round
~5:30 p.m.

8

Room 3655
(Emcees: Gabi Fiedor & Shourya Singh)
(Judges: Tom Mansell & David Murhammer)

- 1st place from 5
- 1st place from 6
- 1st place from 7

Mid-America Regional Champions

1st place from 8

All games will be held in the Seamans Center on Saturday, April 11th

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CONTACT INFORMATION

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Competition Chairs

Cade Machin (ChemE Car): *cade-machin@uiowa.edu*
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Gabi Fiedor (ChemE Jeopardy): *gabriela-fiedor@uiowa.edu*
Shourya Singh (ChemE Jeopardy): *shourya-singh@uiowa.edu*
Klaertje Hesselink (Technical Presentations): *klaertje-hesselink@uiowa.edu*
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Event Chairs

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Evelyn Moorhouse (Awards Banquet): *evelyn-moorhouse@uiowa.edu*
Isabelle Pfeiffer (Awards Banquet): *isabelle-pfeiffer@uiowa.edu*

SPECIAL THANKS

Conference Planning Committee

Chapter Advisor David Murhammer

Staff at the Iowa Memorial Union & the Graduate Hotel

Sponsors

- Procter&Gamble
- Ingredion
- Cambrex
- Emerson
- FM
- cGMP Consulting
- Lesaffre
- International Paper
- OXE
- AIChE ChESS

UIowa AIChE Officers and Chemical Engineering Faculty

AIChE Officers, Judges, Volunteers, & Attendees

ABSTRACTS - TECHNICAL PRESENTATIONS

Basmala Aldamak (Iowa State) - Investigating the Role of Cardiac Allograft Vasculopathy in Heart Transplant Rejection

Heart transplantation remains a life-saving therapy for patients with end-stage heart failure; however, its long-term success is limited by immune-mediated complications, most notably cardiac allograft vasculopathy (CAV). CAV develops in nearly 50% of transplant recipients within ten years and is the third leading cause of death among patients more than three years post-transplant. The disease is characterized by progressive narrowing of coronary arteries caused by neointimal hyperplasia, driven by smooth muscle cell (SMC) phenotypic modulation and immune infiltration. While previous studies have focused primarily on recipient immune responses, emerging evidence suggests that donor-derived immune cells, particularly macrophages, play a critical role in shaping early graft responses and long-term vascular remodeling.

This study investigates how donor-derived macrophages interact with recipient immune cells to influence SMC fate specification and drive vascular remodeling in CAV. To examine these mechanisms, we utilized a murine heterotopic heart transplantation model in which donor hearts were implanted into the abdominal cavity of recipient mice, enabling detailed analysis of immune-stromal interactions within the graft. Findings from the murine model were validated using human cardiac transplant biobank samples to strengthen translational relevance.

Immunofluorescence staining was performed to characterize cellular behaviors and signaling pathways associated with disease progression. Key molecular markers included KLF4 and Sca1, regulators of SMC plasticity; PAR1 and PAR2, mediators of protease-activated inflammatory signaling; phospho-STAT3, a central effector of the JAK-STAT signaling axis; and PTEN, a tumor suppressor that restricts cellular proliferation and migration.

Characterization of these molecular networks revealed how donor- and recipient-derived immune cells converge to modulate SMC phenotype and promote neointimal remodeling.

These findings provide new insight into the mechanisms underlying CAV pathogenesis and highlight potential therapeutic targets for intervention. Current clinical management relies heavily on broad immunosuppressive therapies that reduce rejection but increase susceptibility to infection, malignancy, and systemic toxicity. Our results support a more targeted therapeutic strategy focused on selectively modulating the SMC populations that drive disease while preserving normal vascular function.

One promising avenue involves functionalized nanoparticles engineered to recognize CAV-associated protein signatures. Such systems could enable localized drug delivery directly to modulated or progenitor SMC populations while sparing contractile cells and minimizing systemic exposure. Targeted approaches of this kind have the potential to reduce off-target effects, extend graft survival, and improve long-term outcomes for transplant recipients.

Overall, this study demonstrates that donor-derived macrophages are active regulators of recipient immune responses and SMC remodeling in CAV. By integrating murine transplant models, human tissue validation, and pathway-level profiling, this work establishes a mechanistic framework linking immune-stromal interactions to vascular pathology and lays the foundation for targeted, cell-specific therapies that advance precision medicine in heart transplantation.

Ellie Albertoni (Iowa State) - Surface Driven Defect Migration in Ge and GeSn Slabs

In recent years, germanium-tin (GeSn) alloys have gained significant attention for semiconductor and optoelectronic applications due to their tunable direct bandgap, a characteristic not seen in silicon-based devices. Despite this promise, a major challenge in GeSn integration lies in the limited solubility and lattice mismatch between Ge and Sn, which can lead to phase separation, defect formation, and overall instability in the alloy. Addressing these issues requires a fundamental understanding of defect formation and migration at the atomic scale.

In this work, we utilize density functional theory (DFT) to examine how the formation and diffusion of germanium vacancies are influenced by the surface orientation, surface termination, applied strain, and proximity to the surface. Additionally, we examine the pathway of vacancy-mediated tin diffusion and how the energetics vary with surface orientation and strain. These insights provide a theoretical foundation for controlling defect behavior during synthesis and optimizing the structural stability of GeSn-based materials for optoelectronic device applications.

Lali Nozadze (Iowa State) - Prebiotic-Guided Engineering of E.Coli Nissle 1917 as a Live Biotherapeutic

The composition and balance of the gut microbiota play a crucial role in maintaining human health. Modulation of microbial community through prebiotics has been extensively investigated to elucidate the connections between gut microorganisms and various gastrointestinal disorders. Prebiotic sugars serve as selective substrates for gut microbes that possess the enzymatic machinery required for their hydrolysis. Consequently, prebiotics have garnered significant attention for their ability to selectively promote the growth of beneficial bacterial populations within the gut ecosystem.

In parallel, probiotic strains capable of utilizing these prebiotics have been explored as live biotherapeutic agents for the prevention and treatment of diseases such as inflammatory bowel disease (IBD) and Crohn’s disease.

In this study, we investigated the raffinose utilization profiles for engineering E. coli Nissle 1917 (EcN) as a next-generation live biotherapeutic to mitigate antimicrobial resistance (AMR). Our engineered EcN:pET28a-Inv, harboring a safe levansucrase gene, exhibits unique growth kinetics in varied pH and temperature environments. Remarkably, the recombinant strain exhibited a three-fold increase in maximum cell density compared to the control, indicating enhanced growth driven by raffinose utilization. These findings establish a promising foundation for further rational design of raffinose-responsive, antimicrobial-peptide-releasing live biotherapeutics targeting priority AMR pathogens listed by the Centers for Disease Control and Prevention (CDC).

Kiersten Harris (University of Kansas) - Modeling and Evaluating Drug Release from Hydrogels under Different Storage Conditions

The longevity of medicinal products is critical to providing affordable, accessible healthcare. Alginate hydrogels are an ideal delivery system for affordability and accessibility as they are composed of naturally occurring alginate from algae that is biocompatible and biodegradable. Preliminary results have shown that the chemical structure of alginate beads can protect delicate pharmaceuticals from decomposition (Weng); however, there is uncertainty about their performance following different storage conditions.

Green food coloring was used as a model drug and encapsulated in a calcium-alginate hydrogel and stored under different conditions: immediate-use, 4 °C and 25 °C. The impact of diffusion was studied by submerging the stored beads in water which served as a dissolution solution. The diffusion of food coloring was measured over time using UV-Vis spectrophotometry. Mass transfer from the beads to the surrounding solution was modeled as diffusion through a spherical hydrogel matrix governed by Fick’s second law where the release rate depends on the concentration gradient and the effective diffusion coefficient within the bead. Immediate-use beads exhibited faster rates of diffusion and released a higher quantity of food coloring compared to beads stored at both 4 °C and 25 °C. This behavior is consistent with the mass transfer model, as hydrated beads maintain larger pore channels and have a higher effective diffusion coefficient allowing the dye to migrate faster through the hydrogel matrix. In contrast, water loss during storage likely reduces pore size and increases mass transfer resistance. The differences in diffusion rate without damage to the beads' physical appearance suggest that water loss does not damage the structure of the beads but instead alters transport properties within the hydrogel network.

Bailey Butler (University of Arkansas) - Strengthening the Future of Kidney Dialysis One Cosolvent at a Time

Chronic kidney disease (CKD) affects approximately 850 million people worldwide each year. End-stage kidney disease (ESKD), being the highest stage of CKD, requires dialysis or a kidney transplant. Hemodialysis is the most common ESKD treatment, however it has a significant physical burden on patients. Also, the membranes currently used, Polysulfone (PSF) being the most common, have many limitations, including albumin leakage and a 70% rejection of urea toxins. Nanocellulose membranes are gaining attention due to their unique properties, including mechanical strength, biodegradability, and the natural abundance of cellulose. New research suggests that dissolving 2,2,6,6- tetramethylpiperidinyl-1-oxyl (TEMPO) Oxidized Nanocellulose in 1-Ethyl-3-Methyl Imidazolium Acetate (EMIM-Ac) could be a promising alternative to PSF membranes. Some advantages of membranes made from this solution include improved flux, a sharper molecular weight cut-off, and improved anti-fouling properties. However, the strength must be thoroughly investigated to ensure their durability and reliability for practical use. The strength of the membranes can be influenced by the ionic liquid used, the cosolvents added, and the ratio of the solutions used to cast the membrane.

This study investigates differences in membrane strength when varying cosolvents specifically. The viscosity of the solutions used to cast membranes is also evaluated, using a Brookfield DV2T Viscometer, and related to the strength of the membranes. These solutions are cast into membranes using a Porometer Memcast at a thickness of 500 micrometers. The mechanical strength of each flat sheet membrane is evaluated using a Mark-10 IntelliMESUR F305 Mechanical Test Frame, which measures the different solutions' resistance to tearing or breaking under applied stress.

The viscosity of the solution used to cast the membrane is expected to play a key role in determining membrane strength, with higher viscosity potentially leading to improved mechanical properties. This study hypothesizes that modifying the solution components prior to casting the membrane affects the mechanical strength, and solutions with increased viscosity are directly correlated to increased membrane strength.

Lilly Hutchinson (University of Arkansas) - Design and Characterization of Adipose-Derived Stem Cell Collagen I Scaffold for Regenerative Medicine

The current gold standard for treating nerve injury is the autograft nerve which relies on a second surgery that damages the donor site1–3 . Further work regarding tissue engineered grafts for nerve repair is needed. The extracellular matrix (ECM) of peripheral nerves is primarily made of collagen I, therefore, a hydrogel from this ECM component is a viable option for potential treatment4 . Adipose-derived stem cells (ASCs) express matrix metalloproteinases (MMPs) which naturally degrade and are regulated by tissue inhibitors of metalloproteinases (TIMPs)4,5 . ASCs were also chosen because they have been previously established to increase neural tissue remodeling6 .The increase in MMPs, specifically MMP-2 and 9 have been previously shown to promote neural repair7–9 . MMP-14 activates MMP-2, so its expression could further increase that of MMP-2 4 . However, the over expression of MMPs can lead to tissue damage, so the ratio of TIMPs to MMPs, specifically TIMP-1 in the case of MMP-2, 9, and 14, is of interest to determine if MMP expression promotes neural regeneration8 . Studying the expression of MMP2, 9, and 14 within the cold-cast and warm-cast hydrogels will provide insight into potential nerve graft structures. Due to the dynamic cell/ECM interactions, changing the collagen fiber thickness and alignment should change the cellular interactions within the hydrogel. A temperature dependent casting method coupled with stretching can be used to change the microenvironment of a collagen I hydrogel10–12 . Analyzing the cellular response to different microenvironments will indicate what hydrogel type increases the repair response of a hydrogel nerve graft

Olivia Reid (University of Arkansas) - Turning down the heat: Fine-tuning Nanocellulose Membranes for Kidney Dialysis

TEMPO-oxidized nanocellulose membranes are widely used in both lab and industrial applications. From the ultrafiltration of milk to advancements in kidney dialysis, the potential implementations are vast and continually expanding. This study focuses on investigating the effect of varying coagulation temperatures on the morphology and properties of TEMPO oxidized nanocellulose membranes to enhance their performance in specific filtration applications. It is hypothesized that at higher temperatures, the solvent exchange between the membrane solution and the water bath will occur more rapidly, leading to the formation of larger pore structures. Conversely, at lower temperatures, the slower solvent diffusion will result in smaller, more uniform pores. The oxidized membranes are synthesized using 2,2,6,6-tetramethylpiperidinyl-1-oxyl (TEMPO) to enhance selectivity and antifouling properties. Characterization of the membranes produced at varying coagulation temperatures is crucial to determine their potential applications in future research. Scanning electron microscopy (SEM) was the primary method used for membrane characterization, and alternative rejection experiments were conducted to confirm the results obtained from SEM.

Preliminary results suggest that higher temperatures during phase inversion cause not only larger pore structures but also reduced fiber bonding, resulting in a looser, less compact morphology. In contrast, lower temperatures favor smaller pore size and fibrous crosslinking which create a more consistent pore structure. By understanding how varying temperatures affect membrane morphology, researchers can more effectively tailor membrane casting techniques to suit specific experimental needs.

Sage Paschall (University of Arkansas) - Constructing a Probabilistic Approach to Multiscale Simulation: Evaluating Machine-Learned Backmapping Models of Diphenylalanine

When adjusting state conditions, some peptide chains have demonstrated the tendency to self-assemble into various nanostructures, such as nanovesicles or nanotubes. Diphenylalanine (FF) is an example of these self-assembling peptides, as it has exhibited the ability to form electrically conductive structures, which have many promising potential applications in biotechnology and nanoelectronics. However, the exact mechanisms underlying this self-assembly process remain largely ambiguous. Atomistic-scale molecular dynamics (MD) simulations allow for the evaluation of atomic-level interactions crucial in understanding the driving thermodynamic forces behind self-assembly, but are too computationally expensive to span the necessary timescale to observe the process in action. Coarse-grained (CG) models allow for simulation at the appropriate timescale, but come at the cost of vital atomistic detail. It is therefore important to develop methods of switching between atomistic and CG resolution efficiently in order to probe the necessary characteristics while maintaining computational efficiency. Scaling down to the CG space from the atomistic is relatively straightforward, but scaling up from the CG space to the atomistic (backmapping) remains a significant challenge. While deterministic backmapping methods have been thoroughly studied, they fail to capture the inherent variability present in a CG structure. By incorporating machine-learning methods, a probabilistic backmapping approach can be utilized to better represent this variability. Separate models were trained in internal bond-angle-torsion (BAT) coordinates for each individual MARTINI CG bead. Sampling and analysis of the learned probability distributions demonstrate that the models very accurately replicate diphenylalanine’s atomistic structure. Evaluation of the potential energies of backmapped structures reveals that the model predicts physically viable, low-energy conformations in the majority of cases. While further evaluation and refinement are needed to enable integration into a complete atomistic system, preliminary results demonstrate strong potential. The compartmentalized training procedure additionally allows for a transition to more complex systems, such as long-chain polymers and proteins, with relative ease.

ABSTRACTS - TECHNICAL PRESENTATIONS

Rhea Fisch (University of Iowa) - Development of Polyhydroxyalkanoate Engineering Tools Through Analysis of Cupriavidus necator Wild Type Biodiversity

Traditional plastics present major environmental risk because they are carbon intensive and take centuries to decompose. Bioplastics are an appealing solution, as they solve both problems with similar mechanical properties. One important candidate bioplastic is polyhydroxyalkanoates (PHA), which is produced natively by several bacteria, including Cupriavidus necator. Analysis of PHA production in C. necator is stifled by its nature as an intracellular product, and engineering of it is stifled by the poor plasmid stability of H16, the main type strain. Plasmid stability of other strains were studied, however these more stable strains produce lower molecular weight PHA, limiting their workability in industry. To remedy this, we develop high-throughput methods of analyzing PHA production criteria and use them to study wild type biodiversity in 13 strains of the species. This was done spectroscopically, using kinetic optical density data to measure growth, and a dye called LipidGreen2 to measure PHA concentration. Python was used to analyze these growth data at high throughput and LipidGreen2 fluorescence was calibrated against the traditional method of quantification through gas chromatography. To contextualize the impact of these phenotypic differences, the genomes of each strain were sequenced and assembled, and compared to the observed phenotypic variation to allow for this biodiversity to be exploited for greater PHA production. These findings can be used to accelerate metabolic engineering research on C. necator as the methods used allow for higher throughput analysis of PHA growth criteria and impetus for recombination to be conducted on strains with greater plasmid stability such as DSM 2625.

Brooke Ruff (University of Oklahoma) - Improving Retention and Early Engagement in Chemical Engineering: An AIChE Student Chapter Initiative

Student retention and early engagement remain persistent challenges in many Chemical Engineering programs. Within the American Institute of Chemical Engineers (AIChE) student chapter, enrollment capacity allows for approximately 80 active members; however, cohorts that begin with roughly 60 first-year students typically decline to only 40–45 participants by the sophomore year. This project investigates structural and cultural factors contributing to this loss of engagement and evaluates strategies to strengthen student retention, professional development, and early academic integration. The study focuses on several initiatives: increasing undergraduate research participation, developing articulation agreements with community colleges to broaden the recruitment pipeline, restructuring chapter leadership to improve operational continuity, and creating targeted outreach programs for both first-year and high-school students. Particular attention is given to first-year engagement mechanisms, including a “Lunch and Learn” program that successfully connected freshmen with faculty mentors and upper-class students, leading to increased awareness of research opportunities and scholarship pathways. In addition, the project examines communication effectiveness within student organizations, recognizing that traditional email channels are often ineffective for undergraduate audiences. To support long-term engagement, the work also proposes the implementation of a Chemical Engineering introductory elective modeled after the “ChemE Cube” concept developed at Purdue University School of Chemical Engineering. This course would provide early exposure to chemical engineering concepts, community building, and professional pathways for first-year students who currently lack a dedicated departmental course. Comparative analysis of volunteer and student organizations with strong retention practices will inform best practices in leadership structure, communication strategies, and programming. The outcomes of this research aim to provide a scalable framework for improving student retention, strengthening the undergraduate research pipeline, and enhancing the overall effectiveness of AIChE student chapters in supporting the professional development of future chemical engineers.

Nour Bou Alwan (University of Oklahoma) - Modeling PFAS Adsorption in Zr-Based MOFs using Molecular Simulation

Per- and polyfluoroalkyl substances are long lasting, hazardous chemicals that have garnered significant attention due to their resistance to capture. Widely used and persistent in the environment, these chemicals have been detected in human and animal blood, leading to adverse health effects. Research has recently revealed Metal-organic frameworks, otherwise known as MOFs, to be a promising solution to PFAS capture and removal. These crystalline materials have ultrahigh porosity, large internal surface areas, and high thermal stability, which maximize their potential within capture and degradation. The focus of my research is examining the adsorption efficiency of MOF-808 for long chain PFAS through batch adsorption experiments, evaluating parameters such as temperature and adsorption energies. So far, results generated have shown that long chain PFAS have a strong affinity to the MOF-808 lattice. Specifically , my research on how PFAS of the same chain length and different head groups affect adsorption proved that PFAS with a more polar head group binds more efficiently and form stronger bonds with the MOF. The two main objectives of my research include examining the adsorption capacity of PFOA vs. PFOS and examining how different parameters (specifically temperature) influence the removal of contaminants from water. Promising results have been generated so far, and hopefully, this study will help advance the application toward the removal of these contaminants from water and other harmful sources.

Sarah Barakat (University of Oklahoma) - Assessment of Red Blood Cell Damage in Mechanical Circulatory Support Systems Using Extracellular Vesicles and Hemolysis

This project, completed in collaboration with a team at RIT, investigates red blood cell damage in mechanical circulatory support systems. Blood damage in ventricular assist devices is most commonly evaluated using hemolysis, but hemolysis alone may not fully capture the range of complications associated with device induced blood trauma. Because of this, the production of extracellular vesicles was used in this study as a metric of red blood cell damage, along with hemolysis index for comparision. Porcine red blood cell samples were exposed to varying shear conditions using an axial flow shearing device with a magnetically levitated rotor, which allowed shear stress and exposure time to be controlled through changes in rotor speed and flow rate. Microparticle concentration and hemolysis index were measured and compared across experimental conditions. The effect of each variable on red blood cell damage was then assessed, and results showed an overall positive correlation between microparticle concentration and hemolysis index, with damage generally increasing as shear increased and exposure time decreased.

ABSTRACTS - TECHNICAL PRESENTATIONS

Jacob McCormick (University of Tulsa) - Antioxidative ZrB2/SiC Coating Systems for Carbon/Carbon Composites in High Temperature Applications

Carbon/Carbon (C/C) composites are critical to next-generation technologies, including aerospace propulsion, hypersonic flight vehicles, and atmospheric re-entry systems due to their low density, superior strength, and thermal shock resistance. However, they experience mass loss above 500°C in oxygen-rich environments. This research addresses this challenge through the development and optimization of advanced antioxidative multilayer coatings that integrate pack cementation (PC), chemical vapor deposition (CVD), and slurry-derived barrier systems to enhance oxidation endurance and material reusability under extreme environments.

Silicon carbide (SiC) was selected as the principal protective phase for its high melting point and chemical affinity with carbon. Complementary ZrB_2-based slurry coatings were incorporated to generate refractory oxides (ZrO_2 and B_2O_3). A systematic design of experiments was used with a multilayer coating approach where number of layers, method, chemical composition of the PC layer, and sequence were varied to optimize oxidation resistance. These coated C/C samples were tested in an air atmosphere at 1000 °C to optimize endurance.

The oxidation tests revealed that PC coatings consistently functioned as a robust base layer due to its strong adhesion. In double layer coatings, CVD-SiC slowed the oxidation diffusion and subsequent mass loss while slurry suppressed mass loss due to the formation of refractory oxides. In triple layer coatings, implementing CVD-SiC between the PC base and slurry, improved overall oxidation. Increasing layers in a certain sequence amplified protection: four-layer samples lasted around 250 hours, five-layer samples 400 hours, and six-layer samples lasted 500 hours without degradation. By extending oxidation resistance, this work advances research in high-temperature materials for extreme operational environments.

Andrea Carbonell (Washington University in St. Louis) - Lithium Battery Recycling: Highly Selective Critical Mineral Recovery from NMC Cathodes via Pulsed Electrodeposition in Deep Eutectic Solvents

Critical metals found in lithium-ion batteries (LIBs), nickel and cobalt, need to be recovered from LIB waste to maintain a circular economy of these critical metals in the United States. Current approaches to critical metal recovery are energy-intensive, environmentally taxing, and have limitations on which metals they recover from LIB waste. This study aims to find an electrochemical method to selectively recover metals from LIB waste using an environmentally friendly solvent, a deep eutectic solvent (DES). A 1:2 molar ratio of choline chloride to urea DES was used to dissolve the LIB waste. Ni and Co have very similar electrochemical properties when dissolved in DES and have issues selectively electroplating onto a substrate. In lower applied potentials, both Ni and Co electroplate onto the substrate together. To facilitate this issue, cyclic voltammetry was utilized to calculate the diffusion coefficient for Ni and Co. It was found that Ni has a higher diffusion coefficient in DES than Co, therefore it moves through solution faster. By applying a potential in short increments, with a method called “pulse”, Ni was selectively electroplated (98.8% selectivity) from LIB waste dissolved in DES onto a copper foil, the substrate of choice.

Arthur Benson (University of Kansas) - Interfacial Behavior of Anti-Reductive Electrolytes in Lithium-Sulfur Batteries

Lithium–sulfur (Li–S) batteries are a promising candidate for energy storage applications due to their high energy density and low material cost. In theory, the formation of polysulfides in the electrolyte enables a high energy capacity and power output. In practice, however, parasitic reactions between polysulfides and the lithium anode lead to rapid lithium depletion and battery degradation. The standard electrolyte used for Li–S batteries consists of 1.0 M lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) in a mixture of equal parts 1,3-dioxolane (DOL) and 1,2-dimethoxyethane (DME). Previous studies demonstrated that introducing anti-reductive additives into this mixture significantly improves battery lifespan by encapsulating polysulfides within solvation shells, thereby reducing parasitic reactions at the lithium anode. While these studies provided insight into bulk electrolyte behavior, the molecular organization near electrode surfaces, where critical oxidation–reduction reactions occur, remains poorly understood. In this work, we use molecular dynamics (MD) simulations to investigate the interfacial behavior of several anti-reductive additives, including diisopropyl ether (DIPE), diisopropyl sulfide (DIPS), 1,1,2,2-tetrafluoroethyl-2,2,3,3-tetrafluoropropyl ether (HFE), and hexamethyl ether (HME), under conditions consistent with experimental studies. Graphene nanosheets are used to represent electrode surfaces, and fixed-charge models are applied to simulate different electric potentials. The simulations reveal that anti-reductive additives significantly reshape the interfacial structure by redistributing solvent molecules and ions (Li^+ and $TFSI^-$) near the electrode surface, possibly altering the formation and composition of the solid electrolyte interphase (SEI). These findings provide molecular-level insights into how electrolyte design affects interfacial structure and may help guide the rational design of longer-lasting Li–S batteries

Corey Van Oosbree (University of Kansas) - Genetic Algorithms for Decision Dependent Batch Scheduling Under Yield Uncertainty

Batch scheduling is the process of planning the sequence and timing of batch operations within a production process to maximize production while accounting for factors such as intermediate storage, inventory, and rolling demand. Real-world batch processes are subject to yield uncertainty, and the actual output of a batch operation may deviate from its expected value due to process variability. This project extends a prior comparative study of deterministic and genetic algorithm (GA) scheduling approaches by introducing stochastic yield uncertainty and rolling demand into the batch scheduling framework. Yield uncertainty is modeled as a truncated Gaussian distribution over batch outputs, sampled independently for each task, unit, and output chemical. A scenario-based stochastic programming approach is employed, in which each scenario represents a realization of the yield parameters. Performance across scenarios is evaluated using risk measures including expected value and Conditional Value-at-Risk (CVaR). An extended version of this framework incorporates decision-dependent uncertainty, in which the expected yield of a task varies based on sequencing and duration decisions. The GA scheduler is evaluated stochastically by simulating each candidate schedule across multiple yield scenarios and computing risk measures, comparing schedule quality and robustness under uncertainty. The results were compared to the optimal solution of the mixed-integer linear program (MILP) is solved using the Gurobi solver through the Pyomo library in Python, which is solved for each yield realization scenario. To evaluate both approaches, a multi-stage chemical production problem is considered, involving a shared facility with a heater, reactors, and a distillation column, with constrained intermediate storage and rolling demand for final products. The two methods are compared based on profitability under uncertainty, robustness to adverse yield scenarios, and computational efficiency. Results show that as the time horizon and number of scenarios increase, the performance of the deterministic model decreases and it becomes necessary to utilize the GA.

ABSTRACTS - POSTER COMPETITION

Madison Jones (University of Kansas) - Deep Eutectic Solvents and Ionic Liquids for the Separation of Azeotropic Refrigerant Mixtures Thrust 1, Project 1.1

Nora Jennings (University of Kansas) - Synthesizing Organic Semiconductors from Y6:PM6 Nanoparticles

Currently, organic semiconductors typically require toxic solvents, as the nonpolar molecules can't dissolve in environmentally friendly, polar solvents like water. However, by using nanoparticles, miniemulsions can be formed, thus this allows us to use water as a solvent for organic nanoparticles. One of the most prominent materials for organic semiconductors in current research is a blend of the organic compounds Y6 and PM6. Thus, my research demonstrates the progress being made for creating thin film semiconductors from nanoparticle Y6:PM6 blends.

The poster presentation will include a brief description of the purpose of the selection of Y6 and PM6, as well as the purpose for using nanoparticles. The process for creating a Y6:PM6 nanoparticle solution will be described, including the purpose and use of surfactants. Additionally, it will include various challenges and strategies for creating even thin films. Current focuses include controlling the concentration of surfactants and the annealing temperature. The efficacy of varying these parameters have been determined by optical absorption and photoluminescence spectroscopy.

Directions for future research will be included in the conclusion, including further strategies to implement to try to ensure that these films can easily be replicated under a certain set of conditions.

ABSTRACTS - POSTER COMPETITION

Shomoy Kamal (University of Tulsa) - Removal of Chromium Metal Using One-Step and Two-Step Activated Biochar-Based Adsorbents

The effects of global urbanization and industrialization have led to the pollution of sources of drinking water with heavy metal contaminants. Pollutants such as chromium are released in hazardous concentrations by industries such as leather tannery, posing a threat to the environment and to human health, especially in poorer countries. This research project explores the use of biochar, a renewable carbon-rich material derived from cellulose biomass, as an adsorbent for heavy metals in water. Biochar-based adsorbents have the potential to be low-cost and sustainable solutions to heavy metal pollution, and are adaptable to various needs by different methods of activation and modification. This research project aims to determine the optimal activation conditions for biochar-based adsorbents to adsorb chromium from water.

Biochar used in this project is synthesized by performing hydrothermal carbonization on dry cellulose biomass in a reactor, with a 1:7 ratio of cellulose to water and a temperature and pressure of 300 °C and 1300 psi. The biochar is activated using one-step and two-step activation processes. One-step activation involves only a KOH chemical activation process, with KOH to biochar ratios of 0.5:1, 1:1, or 2:1 and activation temperatures of 700, 750, 800, or 850 °C. Two-step activation includes a thermal pre-activation of the biochar at 1000 °C, followed by the aforementioned KOH chemical activation. Activated biochar adsorbents are tested for adsorption by deployment into chromium solutions of 50, 100, 150, and 200 ppm concentrations. The adsorbent dosage, solution pH, and adsorption time are held constant at 1.5 g/L, pH 2, and 24 hours respectively. Adsorption samples are analyzed in an ICP-OES (Inductively Coupled Plasma Optical Emission Spectroscopy) device to determine the remaining chromium concentration, and the calculated percent adsorptions are used to compare the performance of different activation conditions for adsorbents.

The expected outcomes of the project include results indicating the activation conditions that result in the greatest adsorption of chromium in water. The research also aims to similarly analyze the adsorption of calcium, another heavy metal pollutant, in the future. Ultimately, the results of the research are intended to optimize the adsorption potential of biochar adsorbents, to allow for large-scale deployment of these adsorbents in the future to combat heavy metal pollution in bodies of water.

Sungwon Lee (University of Tulsa) - Parametric Study of Renewable Methanol Production via CO2 Hydrogenation: Process Simulation and Sensitivity Analysis

Catalytic hydrogenation of CO2 to methanol represents a viable pathway for carbon utilization and chemical energy storage, particularly when coupled with direct air capture and renewable hydrogen production. This study presents a parametric analysis of an integrated methanol production process simulated in Aspen Plus, validated against the benchmark of Van-Dal and Bouallou. The process models CO_2 hydrogenation over a $Cu/ZnO/Al_2O_3$ catalyst using the Vanden Bussche and Froment kinetic model in an RPlug reactor at 78 bar and 210°C. Downstream purification employs a two-column distillation sequence targeting 99.85 mol% methanol purity, modeled using the NRTL-RK property method. Sensitivity analyses are performed across three process units: the synthesis reactor, PEM electrolyzer, and direct air capture unit. For the reactor, we examine the effects of H2/CO2 feed ratio, operating pressure, inlet temperature, and recycle ratio on methanol yield and energy consumption. For the electrolyzer, current density, operating pressure, and renewable electricity capacity factors are evaluated in terms of specific energy consumption and hydrogen production cost. For the DAC unit, we assess the impact of sorbent regeneration temperature, air contactor flow rate, and CO2 capture efficiency on the overall carbon and energy balance. Results from this study provide insights into the key operating variables governing integrated plant performance, with the goal of identifying conditions that maximize carbon utilization and minimize total energy penalty for renewable methanol production.

ABSTRACTS - POSTER COMPETITION

Dayton Hartsell (University of Arkansas) - Silver Electrolysis with a Twist

The current wastewater system operating aboard the ISS operates using iodine as a biocide, but overexposure to iodine could lead to hyperthyroidism. An alternative biocide is silver addition, specifically separated by silver electrolysis, but this process is short lived due to dendrite formation shorting the reaction. Dendrite formation might be prevented if there is a large enough shear force acting between the cathode and anode and is the focus of this paper. Because of this a shear force must be induced within the piping system, this can be done with a static mixer. Previous work has determined three static mixer shapes, a baffled mixer, a bowtie mixer, and a spiral mixer are feasible designs. COMSOL Multiphysics simulation for computational fluid dynamics combined with physical experiments will be presented to show if this is a viable strategy to reduce or eliminate dendrite formation.

ABSTRACTS - POSTER COMPETITION

Ian Popp (University of Arkansas) - Next Generation C2C12 Models: Leveraging dCas9 Gene Editing to Accelerate Discovery of Neuromuscular Disease Modifiers

Duchenne muscular dystrophy (DMD) is a genetic disease caused by a dystrophin mutation which results in nonfunctional expression dystrophin. (1,2) This disease impacts 1 in 5,000 male births and results in muscle degeneration leading to a median lifespan of 28 years (3,4). CRISPR-dCas9 recruited enhanced activation model (CRISPR DREAM) targets a specified sequence and regulates gene expression. CRISPR DREAM is a CRISPR-dCas9 system that uses human derived transcriptional activation domain plasmids (TADs) which can elicit a weaker inflammatory response in humans (5). Increased UTRN RNA has been shown to alleviate the impact of dystrophin protein deficiency, and increased UTRN RNA expression causes increased protein production to compensate for the dysfunctional dystrophin (6). Myostatin and myostatin receptor both regulate muscle growth which make these genes of interest for muscular based therapies such as DMD (7,8). Multiple guide sequences were designed for these genetic targets and transformed into CRISPR-DREAM plasmids for genetic regulation. Transcriptional efficacy was observed with quantitative real-time polymerase chain reaction (qRT-PCR), showing increased Utrn expression for both TADs indicating potential as a tool in muscle therapy applications. Due to successful regulations in the C2C12 cell line using CRISPR DREAM, a constitutively expressed CRISPR-DREAM C2C12 model cell line has been developed for rapid testing of genetic targets, requiring fewer plasmids for each test. Through multiplexing, genetic targets in combination are rapidly tested as a more holistic gene therapy approach to treating DMD.

ABSTRACTS - POSTER COMPETITION

Natalie Erickson (University of Arkansas) - A Baseline Study of Artificial Intelligence Use among Chemical Engineering Undergraduates at the University of Arkansas.

In recent years, artificial intelligence (AI) has shifted from a novel innovation to a tool used in daily life, particularly within higher education. While anecdotal evidence suggests high levels of student engagement with AI, empirical data regarding usage patterns remains limited. This baseline study investigates AI integration among undergraduate chemical engineering students at the University of Arkansas. Through an anonymous survey (N=68; comprising 20 freshmen, 14 sophomores, 16 juniors, and 18 seniors), researchers assessed usage frequency, student comfort levels, and their evolving relationship with AI tools. The findings reveal that 75% of respondents utilize AI for coursework at least once a week, with 32% engaging with these tools daily. These results provide educators with a realistic benchmark of student behavior, offering critical insights to help guide the ethical and responsible integration of AI into the engineering curriculum.

Sage Paschall (University of Arkansas) - Constructing a Probabilistic Approach to Multiscale Simulation: Evaluating Machine-Learned Backmapping Models of Diphenylalanine

When adjusting state conditions, some peptide chains have demonstrated the tendency to self-assemble into various nanostructures, such as nanovesicles or nanotubes. Diphenylalanine (FF) is an example of these self-assembling peptides, as it has exhibited the ability to form electrically conductive structures, which have many promising potential applications in biotechnology and nanoelectronics. However, the exact mechanisms underlying this self-assembly process remain largely ambiguous. Atomistic-scale molecular dynamics (MD) simulations allow for the evaluation of atomic-level interactions crucial in understanding the driving thermodynamic forces behind self-assembly, but are too computationally expensive to span the necessary timescale to observe the process in action. Coarse-grained (CG) models allow for simulation at the appropriate timescale, but come at the cost of vital atomistic detail. It is therefore important to develop methods of switching between atomistic and CG resolution efficiently in order to probe the necessary characteristics while maintaining computational efficiency. Scaling down to the CG space from the atomistic is relatively straightforward, but scaling up from the CG space to the atomistic (backmapping) remains a significant challenge. While deterministic backmapping methods have been thoroughly studied, they fail to capture the inherent variability present in a CG structure. By incorporating machine-learning methods, a probabilistic backmapping approach can be utilized to better represent this variability. Separate models were trained in internal bond-angle-torsion (BAT) coordinates for each individual MARTINI CG bead. Sampling and analysis of the learned probability distributions demonstrate that the models very accurately replicate diphenylalanine’s atomistic structure. Evaluation of the potential energies of backmapped structures reveals that the model predicts physically viable, low-energy conformations in the majority of cases. While further evaluation and refinement are needed to enable integration into a complete atomistic system, preliminary results demonstrate strong potential. The compartmentalized training procedure additionally allows for a transition to more complex systems, such as long-chain polymers and proteins, with relative ease.

ABSTRACTS - POSTER COMPETITION

Alex Quast (University of Iowa) - Lithium Uptake by Hydrogen Manganese Oxide: Influence of Particle Size and Solution Properties on Performance

Lithium is classified as a critical material due to its essential role in modern technology and energy systems. Current recovery methods are expensive and environmentally harmful. Given the importance of lithium there is a growing interest in novel methods of recovery. Therefore, there is a need to develop cost effective and environmentally friendly strategies capable of extracting lithium from unconventional sources. In this study we investigated the Li ion uptake and efficiency of 4 different hydrous manganese oxide (HMO) particles with varying particle sizes. LMO powder was converted to HMO through acidification to be used in uptake studies. A lithium stock solution of 1g/L LiCl was buffered at pH 7, 10, and 12. Lithium ion uptake isotherm studies were performed at each pH on each HMO particle to determine the relationship between particle size, specific surface area, and pH with uptake capacity. To test the efficiency of uptake, kinetic studies were performed as well. We observed greater Li uptake at higher pH values. Notably, at pH 7 we observed distinct differences in Li uptake that can be attributed to differences in particle size, consistent with largely a surface driven uptake process. In contrast, at pH 12, all sizes of HMO particles exhibited comparable degrees of uptake, consistent with Li uptake occurring within the bulk of the HMO particle. Collectively, evidence suggests that lithium is removed from solution by HMO particles through a mix of surface adsorption and internal channel absorption. This work yields insights that may help to guide the design of highperformance HMO sorbents for the selective uptake of Li from brines and other waste streams.

Bruce Baker (University of Nebraska-Lincoln) - Fighting Freezing Rain: Surface Texturing for Improved Hydrophobicity

Reduction of droplet-to-surface contact time and area has a wide variety of industrial benefits and is a primary focus of anti-icing technology. It is known that contact dynamics may be affected to some degree by surface texture, droplet radius, variations in the hydrophobic coating, and temperature variation of the droplet or surface, among other factors. The team is dedicated to quantifying the influence of these factors and assessing how strongly they each affect droplet impact. In this study, poly(1H,1H,2H,2H-perfluorodecyl acrylate) (pPFDA) is deposited via initiated chemical vapor deposition (iCVD) on a smooth silicon surface as well as femtosecond lasers roughened aluminum surfaces. The surfaces are each imaged at the millimeter scale to quantify roughness. The coated substrates are placed on a peltier device at varying temperatures, and droplet impacts are then measured and evaluated at a high framerate to yield kinetic information. The roughened surfaces saw a large reduction in contact time and a much more elastic collision between the droplet and the surface. Droplets adhered to chilled surfaces more strongly, and this effect was enhanced on rougher surfaces.

ABSTRACTS - POSTER COMPETITION

Edward Stone (University of Nebraska Lincoln) - Exploring Metabolic Adaptations in Treponema pallidum through Genome-Scale Metabolic Modeling

Treponema pallidum, the causative agent of Syphilis, exhibits unique metabolic characteristics, including the absence of a fully functional TCA cycle, which raises questions about how it sustains its high motility with limited ATP production. Moreover, T. pallidum is difficult to culture in vitro This project aims to reconstruct a genome-scale metabolic model (GEM) of T. pallidum to gain a better understanding of the bacteria, specifically addressing how it achieves high motility with limited ATP generation and whether its uptakes lactate as a carbon source to compensate for its lack of TCA cycle. To build this model, we first conducted a literature review to elucidate the bacterium's metabolism. Using an automated model building pipeline called KBase, we developed a draft model which was later refined by adding and removing reactions to accurately represent T. pallidum's metabolic traits. After developing the model, we validated it using Memote, achieving a score of 92%. To further validate the model, we predicted the essential genes for T. pallidum. Since no information on T. pallidum's essential genes is available, we used gene (enzyme) orthology via BLAST to compare the predicted genes with those of E. coli and Neisseria gonorrhoeae which are phylogenetically close. BLAST revealed that 41 out of the 42 predicted genes had orthologs in E. coli, and 37 had orthologs in N. gonorrhea. Of the E. coli orthologs, 26 were essential for growth, while 28 orthologs were essential in N. gonorrhea, further demonstrating the robustness of our model. Additionally, we used TransportDB to verify the transporter proteins and tested the model's ability to metabolize various carbon sources such as glucose, pyruvate, and mannose. The resulting GEM provides insights into T. pallidum's metabolism and offers a foundation to explore key questions about the bacteria's high motility and its potential to uptake lactate as a carbon source. In the future, it can serve as a powerful tool for studying the bacterium's metabolic adaptations and responses to various environmental conditions.

Alseny Boiro (University of Oklahoma) - Title: Controlling Hydrogel Properties with Polymer Additives

Hydrogels are crosslinked polymers network capable of retaining large amounts of water while maintaining structural integrity, making them highly valuable in biomedical and materials engineering applications. This study investigates the influence of high-molecular weight polyethylene oxide (PEO) additive on the swelling behavior of hydrogels obtained from crosslinking polyethylene glycol diacrylate (PEGDA). PEGDA serves as photo-cross linkable precursor that forms a stable three-dimensional network upon UV exposure, while PEO acts as water-soluble polymer additive. The study hypothesizes that incorporating high-molecular weight PEO enhances hydrogel mechanics and alters phase behavior through physical entanglements and potential phase separation effects. Hydrogels were prepared via UV-induced crosslinking, and their structural physical properties were characterized using swelling measurements. Understanding these precursor and polymer additive interactions provide insight into tailoring hydrogel systems for advanced applications in biomaterials, tissue engineering, and soft matter design.

ABSTRACTS - POSTER COMPETITION

Kate Wattenbarger (University of Oklahoma) - Understanding the Effects of Acid Electrolyte Anions on Pt, Pd, and IrO_2 Surfaces for Oxygen Electrocatalysis

Electrocatalysis plays the central role in electrochemical energy conversion technologies such as fuel cells and electrolyzers, in which the device performance is limited by the Oxygen Reduction Reaction (ORR) and Oxygen Evolution Reaction (OER) due to their intrinsically sluggish kinetics involving multiple proton–electron transfer steps.1,2 Under realistic electrochemical conditions, acid electrolytes are commonly used to control and maintain the pH of the system, resulting in the presence of electrolyte anions in the reaction environment. Although electrolyte anions are often treated as spectators, they can influence electrochemical reactions in several ways. These anions can significantly influence catalytic performance by adsorbing on the catalyst and thus blocking the active sites, modifying the local reaction environments, and altering interfacial electric field interactions.3,4 Consequently, understanding the adsorption behavior of electrolyte anions is critical for improving catalytic activity in electrochemical devices. In this work, the adsorption behavior of ten acid electrolyte anions, including halides (F- , Cl- , Br- , and I-) and oxyanions (ClO4 - , NO3 - , HSO4 - , SO4 2- , H2PO4 - , and HPO4 2-), were investigated using density functional theory (DFT). The adsorption of these anions was evaluated on Pt and Pd metal surfaces, as ORR model catalyst, and IrO2 metal oxide surfaces, as OER model catalyst, to understand their interactions across different catalytic materials. For metallic Pt and Pd electrocatalysts, both terrace and stepped surfaces were considered using (111) and (211) facets. (110), (101) and (100) facets of IrO2 were considered based on the relatively high surface area fractions in the Wollf particle construction and the reported high experimental catalyst activity. Adsorption free energiestogether with preferred adsorption configurations, solvation energies, and Bader charges of the adsorbed anions were analyzed to characterize anion-surface interactions. These calculations provide insight into the role of electrolyte anions in modulating the local interfacial environment and oxygen electrocatalytic activity. Understanding the interactions of the electrolyte anions with metal/metal oxide surfaces can guide the rational design of electrocatalysts and electrolyte environments for optimized electrochemical devices

Mandisa Masonya (University of Oklahoma) - Computational Investigation of Short-Chain PFAS Capture by Zirconium-Based Metal-Organic Frameworks

Per- and polyfluoroalkyl substances (PFAS) are persistent, mobile contaminants that resist conventional remediation due to the strength of their C–F bonds and chemical stability. Although metal–organic frameworks (MOFs) possess high surface areas, tunable pore architectures, and chemically functionalizable nodes that make them promising candidates for adsorption-based remediation, comparatively limited work has examined their application to short-chain PFAS capture at the molecular scale. This study evaluates the adsorption behavior of PFBS and Gen-X within pristine MOF-808, HCOO-capped MOF808, and NU-1000 using molecular modeling and dynamics simulations. All MOF structures were geometry optimized and treated as rigid frameworks. Simulations were conducted in a simplified, solvent-free environment containing only the MOF and PFAS molecules, with future work extending to explicit aqueous systems. The COMPASS III force field was employed for structural optimization and molecular dynamics calculations. Adsorption performance was characterized through calculated adsorption capacities, binding energies, radial distribution functions (RDFs), mean square displacements (MSDs), and diffusion coefficients. Comparative analysis revealed high adsorption strength across the three frameworks, with RDF profiles indicating preferential coordination between PFAS oxygen atoms and metal nodes, while MSD-derived diffusivities demonstrated high mobility within pore environments. These results provide molecular-level insight into shortchain PFAS–MOF interactions, an area that remains underexplored, and establish a computational foundation for rational MOF design in environmental remediation applications.

Nour Bou Alwan (University of Oklahoma) - PFAS Capture Using Zr-MOFs: A Computational Study

Per- and polyfluoroalkyl substances (PFAS) are persistent, mobile contaminants that resist conventional remediation due to the strength of their C–F bonds and chemical stability. Although metal–organic frameworks (MOFs) possess high surface areas, tunable pore architectures, and chemically functionalizable nodes that make them promising candidates for adsorption-based remediation, comparatively limited work has examined their application to short-chain PFAS capture at the molecular scale. This study evaluates the adsorption behavior of PFBS and Gen-X within pristine MOF-808, HCOO-capped MOF808, and NU-1000 using molecular modeling and dynamics simulations. All MOF structures were geometry optimized and treated as rigid frameworks. Simulations were conducted in a simplified, solvent-free environment containing only the MOF and PFAS molecules, with future work extending to explicit aqueous systems. The COMPASS III force field was employed for structural optimization and molecular dynamics calculations. Adsorption performance was characterized through calculated adsorption capacities, binding energies, radial distribution functions (RDFs), mean square displacements (MSDs), and diffusion coefficients. Comparative analysis revealed high adsorption strength across the three frameworks, with RDF profiles indicating preferential coordination between PFAS oxygen atoms and metal nodes, while MSD-derived diffusivities demonstrated high mobility within pore environments. These results provide molecular-level insight into shortchain PFAS–MOF interactions, an area that remains underexplored, and establish a computational foundation for rational MOF design in environmental remediation applications.

ABSTRACTS - POSTER COMPETITION

Alexa Wienhoff (Washington University in St. Louis) - Developing Analytical Methods for Iowa's Emerging Aqueous Contaminants

Herbicides are common aqueous contaminants that can enter surface waters as runoff from agricultural lands, where they are applied to control unwanted vegetation. Herbicides in surface waters pose risks to aquatic ecosystems and human health, particularly when they enter the drinking water supply. The detection of aqueous contaminants like herbicides requires solid phase extraction (SPE), which is a method to isolate analytes from liquids, followed by liquid chromatography-mass spectrometry (LC-MS) for selective quantification. This study aims to optimize an SPE and LC-MS detection method for herbicide contaminants with high surface water concentrations near agricultural sites in Iowa, as well as northern Missouri. LC-MS methods were evaluated to establish quality assurance and quality control (QA/QC) standards and optimize detection parameters for 29 compounds of interest. Initial SPE testing was conducted to understand compound recovery and detection limits. Data from LC-MS and SPE experiments were applied to determine an appropriate method to determine herbicide concentrations in field samples with a concentration greater than 1 ng/L. Federal water and land use data were synthesized to select seven waterways impacted by agricultural runoff for sampling during the 2026 growing season. Overall, this method combined with ongoing field work will enable detection of both conventional herbicides and emerging herbicides newly registered for the 2026 growing season. Identification of these herbicides and their concentrations will contribute to awareness of water quality in Iowa and Missouri by the impacted public and relevant health policymakers.

ABSTRACTS - POSTER COMPETITION

Andrea Carbonell (Washington University in St. Louis) - Lithium Battery Recycling: Highly Selective Critical Mineral Recovery from NMC Cathodes via Pulsed Electrodeposition in Deep Eutectic Solvents

Critical metals found in lithium-ion batteries (LIBs), nickel and cobalt, need to be recovered from LIB waste to maintain a circular economy of these critical metals in the United States. Current approaches to critical metal recovery are energy-intensive, environmentally taxing, and have limitations on which metals they recover from LIB waste. This study aims to find an electrochemical method to selectively recover metals from LIB waste using an environmentally friendly solvent, a deep eutectic solvent (DES). A 1:2 molar ratio of choline chloride to urea DES was used to dissolve the LIB waste. Ni and Co have very similar electrochemical properties when dissolved in DES and have issues selectively electroplating onto a substrate. In lower applied potentials, both Ni and Co electroplate onto the substrate together. To facilitate this issue, cyclic voltammetry was utilized to calculate the diffusion coefficient for Ni and Co. It was found that Ni has a higher diffusion coefficient in DES than Co, therefore it moves through solution faster. By applying a potential in short increments, with a method called “pulse”, Ni was selectively electroplated (98.8% selectivity) from LIB waste dissolved in DES onto a copper foil, the substrate of choice.