

32nd Annual Meeting at Tuscaloosa, AL May 13th – 17th, 2023

NAMS 2023: A New Era of Sustainable Membrane Innovation

OVERVIEW OF WORKSHOPS

CONFERENCE CHAIRS Milad Esfahani, The University of Alabama Steven Weinman, The University of Alabama Jason Bara, The University of Alabama

https://membranes.org/nams-2023/ Embassy Suites by Hilton Tuscaloosa Alabama Downtown

Membranes for Water Treatment & Reuse Saturday May 13th, 2023, 9:00 AM – 5:00 PM

Lecturers:

Dibakar Bhattacharyya, University of Kentucky, <u>DB@uky.edu</u> Yoram Cohen, University of California Los Angeles, <u>yoram@ucla.edu</u> Ben Weaver, Solecta, <u>ben.weaver@solectamembranes.com</u>

ABSTRACT

Membrane processes are finding wide applications ranging from water treatment to reactors to advanced bioseparations. Membranes are particularly useful for material recovery and for permeate reuse (such as, water recycle). The workshop is configured as a one day program of about 6 hours of lectures. Both desalination and toxic pollutant removal/destruction techniques will be discussed. The workshop topics include membrane selection criteria, practical information regarding configuration, performance and operating conditions (including RO process control and fouling aspects) of membrane technology applied to desalination of brackish and seawater, and wastewater reclamation systems, mixed-matrix membranes. and advanced functionalized/responsive membranes from metal capture to emerging pollutants (PFAS) detoxification. Membrane surface and pore functionalization approaches, reactive nanostructured for water detoxification will be part of the advanced membrane topics. The effects of feed water quality, pretreatment options, operating parameters and performance of membrane units and hybrid options will also be discussed. The workshop material will also include information on economics of membrane systems including drivers for membrane selection for various applications, module design, industrial applications, etc.

Membrane Modeling and Simulation Saturday May 13th, 2023, 9:00 AM – 5:00 PM

Lecturers:

Mahdi Malmali, Texas Tech University, <u>Mahdi.Malmali@ttu.edu</u>, Nitish Mittal, ExxonMobil Corporation, <u>Nitish.Mittal@exxonmobil.com</u>, Udit Gupta, Siemens Process Systems Engineering Inc., <u>U.Gupta@siemens.com</u>,

ABSTRACT

This workshop provides the participants an opportunity to connect technical knowledge with modeling practices. We will start the workshop with a detailed introduction of the fundamentals of the transport mechanism in membrane and reviewing the key modeling parameters in modeling. The participants will be then introduced to the simulation software environment. The rest of the workshop will be mostly focused on hands-on practice examples using simple, but insightful, membrane problems. The simulation software will be available for the registrants through a cloudshare environment. Participants will be trained to create a process-level membrane model and conduct a sensitivity analysis using the software features. The developed model will be later imported into a process flowsheet. At the beginning of each hands-on session, a partial model will be provided. A fully-fledged model will be provided at the end of each session, which will be used in the subsequent session. A tentative outline of the workshop is provided below. Notes:

- Participants should bring their own laptops. For hands-on sessions, participants will connect to a cloudshare environment through an online browser (e.g., Google Chrome, Mozilla, Firefox, etc.). The simulations will be run on a remote cloudshare computer.

- Two weeks prior to the workshop, a review package will be made available to participants. This package includes slides, journal articles, and a summary note about the topics that will be discussed in the workshop.

- One week prior to the workshop, a survey will be forwarded to participants. The purpose of this survey is to determine the expertise of the participants in the modeling and simulation packages. Instructors will use this survey to familiarize themselves with the needs and expectations of the participants.

Mahdi Malmali is an assistant professor of Chemical Engineering at Texas Tech University. He received his M.S. in Chemical Engineering from Sharif University of Technology (2010) and his Ph.D. in Chemical Engineering from the University of Arkansas (2014). Dr. Malmali joined the Chemical Engineering and Materials Science department at the University of Minnesota as a postdoctoral research associate (2015-2017). Dr. Malmali joined Texas Tech University in 2018.

His research focuses on developing innovative reactions and separations, with the goal to decarbonize the chemical industry. He is particularly interested in designing advanced membranes, membrane-based separations, and reaction processes that can promote democratizing and decentralizing clean water and sustainable energy. Dr. Malmali utilizes process customized modeling and simulations for the energy analysis of reaction and separation processes.

Nitish Mittal is a Staff Research Engineer in Chemical Process Research division of ExxonMobil Corporation. Before joining ExxonMobil in 2018, he graduated with a Ph.D. in Chemical Engineering from the University of Minnesota where he developed fundamental and process model for inorganic membrane separation with applications in gas, chemicals and biofuels. Dr. Mittal has published eight peer-reviewed papers in high-impact journals and has been invited to present at international membrane conference venues including International Congress on Membranes & Membrane Processes and Gordon Research Conference Membranes: Materials and Processes. At ExxonMobil, Dr. Mittal works on the process development and scale-up of novel reaction and separation systems.

Udit Gupta is a Senior Consultant Engineer in the Energy & Chemicals Horizontal of Siemens Process Systems Engineering Inc. (SPSE). Before joining SPSE in 2019, he graduated with a Ph.D. in Chemical Engineering from the University of Minnesota where he developed microkinetic models for complex reaction networks using automated network generation. He also did postdoctoral research at University of Delaware developing modules for modeling chemical reaction systems. Dr. Gupta has published six peer- reviewed papers in high-impact journals. Dr. Gupta has been delivering technical training for SPSE's gPROMS Advanced Process Modeling Software to various Energy & Chemicals clients as well as conducting workshops at conferences.

Start	End	Туре	Title
9:00 AM	9:15 AM	Introduction	
9:15 AM	9:45 AM	Theory	Session-1: Transport mechanisms and models
9:45 AM	10:15 AM	Modeling	Session-2: Significance of modeling and synergy with experiments
10:15 AM	11:00 AM	Hands-on	Session-3: Introduction to the Simulation environment
11:00 AM	12:00 PM	Hands-on	Session-4: Developing a fundamental membrane model
12:00 PM	1:00 PM	Break	LUNCH
1:00 PM	2:30 PM	Hand-on/Demo	Session-5: Developing a membrane process model

Tentative session schedule:

2:30 PM	3:15 PM	Hands-on	Session-6: Sensitivity analysis and design specification
3:15 PM	3:30 PM	Break	
3:30 PM	4:30 PM	Demo	Session-7: Using membrane process model within a flowsheet
4:30 PM	5:00 PM	Wrap-up	Closing remarks

Note: We plan to use SPSE's gPROMS Advanced Process Modeling Software as the simulation platform as SPSE has agreed to provide free software licenses and cloudshare platform for the workshop. However, the topics and subjects covered in this workshop will be applicable to other software packages.

Session description for membrane modeling workshop

Session-1: Transport mechanism and models

This session will summarize the mechanism of membrane permeation, concept of driving force, and key modeling parameters in different types of membrane materials, and applications. We will compare various mechanisms, their implication on modeling, and scope of model transferability from one application to the other.

Session-2: Significance of modeling and synergy with experiments

We will discuss the advantages and limitations of the modeling, and how the synergy of experiments and modeling can be used to tackle a physical problem. We plan to demonstrate this by using a simple, but insightful, membrane problem that we plan to solve within this workshop. We will discuss how to convert the problem into equations relating key membrane parameters (e.g. permeability, selectivity, etc.), operating conditions (pressure and temperature), and required performance output (recovery, purity, etc.), and the role of experiments and modeling to obtain these quantities.

Session-3: Introduction to Model Simulation environment

Instructors will introduce the participants to the basic capabilities of the simulation software, such as, overview of the layout, how to write equations, simulate the model, and access the results. For this workshop, we will be using SPSE's gPROMS Advanced Process Modeling Software as the simulation platform.

Session-4: Developing a fundamental membrane model

During this session, participants will use the equations developed in Session-2 and incorporate them into the simulation software. In this hands-on activity, instructors will focus on important aspects of the simulation, such as membrane and modeling equations - rather than intricacies of the software itself. Hence, a partially-built model/template will be provided for the participant as the starting point.

Session-5: Developing a process membrane model

This session will cover the equations for integrating a membrane fundamental model into a process-level model. This will be a combination of demonstration and hands-on exercises. We will demonstrate how to implement a distributed model) ordinary differential equation) within the simulation environment. This partially built model will be provided as a template for hands-on exercise focusing on plug-flow model implementation. The concept of stage-cut and boundary layer resistance will be briefly discussed.

Session-6: Sensitivity analysis and design specification

During this session, we will teach how to use the developed model to study the effect of various operating conditions and key membrane parameters. Some of the software features will be used to scan through the output space/vector for the provided input space/vectors. Further, we will show how to back calculate the key membrane parameters or operating conditions for a given design specifications. The completed model from the previous exercise will be provided for this activity.

Session-7: Using membrane process model within a flowsheet

In this session, we will demonstrate how to use a membrane model in a process flowsheet connecting reactors and other separation units.

Membrane Gas Separations Sunday May 14th, 2023, 9:00 AM – 5:00 PM

Lecturers:

Benny Freeman, University of Texas at Austin, <u>freeman@che.utexas.edu</u> Glenn Lipscomb, The University of Toledo, <u>glenn.lipscomb@utoledo.edu</u> Tim Merkel, MTR Inc., <u>tim.merkel@mtrinc.com</u>

ABSTRACT

This workshop will cover the entire spectrum of membrane-based gas and vapor separations: from the materials science of gas separation membranes and the fundamentals of membrane transport to the design and economics of industrial gas separation applications. This workshop should be of interest to membrane researchers as well as membrane practitioners.

Outline:

- 1. Materials: Freeman, 9-10:30 AM
 - Material science of gas separation membranes and transport mechanisms
- 2. Break: 10:30-10:45 AM
- 3. Modules: Lipscomb, 10:45-12 and 1-2:15 PM
 - Module Manufacture (patent review)
 - Scroll/spiral wound module formation
 - Fiber bundle/tubesheet formation and types
 - Header and case design
 - Module Performance
 - Basic design equations for gas separations
 - Hollow fiber versus spiral wound
 - Module inefficiencies: fiber size/property variation & poor shell flow

distribution

- 5. Break: 2:15-2:30 PM
- 6. Applications: Merkel, 2:30-5 PM

Basics of Gas Separation System Design

- Pressure ratio
 - Multi-step and multi-stage configurations

Gas Separation Industry: History and Overview

Air Separation

- Nitrogen enriched Air
- Oxygen enriched Air

Hydrogen Separation

Natural Gas Separation

- Acid Gas Removal
- Nitrogen Removal
- NGL Recovery/Fuel Conditioning

VOC Removal/Recovery

Emerging Applications

Membranes in Bioprocessing Sunday May 14th, 2023, 9:00 AM – 5:00 PM

Lecturers:

John Cyganowski, MilliporeSigma, John.Cyganowski@emdmillipore.com Herb Lutz, MilliporeSigma, herb.lutz@milliporesigma.com

ABSTRACT

This workshop includes the use of membranes in bioprocessing for clarification, harvest, sterilization, virus retention, and protein concentration and buffer exchange.

MORNING SESSION 9AM-12 noon- Intro & Normal Flow Filtration

- 1. Overview (30' -10slides) Herb., key questions
 - History
 - Membrane types- show & tell
 - Bioprocess Applications & role of membranes.
- 2. NFF- clarification (30'-10 slides) Cyg
 - Membranes, devices, applications, operation- pleated/disk/pod devices
 - Pmax selection & sizing
 - Selected implementation topics- ads vs size excl, variability
- 3. NFF- sterilization (20'break, 50'-20 slides) Herb.
 - Membranes, devices, applications, operation-cartridge/pod.
 - Vmax selection & sizing.
 - Validation & Integrity testing.
- 4. NFF- virus retention (50').
 - Membranes, devices, applications, operation.
 - Vmax selection & sizing.
 - Validation & Integrity testing

AFTERNOON SESSION 1PM-5PM- Tangential Flow Filtration & Wrap-up

- 5. TFF- Protein concentration and diafiltration (80'-27slides; 10' break) Herb.
 - Membranes, devices, applications.
 - Operation- UF & DF- demo milk or w PXL50
 - Selection & sizing
 - Selected implementation topics-high conc?, HCUF, donnan, SPTFF?
- 6. TFF- clarification (50'-20 slides; 20' break) Cyg.
 - Membranes, devices, applications, operation- cassette, prostak/fiber/spiral
 - Selection & sizing
 - Selected implementation topics-harvest/cell removal? Perfusion.
- 7. Wrap-up (30').

• Manufacturers, economics, references, trends, selected topics-quiz? Continuous, closed system

After taking the workshop, participants will be able to define process requirements and select among different filters and size and optimize their operation. The workshop is of interest for membrane researchers, process development scientists, plant operators, and technical operations.