Texas A&M Energy Research Society

2023 TEXAS A&M CONFERENCE ON ENERGY

Energy Efficiency: Optimizing Resource Utilization

Sept. 27-29, Memorial Student Center (MSC)

TEXAS A&M UNIVERSITY

Howdy!

Warm greetings from the 2023 Texas A&M Conference on Energy, here at Texas A&M University!

Since 2016, the Texas A&M Conference on Energy has been an annual conference organized by the Texas A&M Energy Research Society (ERS) with the support of the Texas A&M Energy Institute.

Texas A&M ERS is a community of students and researchers who have an interest in energy-related fields. Our mission is to work for students and researchers conducting multi-disciplinary energy research to ensure their needs are understood, advocated, and promoted through education, research, and learning. We aim to create a dynamic and synergistic environment within the university through technical and social events. Texas A&M Conference on Energy is our signature event. We hope you enjoy the conference and attend the wide variety of events offered!

Thanks and Gig'em!

Meet the team

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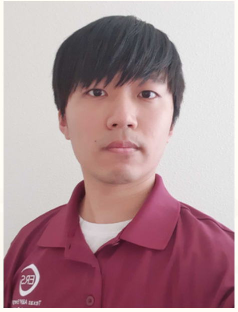
Meet the team



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Guide

Conference Schedule

Day 1 (09/27/23)

6:00 PM	7:00 PM	Registration (Outside Gates Ballroom)
7:00 PM	7:45 PM	Opening remarks and plenary talk (Gates Ballroom) by Dr. Shannon Bragg-Sitton (INL)
7:45 PM	9:00 PM	Networking and dinner reception (Gates Ballroom)

Day 2 (09/28/23)

8:00 AM	9:00 AM	Registration and breakfast (Gates Ballroom)			
9:00 AM	10:30 AM	Oral session 1 (4 tracks)			
		Energy Driven Policy MSC 2500	Safety & Resilience in Energy Systems MSC 2501	Multi-Scale Energy Systems Engineering MSC 2502	Multi-Functional Materials (A) MSC 2503
10:30 AM	10:40 AM	Transition & break			
10:40 AM	11:10 AM	Plenary talk (Gates Ballroom) - Dion Billard (Halliburton)			
11:15 AM	11:45 AM	Plenary talk (Gates Ballroom) - Chase Lansdale (Electric Power Engineers and ENER-i.AI)			
11:45 AM	1:00 PM	Lunch (Gates Ballroom)			
1:00 PM	2:00 PM	Panel discussion (Gates Ballroom): Smart Technologies and Energy Efficiency: Leveraging Digitalization to Optimize Resource Utilization			

Conference Schedule

Day 2 (09/28/23)

2:00 PM	2:15 PM	Transition & break			
2:15 PM	2:45 PM	Keynote address (Rudder Forum) - Alice Jackson (Xcel Energy)			
2:45 PM	3:00 PM	Transition & break			
3:00 PM	4:30 PM	Oral session 2 (4 tracks)			
		Energy Savings MSC 2500	Sustainability MSC 2501	Data Science & Statistical Learning MSC 2502	Multi-Functional Materials (B) MSC 2503
4:30 PM	5:30 PM	Recruiting/networking session (Gates Ballroom)			

Day 3 (09/29/23)

8:00 AM	11:00 AM	Breakfast (Gates Ballroom)
9:00 AM	9:30 AM	Plenary talk (Room 2401) - Dr. Jeremy Pearce (Shell)
9:30 AM	9:45 AM	Transition & break
9:45 AM	11:30 AM	Poster session and recruiting/networking session (Gates Ballroom)
11:30 AM	12:00 PM	Awards & closing remarks (Gates Ballroom)

Keynote Speaker

The Energy Transition: Achieving a Balance Across Customer Needs, Politics and the Laws of Physics

Alice Jackson

Senior Vice President of System Strategy
Chief Planning Officer
Xcel Energy

09/28/23, 02:15 - 02:45 pm
Rudder Forum

Alice K. Jackson is the Senior Vice President of System Strategy and Chief Planning Officer at Xcel Energy, Inc., an investor-owned utility that operates in eight states in the central U.S.

Ms. Jackson leads the Integrated System Planning organization for Xcel Energy. This organization focuses on planning and designing the energy delivery systems for roughly 5 million electric and natural gas customers.

Directly prior to her role as Senior Vice President, Ms. Jackson led the Operating Company team for Public Service Company of Colorado as President. In this role she was responsible for the community, legislative, regulatory activities and held responsibility for delivering on corporate financial outcomes and objectives for Xcel Energy.

Prior to her executive leadership roles within Xcel Energy, Alice held various regulatory positions with Southwestern Public Service Company in Texas and with Public Service Company of Colorado.

Abstract The balancing of customer interests, political interests and the laws of physics in a complex energy system come together to drive quite the debate. Accomplishing the energy transition away from large centralized baseload and dispatchable generation to a system with significantly more variable energy will demand a deliberate and a balanced approach. Ms. Jackson will present thoughts on how Xcel Energy is approaching the clean energy transition across eight central U.S. states. She will share some of her experiences, learnings, and some of the outstanding unknowns yet to be solved.

Plenary Speaker 1

Achieving the Seemingly Impossible Goal of Net-Zero Emissions

Dr. Shannon M. Bragg-Sitton

Director, Integrated Energy & Storage Systems Division

Idaho National Laboratory

09/27/23, 07:00 - 07:45 pm
Gates Ballroom (MSC)

Dr. Shannon Bragg-Sitton is an internationally recognized pioneer in the innovative application of nuclear energy alongside other clean energy generators, seeking to maximize energy utilization, generator profitability, and grid reliability and resilience through systems integration.

Since 2021, Shannon has served as the Director for the Integrated Energy & Storage Systems Division in the Energy & Environment Science & Technology Directorate at Idaho National Laboratory, which includes Power and Energy Systems, Energy Storage and Electric Transportation, and Hydrogen and Electrochemistry departments. In 2014 she helped establish the DOE Office of Nuclear Energy Integrated Energy Systems (IES) program (https://ies.inl.gov), serving as the program National Technical Director from 2014-2023. The IES team has developed novel modeling and simulation tools for technical and economic assessment of multi-input, multi-output IES and supporting experimental capabilities. Shannon is also the Chair of the Generation IV International Forum (GIF) Task Force on Non-electric Applications of Nuclear Heat (NEANH).

Shannon has held multiple leadership roles in DOE Office of Nuclear Energy programs since joining INL in 2010, including program leadership for space nuclear power and propulsion systems, advanced nuclear fuels, used fuel disposition, and microreactor development.

Dr. Bragg-Sitton holds a PhD and MS in Nuclear Engineering from the University of Michigan, an MS in Medical Physics from the University of Texas at Houston, and a BS in Nuclear Engineering from Texas A&M University.

Plenary Speaker 1

Achieving the Seemingly Impossible Goal of Net-Zero Emissions

Abstract Meeting growing energy demands while eliminating emissions, maintaining affordability, and ensuring energy justice is one of the most significant grand challenges of our time. Governments and private industry around the world have established aggressive goals to achieve net-zero emissions by mid-century. In the U.S., this equates to a net-zero electricity sector by 2035 and across all energy use sectors—including electricity, industry, and transportation—by 2050. The key question then becomes: Can we get there from here?

Meeting these aggressive goals demands immediate action, and they require us to think more holistically about our clean energy options. Currently, almost 85% of global energy demands are met by unabated fossil fuels. That means we have a lot of work to do, and we need to consider all of the non-emitting generation options available in each region—including fossil with carbon capture, renewables, and nuclear. And we need to reach our goal while establishing energy justice, which refers to the goal of achieving equity in social and economic participation in the energy system, while remediating past social, economic, and health burdens on communities that have been brought about by our energy system.

This presentation will describe U.S. and global efforts focused on novel energy system solutions that strive to maximize use of all clean energy generation options to meet our energy demands, while ensuring sustainability, customer affordability, and a just energy system.

Plenary Speaker 2

Innovation in Action: How Halliburton is Pioneering Digital Solutions for Tomorrow's Challenges

Dion Billard

Digital Discipline Manager

Halliburton

09/28/23, 10:40 - 11:10 am
Gates Ballroom (MSC)

Mechanical Engineer boasting a quarter-century of expertise in the oil and gas sector, exclusively with Halliburton. Throughout my tenure, I have undertaken various operational and managerial capacities spanning both Canada and the USA.

My professional depth includes a strong foundation in hydraulic fracturing diagnostics, engineering, operations, and business development. In recent years, particularly the last five, I have pivoted towards spearheading digital transformation initiatives within Halliburton, overseeing the successful deployment of digital solutions across multiple business divisions.

Presently, I am affiliated with Testing and Sub-Sea (TSS) in the capacity of Digital Discipline Manager. I have the privilege of leading a global team of over 60 professionals, orchestrating the development and rollout of more than 10 state-of-the-art digital solutions for both TSS and Halliburton at large.

Abstract This presentation delves into the innovative digital solutions implemented by Halliburton to cater to contemporary business challenges. Recognizing the issues posed by an aging and novice workforce, Halliburton has introduced automation for equipment control while streamlining resource management. Emphasis has also been placed on fostering diverse, collaborative teams to enhance synergy and drive results. A pivotal part of the initiative includes the launch of an efficient software development program, and building a infrastructure to incorporate Machine Learning (ML) and Artificial Intelligence (AI). Through these strategic measures, Halliburton demonstrates its commitment to leveraging technology to optimize business operations and prepare for future advancements.

Plenary Speaker 3

Building Confidence in Grid Optimization:
A Step-by-Step Guide to Incorporating Advanced Intelligence into Electric Grid Planning

Chase Lansdale

Engineer and Director of Product Marketing

ENER-i.AI / Electric Power Engineers

09/28/23, 11:15 - 11:45 am
Gates Ballroom (MSC)

A professional engineer by trade, Chase Lansdale helps develop next-generation electrical engineering features and oversees integrations of his company's cloud-based technologies across the electric power industry.

Prior to the formation of ENER-i.AI, Chase worked as a consulting engineer for ENER-i's sister company, Electric Power Engineers, where he worked in a myriad of departments from siting and designing renewable generation to optimizing transmission and distribution power grids.

Throughout his career, Chase has worked with hundreds of generation developers and utilities alike with the aim of enabling a clean and reliable energy future.

Plenary Speaker 3

Building Confidence in Grid Optimization: A Step-by-Step Guide to Incorporating Advanced Intelligence into Electric Grid Planning

Abstract The transition to a sustainable and efficient energy landscape hinges not just on the inception of advanced solutions, but on their practical and confident implementation. Planning engineers, central to this evolution, often grapple with the intricacies of embedding grid optimizations into their workflows. Addressing this challenge, this talk delineates a systematic progression:

1. Modeling the Possibilities: Using advanced software to simulate grid scenarios, predict outcomes, and discern potential efficiency benefits, thereby presenting a preliminary vision of what's attainable.
2. Hardware-in-the-Loop (HIL) Testing: Moving from digital-only models to real-time tests that merge software simulations with physical hardware. This crucial step verifies software predictions, giving a tangible touchpoint of the benefits without full-scale field deployment.
3. Operational Field Proofs: Graduating to on-ground, real-world tests, this phase evaluates the software's recommendations in actual grid environments. It offers invaluable insights into any necessary refinements and potential pitfalls.
4. Integration into Planning Processes: Armed with robust data from the first three steps, planning engineers can seamlessly incorporate the software solutions into their regular planning routines. This final transition is where we harness the full potential of grid optimizations, realizing significant cost savings and efficiency enhancements.

By demystifying the progression from modeling to real-world implementation, this presentation aims to instill confidence in planning engineers. Let's navigate the journey of reshaping power distribution, capitalizing on the untapped savings of advanced grid optimizations.

Plenary Speaker 4

Decarbonization by Electrification

Jeremy Pearce

Industrial Electrification Technology Program Manager

Shell

09/29/23, 09:00 - 09:30 am
MSC Room 2401

Jeremy Pearce started his career with Shell at the Bellaire Technology Center as a Research Scientist developing novel well logging and fiber-optic surveillance technologies.

He joined the Unconventionals organization in 2012 and has held a variety of technical and business roles including as an Asset Petrophysicist in Permian, Business Advisor, Commercial Continuous Improvement Lead, and Business Planning Manager in Appalachia.

In 2019, he returned to PTX and served as the General Manager of Shales Technology maturing and deploying technologies to deliver substantial value to the Unconventionals business. Jeremy is a part of the newly formed Power Technology organization leading the Electrification of Demand Technology Program, which is a multi-year program developing technologies to decarbonize industrial sites through electrification.

Jeremy holds a B.S. in Computer Engineering from Texas A&M University, M.S. & Ph.D. in Electrical Engineering from Rice University, and an M.B.A. from Rice University.

Abstract Industries currently account for a significant portion of global energy demand, largely reliant on fossil fuels. However, a seismic shift is on the horizon as electricity is poised to become the dominant energy source within the next two decades, aligning with decarbonization efforts. Electrification, alongside hydrogen and carbon capture use and storage, plays a central role in this transition. Despite this promise, critical technological challenges hinder the widespread adoption of variable renewable energy (VRE) in industry, including process electrification, flexibility management for VRE variability, and reliable VRE access. Shell has launched a technology program focused on power technologies and Electrification of Demand (EoD) to address these challenges. In this presentation, we explore these key technological areas and their significance in electrifying industry.

Panel Discussion

Smart Technologies and Energy Efficiency:
Leveraging Digitalization to Optimize Resource Utilization

09/28/23, 01:00 - 02:00 pm, Gates Ballroom (MSC)

In the wake of the 21st century, we find ourselves at the intersection of technological innovation and the pressing need for sustainable resource management. Energy, a vital pillar of modern civilization, has transitioned from a commercial commodity to a strategic asset that underpins our societies. Historically, conventional energy sources, primarily petroleum and its derivatives, have been the lifeblood of our global infrastructure, powering the engines of economic growth and technological advancement. However, the challenges posed by conventional energy sources are twofold.

First, their finite nature forces us to confront the inevitable exhaustion of these resources. Second, the relentless exploitation of conventional energy gave rise to an environmental crisis, characterized by pollution and climate change. In reaction to these challenges and many more, the responsibility of guiding society towards a cleaner and more sustainable energy future lies with those entrusted with knowledge and innovation, including engineers and technologists, to list a few.

As we enter the era of smart technologies and energy efficiency, digitalization emerges as a powerful catalyst for change. In our quest for greener and more efficient energy solutions, we must harness the potential of digital technologies to optimize resource utilization. This transition requires a comprehensive re-evaluation of our energy infrastructure, from production and distribution to consumption. By integrating intelligent systems, data analytics, and automation, we can unlock the full potential of our energy resources while minimizing waste and environmental impact. Smart technologies offer unprecedented opportunities for real-time monitoring and control of energy systems, enabling us to respond proactively to fluctuations in supply and demand. Moreover, digitalization facilitates the seamless integration of renewable energy sources, such as solar and wind, into our existing grids, ensuring a reliable and sustainable energy supply. Energy efficiency becomes more than a goal; it becomes a fundamental principle driving our energy landscape.

As we navigate this transition, we must ensure a smooth and equitable distribution of the benefits of digitalization and energy efficiency. Thus, our mission as engineers and innovators is clear: to bridge the gap between conventional and renewable energy sources by leveraging smart technologies to optimize resource utilization. In doing so, we will not only secure the energy needs of the present but also pave the way for a more sustainable and prosperous future for generations to come.

Panelists

Panelist I. Chase Lansdale

Engineer and Director of Product Marketing

ENER-i.AI / Electric Power Engineers

A professional engineer by trade, Chase Lansdale helps develop next-generation electrical engineering features and oversees integrations of his company's cloud-based technologies across the electric power industry.

Prior to the formation of ENER-i.AI, Chase worked as a consulting engineer for ENER-i's sister company, Electric Power Engineers, where he worked in a myriad of departments from siting and designing renewable generation to optimizing transmission and distribution power grids.

Throughout his career, Chase has worked with hundreds of generation developers and utilities alike with the aim of enabling a clean and reliable energy future.

Panelist II. Evan Johnson

Vice President of Energy Transition Solutions

Nabors Industries

Evan Johnson is the Vice President of Energy Transition Solutions. In this role, he leads the R&D team, driving the innovation of and development for all graphene production and new graphene applications. His 15+ years of executive experience in alternative energy has led to over 25 patents.

Panelist III. Satya Amaran

R&D Leader, Operations Research

Dow Chemical

Satya is an R&D Leader in the Machine Learning, Optimization, and Statistics (MiLOS) team at Dow. His passion lies in unlocking degrees of freedom and integrating decision silos through systems thinking. He plays a key role in Dow's digital and analytics journey in the identification of opportunities, technology transfer from external collaborations, nurturing of talent, and the incorporation of optimization/AI in work processes.

During his PhD at CMU, he worked on optimization under uncertainty and applications to the chemical industry. He has authored/co-authored 15 refereed papers, 1 book chapter, and 25+ invited conference presentations.

Panelists

Panelist IV. Karen L. Butler-Purry

Professor, Electrical and Computer Engineering

Texas A&M University

Dr. Karen L. Butler-Purry was awarded a B.S. (summa cum laude) from Southern University in Baton Rouge, a M.S. degree from the University of Texas at Austin, and a Ph.D. from Howard University in Washington, D.C., all in Electrical Engineering.

During her over 25 years at Texas A&M University, Dr. Butler-Purry has vast experiences as an administrator and program leader at Texas A&M. Dr. Butler-Purry's research interests are in the areas of modeling and simulation, protection and control of electric power distribution systems and isolated power systems such as all electric power systems for ships, smart grids, and power microgrids, cybersecurity protection, intelligent systems for power system equipment deterioration and fault diagnosis, and engineering education. She received the National Science Foundation Faculty Career Award (1995) and the Office of Naval Research Young Investigator Award (1999).

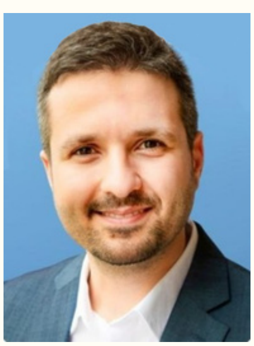
Panelist V. David E. Claridge

Professor, J. Mike Walker '66 Department of Mechanical Engineering

Texas A&M University

Dr. Claridge is internationally known for his work over the last 20 years directing the development and participating in the implementation of the Continuous Commissioning® process for improving the comfort and energy efficiency of buildings. He has made major contributions to the analysis of heat transfer between buildings and ground and to the analysis of air leakage in buildings.

Dr. Claridge has over 400 publications, including technical journals, books, book chapters, and conference publications, including over 100 dealing with monitoring of buildings, analysis of monitored building data, or building diagnostics. He is also an author of well over 100 reports and holds 12 patents. His professional services include serving as President of the ASHRAE College of Fellows, Deputy Editor of the International Journal of Energy Research, Editorial Board of the Journal of Building Performance and Simulation.



Moderator. Bassel Daher

Research Scientist

Texas A&M Energy Institute

Bassel Daher is a Research Scientist at Texas A&M Energy Institute with more than 12 years of experience developing policy-oriented research geared toward guiding evidence-based decision making for water-energy-food system transformation, as evidenced by more than 55 publications covering case studies based in the United States, Lebanon, Qatar, Turkey, Jordan, Morocco, and Bangladesh. Daher is also dedicated to improving Water-Energy-Food nexus governance and facilitating the localization and implementation of the Sustainable Development Goals through community engaged participatory approaches. Daher is also a Research Fellow at the Institute for Science Technology and Public Policy and Adjunct Assistant Professor at the Department of Biological and Agricultural Engineering.

Oral Presentations 1

Oral Session Morning Session
MSC 2500, 2501, 2502, 2503

Thursday
September 28

	Energy Driven Policy (MSC 2500)	Safety & Resilience in Energy Systems (MSC 2501)	Multi-Scale Energy Systems Engineering (MSC 2502)	Multi-Functional Materials A (MSC 2503)
9:00 am – 9:15 am	Optimal Investment Policy in Sharing and Standalone Economy for Solar PV Panel under Operational Cost *Subhojit Biswas*	A Model for Fortifying Distribution Network Nodes Subject to Disruptions *Pelin Kesrit*	Energiapy - An Open Source Python Package for Multiscale Modeling & Optimization of Energy Systems *Rahul Kakodkar*	Optimizing the Reactivity of Ti_2N MXene Through Decoupling Surface and Bulk Structure and Phenomena *Ray Yoo*
9:15 am – 9:30 am	Distributed energy resources as means to manage organizational environment: A resource dependence theory perspective *Aaron Heinrich*	How to benchmark the safety of different types of lithium-ion batteries? *Sankhadeep Sarkar*	Multiscale simulations enabling rational design for the next-gen battery materials *Dacheng Kuai*	The influence of CNT fillers and silanization on mechanical properties of ceramic composites *Laxmi Sai Viswanadha*
9:30 am – 9:45 am	Geospatial Trends in Emissions Reduction Capability of Future All-Electric Aircraft *Jacob Eaton*	Experimental and Kinetics Modeling Study of Tri-Methyl-Phosphate Pyrolysis: Toward P-Containing Fire Suppressants for Lithium-Ion Battery Electrolytes *Claire Gregoire*	Multi-Scale Energy Analysis of Micro-Channel Heat Sink in a Datacom Facility *Amin Isazadeh*	Nanowire-Assisted Photocatalysis for Water Remediation *Bhupesh Pydiraju Yanda*
9:45 am – 10:00 am	Green Transportation in Texas with Electric and Hydrogen Fuel Cell Cars *Hongbo Du*	Location-allocation optimization for EV infrastructure planning: Computational challenges and advances *Benjamin Auer*	A framework for the combined evaluation of economic and CO_2 fixation feasibility of Carbon Capture and Utilization (CCU) reaction pathways *Gasim Ibrahim*	Electrochemical properties of diglyme based structural battery electrolytes for low temperature applications. *Sayyam Sawant Deshpande*
10:00 am – 10:15 am	A mechanism to account for locational carbon impact in electricity market *Subir Majumder*	A Systematic Methodology for Resilience Analysis of Energy Systems *Natasha Jane Chrisandina*	Advancing Grid Infrastructure: A Machine Learning-Driven Prediction and Optimization Approach *Harsh Birenkumar Shah*	Intermediate Transfer Rates and Solid-State Ion Exchange are Key Factors Determining the Bifunctionality of a Tandem CO_2 Hydrogenation Catalyst *Fatima Mahnaz*
10:15 am – 10:30 am	Multiphase Pumping: A Transformative Approach Towards Methane Emissions Reduction and Production Optimization in Oil&Gas Fields *Mohamed Gamal* *Mohamed Abdalla*		Probabilistic Considerations of Equipment Availability for Multi-Scale System Optimization *Marcello Di Martino*	Surface Terminations of Ti_4N_3 MXene and their Effect on HER/ORR Reactivity *Eugenie Pranada*

Oral Presentations 2

Oral Session Afternoon Session
MSC 2500, 2501, 2502, 2503

Thursday
September 28

	Energy Savings (MSC 2500)	Sustainability (MSC 2501)	Data Science & Statistical Learning (MSC 2502)	Multi-Functional Materials B (MSC 2503)
3:00 pm – 3:15 pm	Impacts and Methodology of Outside Air Temperature based Supply Air Temperature Reset Luke Madden	Biogas Production from Solid-State Anaerobic Digestion of Poultry Waste Faryal Fatima	Rapid Forecasting of CO_2 Plume Migration in Varied Geological and Engineering Scenarios Utilizing Transfer Learning Yusuf Falola	Multifunctional Shape Memory Polymer Composites (SMPCs): Bottom-up Design of Next-Generation Adaptive Materials Jitendra Choudhary
3:15 pm – 3:30 pm	Multi-period optimization of heat integration for chemical plant electrification with thermal energy storage Mengdi Li	Numerical Study on Motion Effects of Floating Offshore Wind Turbines Haidong Lu	Physics-informed Neural Networks on High-Dimensional Partial Differential Equations David Rodriguez Sanchez	Freeform additive manufacturing of carbon fiber reinforced composites using dielectric barrier discharge-assisted Joule heating Smita Shivraj Dasari
3:30 pm – 3:45 pm	Development and Analysis of Novel Chiller Modeling Strategies for a More Cost-friendly Process for Determining Energy Savings from Chiller Retrofit Measures Martin Ssembatya	A Modified Overset Method in OpenFOAM for Simultaneous Motion and Deformation: A Case Study of a Flexible Flapping Foil hydrokinetic turbine Ahmed A. Hamada	Detecting anomalous motions in the Shell-polishing process using sensor fusion and Machine Learning Shashank Galla	Effects of Aluminum Foam on Boiling Heat Transfer for Thermosyphon Evaporator Digvijaysinh Barad
3:45 pm – 4:00 pm	Effect of surfactant on polymer flooding with and without shear-thinning polymer in chemical enhanced oil recovery Carlos Acosta	Comparing Numerical Methods for the Hydrodynamic Analysis of Floating Offshore Wind Turbines Lubna Margha	Optimal Performance Objectives in a Conserved Cell-Cell Signaling Pathway Razeen Shaikh	In-Situ Spectroelectrochemistry to Unveil the Mechanism of Green Ammonia Production on the Ti_2N Nitride MXene Denis Johnson
4:00 pm – 4:15 pm	Intelligent Compressed Air Storage System for Intermittent Demand of Compressed Air Taeksoo Kim	Process Design Of Green Hydrogen Production Systems From Offshore Wind Energy Vy Nhat Le	Intersection of Data Science and Stats with Nuclear Energy Policies Shaina Nair	Investigation into the Reaction Pathways and Catalyst Deactivation for Polyethylene Hydrogenolysis over Silica-Supported Cobalt Catalysts Ryan Helmer
4:15 pm – 4:30 pm	Impact of Entrained Air on Chilled Water/Hot Water System Performance Di Lu	Photocatalytic Integrated Design for Hydrogen Production with Combined Solar and LED Light Sources Ahmed Abbas	Numerical Investigation of Surface Tension Effects on Transcritical Liquid Breakup in High-Pressure Supercritical Propulsion Systems Prajesh Jangale	Structural and Fast-Charging Organic Battery Cathodes Based on Redox-Active Polymers and Carbon Fiber Fabric Suyash Oka

Oral Session 1: Abstracts

I. ENERGY DRIVEN POLICY

1. Optimal Investment Policy in Sharing and Standalone Economy for Solar PV Panel under Operational Cost

Subhojit Biswas[1]

1. *Wm Micheal Barnes '64 Department of Industrial and Systems Engineering, Texas A&M University, College Station, TX 77843, USA.*

Corresponding author: subhojit.biswas@tamu.edu

The transition to sustainable energy sources, driven by the need to address climate change and resource depletion, has led to the increasing adoption of solar PV panels. These panels align with various Sustainable Development Goals (SDGs) by providing clean and affordable energy, promoting climate action, and supporting sustainable communities. Solar PV panels face challenges despite their advantages, including susceptibility to natural disruptions like hurricanes, hailstorms, and extreme temperatures. The research explores the viability of a sharing economy business model that allows multiple participants to collectively invest in solar PV systems and share the benefits to ensure the future expansion of solar PV installations. The study formulates the problem as a game theory model to strategize and find optimal solutions for both the standalone economy and sharing economy scenarios, considering operational costs, net metering, and the unpredictability of natural disasters. By providing valuable insights into the dynamics of the PV market with the help of computational results, the research aims to enhance the resilience of solar installations and promote sustainable energy practices. Through this work, individuals and communities can make informed investment decisions, contributing to a cleaner, greener, and more sustainable world.

Oral Session 1: Abstracts

I. ENERGY DRIVEN POLICY

2. Distributed energy resources as means to manage organizational environment

Aaron D. Heinrich[1], *Trevor S. Hale*[1 3], *Jennifer J. Blackhurst*[2], *William W. Anderson Jr.*[3]

1. *Information and Operations Management Department, Texas A&M University, College Station, Texas, 77845*
2. *Business Analytics Department, University of Iowa, Iowa City, IA 52242*
3. *Naval Facilities Engineering Systems Command, Naval Base Ventura County, Port Hueneme, CA 93043*

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As the electric bills of residential, commercial, and industrial sector consumers continue to rise, managers of businesses operating in these sectors have vested interested in mitigating the resultant, erosive effect to their bottom lines. Since the advent of behind-the-meter distributed energy resources (DERs), researchers have developed various strategies aimed at leveraging such resources as means to not only reduce electric bills, but also drive them negative, viz., arbitrage. We present a framework through which we describe the as-is and to-be electric grids to do just that. We also delineate a nonlinear program for consumers.

Keywords: Distributed energy resources (DERs), energy storage, energy arbitrage

Oral Session 1: Abstracts

I. ENERGY DRIVEN POLICY

3. Geospatial Trends in Emissions Reduction Capability of Future All-Electric Aircraft

Jacob Eaton[1], Mohammed Naraghi[1], James.G. Boyd[1]

1. *Department of Aerospace Engineering, Texas A&M University, College Station, Texas.*

Corresponding author: jeaton995@tamu.edu

Greater than 28% of US greenhouse gas (GHG) emissions originated from the transportation sector in 2018. While the emissions footprint of ground-based transportation is projected to decline over upcoming decades, aviation sector emissions conversely are projected to increase by more than 50% by mid-century. Adoption of 'zero-emissions' all-electric aircraft offer one pathway to curtail this growth as they are net-zero emissions during operation. However, their potential impact is directly constrained from a technological perspective by battery specific energy, and indirectly constrained from an emissions perspective by net emissions intensity including indirect, upstream emissions. This work explores the suitability of AEA to operate specific flight routes in the United States, with the intent of identifying geospatial trends in future AEA viability. Early research indicates that substantive (>5%) emissions reductions could be achieved regionally in the United States via adoption of AEA, with exponentially greater emissions reductions resulting from a sustained transition to reduced-emissions-intensity power sources.

Oral Session 1: Abstracts

I. ENERGY DRIVEN POLICY

4. Green Transportation in Texas with Electric and Hydrogen Fuel Cell Cars

Hongbo Du[1], *Sunith B. Madduri*[1], *and Raghava Kommalapati*[1 2]

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Transport consumed about 28% of all energy in the U.S. in 2021, and its emissions strongly influence air quality. On the other side, Texas is the NO.1 generator of renewable energies, including solar and wind power, accounting for one-fourth of the total renewable energies in the U.S. Green mobility in Texas targets to reduce air pollution from transport and to address climate change through mitigation and adaptation of modern vehicle technologies, such as hybrid powertrain, vehicle electrification, and fuel cell. Our research addressed this critical gap and developed environmental impacts and cost assessments for hybrid gasoline cars, battery electric cars, and hydrogen fuel cell cars in Texas under several possible energy scenarios from 2022 to 2040 using some lifecycle assessment tools and lifecycle cost analysis. The carbon footprint of battery electric cars and hydrogen fuel cell cars was determined with respect to the transport, logistics, and supply chain sectors for two major components: Vehicles and Fuels/power such as gasoline, electricity, and hydrogen. Greenhouse gas (GHG) emissions of hydrogen fuel cell cars powered by green hydrogen are lower than those of conventional passenger cars. The emissions associated with hydrogen production via the current electricity mix are higher than those of traditional cars. The emissions are significantly lower when hydrogen is produced via biomass pyrolysis, and water electrolysis driven by solar or wind power electricity. Hydrogen production cost varies with respect to many factors, and it varies between $2.6 - $6.0 via different production technologies, such as water electrolysis, biomass gasification, and biomass dark fermentation.

Keywords: Electric car; hydrogen fuel cell car; greenhouse gas emissions; lifecycle cost

Oral Session 1: Abstracts

I. ENERGY DRIVEN POLICY

5. A mechanism to account for locational carbon impact in electricity markets

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There are several challenges in existing mechanisms to recover the cost of carbons in the electricity market. For example, carbon pass-through incentivizes reduction in energy use, with challenges in terms of social equity. Both costs of carbon and energy are embedded in the cap & trade mechanism, resulting in difficulties in monitoring electricity prices and tracking the locational aspects of carbon emissions. The proposed method solves both challenges by considering coupled power and carbon flow markets. The power flow model could be utilized for calculating electricity transport, and the atmospheric dispersion model to track carbon flow. The participants in the energy market can now participate in the carbon market with their cost to not inject carbon into the environment, and the customers can bid their willingness to pay for reduced carbon available at their premises. Here, we assume the presence of an external entity that generates the demand function based on the social cost of carbon and regulation standards. This mechanism would provide an additional mechanism to recover the cost of infra-marginal renewable resources. Instead of subsidizing renewable energy producers, marginalized communities could be directly subsidized regarding their carbon costs. Therefore, this mechanism is Environmental, Social, and Governance (ESG) compliant. Given that the scope of market clearing in the electricity market would be limited to individual resource nodes, the granularity for calculating the impacts of carbon on the consumers would be limited to the span of the distribution network within a resource node. This mechanism could be extended to air pollution in general.

Keywords: Climate Change, Electricity Sector, Equity, Market Mechanism

Oral Session 1: Abstracts

I. ENERGY DRIVEN POLICY

6. Multiphase Pumping: A Transformative Approach Towards Methane Emissions Reduction and Production Optimization in Oil & Gas Fields

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The detrimental impact of greenhouse gases on global warming has prompted urgent measures to address methane emissions, a potent greenhouse gas contributing to climate change. Methane gas, with its significantly higher heat-trapping capability compared to carbon dioxide, is a major environmental concern and its emissions reduction efforts are essential to slow the rapid rate of climate change. Oil and gas production facilities represent a major source of methane emissions; one of such are marginal (stripper) wells. According to the 2023 report by the US EIA, 80% of US oil and gas wells are marginal wells representing approximately 6% of US oil and gas production. Surprisingly, these wells represent disproportionately large sources of methane emissions, emitting nearly 1.5 times the methane emissions from Permian Basin, which contributes to 44% of US oil production.

This study explores the techno-economic analysis of using multiphase pumping technology to eliminate flaring and methane emissions. Multiphase pumping (MPP) not only boosts total production from the field to a central processing facility, whether located onshore, offshore, or through long-distance tiebacks in a single flow stream, but it also lowers wellhead and bottom-hole pressures, enhancing liquid inflow from the reservoir to the wellbore. Furthermore, MPP eliminates the need for separators, compressors, and flares. The adoption of multiphase pumping technology to increase production efficiency and reduce emissions; by eliminating gas flaring or venting during production, blow-down operations, and well testing, can lead to additional revenue streams, making it a win-win solution for both the environment and the industry stakeholders.

Keywords: Methane Emissions Reduction, Multiphase Pumping, Production Optimization, US Climate Policy, Techno-Economic Analysis.

Oral Session 1: Abstracts

II. SAFETY & RESILIENCE IN ENERGY SYSTEMS

1. A Model for Fortifying Distribution Network Nodes Subject to Disruptions

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We consider a distribution network for delivering a natural resource or physical good to a set of nodes, each of which serves a set of customers, in which flow disruptions may occur at one or more nodes. Each node receives flow through a path from one or more source nodes, implying that a node experiences a disruption if a disruption occurs at one or more nodes on each path from a source node. All nodes in the network are subject to a future disturbance of an uncertain degree of severity, and we assume we can quantify the degree of severity, and that it follows some well-defined probability distribution. For each node in the network, we wish to determine a fortification level that enables the node to withstand a disturbance up to some level of severity. The cost of fortification is nondecreasing in the maximum-severity fortification level chosen, and we wish to maximize the expected number of customers who do not experience a disruption following the occurrence of a disturbance, given a limited fortification budget. We formulate this problem as a mathematical program, characterize useful properties of optimal solutions, and provide methods for determining optimal fortification levels under various assumptions on the probability distribution of the disturbance severity and the network structure.

Keywords: Power network, fortification

Oral Session 1: Abstracts

II. SAFETY & RESILIENCE IN ENERGY SYSTEMS

2. How to benchmark the safety of lithium-ion batteries?

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The wide acceptability of lithium-ion batteries (LIB) is hinged upon safety, energy, and economics. Given the different types of batteries existing today, generally defined by the cathode type (namely Lithium iron phosphate, Lithium Cobalt Oxide, Lithium Nickel Manganese Cobalt Oxide). Though a lot of research studies have focused on the energy density and power density for different applications, limited studies have focused on characterizing different types of lithium-ion batteries in terms of safety and its influence on economics.

Thus, this study shows the technique and identifies indicators (e.g., self-heating rate) needed to benchmark battery safety based on design and operating conditions. LIB safety is influenced by several operating conditions (e.g., lower temperature leads to lithium metal formation which may lead to dendrite formation with time) and battery's material properties, including electrode, electrolyte and separator (e.g., heating release rate, ignition time). All these factors are collated and interconnected to provide battery reliability given there are uncertainties in design or operation variables.

Keywords: battery, safety, benchmarking, quantification.

Oral Session 1: Abstracts

II. SAFETY & RESILIENCE IN ENERGY SYSTEMS

3. Experimental and Kinetics Modeling Study of Tri-Methyl-Phosphate Pyrolysis: Toward P-Containing Fire Suppressants for Lithium-Ion Battery Electrolytes

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The highly flammable electrolytes in lithium-ion batteries (LIBs) have been the source of numerous and significant fire incidents due to various factors such as a default in the conception of the battery or operational abuse. While halogenated options have been widely used for many years, their implication in the tropospheric ozone layer destruction led to their banishment, driving the need for replacement. For instance, MacDonald et al. showed that phosphorus compounds demonstrated a two-to-four times higher suppressant effect than CF_3Br. Phosphorus-containing combustion intermediates enable catalytic quenching mechanisms of combustion radicals that promote flame extinction Tri-methyl-phosphate (TMP) is a candidate fire suppressant, which could possibly allow for an integration in the electrolyte without excessive degradation of the battery performance. The aim of this study is to provide new experimental data to further validate the only TMP detailed chemical kinetics mechanism available in the literature. Pyrolysis experiments were performed using a shock tube to measure CO time histories via laser absorption with temperatures ranging from 1433 to 1695 K near 1.3 atm. These new sets of data provide valuable targets to improve the performance of the model, which is not able to reproduce the experimental results with high accuracy. While more work is needed to refine the predictions, reaction analyses for CO formation showed that the main TMP pyrolysis reaction pathway ($PO[OMe]_3$ in the model) can be identified as $PO[OMe]_3 \rightarrow PO[OMe]_2[OCH_2] \rightarrow CH_2O \rightarrow HCO \rightarrow CO$.

Keywords: Fire Suppressant; Battery; Shock Tube, CO Time History; Kinetics Modeling

Oral Session 1: Abstracts

II. SAFETY & RESILIENCE IN ENERGY SYSTEMS

4. Location-Allocation Optimization for EV Infrastructure Planning: Computational challenges and advances

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Electric vehicle (EV) share is expected to increase, thus corresponding to an increase in charging demand. Thus, there is a marginal utility of EV infrastructure allocation and its location, that will serve a future demand in an optimal way, known as the EV infrastructure planning problem. One major challenge in solving this problem is its inherent uncertainty due to different growth models of EV technology adaptation. Therefore, defining where to place charging infrastructure and of which capacity for a forecasted demand is a delicate step to solve the overall problem. Such an EV infrastructure planning problem can be modeled as a multi-stage stochastic location-allocation optimization problem, typically rendered as large-scale mixed-integer linear programming (MILP) problem, the solution of which yet poses another major challenge. Due to the MILP's computational complexity, it might not successfully be incorporated in the main problem's solution approach. Thus, it is desired to reformulate the problem into an approximation that is easier to solve by relaxing the integrality constraints, yielding a linear programming (LP) problem. The difference between the MILP's and the LP's solution is known as the integrality gap. It does not explicitly provide insight in how changes in integer variables influence optimal decision making, e. g. trigger different demand-supply matching or alter infrastructure allocation, leading to potentially false conclusions when trusting the relaxation. Thus, we propose a quantification of the relaxation error that does not only incorporate the objective function value but also the decision variables, rendering the effect of relaxation onto the integer variables visible. Also, this error can be carefully incorporated in bespoke branch-and-bound search algorithms.

Keywords: Location-Allocation Optimization, Planning Problem, Integrality Gap, Relaxation, Mixed-Integer Linear Programming

II. SAFETY & RESILIENCE IN ENERGY SYSTEMS

5. A Systematic Methodology for Resilience Analysis of Energy Systems

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Disruptions to the energy sector have increased in both frequency and impact, causing massive losses of life and livelihood. It is critical that energy systems are designed to withstand unforeseen disturbances to ensure a steady and reliable energy supply in the long-term. However, the upfront investment required to design resilient energy systems can be prohibitive, and the return on this investment can be uncertain because future disruptions are often unforeseen in both timing and impact ("unknown-unknown" disruptions). Therefore, a systematic methodology for analyzing potential future scenarios and the impact of various design decisions on post-disruption system behavior is needed.

In this work, we expand upon the existing multiscale framework for energy system design by conducting a resilience assessment on the system to identify the decision variables on the supply chain and process levels that have the greatest impact on system performance during disruption and recovery. Using the key decision variables identified in this step, a surrogate model of the process can be introduced to provide more insights into individual node and arc behaviors and their interplay with the supply chain at large. Constructing surrogate models around the key decision variables allows for an accurate but computationally efficient representation of supply chain components. A mixed-integer non-linear programming (MINLP) model is then constructed to obtain the optimal supply chain network design with consideration of process design and operations. The proposed methodology can inform simultaneous process and supply chain design while balancing current economic investment with expected future performance. To illustrate the methodology, we present a case study on a distributed biomass value chain for small-scale energy carrier production.

Oral Session 1: Abstracts

III. MULTISCALE ENERGY SYSTEMS ENGINEERING

1. Energiapy - An Open Source Python Package for Multiscale Modeling & Optimization of Energy Systems

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The energy transition poses formidable challenges, such as a plethora of technology and resource options, renewable intermittency, uncertainty of future scenarios, a dearth of materials to establish technology pathways, resiliency to disruptions, the accounting of carbon emissions over the life cycle of technology use, interaction and competition with vital chains such as food and water. Tools that support data-driven decision making are essential to achieve net-carbon neutrality over the coming decades. To this end, numerous energy systems modeling frameworks have been developed utilizing disparate architectures and programming languages such as AMPL, Python, Julia, etc. Here, we present energiapy, a decisions making and risk analysis tool for the design and optimization of energy systems. The novelty of energiapy lies in the highly configurable system agnostic component-based approach. Notably, formulations can span from the level of individual processes to networks spanning multiple regions. The object-oriented approach allows deterministic factors to be assigned at the appropriate level, viz. localization factors at the location level, and process parameters at the process level. The components involved follow a suggested hierarchy which allows the formulation of models ranging from multi-scale mixed integer programs (MIPs) to multi-parametric, and robust stochastic programs. This lends significant flexibility to the user in both developing network models, as well as the scenarios over which these models are tested. Moreover, scenarios can also be aggregated and solved over a set of representative temporal periods, used to generate graphs for network analysis, and both the data input and solutions can be visualized. These developments are demonstrated over a detailed hydrogen economy case study which is solved through different approaches. First as a deterministic mixed integer linear program (MILP), then as a multi-parametric linear program (mpLP), and then as its robust equivalent. The key applications illustrated in the study include: 1) the design of future energy systems (network design), 2) scheduling under uncertainty, 3) life-cycle and environmental impact assessment, 4) techno-economic analysis, 4) system resiliency and reliability characterization.

Oral Session 1: Abstracts

III. MULTISCALE ENERGY SYSTEMS ENGINEERING

2. Multiscale simulations enabling rational design for the next-gen battery materials

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After decades of innovation and development, state-of-the-art lithium-ion batteries (LIBs) are approaching their theoretical energy density. Meanwhile, the worldwide sustainable energy transformation brings ever-growing demands for advanced energy storage devices. Lithium metal batteries (LMBs), which directly apply lithium metal as the major anode material without graphene, shed light on breaking the specific capacity bottleneck. Upon contacting, the electrolyte and anode materials react during the fabrication and generate a dense layer on anode, namely solid electrolyte interphase (SEI) which keeps evolving during battery operation. SEI protects cell materials from further degradation and regulates the lithium-ion deposition and dissolution, which is the key to safe and efficient battery performance. Aimed at rationally designing the battery materials, we present a multiscale simulation framework for elucidating the SEI formation mechanisms near the LMB anode surface. To resolve the complex electrochemistry in forming SEI based on limited experimental evidence, we studied the plausible electrolyte degradation and polymerization pathways based on atomistic simulations. The ultra-fast decomposition reactions of the classical electrolyte components including ethylene carbonate (EC), vinylene carbonate (VC), and lithium hexafluorophosphate (LiPF6), were emulated in ab initio molecular dynamics (AIMD). The corresponding thermodynamic profiles were determined at a higher level of density-functional theory (DFT). Polymerization pathways of EC and VC were also systematically evaluated for the foundation of kinetic Monte Carlo (kMC) simulations. The determined reaction network together with the quantified thermochemistry was integrated into the coarse-grained scale kMC model. After accumulating the sub-nanosecond events to the second-level timescale, we obtained the evolution of SEI morphology under various reaction environments. With the substantial SEI configurations, we can further elaborate with a series of follow-up studies such as ionic diffusion and mechanical property predictions. This framework not only bridges atomistic and continuum scale simulations, but also brings bottom-up electrolyte tuning into possibility.

Keywords: multiscale simulation, density-functional theory, kinetic Monte Carlo, lithium metal battery

III. MULTISCALE ENERGY SYSTEMS ENGINEERING

3. Multi-Scale Energy Analysis of Micro-Channel Heat Sink in a Datacom Facility

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Datacom infrastructures operate on multiple scales, ranging from individual chips to entire data centers. Efficient thermal management systems must be designed considering these different scales. However, the thermal performance at one scale can significantly impact the performance of others due to their interdependence. Moreover, the increasing prevalence of high-performance CPUs generating heat at rates exceeding 100 W/cm² has rendered air-cooled systems impractical and expensive, as they possess a limited heat removal capacity of less than 50 W/cm².

To address these challenges, liquid-cooled systems with superior heat removal capacity, which offer numerous advantages such as environmental friendliness, scalability, and high precision can be utilized. This study investigates the energy impact of an advanced liquid-cooled micro-channel heat sink, used for dissipating heat from a 10-cm2 electronic chip, across various scales of a data center including chip, server, and rack levels. Both single-phase and two-phase cooling systems are numerically analyzed under different operating conditions, including coolant type with low global warming and ozone depletion potentials, flow rate, micro-structured surface enhancements like microcavities, and heat flux.

The research encompasses a multi-scale energy analysis of the liquid-cooled system, with a focus on evaluating flow performance and thermal performance. Parameters such as surface temperature, coolant-to-chip thermal resistance, inlet-to-outlet differential pressure, channel-wise pressure oscillation, and temperature stability within the micro-channels are assessed. Through extensive analysis, it was observed that liquid-cooled micro-channels not only significantly reduce the overall energy usage and carbon footprint of a data center facility, but that the thermal resistivity of such heat sinks can be less than 0.1 K/W/cm², which is less than half the thermal resistance of conventional heat sinks.

By adopting liquid-cooled micro-channel heat sinks, data centers can effectively mitigate thermal challenges associated with high-performance CPUs, and enhance energy efficiency, paving the way for sustainable and environmentally responsible data center operations.

Keywords: Data center, micro-channel heat sink, multi-scale energy analysis

Oral Session 1: Abstracts

III. MULTISCALE ENERGY SYSTEMS ENGINEERING

4. GASEF: A Framework for the Combination Evaluation of Economics and CO_2 Fixation Potential of CCU Pathways

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This presentation will highlight a novel framework for early-stage assessment of CCU reaction technologies. The greenhouse gas abatement, economics, and sustainability framework (GASEF) assesses commercial viability by analyzing a CCU technology's economic and CO_2 fixation potential. The framework is then used to discuss the possible implications of providing CO_2 subsidies for CCU processes based on the total amount of CO_2 fed, versus providing CO_2 subsidies based on the net CO2 fixation of the process. The developed framework utilizes the CO2Fix parameter and the metric for inspecting sales and reactants (MISR) to estimate CO_2 fixation and economic potentials. Both metrics can be estimated using limited information obtained from the stoichiometry of the CCU reaction. Two case studies are presented to demonstrate the framework, representing two standard CCU technologies: the dry reforming of methane and CO_2 hydrogenation to methanol. The dry reforming of methane was found to have the potential for commercial viability even when the technology includes financial considerations for carbon capture and sequestration efforts to achieve a net-zero process. The CO_2 hydrogenation to methanol process was also found to have the potential for commercial viability; however, at low values of CO_2 credit (0.05 $/kg$CO_2$), the commercial viability becomes tenuous.

Keywords: CCUS, CO_2 fixation, modeling, technoeconomic

Oral Session 1: Abstracts

III. MULTISCALE ENERGY SYSTEMS ENGINEERING

5. Advancing Grid Infrastructure: A Machine Learning-Driven Prediction and Optimization Approach

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The effective integration of renewable sources into the energy mix is essential towards achieving sustainable energy goals, especially the decarbonization of the energy grid. Nevertheless, the inherent variability of renewables, such as solar and wind, presents significant challenges to grid stability. Energy storage while offering a modest solution, can be expensive. Moreover, the materials required in some dynamic energy storage technologies have a high environmental impact. Decision makers can benefit from insight into future energy markets, e.g. better risk management, informed investment, robust energy policy formulation, energy trading, etc. Energy systems designed with awareness to the underlying dynamics with respect to weather patterns, technology costs, and resource availability can be resilient to future demand surges, resource limitations, while also minimizing cost and limiting the need for additional infrastructure. To this end, we present a comprehensive framework to posit energy transition scenarios based on forecasted parameters. The framework leverages advanced predictive models, such a Long Short-Term Memory (LSTM), to predict parameters such as cost and resource availability. The energy system itself is modelled as a multiscale mixed integer program using the energiapy python package. Scenarios can be tested to maximize storage utilization, minimize cost, and maximize power production. Further, the trade-offs between competing objectives can be determined, as also optimal infrastructure sizing, and storage capacities.

Keywords: Forecasting, Energy transition, Neural networks

Oral Session 1: Abstracts

III. MULTISCALE ENERGY SYSTEMS ENGINEERING

6. Probabilistic Considerations of Equipment Availability for Multi-Scale System Optimization

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In resiliency modeling and optimization studies, the availability of process units represents the likelihood that a process is operational and can recover from failures quickly. This key performance indicator is usually considered via constant reliability metrics such as the mean-time-to-failure (MTTF) and the mean-time-to-recovery (MTTR) of each equipment. It is assumed that the higher the equipment availability, the higher the equipment cost. Then, the cost-optimal process units can be selected by typically solving an optimization problem to minimize cost while satisfying a given process demand. Obtained results, however, are not applicable to real-world processes and supply-chains since the probabilistic nature of the equipment availability is ignored. In turn, this work introduces the equipment availability as a random variable. Based on sampling the distributions of the MTTF and the MTTR, probability distributions for each process equipment cost and the overall process can be obtained as a function of availability. Two sampling strategies are evaluated to consider the uncertain dependency between process availability and cost: (i) The equipment availability is realized and then, based on the obtained value, equipment cost is assigned, and (ii) The equipment availability is realized from three overlapping intervals, representing low-, medium-, and high-cost equipment. Both approaches are evaluated via a Monte-Carlo approach coupled with the optimization model, resulting in cost vs. process availability distributions. It is also shown how this approach can be leveraged to reduce the computational complexity of the original optimization problem.

Keywords: Statistics, Optimization, Resiliency

Oral Session 1: Abstracts

IV. MULTI-FUNCTIONAL MATERIALS (A)

1. Optimizing the Reactivity of Ti_2N MXene Through Decoupling Surface and Bulk Structure and Phenomena

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The continued rise in global energy consumption, along with the associated environmental hazards, pose a significant risk to our society's infrastructure unless the main source is changed. Electrocatalysis involving hydrogen evolution reaction (HER), nitrogen reduction reaction (NRR), and oxygen reduction reaction (ORR), provide a pathway for energy storage and conversion due to their enhanced environmental friendliness and efficient energy input compared to their thermocatalytic counterparts. Currently, the state-of-the-art electrocatalysts suffer from scarcity and high cost. MXenes, a novel family of two-dimensional (2D) transition metal carbide and nitride materials, show potential as cost-efficient and highly abundant electrocatalysts with limited knowledge on their electrocatalytic mechanisms. This is especially true when considering the often-overlooked nitride family of MXenes. Herein, we investigate the electrocatalytic performance of a Ti_2N nitride MXene under different electrolytic mediums. The effect of surface phenomena is investigated through manipulation of the surface passivation layer, as evidenced by Raman and Fourier-transform infrared (FTIR) spectroscopies, scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS). Successful decoupling of the bulk and surface phenomena is achieved through Raman laser power attenuation. Under acidic medium, the surface reactivity towards HER is poor but the bulk reactivity for NRR is favored, making it an optimal NRR catalyst. Under alkaline medium, the surface reactivity of the pristine Ti_2N MXene for ORR is high, but also leads to surface passivation and thus hinders the electrocatalytic activity. Overall, these results provide fundamental insights into future optimization strategies of the Ti_2N nitride MXene, along with other electrocatalysts, towards electrocatalytic applications.

Oral Session 1: Abstracts

IV. MULTI-FUNCTIONAL MATERIALS (A)

2. The influence of CNT fillers and silanization on mechanical properties of ceramic composites

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In this study, the effects of pristine, functionalized (-OH and -COOH) and silanized MWCNTs on polycarbosilane SMP-10 were studied. The interfacial bonding of 3-glycidoxypropyltrimethoxy organosilane with MWCNTs and the extent of functionalization was investigated. EDX results indicated a higher Si% for functionalized CNTs. Zeta potential studies revealed an increased dispersion stability of silane treated CNTs in acidic and neutral pH regions. The ceramic composites were developed using SMP-10 and divinylbenzene as matrix with 3 wt% filler content and exhibited a shrinkage of 30%. The pyrolyzed samples were characterized using SEM and nanoindentation. Composites with CNT fillers exhibited a significant increase in modulus, hardness, and fracture toughness of up to 1.5 x - 2 x than the pristine composites. The improvement in elastic properties due to the addition of CNTs exceeded the predictions of Rule of Mixture, suggesting a considerable change in the morphology of the material as a result of the addition of CNTs. Possible reasons were discussed. These findings hold the promise of advancing material properties of ceramic composites in significant ways, increasing potential for their future applications.

Oral Session 1: Abstracts

IV. MULTI-FUNCTIONAL MATERIALS (A)

3. Nanowire-Assisted Photocatalysis for Water Remediation

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Wastewater remediation is a global issue that is drawing renewed attention due to the rapid increase in water scarcity, pollution of water from both traditional and emerging contaminants. Moreover, water availability is closely related to energy generation. The water-energy nexus is well documented by the Department of Energy (DOE) and indicates that producing energy needs fresh water and producing fresh water needs energy. So, reuse of water requires next-generation remediation techniques, that are energy-efficient and offer the ability to complement techniques employed within the current water treatment trains. One such process, photocatalysis suffers from both technical drawbacks and also poor public perception. For example, as photocatalysis employs light activation of nanostructured semiconductors, process for implementing this in a manner that allows for the safe removal of the semiconductors from water following its remediation will solve both process implementation drawbacks and improve public perception of the process. Our group has been working on such strategies, namely the safe implementation of photocatalysis. In this presentation, benign modes of implementing photocatalysis for removing pathogenic bacteria from water will be discussed in detail. Future direction of these strategies for removing industrial chemicals, such as 'forever chemicals' from water will also be discussed.

Keywords: Wastewater remediation, Photocatalysis, Nanomaterials, semiconductors, Pathogenic bacteria, Forever chemicals

Oral Session 1: Abstracts

IV. MULTI-FUNCTIONAL MATERIALS (A)

4. Diglyme-based structural battery electrolytes produced by polymerization-induced phase separation for low-temperature applications

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Structural batteries have generated significant interest in recent years due to the increasing electrification of the transportation sector. Structural electrolytes are typically composed of a composite material with both efficient ion transport and excellent mechanical strength with light weight. In addition, modern automobiles, aircraft, and spacecraft are required to operate at extremely low temperatures (< -40 ℃). These temperatures are lower than the freezing point of most liquid electrolytes. Further, ion diffusion becomes extremely sluggish at lower temperatures. Liquid electrolytes provide high ionic conductivity but negligible mechanical strength, while solid electrolytes are mechanically robust but have slow ion diffusion kinetics. Bi-continuous electrolytes containing both a solid phase and a liquid phase have previously been created using different phase separation techniques. We have designed a diglyme-based liquid electrolyte having high ionic conductivity of 4.49 x 10-4 S/cm at a temperature of – 40 ℃ and a bicontinuous structural electrolyte containing epoxy and liquid electrolyte capable of operating at a temperature of -40 ℃ with an ionic conductivity of 7.44 x 10-6 S/cm. Furthermore, we show the optimum composition of liquid electrolyte and epoxy in the bi-continuous electrolyte. This optimum corresponds to the trade-off between mechanical strength and ionic conductivity. These results have immediate relevance to the electrification of cars, spacecraft, and aircraft.

IV. MULTI-FUNCTIONAL MATERIALS (A)

5. Intermediate Transfer Rates and Solid-State Ion Exchange are Key Factors Determining the Bifunctionality of a Tandem CO_2 Hydrogenation Catalyst

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Probing the interaction between different active sites and transfer of reaction intermediates in bifunctional catalysts for tandem hydrogenation of CO_2 is crucial for optimal catalyst design that maximizes synergy to achieve high rates and product selectivity. Herein, thermocatalytic conversion of CO_2 to hydrocarbon (HC) via methanol (CH_3OH) intermediate was investigated by modulating the placement of In_2O_3 and HZSM-5 in bifunctional admixtures at temperatures between 350 to 450 °C and 500 psig, to probe the key factors that drive synergy in these bifunctional systems. Analysis of the intermediate CH_3OH transfer rates showed that although a millimeter scale placement of In_2O_3 and HZSM-5 yields a simple tandem reaction with a total HC and methanol CH_3OH space-time yield of $8x10^{-6}$ $mol_c g_{cat}^{-1} min^{-1}$, a microscale placement exhibits a ten-fold increase in catalytic activity with a total HC and CH_3OH space-time yield of $8x10^{-5}$ $mol_c g_{cat}^{-1} min^{-1}$ (at 400 °C) due to a faster transfer rate of intermediate CH_3OH (10× and 100 faster advection and diffusion, respectively). A combination of reactivity, spectroscopy with Raman, X-ray photoelectron spectroscopy (XPS), powder X-ray diffraction (PXRD) patterns, microscopy with scanning electron microscopy (SEM) and transmission electron microscopy (TEM), and control experiments on methanol to hydrocarbons (MTH) revealed that further enhancing the reaction intermediate transfer at a nanoscale placement was counteracted by solid-state ion exchange (SSIE) between Brønsted acid sites (H^+) of the HZSM-5 with the $In^{\delta+}$ ions from In_2O_3, and that the formation of CH_4 at the nanoscale placement occurs through CH_3OH hydrogenolysis and CO_2 methanation. Overall, our data show the interconnected and subtle ways through which the bifunctionality of catalysts could be regulated and pave the way for the development of design principles for designing more effective bifunctional catalysts for tandem CO_2 hydrogenation.

Keywords: C-C coupling, Sustainable Chemistry, Zeolites, Carbon dioxide hydrogenation, Tandem catalysis, Fuels, Methanol route.

Oral Session 1: Abstracts

IV. MULTI-FUNCTIONAL MATERIALS (A)

6. Modulating MXene Surface and Testing its Bifunctional ORR/HER Reactivity

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MXenes, a class of two-dimensional (2D) carbides and nitrides, have been used for many electrochemical reduction reactions owing to their electronic conductivity, specific surface area, and tunable surface chemistry. The performance of MXenes in catalyzing these reactions, specifically the hydrogen evolution reaction (HER) and oxygen reduction reaction (ORR), is heavily dependent on the aforementioned properties, especially the surface chemistry. However, there are limited experimental works that control the surface chemistry of MXenes for these reactions. This work presents the effects of termination group modulation on the HER and ORR activity and electrochemical stability of Ti_4N_3 nitride MXene in an alkaline medium. The Ti_4N_3 MXene was synthesized via molten salt etching and delaminated using tetramethylammonium hydroxide (TMAOH), dimethyl sulfoxide (DMSO), water (H_2O), or tetrabutylammonium hydroxide (TBAOH). Findings from FTIR, EDS, and XPS show the MXene has -OH, and -F terminations. In terms of HER activity, the delamination process did not affect onset potential as all materials had an onset potential of approximately -0.45 V vs RHE. However, after activation through chronopotentiometry, the HER performance of each Ti_4N_3 material improved differently. Ti_4N_3-TMAOH exhibited a 345-mV improvement for V_j=10 and we attribute this to the low -F coverage on the basal plane. For ORR activity, Ti_4N_3-TBAOH had the most positive onset at 0.73 V vs RHE and the greatest current retention with 76.4% after 18 hours chronoamperometry. Compared to the other materials, Ti_4N_3-TBAOH had the highest -OH surface coverage and the largest flake size. These results provide a framework for the exploration of the surface tuning of nitride MXenes for its advancement in fuel cell and water splitting applications.

Keywords: nitride MXene, surface tunability, delamination, oxygen reduction reaction, hydrogen evolution reaction

Oral Session 2: Abstracts

V. ENERGY SAVINGS

1. Impacts and Methodology of Outside Air Temperature based Supply Air Temperature Reset

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Commercial and residential sector buildings accounted for almost half of end-use energy consumption in the United States in 2021. Air handling units (AHU) are some of the largest energy consumers within these buildings. Temperature and humidity must both be controlled by AHUs to ensure occupant comfort and is accomplished in large part by the supply air temperature. In order to reduce energy consumption and maintain humidity control for the AHU, the supply air temperature can be reset based on outside air temperature. An energy plus simulation was developed for large commercial office buildings in the U.S. and each variable of an outside air based reset was investigated across a 10 oF range in terms of energy savings and uncomfortable hours. This investigation showed the low supply air temperature in the reset had the greatest impact with savings ranging from -0.4% to 3.9% total savings and 9 to 1,390 uncomfortable occupied hours where the space relative humidity was greater than 60%. An analysis of Dry and Humid climates was also completed to present a methodology for calculating the high outside air temperature to assign to the low supply air temperature based on local climate. Annual cost savings ranged from 1.2%-8.9% with uncomfortable occupied hours varying between resets. Humid climates generally had lower high outside air temperature values (60 to 75 °F) as the higher humidity of these climates requires a lower supply air temperature to ensure comfort. Dryer climates allow for higher outside air temperature values, however the trade-off in energy consumption between the cooling coil and the AHU fan can negatively impact achievable savings.

Oral Session 2: Abstracts

V. ENERGY SAVINGS

2. Multi-period optimization of heat integration for chemical plant electrification with thermal energy storage

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To align with the net zero emissions goal, it becomes vital and unavoidable to decarbonize chemical industry. The industry is the second largest greenhouse gas (GHG) emission source. Electrification of the chemical industry enables integration of cleaner energy sources such as renewables. However, the variation in renewable energy supply is a key challenge in electrifying industrial processes. Thermal energy storage (TES) utilizes low-cost storage mediums such as molten salt, rock, and sand that are non-toxic and more accessible, making it easier to scale up for industrial integration. Methods of mathematical optimization can be used to synthesis and design of utility systems. Papoulias and Grossmann (1983) proposed an MILP approach based on LP transshipment model for the synthesis of flexible utility for changing process demand. So far, MPHI is applied for several operating models for utility system and energy storage. In this work, we first extend the LP transshipment model to minimize the TES size while maximizing the heat integration between hot and cold process streams under a time-varying renewable supply. The objective is to minimize levelized cost of the electrical heating (LCOEH) to obtain the optimal TES capacity and design, the amount of green hydrogen for backup heating, and hourly scheduling of TES charging and discharging. that flexibility in changing electricity demand allows the plant to encounter variation in renewable power while taking advantage of variation in price. The cases study shows TES integrated electric heating system can save up to 65% energy cost based on wind power and electricity price in Texas 2021.

Keywords: Thermal Energy Storage, Industrial Decarbonization, Multi-period optimization, Electrification of the chemical industry

V. ENERGY SAVINGS

3. Development and analysis of novel chiller modeling strategies for a more cost-friendly M&V process of the Chiller Retrofit Measure (CRM)

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Commercial and residential buildings in the United States account for about 40% of the country's total primary energy consumption. Without considering the electrical losses, about 35% of this energy is used for the provision of space cooling, heating, and ventilation. Space cooling in commercial buildings is commonly provided by a central chiller. Chiller plants can consume more than 35% of the commercial building's total electrical energy with more than 60% of it used to run chillers. Therefore, improving the chiller energy efficiency enhances the overall energy performance of the building sector in the country and the world over. The energy efficiency of chillers can be improved by either replacement of chiller plant equipment with more efficient ones or upgrading chiller control systems. M&V of energy savings from energy efficiency projects such as the CRM is an important step for stakeholders. However, M&V is usually a budget-constrained process for most energy efficiency projects. The process should be implemented using measured parameters that are readily available and less expensive to measure. This helps to address the time and budget constraints challenges of the M&V process. In this study, we investigate the possibility of using readily available measured parameters such as outdoor air temperature and humidity to predict the year-round energy performance of chillers for a more cost-friendly M&V process. The commonly used M&V modeling strategies use measured parameters such as chilled water and condensing water temperatures that are rarely available for most building sites in the commercial sector.

Oral Session 2: Abstracts

V. ENERGY SAVINGS

4. Effect of surfactant on polymer flooding with and without shear-thinning polymer in chemical enhanced oil recovery

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Chemically enhanced oil recovery by surfactant-polymer(SP) flooding is a tertiary recovery method that is used to increase the amount of oil that can be extracted from reservoirs after primary and secondary recovery. SP flooding involves injection of an aqueous phase with surfactants and polymers into an oil reservoir to displace resident oil. Surfactants reduce capillary forces and residual saturation whereas polymers allow control of mobility ratio across displacing and displaced phases, thus making the displacement of oil more efficient. Daripa and Dutta have developed an in-house code for modeling surfactant-polymer flooding which did not incorporate shear-thinning effect of polymer. Subsequently, Daripa and Mishra extended the code to shear-thinning polymer-surfactant flooding code. Simulations for shear-thinning polymer flooding without surfactants were performed with this code. This talk focuses on the effect of surfactant with and without shear-thinning polymer using two natural polymers (Xanthane,Schizophyllan used widely in industry). This research is currently in progress and in no way complete. Some preliminary results will be presented at this conference.

V. ENERGY SAVINGS

5. Intelligent Compressed Air Storage System for Intermittent Demand of Compressed Air

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An average of 900 million megawatthours (MWh) of energy is consumed annually by the manufacturing industries in US, figure estimated by the US Census Bureau and Department of Energy. It is estimated that 10% of the consumed electricity is used for the generation of compressed air. As 20~30% of the electricity utilized for compressed air is simply wasted for compensating leaks, it is important to save energy in the compressed air system. To save energy while ensuring the adequate pressure to the compressed air system, an intelligent compressed air storage system for the manufacturing facilities with an intermittent demand is introduced. The proposed system would be able to adapt to the varying demand requirements while reducing the operation time of the compressors during the production downtime. Control system, sizing of a reserve tank and flow detection need to be examined to successfully develop the proposed system. In this paper, however, the development of the control system and the sizing of reserve tank are mainly discussed. Control states in the proposed system are defined to design the control system. Simulation models calibrated to the experimental setup and industrial systems are developed to examine the sizing effect of the reserve tank on the system. As a result of the sizing simulation, installing the reserve tank and applying the proposed control system showed reductions in the compressor's electricity consumptions. Reducing the leak rate and changing the setpoints of operation and downtime pressure levels in addition to applying the proposed system showed a possibility of maximizing the energy saving.

Keywords: Energy saving, compressed air storage system, reserve tank, intermittent demand, control state, sizing simulation

Oral Session 2: Abstracts

V. ENERGY SAVINGS

6. Impact of Entrained Air on Chilled Water/Hot Water System Performance

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The chilled water /hot water system in a building heating and cooling system uses water as the primary medium of transfer heat because of its low cost and environmental impact and its relatively high thermal conductivity. However, few studies have considered the impact of entrained air in the water on the performance of the chilled water/hot water system. Studies suggest that entrained air in the water system will cause significant pressure loss in the centrifugal pump and the piping system.

In this study, we conducted experimental tests to determine the pump differential pressure required to maintain a consistent water flow rate while varying the total air volume fraction from 0% to 9.8%. The differential pressure at different locations is recorded to study the impact of the preferential accumulation of air. The study findings indicate that the presence of air in the system required additional pumping power to sustain the water flow rate. Specifically, at high water velocity and low air volume fraction, the primary factor contributing to the system's performance degradation is the pressure drop in the centrifugal pump. On the other hand, at low water velocity and high-volume fraction, the preferential accumulation of air leads to further pressure loss in both the centrifugal pump and the piping systems. Compared to 0% air volume fraction at 3600 RPM centrifugal pump rotational speed, the differential pressure provided by the pump was reduced by 25.8% at 1.6% air volume fraction. At the same time, the piping system pressure loss at 1.6% air volume fraction increased by 1.8% compared to the 0% air volume fraction evaluated at the same water flow rate. As the air volume fraction increased to 9.8% at 3600 RPM pumps rotational speed, the differential pressure provided by the centrifugal pump was reduced by 88.2%; The piping system's pressure loss increased by a factor of around 3.76.

Keywords: Energy efficiency, Chilled water/ hot water system, two phase flow

VI. SUSTAINABILITY

1. Biogas Production from Solid-State Anaerobic Digestion of Poultry Waste

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Poultry waste, a significant byproduct of the poultry industry, poses environmental concerns while presenting an untapped resource for potential biogas production. This study aimed to investigate the feasibility of utilizing poultry waste for biogas production through Solid-State Anaerobic Digestion (SS-AD) and to explore the influence of substrate-to-inoculum (S/I) ratios on process efficiency. The research examined the SS-AD process using three different S/I ratios, including 0.5, 0.75, and 2. The experimental setup utilized batch reactors operating at mesophilic conditions with an organic loading rate of 20%. The reactors were operated for 15 days to assess the biogas production. Results demonstrated that the S/I ratio played a significant role in determining biogas production efficiency. Among the tested ratios, the S/I of 2 exhibited the highest biogas yield, approximately 1257 ml. Biogas yields for S/I of 0.5 and 0.75 were similar, around 760 ml and 777 ml, respectively. Moreover, the biogas production from SS-AD was found to be twice that of the previous studies of wet anaerobic digestion of poultry waste. The findings of this study underscore the potential of SS-AD as a more efficient method for biogas production from poultry waste compared to conventional wet anaerobic digestion. By maximizing biogas yields through proper S/I ratio optimization, SS-AD offers a promising solution for sustainable waste management and energy production.

Keywords: Solid-State Anaerobic Digestion, biogas, substrate-to-inoculum

VI. SUSTAINABILITY

2. Numerical Study on Motion Effects of Floating Offshore Wind Turbines

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Floating offshore wind turbines (FOWTs) have been favored as the ultimate solution for offshore wind development, particularly with recent successful installations in Europe for pilot and demonstration purposes. It is understandable that the new development still encounters great challenges from analysis and design to installation to operations. Compared with inland or fixed-based offshore wind turbines, in particular, one challenge is that the overall performance of an FOWT is largely affected by the motion of its floating structures/platforms that are subject to the combined influence of wind and waves at sea. Previous studies have shown that the surge and pitch motions could lead to significant changes in aerodynamics on the turbine blades. In this study, an IEA 15 MW reference wind turbine is used as the baseline turbine model and is integrated with a semisubmersible-type platform with varied mooring systems to complete the whole model FOWT. A numerical simulation of this FOWT is conducted using the commercial software OrcaFlex, where the aerodynamics of turbine blades is solved based on BEM theory, and the whole structure consists of the tower and floating platform are modeled with 6-degree-of-freedom movement subject to wind and waves at sea. This setup is first verified and validated with benchmark cases. In particular, the motion effects on wind turbine performance will then be investigated with focuses on surge and pitch motions. A mooring analysis of this FOWT will then be carried out to find an effective mooring solution to mitigate the possible side effects due to the motion of floating platform.

Keywords: Floating offshore wind turbines; numerical simulation; motion effects

Oral Session 2: Abstracts

VI. SUSTAINABILITY

3. A Modified Overset Method in OpenFOAM for Simultaneous Motion and Deformation: A Case Study of a Flexible Flapping Foil Hydrokinetic Turbine

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The influence of wing deformation in animal propulsion and motion is an intriguing phenomenon that has contributed to a growing interest in biomimetics in both academia and industry. Among the techniques used to simultaneously simulate body motion and deformation in computational fluid dynamics, Overset (or chimera) can be seen as a promising solution that can handle any arbitrary motion. In OpenFOAM, a free open-source CFD toolbox, the Overset approach has undergone a series of developments. However, it is not yet designed to simulate a deformable moving body, such as a flexible flapping foil, fish-like swimming, and droplet formation. In this work, the OpenFOAM Overset module has been enhanced to handle combined motion and deformation. To verify the newly built solver, a flexible flapping foil problem is solved based on literature work. A NACA0012 foil is forced to heave and pitch in uniform flow using the Overset technique, while its leading edge deforms during each flapping cycle using the Arbitrary Lagrangian-Eulerian (ALE) technique. Eventually, by managing the multiple mesh zones in the motion solver, this contribution offers the possibility to apply deformations to the desired moving mesh zones without altering the other (non-deformable) zones.

Oral Session 2: Abstracts

VI. SUSTAINABILITY

4. Turbulence modeling approaches for the Hydrodynamic Analysis of Floating Offshore Wind Turbines

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Over the last two decades, interest in Floating Offshore Wind Turbines (FOWTs) has increased significantly; responding to the calls of the Blue Economy to harvest wind energy in the deep ocean. In the context of the design and optimization of floating offshore wind turbines, accurate prediction of the flow characteristics around these structures is crucial. The turbulent flow is highly complex and challenging to model accurately. While it is widely known that the chosen turbulence modeling approach has implications for the viscous wake and boundary layer, it is shown here that wave propagation and resulting wave loads are also sensitive to the chosen approach. Here, we compare the performance of a series of RANS standard k-epsilon, realizable k-epsilon, and scale-resolving PANS k-epsilon models when predicting wave loads on a suspended cylinder subjected to regular waves. All numerical results are compared to available experimental data. All simulations are conducted with the OpenFOAM solver interFoam, using the Volume Of Fluid (VOF) method. It is concluded that the turbulence model, as well as the assumed far-field turbulence level in the tank, have a large impact on the resulting wave loads. Most previous literature on multi-phase flows uses properties of the primary phase (water) to estimate initial and inflow turbulent quantities. It is shown here that by using different initial eddy viscosity for each phase, the results can be significantly improved. These results have consequences for the numerical simulations of FOWT hydrodynamics and the enhancement of accurate and reliable models to predict the behavior of offshore wind power systems.

Keywords: Floating Offshore Wind Turbines, Hydrodynamics, CFD, PANS, OpenFOAM, Fixed Cylinder.

VI. SUSTAINABILITY

5. Process Design of Green Hydrogen Production System from Offshore Wind Energy

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Recently, there have been various efforts underway to transition from fossil fuels to renewable energy to combat global warming due to the production of greenhouse gases and meet the targets of the Paris Agreement of net zero (decarbonization) by 2050. Among several options of renewable energy resources being explored, one of them is based on the production of hydrogen energy using green energy resources, such as offshore wind energy. This involves the electrolysis of water using electricity generated from offshore wind turbines without any carbon footprint. This study presents a conceptual design of the green hydrogen production system using the electrolysis process of water by supplying power from offshore wind energy resources. First, the availability of sufficient power from the offshore wind turbine substation is evaluated in order to produce green hydrogen in a cost-effective way. This is followed by designing an offshore subsea hub devoted to the hydrogen production system using water electrolysis, including hydrogen compression/liquefaction, storage, and transport to onshore facility for the commercial usages, such as the power plants, refueling stations, chemical plants (ammonia production, e-fuels), refineries, among others. The various technical specifications including the system functionality, system efficiency, cost, and risks in producing, storing, and transporting hydrogen to onshore facilities are evaluated. Finally, the economics of operating and producing green hydrogen from the system powered by offshore wind energy is summarized.

Keywords: Green hydrogen; Offshore wind; Electrolyzer; Renewable Energy; Hydrogen Process Design.

VI. SUSTAINABILITY

6. Photocatalytic Integrated Design for Hydrogen Production with Combined Solar and LED Light Sources

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This abstract introduces an integrated system that combines a photoreactor and heat exchanger to continuously produce hydrogen using solar and LED light sources. The research focuses on a lab-scale setup, aiming to design an efficient pilot-scale system. The proposed design harnesses solar and LED light sources for the photocatalytic conversion of water into hydrogen, using ascorbic acid as a sacrificial agent. During daylight hours, the photoreactor utilizes abundant and renewable solar energy, seamlessly transitioning to LED light sources at night for continuous hydrogen generation. An integrated heat exchanger optimizes temperature control, enhancing overall system performance and maintaining optimal operating conditions for the photocatalytic reaction.

This research contributes to clean energy technologies, capitalizing on the combined benefits of solar and LED light sources for continuous hydrogen production. The seamless transition between different light sources makes the design suitable for diverse geographic locations and varying daylight conditions. Future work involves evaluating the proposed design at the pilot scale to assess efficiency, scalability, and economic viability, providing insights for sustainable hydrogen production systems, and achieving a carbon-neutral energy future.

Keywords: Solar, LED, Green Hydrogen, Photocatalysis.

Oral Session 2: Abstracts

VII. DATA SCIENCE & STATISTICAL LEARNING

1. Rapid Forecasting of CO_2 Plume Migration in Varied Geological and Engineering Scenarios Utilizing Transfer Learning

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Carbon sequestration is a common technique for combating CO_2 emissions. Usually, CO_2 sequestration is modeled using commercial Numerical simulators. Results from reservoir simulators – saturation distribution and pressure plume forecast – are used to determine Area of Review (AoR), assess risks such as contamination of underground water and micro seismicity. Numerical simulators, however, mostly require high computational time for complex problems. In this work, Fourier Neural Operator (FNO) – based machine learning (ML) model was applied to rapidly forecast the CO_2 pressure and saturation distribution, under fixed injection locations and limited injection rates. Subsequently, the capability of transfer learning to "transfer" knowledge gained from limited scenarios to broad scenarios was demonstrated. The pre-trained FNO based model was leveraged to make a rapid forecast of CO_2 pressure and saturation distribution under variable geological and operational (injection rates, injection location) conditions. Additionally, we considered a scenario of injecting CO_2 for 30 years and monitoring for 50 years. The ML model was able to forecast in less than 30 seconds compared to reservoir simulation which takes about 40 mins. Further, the overall mean relative error of ML predictions is less than 3% and 10% for pressure and saturation respectively. Applying transfer learning for prediction under uncertain conditions, data generation and model training times were reduced by 50% and 75% respectively, compared to the base model. Further, total trainable parameters were reduced 99.9%. Lastly, the mean relative error of TL predictions on the test set is less than 6% and 26% for pressure and saturation respectively.

Oral Session 2: Abstracts

VII. DATA SCIENCE & STATISTICAL LEARNING

2. Physics-informed Neural Networks on High-Dimensional Partial Differential Equations

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The realm of fluid dynamics is governed by a variety of partial differential equations. Some of these equations do not have an analytical solution or a computationally efficient numerical solution. Thus, the creation of Physics-informed Neural Networks (PINNs) was introduced. This set of neural networks works as function approximators for highly complex partial differential equations and uses machine learning concepts to approximate such equations at an impressive accuracy. Nevertheless, the computational cost for these neural networks increases exponentially as higher-dimensional partial differential equations are introduced. This project thus introduces a novel scheme able to efficiently approximate higher-order partial differential equations relevant to the realm of fluid dynamics. Our approach employs and combines two previous methods which further increase the speed and accuracy of higher-dimensional partial differential equations. This new High-Dimensional Physics-informed Neural Network (HD-PINN) first decomposes a partial differential equation into a set of lower-dimensional equations. These sets of equations are then parsed through multiple multi-layer neural networks which predicts these sets of equations to then be merged into the original equation. The predicted results are then parsed through a stochastic dimensional gradient descent optimizer to efficiently and accurately optimize the gradients for each network to be optimized again for the next training loop. Thus HD-PINN can approximate high-order complex partial differential equations such as Burger's and Euler's n-dimensional equations. Such equations have a relevant impact on the realm of fluid dynamics and are tied to a variety of real-life applications.

VII. DATA SCIENCE & STATISTICAL LEARNING

3. Detecting anomalous motions in the Shell-polishing process using sensor fusion and Machine Learning

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We present a novel approach to fuse in-situ imaging and vibration signals to interrogate the fine-abrasive polishing process for finishing ~2mm spherical high-density carbon-coated silicon spheres that end up as targets for Inertial Confinement Nuclear Fusion (ICF) experiments underway at Lawrence Livermore National Labs. The polished shell's surface quality is determined by surface pits and cracks, that can be important determinants of the final energy yield. This study employs an experimental machine tool that emulates LLNL's polishing process and is instrumented to acquire video images and vibration sensor signals synchronously with 0.1-sec resolution. The video images of fast-moving balls were processed using the Convolutional Neural Network (CNN) model to classify shells as close and apart at every frame. These multimodal data streams were used to train an unsupervised EGO-MDA model developed earlier by authors to entity spectral bands of vibration signals that can discern between the frames (or times) when shells were together versus far apart. The results suggest that just 2-3 spectral bands of vibration signals are sufficient to classify when shells are together versus apart, with an accuracy of ~80%. Additionally, they indicate significant differences in median energy levels when shells are together versus apart in the identified spectral bands of vibration signals. The waveform patterns in the key frequency bands suggest that these energy changes result, almost 100% of the time, due to strong collisions and momentum exchange between the shells.

Keywords: CNN, EGO-MDA

Acknowledgement: This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and by the LLNL LDRD program under Project Number 23-ERD-014.

Oral Session 2: Abstracts

VII. DATA SCIENCE & STATISTICAL LEARNING

4. Intersection of Data Science and Stats with Nuclear Energy Policies

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The intersection of data science and statistics in nuclear energy policies can play a crucial role in enhancing the safety, efficiency, and overall decision-making process within the nuclear energy sector. Here are some key areas where data science and statistics can be applied in the context of nuclear energy policies:

1. Safety Analysis and Risk Assessment: Data science techniques can be used to analyse vast amounts of data from sensors, monitoring systems, and historical records to assess the safety of nuclear facilities. Statistical models can help quantify risks associated with various operational scenarios and guide policymakers in establishing safety protocols and regulations.
2. Predictive Maintenance: Data science can enable predictive maintenance strategies by analysing sensor data and historical maintenance records to identify patterns and predict potential equipment failures. This proactive approach can help prevent critical failures, reduce downtime, and optimize maintenance schedules, ensuring safer and more reliable operations.
3. Nuclear Reactor Modelling and Simulation: Utilizing data science and statistical methods in nuclear reactor modelling and simulation can lead to more accurate predictions of reactor behaviour under different conditions. These simulations can be instrumental in assessing the feasibility of policy decisions, understanding safety implications, and optimizing reactor operations.
4. Radioactive Waste Management: Data science can aid in optimizing the management and disposal of radioactive waste by analysing historical data and simulating potential waste storage scenarios. Statistical techniques can help estimate the potential risks associated with different disposal methods and guide policymakers in making informed decisions.
5. Environmental Impact Assessment: Data science and statistical analysis can be employed to assess the environmental impact of nuclear energy facilities. This involves monitoring emissions, studying the dispersion of radioactive materials, and analysing the effects on surrounding ecosystems and communities.
6. Policy Impact Evaluation: Data science techniques can be utilized to evaluate the effectiveness of existing nuclear energy policies and regulations. By analysing relevant data, policymakers can assess the impact of different policies on safety, efficiency, and environmental aspects to make data-driven policy decisions.
7. Public Perception and Communication: Data science can help analyse public sentiment and opinions related to nuclear energy policies through social media and public surveys. Understanding public perceptions can aid in crafting better communication strategies and addressing concerns effectively.
8. Energy Demand Forecasting: Data science and statistical methods can be used to forecast energy demand, including the role of nuclear energy in the energy mix. Accurate predictions can help policymakers plan for future energy needs and make informed decisions about nuclear energy policy.

Overall, the application of data science and statistics in nuclear energy policies can lead to more informed decision-making, increased safety, and improved efficiency in the nuclear energy sector. However, it is essential to handle sensitive data responsibly and ensure transparency in policy-making processes to build public trust and confidence in nuclear energy policies.

Keywords: Data Science , Risk Assessment , Nuclear Reactive Modelling , Environmental Impact Assessment , Policy Impact Evaluation , Public Perception , Energy Demand Forecasting , Sustainability and Predictive Maintenance.

VII. DATA SCIENCE & STATISTICAL LEARNING

5. Numerical Investigation of Surface Tension Effects on Transcritical Liquid Breakup in High-Pressure Supercritical Propulsion Systems

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In the pursuit of enhanced engine performance and reduced emissions, the design of liquid-fueled propulsion systems is shifting towards much higher combustor pressures, surpassing the nominal critical pressure of the fuel and air. This trend leads to the adoption of supercritical conditions, wherein the liquid fuel is injected into the ambient air at supercritical pressure and temperature, causing the fuel temperature to exceed its nominal critical point. This transition from a liquid-like to a gas-like behavior, known as "transcritical behavior," is a crucial aspect governing the operation of modern high-pressure propulsion and energy conversion systems. In these systems, the primary liquid jet breakup and the subsequent breakup of the resulting droplets into smaller ones, called secondary breakup, significantly impact mixing and combustion processes. Despite its importance, there has been a limited focus on droplet breakup at supercritical conditions, particularly at higher flow speeds relevant to high-speed liquid fuel propulsion systems. To gain insight into these phenomena, we have developed a fully compressible multiphase Direct Numerical Simulation (DNS) approach that accounts for real-gas and surface effects. The diffuse interface method is employed to accurately represent transcritical interfaces, accounting for surface tension effects, a critical factor often neglected in previous simulations. A data-driven molecular model predicts the surface tension coefficient to accurately capture surface tension behavior. This approach is employed to investigate the behavior of subcritical n-dodecane droplets in a supercritical nitrogen environment interacting with a shockwave, aiming to identify the governing breakup regimes at transcritical conditions. The development of quantitative measures enables the generalization of droplet breakup regimes, ultimately culminating in the creation of a comprehensive breakup regime map for transcritical droplets. The insights gained from this study contribute to advancing the understanding of transcritical liquid breakup, providing valuable knowledge for designing and optimizing high-speed propulsion systems.

Oral Session 2: Abstracts

VIII. MULTI-FUNCTIONAL MATERIALS (B)

1. Multifunctional Shape Memory Polymer Composites (SMPCs): Bottom-up Design of Next-Generation Adaptive Materials

Jitendra Choudhary[1], *Niraj Ashutosh Vidwans*[1], *Sreeram Vaddiraju*[1 2]

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Designing next-generation multifunctional composites requires the ability to independently tailor their properties, which is not possible with the current state-of-the-art materials. For example, tuning thermal conductivity independent of electrical conductivity, or tuning mechanical strength independent of the density of the composite. The pursuit of such composites, which also have the added function of responding to external stimuli, led our group towards the bottom-up assembly of nanowires into shape memory polymer composites (SMPCs). In the designs pioneered by our group, the key component of the composites are interconnected nanowires networks (obtained by either nanowire welding or nanowire bonding). These nanowire networks can be obtained with varying packing densities, without compromising their mechanical strengths. Moreover, the diameters of the nanowires in the networks can be controlled to tune the electrical, optical, optoelectronic, mechanical, and thermal properties of the resulting nanowire networks. Finally, infiltration of the networks with polymers can lead to hybrids, whose properties can be controlled using external stimuli. In this presentation, specifically, SMPCs and multifunctional composites based on Zn3P2 nanowires will be discussed in detail. Here, Zn_3P_2 nanowires were interconnected nanowire networks using suitable organic molecules such as 4-amino thiophenol (4-ATP) and 1,4 Benzene dithiol (1,4-BDT). Fabrication of SMPCs was then accomplished by infusing shape memory polymers (SMPs) into these pre-fabricated nanowire networks. Key to the novelty of the SMPCs thus obtained are the presence of covalent bonds not only between the nanowires in the networks, but also the infused polymers and the underlying nanowire networks, and finally the crosslinks between the infused polymers. The application of these all covalently-bonded-nanowire-networks in mechanically-strong thermal insulation and energy conversion will be also discussed in this presentation.

Keywords: Zinc phosphide nanowires, nanowire networks, epoxy, shape memory polymers, composites, shape memory polymer composites (SMPCs).

Oral Session 2: Abstracts

VIII. MULTI-FUNCTIONAL MATERIALS (B)

2. Freeform additive manufacturing of carbon fiber reinforced composites using dielectric barrier discharge-assisted Joule heating

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In this work, we have developed a novel out-of-oven additive manufacturing (AM) technique to rapidly print and cure thermosetting carbon fiber reinforced composites (CFRCs) using dielectric barrier discharge (DBD)-assisted Joule heating. Conventionally, CFRCs are produced by automatic fiber placement machines (AFPs) that use large, cumbersome molds and time-consuming oven treatments to cure CFRCs in the desired shapes. Recently, out-of-oven AM has garnered attention as a method to manufacture CFRCs without the use of molds. AM allows for on-the-fly printing and curing of thermosetting CFRCs; however, current out-of-oven AM techniques are limited to UV-curable or rapid-curing resins. Here, we use DBD for in-situ heating and curing during AM of continuous CFRCs; this method is resin-agnostic, applying to most commercially available thermosetting resins. As the partially cured composite (prepreg) is deposited, Joule heating (with the DBD as a non-contact conductor) allows the part to cure in the desired shape; this is possible because of the conductive carbon fibers inside the part. Composites manufactured by this method show properties similar to those manufactured in conventional ovens. With the help of this technique, we can print composites in free space or on 2D, and 3D substrates. We can print 2D structures, and 3D multilayered structures. We also demonstrate that this process can be automated. This technology leverages the advantages of AM techniques to enable the printing of high-performance and lightweight materials in any desired shape.

Keywords: Thermoset, Additive Manufacturing, Joule heating, Plasma

Oral Session 2: Abstracts

VIII. MULTI-FUNCTIONAL MATERIALS (B)

3. Effects of Aluminum Foam on Boiling Heat Transfer for Thermosyphon Evaporator

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Open cell metal foams are found to be one of the better solutions for heat transfer enhancement; especially for two-phase heat transfer like pool boiling. This is due to their ability to provide a higher number of nucleation sites with a greater amount of surface area. Due to additional advantages like high thermal conductivity, compact size, and lightweight, it has potential in a host of several thermal applications. However, the utilization of open cell metal foams in thermosyphon systems has not been fully explored yet. In this study, uniform aluminum metal foam substrates with different pore densities (10 and 40 PPI), as well as composite metal foam substrates were investigated in terms of two-phase heat transfer enhancement in a vertical orientation. Each experiment considered different liquid fill ratios of (10%, 30%, 60% and 100%) and different heat flux levels (2.56 kW/m², 8.67 kW/m², 16.82 kW/m² and 26.68 kW/m²). The working fluid used for this study was 3M Novec-7000.

This investigation employed comprehensive experimental methods, utilizing IR thermometry to gain an in-depth understanding of the distribution of surface temperatures of each substrate. This study also involved a comparative analysis between all substrates and baseline condition (plain substrate) using the heat transfer coefficient (HTC) and enhancement HTC ratio as performance indicators. The findings unveiled that the 40 PPI foam performed consistently better at low fill ratios and at different heat flux values. However, under specific conditions such as a fill ratio of 100% and heat flux of 26.68 kW/m², the composite foam led to superior performance when compared to the other cases. Notably, all metal foam substrates exhibited greater enhancement over baseline at low heat flux of 8.67 kW/m² (near the onset of nucleate boiling) compared to high heat flux of 26.68 kW/m². In summary, use of aluminum metal foams in an evaporator should help improve the performance of thermosyphon.

Keywords: Metal foam, thermosyphon, two phase heat-transfer

Oral Session 2: Abstracts

VIII. MULTI-FUNCTIONAL MATERIALS (B)

4. Green Ammonia Production on Ti2N Nitride MXene: Mechanistic Analysis Through In-Situ Spectroelectrochemistry

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Electrochemical nitrogen reduction reaction (NRR) is used to convert nitrogen (N_2) to ammonia (NH3) at ambient conditions. In general, acidic electrolytes are used to provide protons (H^+) for the reduction process. However, this leads to a low NH_3 selectivity because of H_2 by-product formation. Recently, we showed that a Ti_2N MXene is active and selective for NRR, and provided preliminary evidence that this catalyst works through a Mars-van Krevelen (MvK) mechanism rather than conventional associative/dissociative mechanisms. To improve the selectivity of the NRR process, the electrolyte was shifted from acidic to neutral pH values. From this, it was seen that NRR in 0.1M Na_2SO_4 was able to achieve a high selectivity of 47%. We also observed that at more cathodic potentials, the material begins to irreversibly decompose into TiO_2 as evidenced by cyclic voltammetry analysis before and after chronoamperometry experiments. To further understand the performance of this material, we use in-situ/operando techniques, including X-ray absorption spectroscopy (XAS) and Fourier-transform infrared (FTIR) spectroscopy, to deconvolute the mechanism of NH_3 production. We use XAS to track the Ti oxidation state as a function of reaction time and applied potential. We also use XAS to track the change in the local coordination environment of the Ti atoms. Furthermore, we use FTIR to elucidate the adsorption of NRR reactive species and intermediates on the MXene surface. All findings are further corroborated with density functional theory (DFT) calculations to track the reaction energy pathway over each intermediate. We plan to expand these findings to other materials and systems, and use the knowledge obtained from these studies to design optimal electrolytic conditions to produce NH_3 through NRR.

VIII. MULTI-FUNCTIONAL MATERIALS (B)

5. Investigation into the Reaction Pathways and Catalyst Deactivation for Polyethylene Hydrogenolysis over Silica-Supported Cobalt Catalysts

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Chemical repurposing has emerged as a promising route to valorize “end-of-use” plastic waste and mitigate its release to the environment. In this work, we applied silica-supported cobalt (5 wt % Co/SiO_2) catalysts to produce liquid-range hydrocarbons (C5–C30) in the batch phase at 200–300 °C, 20–40 bar H_2, and 2–36 h with high selectivity and investigated the reaction pathways, the influence of catalyst phase on the product yields and selectivity, and the catalyst deactivation mechanisms. Reaction conditions were optimized for improving liquid product yields at 275 °C, 30 bar H_2, and 8 h reaction time, giving a 55% liquid product yield (C-mole basis), comprising 75% of nonsolid products, with gas yields limited to 19%. By tracking product evolution over time and with varying cobalt surface density, we propose a multipathway mechanism, including a dominant, nonterminal C–C cleavage route on the polymer chain over the catalyst, which drives the high liquid product selectivity. The catalyst also showed recyclability over four reactions with reduced activity and a shift in yield toward liquid products after the first reaction. It was effectively regenerated by calcination under air at 450 °C. We combined the reactivity data with powder X-ray diffraction (PXRD), thermogravimetric analysis coupled with mass spectrometry (TGA-MS), and catalyst surface areas via N_2 physisorption of various fresh, spent, recycled, and regenerated catalysts to attribute the reduced activity and selectivity shift mainly to the presence of a recalcitrant polymer species embedded on the catalyst, comprising 10.5–18.5 wt % of the spent catalyst, which obstructs access to active sites and increases liquid selectivity and overshadows the influence of carbonaceous coke or catalyst phase reduction to Co. Moreover, we successfully applied the catalyst to various postconsumer polyethylene (HDPE and LDPE) samples. These results move the field toward more sustainable and economically viable catalysts for the chemical upcycling of waste plastics.

Keywords: Catalysis, plastics upcycling, circular economy

Oral Session 2: Abstracts

VIII. MULTI-FUNCTIONAL MATERIALS (B)

6. Structural and Fast-Charging Organic Battery Cathodes Based on Redox-Active Polymers and Carbon Fiber Fabric

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Structural energy storage requires optimized batteries with significant energy storage together with excellent mechanical properties. This technology may lead to substantial mass and volume savings in electrified transportation and aerospace applications by storing energy within the object's structural elements. However, until now, most studies on structural energy storage have focused on conventional, inorganic cathode materials such as lithium iron phosphate (LFP), lithium cobalt oxide (LCO), or nickel manganese cobalt oxide (NMC). These materials are usually cast on malleable metallic current collectors that render the battery to be mechanically weak. Further, they exhibit poor rate capabilities at higher C-rates and low capacity retention during the long-term life of batteries while also being potential environmental hazards. Organic radical polymers are a promising alternative because they possess rapid kinetics, charge transfer ability, and good cycling stability while being environmentally benign. Carbon fiber fabrics possess excellent tensile strength and modulus and are increasingly used in automobiles, aviation, and aerospace objects. In this work, we report PTMA (poly (2,2,6,6-tetramethyl-piperidenyloxyl-4-yl methacrylate)) redox-active polymer-based structural battery electrodes containing a carbon fiber (CF) fabric current collector platform. PTMA, super P carbon, and polymethyl methacrylate (PMMA) binder were cast on carbon fiber plain weave fabric, providing excellent structural support while also being a current collector. A full-cell battery containing the structural organic battery electrode, as well as a graphite-based anode, was also prepared. These half and full-cells were investigated for fast charging capability and low temperature (about -20°C) operability tests. This work provides a pathway for utilizing environmentally benign, redox-active polymer-based electrodes in structural and fast-charging organic batteries.

Keywords: Structural organic battery, redox-active polymers, energy storage

Poster Presentations 1

Poster Presentations: 9:45 AM - 11:30 AM
Gates Ballroom, MSC

Friday
September 29

Poster #	Name and Authors
1	Plastic Recycling Pathways Toward the Circularity, Techno-Economic Assessment and Degree of Circularity Evaluation *Wafaa Majzoub*
2	Analysis of Polymeric Materials Energy Consumption in Vehicle Production *Betsie Montano Flores*
3	Harnessing the Moon: Tidal Energy Generation with Hydraulic Multiplication *Francesco Romano*
4	$Ti_4N_3T_x$ MXene as a Highly Stable Universal Aqueous Energy Storage Material *James Kasten*
5	A multi-scale approach for carbon accounting and in-depth LCA *Marco De Sousa*
6	Design and Development of a Stable 1KW Portable Micro Hydro Power Plant for Low-Head Canal Applications in Pakistan *Umer Farooq*
7	Synthesis of h-BN/Nanosilica Hybrid Reinforced Room Temperature Vulcanizing Silicone Rubber (RTV SiR) Nanocomposites for High Voltage (HV) Insulators *Muhammed Zeeshan Ahmed*
8	Optical Bandgap Diagnostics for Assessing Nitride MXenes Stability in Various Solvents *Bright Ugochukwu Ngozichukwu*
9	Dual layered, Zwitterionic coated Forward Osmosis Membrane for the Treatment of Produced Water *Sunith Madduri*
10	Enhanced Photocatalytic Degradation of Azo Dyes Using Metal-Doped TiO_2 *Gladstone Ukoima*
11	Evaluation of Microfiltration and Ultrafiltration Pretreatment on the Performance of Followed Reverse Osmosis for Recycling Poultry Slaughterhouse Wastewater *Sana Fatima*
12	Improving energy storage through nonaqueous electrolytes *Laura Hoagland*
13	Prediction of Offshore Wind Farm Output Power based on SCADA Data with Supervised Machine Learning *Angel Randall*
14	Harnessing social media to understand public perspectives on solar energy in the United States *Sejal Sanjay Shanbhag*

Poster Presentations 2

Poster Presentations: 9:45 AM - 11:30 AM
Gates Ballroom, MSC

Friday
September 29

Poster #	Name and Authors
15	The impacts of energy imbalance on the performance of aquifer thermal energy storage *Zehao Chen*
16	Application of Conversion Function Theory to the Modeling of Multi-Converter Islanded DC Microgrids *Hesam Mazaheri*
17	Bayesian Risk Assessment Modeling of the Electric Power Supply Chain: A Case of Study in the North American Region *Guillermo Duran Sierra*
18	Towards Energy-Efficient Residential Power Systems: A Virtually Islanded Hybrid AC/DC Nanogrid Approach *Debjyoti Chatterjee*
19	Carbon-Negative Hydrogen Production Through Plasma Processing of Waste Bio-oils *Alex Gutenberg*
20	Enhancing HVAC Efficiency: PIR Sensor with Solid State Optical Shutter for Indoor Occupancy Detection *Xin Zhao*
21	Dielectric-based field enhancement in a subwavelength cavity and its application to enhance near-infrared photon upconversion *Arun Bhaskar*
22	Impact of Using Horizontal Wells on Aquifer Thermal Energy Storage System Efficiency *Yinuo Wang*
23	Stable A_2BIrO_6 perovskite catalysts for improved oxygen evolution performance in acidic electrolytes *Harrison Lippie*
24	Atomistic simulations of chemomechanics at electrified interfaces *Veerendra Naralasetti*
25	High resolution modeling and analysis of cryptocurrency demand's impact on power grids *Ranyu Shi*
26	Experimental investigation of the Nano-Fin Effect (NFE) during thin film evaporation from nanopores using temperature nano-sensors *Juliet Shafer*
27	Process Design and Intensification of Catalytic Fluidized Bed Membrane Reactor for Oxidative Coupling of Methane *Moustafa Ali*
28	Learning for Interval Prediction of Electricity Demand: A Cluster-based Bootstrapping Approach *Rohit Dube*
29	Multifunctional materials for sustainable operation of Fluid Catalytic Cracking (FCC) process in petroleum refineries *Anuja Dnyaneshwar Patil, Utkarsh Mahajan*

Poster Session: Abstracts

1. Circular Economics of Plastic Waste Recycling: An Optimization Approach of Waste-to-Energy and Closed-Loop Recycling

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The escalating levels of plastic waste over the last decades posing severe environmental consequences on a global scale have led to an urgent need for sustainable recycling methods. A holistic evaluation of each technology's circular network is critical for advancing energy recovery from plastic waste to achieve a sustainable circular economy. The transition toward CE can be enhanced with process systems engineering, by promoting sustainability problem-solving, optimizing the processes framework for analysis, and providing a circular approach towards sustainable and energy-efficient solutions. In this study, a novel mathematical model is used to optimize different recycling technologies including pyrolysis, gasification, mechanical recycling, and incineration. Chemical recycling products such as pyrolysis oil or synthesis gas are excellent raw materials for many diverse technologies. The model reveals the potential of plastic waste for energy production, while also assessing the effectiveness of various recycling pathways and the most efficient use of the chemical products of these technologies such as methanol, ammonia, hydrogen, and olefines. In addition, a novel degree of circularity indicator is proposed based on energy efficiency and other elements to assess all the processes involved. Taking energy recovery by incineration as a baseline, 20 different scenarios have been evaluated with a multi-criteria analysis to validate the model. Our findings reveal that combined pyrolysis -steam cracking/refinery technologies offer promising avenues for producing sustainable fuels and olefins. This aligns with CE principles and energy-related objectives set by various nations, including the United States. This paper highlights the potential of emerging energy technologies from plastic waste. It also emphasizes the vital role of circularity in transforming waste management into a sustainable and energy-efficient endeavor.

Keywords: Plastic waste recycling, Waste to Energy, Circularity, Optimization.

2. Analysis of Polymeric Materials Energy Consumption in Vehicle Production

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To effectively support the ongoing energy transition, it is also crucial to address the mobility and materials transition. While progress has been made in transitioning from traditional fossil fuel feedstocks to renewable energy sources, commercially feasible solutions that can successfully supplant the existing petrochemical plastic products are yet to be identified. Accordingly, there exists an opportunity to drive a materials transition toward sustainable and durable polymers, which can contribute to the production of lighter and more fuel-efficient vehicles. This challenge is illustrated based on internal combustion engine (ICE) vehicles due to their significant (i) contribution to emissions and (ii) use of energy resources. This work aims to identify the most energy and carbon-intensive stages in the life cycle of an ICE vehicle through an analysis of the materials flow from the mining stage to the end-of-life. The analysis reveals that in the production stage, the exploration of alternative and innovative technologies for mining/extraction is imperative, as it is the most energy-intensive part accounting for nearly 79% of the energy consumed. For further decarbonization, carbon capture, utilization, and storage (CCUS) processes can be integrated into both energy systems and the materials production sector to decarbonize them.

Keywords: Energy transition, Mobility transition, Energy consumption, Emissions analysis, Critical materials

3. Harnessing the Moon: Tidal Energy Generation with Hydraulic Multiplication

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This research introduces a novel approach to tidal energy harvesting, utilizing mechanical methodologies and hydraulic multiplication within a gravity battery-based system for enhanced power output. The study outlines a system where rising tides increase the water pressure in an ocean-connected chamber. This increase in pressure drives water through a conduit into an adjacent tower, creating a hydraulic lift significantly higher than the tidal range. Concurrently, a substantial counterweight is floated, storing considerable potential energy. The counterweight's elevation during rising tides stores vast potential energy, later converted to electricity during low tide periods via an electromagnetic generator. Current tidal energy make use of the kinetic energy from the ebb and flow of the tide and are limited by the variance of the high and low tide. The largest tidal power installation is the Shihwa Lake Tidal Power Plant in South Korea with an output of 254MW. The key novelty lies in the incorporation of a hydraulic multiplication mechanism to increase the variance of water level. The mechanism exploits the area discrepancy between the large seawater inlet and the relatively smaller displacement area beneath the counterweight, similar to a hydraulic lift. This discrepancy enables the counterweight's lift to exceed the standard tidal range, thereby magnifying stored energy. With a counterweight mass of 'M' and a lift height 'H', energy storage per tidal cycle can be computed as $E = MgH$, where 'g' is the gravitational constant. For a series of 22 one-million kg counterweights with 100m of oscillation the output would be 1000 MW. This energy is consistently discharged during the low tide phase, ensuring a stable, grid-compatible power supply. Additionally, the system exploits the buoyant force during rising tides to provide mechanical energy, doubling daily power output. A comprehensive quantitative analysis illustrates the system's economic viability, factoring in material cost (C per cubic meter) and showing minimal operational costs. Assuming C= $100 and material at 50% of total initial cost, the projected cost per GW is $5 billion, $1-4 billion cheaper per GW than Nuclear at $6-9 billion per GW. This positions the plant as a reliable, affordable, and scalable clean energy solution. The research also addresses potential environmental impacts, changes to local ecosystems, and proposed mitigation strategies. Operational challenges, including system maintenance and resilience against extreme weather conditions, are also discussed. Given tidal movements' predictability, this energy source can contribute to a reliable base load power, addressing the intermittency issues common with other renewables, such as wind and solar power. The coastal location also offers potential integration with systems like hydrogen production and ocean water desalination. By leveraging consistent tidal dynamics, we propose a promising renewable energy alternative that could revolutionize the future of power generation.

Keywords: Clean Energy, Tidal Energy, Hydraulics

Poster Session: Abstracts

4. High Performing pH-Universal Electrochemical Energy Storage using 2D Titanium Nitride MXene

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The need for reliable renewable energy storage devices has become increasingly important. However, the performance of current electrochemical battery and supercapacitor devices is limited by either low energy or power densities and short lifespans. Recently, a 2D class of transition metal carbides and nitrides known as MXenes have emerged which demonstrates promise as future materials in energy storage devices. In this presentation, we report the synthesis and characterization of multilayer $Ti_4N_3T_x$ MXene in various aqueous electrolytes. We demonstrate that $Ti_4N_3T_x$ can be electrochemically activated through continuous cation intercalation over a 10-day period (15,000 cycles) using cyclic voltammetry. A wide operating window of 2V is maintained throughout activation. After activation, capacitance increases by 240%, 220%, and 125% in 1M H_2SO_4, 1M $MgSO_4$, and 1M KOH, respectively and reaching over 575 F g^{-1} at 2 mVs^{-1} in H_2SO_4. Moreover, activation in H_2SO_4 electrolyte leads to a switch in the charge storage mechanism from capacitor to capacitor-battery hybrid behavior as a result of hydronium ion intercalation accompanied by changes in the oxidation state of Ti. To date, this is one of the most electrochemically stable MXenes reported in aqueous electrolytes and provides the highest capacitance universally across different pH environments among MXenes. These findings may offer a new and reliable option for reliable energy storage devices with potential applications in large-scale grid storage and electric vehicles.

Keywords: Energy Storage, Intercalation, MXene, Battery, Supercapacitor

5. A Multi-scale Approach for Carbon Accounting and In-depth LCA

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Global anthropogenic greenhouse gas emissions have been increasing since the onset of industrialization. Presently, carbon dioxide (CO_2) emissions account for roughly 80% of the total anthropogenic greenhouse gases released. Notably, CO_2 emissions exhibit a linear relationship with the rise in global temperatures. Many strategies have been proposed to mitigate or at least reduce carbon emissions. With this in mind, approaches to carbon accounting regarding industrial systems are being investigated to achieve a well-informed energy transition. Carbon accounting methods must be accurate as well as reliable to ensure realistic target setting for emission reduction policies. The current state of the art in carbon accounting tools involve black-box approaches which can lead to vagueness as well as inconsistent and at times even conflicting results when using different calculation methods. Given the market competition between dynamic renewable and storage technologies with conventional systems, decision makers need to make decisions at shortened temporal scales. This motivates the integration of real-time carbon accounting with decision-making frameworks. Moreover, a carbon emission database with a finer spatiotemporal resolution is needed. Near real-time carbon accounting has already been applied on a national level, but the integration with decision-making frameworks is novel. This work investigates the uncertainty when working with different impact assessment methods and sheds light on the black-box perspective of present-day carbon accounting and life cycle analysis (LCA) tools. To do so, a detailed near-real-time carbon accounting and decision-making framework has been developed, with the latter being done in energiapy. The multi-scale approach determines emissions on an hourly, daily, weekly, monthly or even yearly basis and avails from them to provide informed decisions on resource allocation.

Keywords: Carbon accounting, Life cycle analysis, Multi-scale, Near-real-time

6. Design and Development of a Stable 1KW Portable Micro Hydro Power Plant for Low-Head Canal Applications in Pakistan

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Pakistan, being a developing nation, faces persistent electricity challenges, particularly in rural and far-flung regions where access to electricity is limited or non-existent. Load shedding remains a significant hurdle in the country's development, affecting both industries and rural communities. To address the issue, we propose the design and development of a prototype 1KW micro hydro power plant that is portable, easy to install, and suitable for utilization on local canal distributaries, even with zero head. The proposed micro hydro power plant aims to harness the kinetic energy of the natural flow of water in canals at zero head, tapping into the vast renewable energy potential offered by Pakistan's extensive canal system primarily used for irrigation purposes. However, conventional zero-head micro hydro turbines have faced stability issues due to their small size and the variable flow rate of the canals, resulting in fluctuating voltages and frequencies that hinder reliable power generation. Our primary objective is to engineer a stable, clean, and reliable energy output from the micro hydro power plant. To achieve this, we plan to integrate the supercapacitors in the power plant and fabricate an innovative turbine design tailored to low-head canal applications. This design will optimize energy conversion efficiency and ensure steady power generation despite the varying flow rates. We aim to minimize the capital costs associated with our micro hydro power plant, making it an affordable and viable solution for the local market. The successful implementation of this project would not only alleviate energy shortfalls in rural areas and support the farming communities but also contribute to sustainable and eco-friendly energy generation. We recognize the scarcity of expertise in this domain and seek to fill the gap by commercializing this product.

Keywords: Micro Hydro Power Plants, Low-head Canal, Clean Energy

7. Synthesis of h-BN/Nanosilica Hybrid Reinforced Room Temperature Vulcanizing Silicone Rubber (RTV SiR) Nanocomposites for High Voltage (HV) Insulators

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High voltage (HV) insulators play a crucial role in power transmission, microelectronic components, transformer systems, and other energy applications. However, they often face challenges related to the surface accumulation of moisture and solid contaminants, which can lead to thermal runaways and flashovers. Such problems ultimately reduce the insulator's durability and overall efficiency. To address these concerns and minimize maintenance costs, polymeric composite-based coatings have become a popular solution. This study focuses on the fabrication of room temperature vulcanizing silicone rubber (RTV SiR) based nanocomposites as external coatings for HV insulators. The primary objective is to enhance the thermomechanical and degradation-resistant properties of RTV SiR using hexagonal boron nitride (h-BN) and nanosilica reinforced hybrid filler. Using perflouro-octyl-triethoxysilane (FTS) functionalized h-BN (hBNNS), improved filler dispersion is achieved within the SiR matrix, which offers increased mechanical strength and hydrophobicity. Different loadings of h-BNNS, h-BNNS-SiO_2, and SiO_2 are prepared using a facile synthesis method and dispersed homogeneously into the RTV SiR matrix. The resulting nanocomposite is spray-coated onto ceramic tiles to evaluate the impact of filler type and loading amount on thermomechanical stability, surface wettability, and resistance to surface tracking. Through characterization, h-BN/nanosilica-reinforced RTV SiR nanocomposites exhibited a manifold increase in electrical breakdown strength in the Inclined Plane Test (IPT) in comparison to pristine RTV SiR, while also showing uniform filler dispersion using Scanning Electron Microscopy (SEM). It also outperformed pristine RTV SiR in Thermogravimetric Analysis (TGA), Water Contact Angle (WCA), and Dynamic Mechanical Analysis (DMA), indicating the nanocomposite's superior thermal stability, dielectric properties, interfacial interactions, and minimal agglomeration, rendering it ideal for energy applications in harsh environments.

Keywords: Nanocomposite; Polymer science; Silicone rubber

Poster Session: Abstracts

8. Optical Bandgap Diagnostics for Assessing Nitride MXenes Stability in Various Solvents

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Two-dimensional transition metal nitride and carbide MXenes have attracted increasing attention for various applications, including optoelectronics, sensing, and energy storage and conversion, due to several unique properties including high conductivity, high surface area, and tunable electronic structure. However, the reliable evaluation of the oxidation stability for these MXenes, which is a crucial factor for their industrial applicability, has been a source of debate, primarily due to the lack of a consistent and reliable diagnostic tool. In this work, we synthesize and characterize $Ti_4N_3T_x$, nitride-based MXene, using the oxygen-assisted molten salt fluoride etching (O_2-MSFE) method. We determine the stability of the synthesized material dispersed in various solvents including water, ethanol, N-N dimethylformamide (DMF), dimethyl sulfoxide (DMSO), hexane, and acetonitrile (ACN). We examined the stability of our delaminated $Ti_4N_3T_x$ (d-$Ti_4N_3T_x$) MXenes by studying the changes in optical energy band gap (*Eg*) using the Tauc and Kubelka-Munk model. Our findings reveal that the high-quality d-$Ti_4N_3T_x$ flakes show resistance to oxidation and retain its optical properties (*Eg*, absorption coefficient, optical conductivity) for a period of 50 days in water, DMSO, and ethanol with mild formation of TiO_2 nanoparticles. These results show that nitride MXenes can be used in lieu of carbides MXenes in applications where oxidative stability is a prerequisite. Both Tauc and Kubelka-Munk methods showed a direct *Eg* irrespective of the solvents used. Since oxidation can affect MXene's intrinsic properties, increase in the *Eg* over time can be used as a more reliable indicator to monitor the oxidation stability of MXenes and this method can be expanded to other materials and systems.

Keyword: MXenes, Oxidation stability, Optical bandgap energy, Tauc model, Kubelka Munk model

9. Dual layered, Zwitterionic coated Forward Osmosis Membrane for the Treatment of Produced Water

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In recent years, the treatment of produced water from industrial processes, particularly the oil and gas industry, has become a pressing environmental challenge. In this study, we present a novel approach to enhance the efficiency and selectivity of forward osmosis (FO) membranes for produced water treatment. The proposed approach involves the development of dual-layered FO membranes, where the selective layer is coated with zwitterionic materials. Zwitterionic coatings are known for their unique surface properties, combining positive and negative charges, resulting in an enhanced resistance to fouling and improved antifouling capabilities. The fabrication process of the dual-layered membranes incorporates state of the art techniques, ensuring a uniform and stable zwitterionic coating on the membrane's selective layer. The characterization of these membranes involves evaluating their morphology, surface charge, hydrophilicity, and structural integrity. The performance of the dual-layered, zwitterionic coated FO membranes is assessed through comprehensive forward osmosis experiments using produced water samples. The evaluation includes studying water flux, reverse solute flux, rejection of contaminants, and long-term stability under various operating conditions. The results demonstrate that the zwitterionic coatings significantly enhance the membrane's resistance to fouling and reduce the adverse effects of organic and inorganic foulants in produced water. The interactions between zwitterionic moieties and various foulants are analyzed, providing valuable insights into the antifouling mechanisms. The findings of this study offer a promising solution for the treatment of produced water, contributing to the advancement of sustainable and efficient membrane technologies. The dual-layered, zwitterionic coated FO membranes demonstrate great potential for practical applications in the oil and gas industry and other industrial sectors, leading to reduced environmental impact and enhanced water quality.

Keywords: Produced water treatment; Forward osmosis membranes; Zwitterionic coatings; Environmental impact; Water quality improvement

10. Enhanced Photocatalytic Degradation of Azo Dyes Using Metal-Doped TiO_2

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The photocatalytic degradation of azo dyes in the presence of titanium dioxide (TiO_2) doped with selective metals has been a topic of growing interest due to its potential for efficient and eco-friendly dye removal. Azo dyes are widely used in various industries, including textiles, cosmetics, and food, but their release into the environment poses significant environmental and health concerns. Photocatalysis, particularly using TiO_2 as a catalyst, has emerged as a promising method to address this issue. This study explores the enhanced photocatalytic activity of TiO_2 through the introduction of selective metal dopants. The incorporation of specific metals into the TiO_2 lattice aims to optimize its photocatalytic properties, including bandgap engineering, charge carrier separation, and surface reactivity. The unique combination of metal dopants and TiO_2 is expected to boost the degradation efficiency and reduce the reliance on expensive and potentially harmful sensitizers. The experimental investigation involves the synthesis and characterization of TiO_2-based photocatalysts doped with various metals. The photocatalytic degradation of different azo dyes is assessed under controlled laboratory conditions, studying the influence of metal dopants on the degradation kinetics, degradation efficiency, and by-product formation. Furthermore, the mechanism of the photocatalytic degradation process is elucidated through advanced analytical techniques, including spectroscopy, microscopy, and surface area analysis. Insights into the photoexcitation and charge transfer processes shed light on the role of metal dopants in enhancing photocatalytic performance. The results demonstrate the significant potential of metal-doped TiO_2 photocatalysts for efficient azo dye degradation. The findings contribute to the understanding of the fundamental principles underlying the photocatalytic process and provide valuable guidance for the design and optimization of advanced photocatalytic systems. Ultimately, this research contributes to the development of sustainable and effective technologies for the removal of azo dyes from various wastewater, promoting environmental preservation and human well-being.

Keywords: Photocatalysis; Wastewater; TiO_2; Graphene Oxide; Cu_2O

11. Evaluation of Microfiltration and Ultrafiltration Pretreatment on the Performance of Followed Reverse Osmosis for Recycling Poultry Slaughterhouse Wastewater

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Poultry slaughterhouse wastewater (PSWW) requires conventional treatments like preliminary, primary, and secondary treatments for discharging into the environment. These traditional methods face drawbacks, e.g., the inability to recover essential nutrients from the water, recycle and reuse it in the industry. Reverse osmosis (RO) is an advanced technology that can produce potable water from municipal wastewater, similar to PSWW. However, the presence of diverse pollutants in the raw PSWW necessitates effective pretreatment to ensure successful RO implementation. This study evaluated the efficacy of microfiltration (MF) and ultrafiltration (UF) as standalone pretreatment processes for PSWW prior to RO. Key parameters, including total solids (TS), total volatile solids (TVS), total fixed solids (TFS), chemical oxygen demand (COD), total nitrogen (TN), and total phosphorus (TP), were closely monitored throughout the evaluation. Results showed that both MF and UF pretreatments effectively reduced TS, TVS, and TFS. MF outperformed UF in COD removal, achieving a 34.2% reduction compared to UF's 18.8% removal efficiency. The later RO treatment achieved 100% removal efficiency of COD and TP and over 96% of TS for both UF and MF permeates. After RO treatment, the final permeate from UF pretreatment had a TN level of 5 ± 0.04 mg/L, while the MF-pretreated case had a TN level of 10 ± 0.02 mg/L. Both types of treated water (MF-RO and UF-RO) meet the standards for non-potable uses in the poultry industry. Our study concludes that MF can be a preferable option for pretreatment and MF-RO is more cost-effective than direct RO treatment.

Keywords: poultry slaughterhouse wastewater; microfiltration; ultrafiltration; reverse osmosis.

12. Improving energy storage through nonaqueous electrolytes

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The rise in energy demand requires innovative energy storage devices. Aqueous electrolytes in batteries are safer and more accessible but are limited by water splitting at 1.2V. Nonaqueous electrolytes circumvent this by removing water from the system to increase the voltage window. One category of nonaqueous electrolytes is ionic liquids: molten salts that are liquid at atmospheric temperature and pressure. Protic ionic liquids (PILs) are acidic with excess hydrogen atoms for proton transfer. These PILs have an increased voltage window which leads to an increased capacitance. Additionally, a 2D class of transition metal carbides and nitrides known as MXenes have emerged which demonstrates promise as future materials in energy storage devices. In this presentation, we report the characterization of multilayer $Ti_4N_3T_x$ MXene in trifluoracetic acid and 2-methylpyradine in a 2:1 molar ratio. Electrochemical measurements such as cyclic voltammetry, electrochemical impedance spectroscopy, and galvanic charge discharge, were used to analyze the cell. The $Ti_4N_3T_x$ was blended with Super P conductive carbon and polyvinylidene fluoride in an 80:10:10 mixture and coated onto titanium foil. The counter electrode was conductive carbon cloth and a gold reference electrode. While voltage windows can extend up to 14 V, the maximum specific capacitance arose at 5 V with 66 F g^{-1} at 20 mV s^{-1}. This system needs to be further characterized to determine the stability window in cyclic voltammetry and charge discharge.

Keywords: Batteries, Two-dimensional Materials, MXenes, Ionic Liquids

13. Prediction of Offshore Wind Farm Output Power based on SCADA Data with Supervised Machine Learning

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Renewable energy is gaining prominence as the harms of climate change and fossil fuel scarcity become more apparent. Wind energy in particular can be generated from both inland and offshore installations. Offshore wind farms (OWF) have high potential to generate more electricity than their inland counterparts because their location provides access to greater wind velocity. However, OWF are subject to certain environmental hazards that significantly impact their ability to produce power, making them costly to implement and difficult to repair. Various machine learning applications have been employed in existing research to improve efficiency and resilience on OWF. This research concerns the usage of supervised machine learning through the development of an artificial neural network to predict the rated power output of an offshore wind farm using several environmental variables as recorded via an open-source SCADA dataset. To reduce overfitting, the prediction of the model is compared against four datasets. The application of this model will lend support to OWF in anticipating whether electricity generation will be high or low, and in identifying how certain combinations of environmental factors will contribute to power output.

Keywords: offshore wind farms, machine learning, artificial neural network

Poster Session: Abstracts

14. Harnessing social media to understand public perspectives on solar energy in the United States

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In the face of global climate change and the pressing need for sustainable energy sources, understanding public attitudes toward renewable energy is paramount. This study leverages the power of social media discussions to gain insights into the public's perspective on the use of renewable energy in their homes across the United States. Utilizing text mining techniques, we scrutinize the discourse around renewable energy, identifying both sentiments and challenges faced by citizens in adopting such technologies.

We further enhance our research with geographical analysis to understand region-specific viewpoints and challenges, offering a more nuanced understanding of the nation's stance on renewable energy. Our findings also highlight instances of peer-to-peer advice and support within these discussions, underscoring the role of the community in driving renewable energy adoption.

The knowledge gained from these insights will help to advance energy security in the United States and shape future energy strategies. We aim to promote a more inclusive and efficient approach to the transition to renewable energy by giving voice to the ideas and experiences of the public.

Policymakers can create more tailored and effective policies for the adoption of renewable energy by recognizing the challenges faced by homeowners. The study ultimately underscores the potential of social media as a rich, real-time source of public sentiment, capable of shaping a more sustainable and secure energy future.

Keywords: Renewable Energy, Text Mining, Energy Transition, Social Media, Energy Policy.

15. The Impacts of Energy Imbalance on the Performance of Aquifer Thermal Energy Storage

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The energy balance ratio is a significant indicator for aquifer thermal energy storage (ATES) system thermal performance, which is the ratio of the difference between the energy that is extracted in cooling and heating mode to the total extracted energy over a certain period. A thermal balance ratio that is closer to zero is usually regarded as a better-performed ATES system. However, there are some areas where the demand for cold and heat is not matched, thus more heat or cold energy accumulates as time goes by, which may reduce the efficiency and suitability of the system. This paper intends to discuss the impacts of the energy imbalance of ATES systems on thermal recovery efficiency and payback time and their environmental influences. In this research, both numerical and analytical models would be used to investigate the effects of different imbalance situations. This paper will achieve the following objectives: 1) quantifying the impacts of different imbalance situations on recovery efficiency and payback time; 2) comparing with previous field studies to verify the findings of the numerical and analytical models; 3) discussing how the energy imbalance of ATES system would affect the environmental performance, and to what extent the energy imbalance ratio is acceptable.

Keywords: Energy imbalance, ATES, recovery efficiency

16. Application of Conversion Function Theory to the Modeling of Multi-Converter Islanded DC Microgrids

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The use of renewable energy sources (RES) in energy systems is increasing. Despite their advantages and decreasing price, their unpredictable availability has adversely impacted their users that may pay higher price for energy. In this regard, power engineers have tried to design systems with multiple power converters to compensate for RES's unpredictability. Although this technology may help the users, this design is difficult to model and control because it has multiple converters for simulation even on supercomputers. Therefore, we are applying the power electronic conversion function theory, developed by our group, to microgrids in order to model multi-converter microgrids for simulation and real time control.

Keywords: Conversion Function Theory, DC Microgrids

17. Bayesian Risk Assessment Modeling of the Electric Power Supply Chain: A Case of Study in the North American Region

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Global electricity demand is expected to increase as population grows, climate change intensifies, and economic and human-related activities develop. To satisfy the demand, fossil fuels such as natural gas, coal, and petroleum are still the main sources for electricity production, although renewable energy contributions to electricity supply have been expanding since the last decades. Moreover, power outages have been escalating in frequency due to disruptions in the electricity supply chain caused by severe weather, vegetation growth, animal interference, physical and cyber-attacks, aging infrastructure, among others. To sustain electricity supply and meet future demands, it is critical to address and identify potential threats to the power supply chain, but also accounting for the vulnerabilities of the systems that are vital parts of the supply chain, as well as the corresponding social, economic, and environmental impacts that can result as consequences of such posing threats on the supply chain systems. In this study, a Bayesian Risk Assessment model was formulated to assess the state of Risk of the electricity supply chain with a special interest on the North American Region (U.S.-Canada-Mexico). The model accounts for variables such as anthropogenic and natural threats, supply chain components and systems including raw materials and sources, suppliers, manufacturing and production, retailers, customers, logistics, and social, economic, and environmental metrics of impact. The Risk model is intended to be used to run Risk scenarios to inform decision-makers about the current state of Risk in the supply chain and can be used to strategize mitigating measures to reduce Risks to a desirable threshold.

Keywords: Risk Assessment, Bayesian Network, Electric Power, Supply Chain, Decision-making

18. Towards Energy-Efficient Residential Power Systems: A Virtually Islanded Hybrid AC/DC Nanogrid Approach

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Global urbanization, driven by population and economic growth, has notably escalated residential energy demand. Solar photovoltaic and other renewables generate DC power, necessitating DC/AC inverters for AC grid compatibility. Many residential appliances like mobile chargers, LED lights, and electric vehicles also run on DC power, interfaced with AC systems via AC/DC rectifiers. These stages introduce AC to DC conversion losses, impairing efficiency. Establishing a DC residential system and directly powering DC loads from DC renewable sources emerges as a cost-effective solution. In an all-DC building, bypassing conversion stages can conserve 10–18% of energy. Despite growing DC adoption, a complete shift from 100% AC to 100% DC utility distribution remains unlikely. This study introduces a novel concept: the hybrid AC/DC nanogrid for residential structures. This technology seamlessly integrates the DC grid with existing AC infrastructure. The hybrid approach connects only DC loads to DC sub-grid, reducing intermediate AC-DC conversions. Hybridizing the AC grid enhances efficiency by minimizing conversion losses, improves system frequency and voltage profile, and boosts overall reliability. This hybrid architecture maximizes the advantages of both AC and DC, resulting in an efficient and cost-effective residential power system. The paper proposes an optimization-driven control enabling the community nanogrid to operate nearly independently, reducing reliance on the utility grid. Employing Pyomo and the Interior Point Optimizer (IPOPT) solver, a multi-objective optimization problem is solved to enhance efficiency and reliability. The efficacy of the approach is demonstrated on a 12-bus hybrid AC-DC nanogrid, highlighting its potential for residential power distribution network.

Keywords: Photon Upconversion, Dielectric resonator, Trapped mode

19. Carbon-Negative Hydrogen Production Through Plasma Processing of Waste Bio-Oils

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As the energy sector continues to move away from fossil fuels in search of a more reliable, renewable energy source, energy derived from hydrogen has proven to be a promising candidate. Specifically, the elimination of carbon emissions through carbon-neutral and carbon-negative hydrogen production allows for the continued combatting of greenhouse gas emissions while producing a sustainable method for storing renewable energy. Through the use of a multi-phase non-thermal plasma reactor and electrical discharges at ambient pressure and a temperature of 100˚C, waste bio-oil in the form of used soybean oil was processed and converted into liquid and gaseous products. Using a 90-10% by volume mixture of methane and hydrogen gas and 500 kJ/kg of energy input to the reactor results in the conversion of the waste bio-oil into hydrogen, other gaseous products, and potentially useful biofuels including gasoline and diesel left in the liquid phase at a higher efficiency than current traditional processes. Additionally, as this conversion process is carbon-negative it offsets more carbon than it contributes to the environment making it well suited for the changing environmental protection requirements for energy production.

Keywords: Carbon-Negative, Bio-oil, Hydrogen, Waste Oil, Plasma

20. Enhancing passive infrared sensing with solid state optical shutter for occupancy-based building energy control

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Efficient energy utilization within indoor environments is a pressing concern, especially for heating and cooling, which contribute to over 50% of household energy consumption. While conventional pyroelectric infrared radiation (PIR) sensors have been used to save energy through the detection of human motion, they fall short in identifying stationary occupancy, resulting in low accuracy, typically around 60%, in occupancy sensing, since it only responds to human motion. To address this limitation, our innovation leverages the polymer-directs liquid crystal (PDLC)-based solid-state optical shutter, optimized for mid-range Infrared (IR) wavelengths, replacing the standard Fresnel lens. This enhancement empowers the PIR sensor to discern even subtle stationary presence within indoor spaces with a high accuracy of 97.8%. This study introduces a novel AI powered sensor system poised to optimize Heating, Ventilation, and Air Conditioning (HVAC) smart control strategies while maintaining occupant privacy. This innovation holds promise for sustainable energy optimization, cost savings, and elevated occupant-centric comfort, especially in the face of energy cost saving, carbon emissions reduction goals, and mounting climate challenges.

Keywords: HVAC, Occupancy Sensing, PIR, PDLC, Optical Shutter

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Poster Session: Abstracts

21. Dielectric-Based Field Enhancement in a Subwavelength Cavity and its Application to Enhance Near-Infrared Photon Upconversion

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The ability to confine light is crucial in science and technology. Here we confine and concentrate electromagnetic field from incident light into a subwavelength layer, formed between an omnidirectional perfect reflector and an array of dielectric resonators (fig 1a). The confinement is obtained by enhanced forward scattering by the dielectric nano resonator array combined with perfect reflection at all angles (fig 1b) from the omnidirectional mirror at the incident wavelength. The electric field enhances (fig 1c) due to the excitation of resonance modes (Fabry Perot, waveguide-like modes) within this subwavelength spacing. Current field confinement techniques, however, rely on either plasmonic structures or metal nanoparticles, which suffer resistive losses and can quench excited electronic states. On the other hand, dielectric resonators are nearly free of such losses, do not provide relaxation pathways for excited electrons, and can simultaneously excite electric and magnetic resonances. The omnidirectional perfect reflector is also formed entirely of dielectric material. Here we design this novel cavity in the near-infrared wavelength and use the field enhancement to improve the photon upconversion (UC) luminescence (1540nm to 980nm) of the Erbium, Er3+, ion. Upconversion of infrared photons can be used to improve the efficiency of a silicon solar cell.

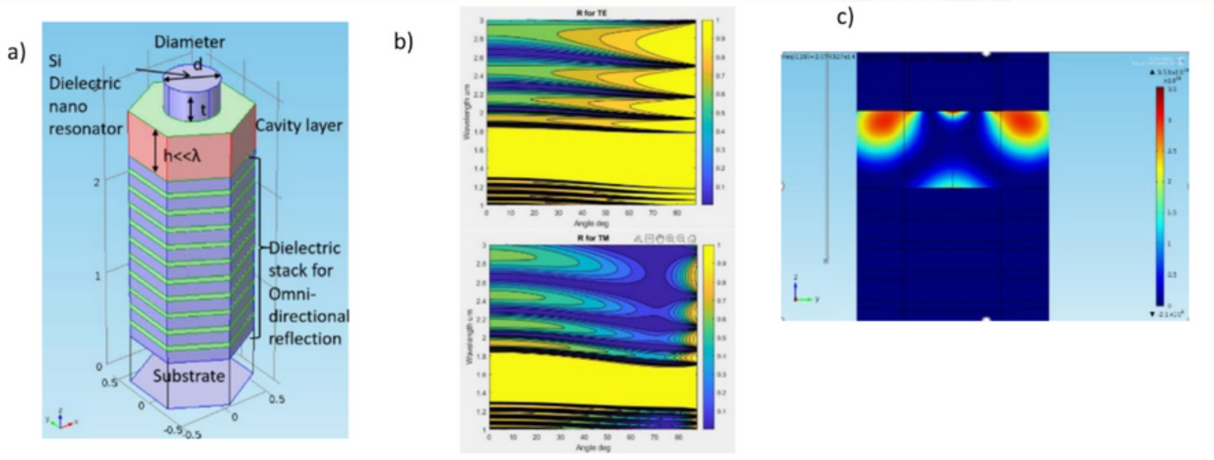

Figure 1: a) Unit cell of a hexagonal array of dielectric silicon(blue) nano resonator discs, the subwavelength cavity (red) of thickness h, and bottom omnidirectional perfect reflector on a silicon substrate. b) Reflectivity of dielectric stack as a function of incident angle and wavelength. Note that reflection =1 for all angles and polarization around 1.5µm. c) Enhanced electric field profile inside the cavity at resonance along y-z plane

Keywords: Photon Upconversion, Dielectric resonator, Trapped mode

22. Impact of Using Horizontal Wells on Aquifer Thermal Energy Storage System Efficiency

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Aquifer thermal energy storage (ATES) is a technique to conserve thermal energy while being environmentally friendly. ATES system stores excess thermal energy in the form of hot or cold water in groundwater aquifers. When there is a heating or cooling need, the stored water can be recovered from the aquifer and utilized. In recent decades, interest in implementing ATES systems and reducing carbon dioxide emissions has grown worldwide. However, more research is still needed to evaluate the feasibility of this system. This study aims to investigate the energy storage and production efficiency of ATES systems when horizontal wells are used. Though horizontal wells have never been applied in ATES practices, the technique is relatively mature and gained popularity due to its decreasing cost. By coupling horizontal and conventional vertical wells, we found the potential for the ATES system to cope with more complex or restraint subsurface environments. Various well-arrangement scenarios are simulated in COMSOL, a numerical modeling software. After comparing the resulting data, conclusions and suggestions are given on well-arrangement to maximize system efficiency under certain subsurface conditions.

Keywords: Geothermal, ATES, Numerical Modeling

23. Stable A_2BIrO_6 perovskite catalysts for improved oxygen evolution performance in acidic electrolytes

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Electrocatalytic water splitting for carbon neutral H_2 production is currently limited by the sluggish oxygen evolution reaction (OER). While high performance can be obtained in proton exchange membrane electrolyzers, the oxidizing potential and acidic conditions at the anode lead to rapid dissolution of most active OER catalysts. IrOx is one of few commercial catalysts with both high activity and stability, but its high cost prevents economical water splitting. Highly stable double perovskite catalysts with the stoichiometry A_2BIrO_6 exceed the activity of IrOx with a 60-70% decrease in Ir content by mass and limitless possibilities for tuning catalyst composition. Here, a series of double perovskites with A = Sr, Ba and B = Fe, Co, Y, In, La, Ce, Pr, Nd, Tb were synthesized via solid state reactions, tested for the OER using chronoamperometry in 0.1M $HClO_4$, and normalized by the electrochemical surface area to determine activity trends. Our goal is to relate the bond strength and coordination of Ir with OER intermediates to catalyst activity. Therefore, all perovskites were also characterized with H_2 temperature programmed reduction (TPR), O_2 temperature programmed oxidation (TPO), and CO chemisorption to understand surface oxygen lability. Together, these studies establish links between surface oxygen lability and OER activity in acid.

Keywords: Iridium, Double Perovskite, Oxygen Evolution, Water Splitting, Electrocatalysis

24. Atomistic simulations of chemomechanics at electrified interfaces

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As the world transitions to a more electrified future, the efficiency of a wide range of systems ranging from electric vehicles to power sources depends on our fundamental understanding of molecular mechanisms occurring at electrified interfaces. Deeper insights into reactivity and chemomechanics of interfaces in mechanical and electrical contact will enable us to design better surface structures and lubricants for efficient mechanical energy transmission across electric powertrains. Here, we perform ab initio density functional theory (DFT) calculations and reactive molecular dynamics (RMD) simulations to understand the surface reactivity and evolution of tribolayers at lubricant-substrate interfaces in electrified and non-electrified contact. DFT and RMD simulations also describe the composition and atomic structure of tribolayers, as well as the role of temperature, lubricant and surface chemistry, and electrification on the tribology of the surface. Specifically, atomistic simulations of polyalphaolefin (PAO) lubricants in contact with naturally-oxidized steel surfaces describe the decomposition of lubricant molecules leading to the formation of amorphous, non-protective FeC-rich tribolayers, which degrade upon mechanical loading. The formation of Fe-C bonds is enhanced by higher temperatures, presence of electric fields, and reducing agents in the PAO lubricant. Insights from these simulations can provide design rules for realizing more protective and crystalline tribolayers stable under extreme conditions of friction, temperature, and electrification.

Keywords: Atomistic simulations, Chemomechanics, Interface

Poster Session: Abstracts

25. High resolution modeling and analysis of cryptocurrency mining's impact on power grids: Carbon footprint, reliability, and electricity price

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Blockchain technologies are considered one of the most disruptive innovations of the last decade, enabling secure decentralized trust-building. However, in recent years, with the rapid increase in the energy consumption of blockchain-based computations for cryptocurrency mining, there have been growing concerns about their sustainable operation in electric grids. This paper investigates the tri-factor impact of such large loads on carbon footprint, grid reliability, and electricity market price in the Texas grid. We release open-source high-resolution data to enable high-resolution modeling of influencing factors such as location and flexibility. We reveal that the per-megawatt-hour carbon footprint of cryptocurrency mining loads across locations can vary by as much as 50% of the crude system average estimate. We show that the flexibility of mining loads can significantly mitigate power shortages and market disruptions that can result from the deployment of mining loads. These findings suggest policymakers to facilitate the participation of large mining facilities in wholesale markets and require them to provide mandatory demand response.

Keywords: Cryptocurrency mining; Carbon footprint; Reliability; Electricity market; Demand flexibility

26. Experimental Investigation of the nanoFin Effect (nFE) during Thin Film Evaporation from Nanopores using Temperature Nano-Sensors

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Recent advances in micro/nano-fabrication has enabled the deployment of nanostructured surfaces, nanochannels, and nanoporous membranes for development of new generation thermal management devices with remarkable potential for heat transfer enhancement. Anomalous heat transfer has been reported in studies involving heaters with nanostructured surfaces. For example, nanofins with lower thermal conductivity values can cause higher levels of enhancement in heat flux values, especially during phase change (such as for boiling on heaters with nanostructured surfaces). In addition, confinement of fluid in nanopores can also result in anomalous properties. This is manifest in anomalous production curves during hydraulic fracturing operations in oil and gas applications. A transport model that resolves these conundrums is termed as the "nanoFin Effect (nFE)". nFE is governed by interfacial phenomena, i.e., the formation of thermal impedances in parallel circuit configuration: (a) interfacial thermal resistance (also known as "Kapitza resistance"); (b) thermal capacitor; and © thermal diode (that form at the interface between each nanoparticle and the surface adsorbed thin-film of solvent molecules). nFE (i.e., primarily the interfacial thermal diode effect) also leads to preferential trapping of ions on the surface adsorbed thin film of solvent molecules leading to very high concentration gradients causing drastic reduction in corrosion. The motivation of this study was to explore nFE during thin film evaporation from nanopores. The methods used in this study include mounting a nano-thermocouple array (also termed as Thin Film Thermocouples or "TFT") on a hot plate and observing the transient response recorded by the TFT array when a small liquid droplet (of fixed mass or volume) is dispensed on to an isotropic AAO membrane containing nanopores. In this study, two different pore sizes were explored: 200 nm and 10 nm. The experiments were performed using acetone and isopropyl alcohol droplets for four different temperature settings of the heated membrane (containing the nanopores)

Keywords: Thin film evaporation; nanoFin Effect; Nano-sensors

27. Process Design and Intensification of Catalytic Fluidized Bed Membrane Reactor for Oxidative Coupling of Methane

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The catalytic oxidative coupling of methane (OCM) process has received intense interest in the literature due to the potential to directly convert natural gas to value-added chemicals at a reduced cost, energy consumption and carbon emissions when compared to more conventional processes, Tiemersma (2012); Onoja (2019). However, major challenges such as low yield, catalyst deactivation, and reactor scale-up still challenge the commercialization of this process. A promising solution to address these challenges is to develop innovative OCM reactor designs leveraging the recent advances in modular process intensification, e.g. micro-channel reactors and membrane reactors, Serres (2012); Patcharavorachot (2014). Moreover, the investigation of OCM reaction systems has mostly been focused on steady- state conceptual design, while ignoring the process dynamics which limits the applicability of evaluating the implementation for commercial use.

The aim of this work is to design an optimal OCM process at commercial scale leveraging the concept of modular process intensification, Pistikopoulos (2022). We investigate an intensified fluidized bed membrane reactor (FBMR) catalyzed by La_2O_3/CaO, and compare its performance to a conventional fluidized bed reactor (FBR). The use of membrane for oxygen feed distribution has been reported to result in better ethylene yield and selectivity by selectively enhancing the desired reactions, but also adds to capital cost investment and scaling up challenges. To systematically identify the optimal design solution, high fidelity FBMR and FBR models are developed in gPROMS ModelBuilder, which comprise partial differential algebraic equations accounting for mass balances, hydrodynamics, catalyst solid distribution, etc. detailed 10-step reaction kinetic model is adopted from Cruellas et al. (2020). The two reactor configurations are enhanced to obtain maximum performance, with the corresponding design parameters on reactor sizing, temperature, catalyst particle velocity, and membrane tube design (for FBMR).

Keywords: OCM, Dynamic Modeling, FBMR

28. Learning for Interval Prediction of Electricity Demand: A Cluster-based Bootstrapping Approach

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Accurate predictions of electricity demands are necessary for managing operations in a small aggregation load setting like a Microgrid. Due to low aggregation, the electricity demands can be highly stochastic and point estimates would lead to inflated errors. Interval estimation in this scenario, would provide a range of values within which the future values might lie and helps quantify the errors around the point estimates. This paper introduces a residual bootstrap algorithm to generate interval estimates of day-ahead electricity demand. A machine learning algorithm is used to obtain the point estimates of electricity demand and respective residuals on the training set. The obtained residuals are stored in memory and the memory is further partitioned. Days with similar demand patterns are grouped in clusters using an unsupervised learning algorithm and these clusters are used to partition the memory. The point estimates for test day are used to find the closest cluster of similar days and the residuals are bootstrapped from the chosen cluster. This algorithm is evaluated on the real electricity demand data from EULR (End Use Load Research) and is compared to other bootstrapping methods for varying confidence intervals.

Keywords: Time Series, Load Forecasting, Confidence Intervals, Machine Learning, Residual Errors.

29. Multifunctional materials for sustainable operation of Fluid Catalytic Cracking (FCC) process in petroleum refineries

Anuja Dnyaneshwar Patil, Utkarsh Mahajan

In the quest for sustainable and efficient petroleum refining, the Fluid Catalytic Cracking (FCC) process stands at the forefront of innovation. The energy sector's reliance on refined petroleum products underscores the critical role of FCC units in meeting global energy demands. This abstract explores the transformative potential of multifunctional materials in enhancing the sustainability and operational efficiency of FCC units in petroleum refineries. From catalyst design and coke management to heat recovery, emissions reduction, and resource efficiency, multifunctional materials offer versatile solutions that address diverse challenges. By fostering interdisciplinary collaboration and prioritizing sustainability assessments, these materials pave the way for a greener, more efficient, and economically viable future for FCC operations, aligning with the evolving energy landscape.

Venue Map

Memorial Students Center (MSC) Building
Level 2
Registration desk
Bethancourt Ballroom (2300A & B)
Gates Ballroom (2400)
Oral presentations (2404, 2405, 2500)
Poster Sessions /Networking (2406)
Bridge to Rudder Tower
Multicultural Services 2200
MSC Student Programs 2440
DoIT 2256
Reynolds Gallery 2221
Forsyth Galleries 2428
Forsyth Offices 2440
2401
2400
2460
2463
2406 A
2406 B
2405
2404
2403
2402
Kitchen 2311
2302
2301
2300 A
2300 B
2300 C
2300 D
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2503
2504
2505
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