PSTC Spring 2025 Meeting Abstracts

Automating Distillation Column Operations through Imitation and Reinforcement Learning

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This project will develop an intelligent system that can automate the role of human operators in distillation column operations at the Process Science and Technology Center (PSTC). By combining imitation learning and reinforcement learning techniques, a system will be created that can not only perform routine operations but also handle unusual interventions that typically require human expertise. The project will leverage existing operational data, the Aspen simulator, and novel machine learning (ML) approaches to create a robust automation solution that maintains safety and product quality while optimizing energy usage and throughput. This research represents a significant step toward autonomous operations at PSTC and, in general in the integration and exploitation of recent ML advances for industrial engineering and will generate fundamental insights into human-aligned reinforcement learning.

Facilitated Transport Membranes for Olefin/Paraffin Separation

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Historically, silver salt-based facilitated transport membranes for olefin/paraffin separation have been studied but not reduced to practice, due in large part to the chemical instability of the silver salts to contaminants that can be in such process streams, such as hydrogen and acetylene. We have recently discovered that certain silver salts, when added to rubbery polymers, have outstanding separation performance and are highly stable to the presence of compounds like hydrogen and acetylene. This presentation will focus on the scientific basis for this stability and discuss initial steps to reduce these membranes to practice.

Electrfied Distillation Processes

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We discuss opportunities in electrifying distillation processes. The presentation will cover speculative new diabatic column architectures enabled by electric heating, featuring fast startup/shutdown cycles and higher energy efficiency due to lower entropy creation. Further, the operation of these devices in the context of integrated chemical processes, and their interaction with the power grid will be discussed. Finally, we provide an update on the progress of the PSTC electrification upgrade.

Microporous Materials and Polymeric Membranes for Low Energy Separations

Kurtis Carsch

Department of Chemistry
The University of Texas at Austin

Abstract: The Carsch Research Group focuses on the design, characterization, and application of microporous materials and polymeric membranes for low-energy separation processes of major societal importance. Our approach centers on: (1) leveraging unconventional mechanisms with inspiration from fundamental chemical design principles, (2) developing sorbents that are intrinsically liquid or maintain porosity in the presence of liquids, and (3) engineering novel composites with robust physical properties. In this seminar, I will discuss the synthesis of a class of microporous materials capable of reversibly separating CO2 and CO at high temperatures, an unprecedented demonstration for adsorbents. Additionally, I will highlight the discovery of sorbents with record-breaking CO sorption capacities, enabled through an unusual mechanism of cooperative adsorption confined to a single metal site.

Post-Combustion CO_2 Capture with Amine Solvents

Fred Closmann, Gary Rochelle

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Dr. Closmann and Dr. Rochelle oversee research related to lowering the risk of post-combustion CO_2 capture with amine solvents by studying the mechanisms of amine degradation and emissions. Solvent degradation can occur through oxidation from high oxygen and NO_2 levels in incoming flue gases. Both flue gas constituents absorb into the solvent in the absorber packing and sump, resulting in free radical reactions, amine oxidation, and solvent loss. Oxidation products include compounds classified as hazardous air pollutants (HAPs) and ammonia which would likely be regulated under a CO_2 capture process plant permit. The current and future research conducted at the Pickle Research Center is designed to understand and mitigate these mechanisms."

Electromagnetic Heating for High Temperature Reaction Processes

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Texas A&M University

Electrified heating of chemical reactors represents a significant opportunity to reduce the carbon footprint of the chemical process industries. Specifically, endothermic reaction processes require energy input at high temperatures (> 500°C) that today is delivered by combustion of carbon-containing energy sources. Prominent high-volume examples include thermal cracking of hydrocarbons to produce ethylene, dehydrogenation of alkanes to produce light olefins, steam methane reforming, and catalytic reforming of naphtha to produce aromatics.

Electrification of these processes will require new methods of electrical energy input and new reactor and catalyst configurations. We are currently exploring radio frequency (RF) and induction strategies that can heat catalysts volumetrically, potentially reducing reactor volume by enabling isothermal operation. The biggest challenge, regardless of the electrification method chosen, is delivery of electrical energy inside the reactor, and we are prototyping designs to address this challenge.

Adsorption Process and Adsorbent Materials Research at USC

James A. Ritter

Department of Chemical Engineering
The University of South Carolina

This presentation will discuss on-going projects on pressure swing adsorption (PSA) in the Ritter Lab at USC. Some of the applications his group is studying include a new commercial 4-bed PSA system for natural gas conditioning, a bench scale demonstration of a 3-bed PSA system designed for CO2 capture and a novel pressure swing adsorption reactor for NH3 synthesis. Both experimental and process modeling results will be discussed. Other on-going and future projects will also be briefly discussed.

Membrane Technologies for Resource Recovery from Waste Water Streams

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Domestic and industrial wastewater reuse is a key component of a circular economy. In many cases, the economic viability of water reuse depends on the ability to recover value-added resources from these waste streams. To this end, membrane processes offer significant potential for selectively recovering resources such as critical minerals, nutrients, and salts. However, these processes are often hindered by membrane fouling, inadequate selectivity, and insufficient pretreatment. While previous studies have focused on membrane fouling in waters containing a single foulant, this presentation will explore the synergistic and antagonistic interactions among background water constituents, resources and foulants in complex waters typical of industrial wastewater.