Scientific Schedule

UCTEA
CHAMBER OF CHEMICAL ENGINEERS
ISTANBUL BRANCH

4TH INTERNATIONAL PROCESS SYSTEMS ENGINEERING WORKSHOP ISTANBUL

4. ULUSLARARASI PROSES SİSTEMLERİ MÜHENDİSLİĞİ ÇALIŞTAYI İSTANBUL

PSE 2026 brings together world-leading researchers, candidates, and emerging scientists.

30.03-01.04
2026

Koç Üniversitesi
Anadolu Medeniyetleri
Araştırma Merkezi

The workshop will focus on integrating artificial intelligence, data-driven optimization, process intensification, and sustainable systems design, shaping the next generation of process engineering innovations.

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Kimya Mühendisleri Odası İstanbul Şubesi

March 30, 2026 (Monday)

Welcome and Introduction			
08:30-08:45	Welcome		Metin Türkay / Rafiqul Gani
08:45-09:00	Chamber of Chemical Engineers		Serkan Küçük

Session 1: Advances in PSE			
09:00-09:30	S1.1	Computational Strategies for the Optimization of Supply Logistics and Field Management of Carbon Dioxide Capture and Storage	**Ignacio E. Grossmann** CMU
09:30-10:00	S1.2	Federated Learning for Process Systems Engineering: Foundations, Quantum Enhancements, and Applications	**David E. Bernal Neira** Purdue Univ.
10:00-10:30	S1.3	Multiscale Design Strategies for Process and Product Design. Energy and Consumer Product Applications	**Mariano Martin** Univ. of Salamanca
10:30-10:45	Discussion		
10:45-11:00	**Coffee / Tea Break**		

Session 1: Advances in PSE			
11:00-11:30	S1.4	A General Optimization-Based Framework for Designing Flexible Chemical & Energy Systems	**Christos Maravelias** Princeton Univ.
11:30-12:00	S1.5	Optimizing Processes with Hybrid Models: Energy and Biomedical Case Studies	**Selen Cremaschi** Auburn Univ.
12:00-12:30	S1.6	Advances in Process Scheduling and Control for Chemical and Energy systems using Deep Reinforcement Learning Strategies	**Luis Ricardez-Sandoval** Univ. of Waterloo
12:30-12:45	Discussion		
12:45-13:45	**Lunch**		
13:45-14:30	**Free Social Time**		

Session 2: Artificial Intelligence			
14:30-15:00	S2.1	AI for Science and the Science of AI	**Venkat Venkatasubramanian** Columbia Univ.
15:00-15:30	S2.2	AI for Science and Sustainability: A Journey from Process Systems Engineering	**Fengqi You** Cornell Univ.
15:30-15:45	Discussion		
15:45-16:15	**Photo & Coffee/Tea Break**		

Session 3: AI-based PSE Tools			
16:15-16:45	S3.1	Digital Twins for Production/Distribution Systems	**Metin Türkay** Koç Univ.
16:45-17:15	S3.2	Leveraging LLMs in PSE Applications: from Prompt Design to Iterative Generation	**Xi Chen** Zhejiang Univ.
17:15-17:45	S3.3	Agent-based AI Augmented PSE Software Tools with Problem Solving and Learning Options	**Rafiqul Gani** PSE for Speed
17:45-18:00	Discussion		
18:30-19:30	**Banquet**		

March 31, 2026 (Tuesday)

Session 4: Integrated PSE			
09:00-09:30	S4.1	Protocol for Safety-Intelligent Cyber-Physical Monitoring and Control System in Energy Management Applications	**Stratos Pistikopoulos** Texas A&M
09:30-10:00	S4.2	Bridging Process Models and Practice: Model Based Design of Experiments Enabled Digital Twins for Biomanufacturing	**Marianthi Ierapetritou** Univ. of Delaware
10:00-10:10	Discussion		
10:10-10:30	**Coffee/Tea Break**		
10:30-11:00	**Special Session: Honoring Prof.Dr. Yaman Arkun**		

Session 4: Integrated PSE (continued)			
11:00-11:30	S4.3	Optimal Design and Operation of Renewable-Energy-Integrated Microgrids under Uncertainty	**Erdal Aydın** Koç Univ.
11:30-12:00	S4.4	Toward Scalable Lithium Extraction from Unconventional Feedstocks: A Process Systems Engineering Perspective	**Burcu Beykal** Univ. of Connecticut
12:00-12:30	S4.5	Process Systems Engineering Approaches for Sustainable Apparel Manufacturing	**Mohidus Samad Khan** BUET
12:30-12:45	Discussion		
12:45-13:45	**Lunch**		
13:45-14:30	**Free Social Time**		

Session 5: Augmented PSE			
14:30-15:00	S5.1	AI-Driven Multi-Scale Frameworks for Net-Positive Housing and WEFE Nexus Governance in the Global South	**Iqbal Mujtaba** Univ. of Bradford
15:00-15:30	S5.2	Physics Constrained Machine Learning for PSE Applications	**Faruque Hasan** Texas A&M
15:30-16:00	S5.3	Digital Twins for Health: A Process Systems Engineering Perspective with Applications in Drug Delivery	**Luke Achenie** Virginia Tech
16:00-16:30	S5.4	Artificial Intelligence-assisted Small Molecule Drug Design	**Lei Zhang** DUT
16:30-16:45	Discussion		

Session 6: Industry Presentations			
16:45-17:05	S6.1	Refinery-Wide Diesel Network Optimization	**Ahmet Can Serfidan** Socar Tech Türkiye
17:05-17:25	S6.2		**Emre Kuzu**
17:25-17:55	S6.3	From MILP to Learned Policy Constraint Aware Imitation Learning for Industrial Scheduling	**Mert Can Özcan** SmartOpt
17:55-18:15	S6.4	Application of Artificial Intelligence for Quality Prediction in Refineries	**Gizem Kuşoğlu Kaya** Tüpraş
18:15-18:35	S6.5	Process Simulation and Sustainability Assessment of Biohydrogen Production Integrated into an Istanbul Wastewater Treatment Plant: An Aspen Plus Study	**Sevim Özgül** Bahçeşehir Univ.

April 1, 2026 (Wednesday)

Session 7: PSE Perspectives			
09:00-09:30	S7.1	Next Generation Process Simulators: Hybrid and Agent-oriented Systems	**Seyed Mansouri** DTU
09:30-10:00	S7.2	Impact of Modeling Research on Pharmaceutical Process Development	**Hirokazu Sugiyama** Tokyo Univ.
10:00-10:30	S7.3	Probabilistic Deep lLearning-based Modeling for Thermal and Exergy Prediction in Organic Rankine Cycles	**Alfonso Mauricio Sales Cruz** UAM
10:30-10:45	Discussion		
10:45-11:00	**Coffee/Tea Break**		

Session 7: PSE Perspectives (continued)			
11:00-11:30	S7.4	Symbolic Regression and its Applications in Chemical Engineering	**Lakshminarayanan Samavedham** NUS
11:30-12:00	S7.5	On the Techno-Economics of Three Emerging Desalination Technologies: Adsorption, Hydrate-Based, and Membrane Distillation Systems	**Hassan Baqeel** KFUPM
12:00-12:30	S7.6	Mechanistic and Machine Learning Combined Examples from Health, Energy and Formulations	**Joan Cordiner** Univ. of Sheffield
12:30-12:40	Discussion		
12:40-12:50	**Closing Remarks**		
12:50-13:40	**Lunch**		

Computational Strategies for the Optimization of Supply Logistics and Field Management of Carbon Dioxide Capture and Storage

Ignacio E. Grossmann
Rudolph R. and Florence Dean University Professor,
Department of Chemical Engineering
Carnegie Mellon University

In this presentation, we first address in collaboration with TotalEnergies the profit maximization for shipping cryogenic carbon dioxide in Carbon Capture and Storage from emitters to a port for injection in depleted oil fields. For the supply logistics an MILP model is proposed based on a discrete-time Resource Task Network (RTN) where inventory levels of carbon dioxide at the ports are obtained along with the decision variables determined at each time interval. To solve the resulting large-scale MILP model, decomposition techniques based on bilevel decomposition and two-stage optimization decomposition are first proposed for the simpler case where trips (or milk runs) between emitter ports are not considered. For the real-life case that allows milk runs, a Lagrangean decomposition is proposed with a shrinking time horizon strategy for the solution of subproblems for long time horizons. As alternative solution strategies we also consider discrete-event simulation (DES) integrated with a simplified MILP model as well as a discrete-time constraint programming (CP) model. Several instances based on real data are solved by all five methodologies to compare their computational expense and solution obtained. The presentation next describes an advanced multiperiod MINLP model for reservoir simulation for CO_2 capture and storage. The system is defined with a fixed number of wells, well topography, well injection potential as a function of reservoir pressure, and reservoirs' pressure evolution as a function of cumulative injected volume. The problem is formulated as an MINLP model to determine an optimal field management plan over a long-time horizon, optimizing the number of injection wells and buffer tanks including penalizing the cost of venting. The output is a timeline of operations to open and close the wells as required, and the wellhead flowing pressures of each active well. We propose first a shrinking horizon approach to reduce the computational cost. Since the goal is to optimize over longer time horizons, this is followed using a sampling time indices approach, which when combined with a greedy heuristics algorithm allows the solution of practical problems with time horizons of up to 25 years.

Ignacio E. Grossmann is the Rudolph R. and Florence Dean University Professor in the Department of Chemical Engineering, and former department head at Carnegie Mellon University. He obtained his B.S. degree at the Universidad Iberoamericana, Mexico City, in 1974, and his M.S. and Ph.D. at Imperial College in 1975 and 1977, respectively. He is a member and former director of the Center for Advanced Process Decision-making, an industrial consortium that involves 20 petroleum, chemical, engineering, and software companies.
He is a member of the National Academy of Engineering, and Fellow of AIChE and INFORMS. He has received the INFORMS Computing Society Prize and the following AIChE awards: Computing in Chemical Engineering, William H. Walker for Excellence in Publications, Warren Lewis for Excellence in Education, Research Excellence in Sustainable Engineering, Founders Award for Outstanding Contributions to the Field of Chemical Engineering. In 2015 he was the first recipient of the Sargent Medal by the IChemE. He has honorary doctorates from Abo Akademi in Finland, University of Maribor in Slovenia, Technical University of Dortmund in Germany, University of Cantabria in Spain, Russian Kazan National Research Technological University, Universidad Nacional del Litoral, Argentina, Universidad de Alicante in Spain, RWTH Aachen, Germany, and Universidad Nacional del Sur, Argentina.
He has authored more than 700 papers, the recent textbook *Advanced Optimization for Process Systems Engineering, and the textbook Systematic Methods of Chemical Process Design*, which he co-authored with Larry Biegler and Art Westerberg. He has also organized the virtual library on process systems engineering. Grossmann has graduated 69 Ph.D. and 40 M.S. students. His main research interests are in the areas of mixed-integer and disjunctive programming, optimal synthesis and planning of chemical processes, sustainable energy and power systems, supply chain optimization, and stochastic programming.

Federated Learning for Process Systems Engineering: Foundations, Quantum Enhancements, and Applications

David E. Bernal Neira
Asst. Prof., Davidson School of Chemical Engineering
Purdue University

Federated learning (FL) is gaining recognition as a collaborative model development approach in process systems engineering, allowing organizations to train predictive models without sharing proprietary data. A recent tutorial (https://doi.org/10.1021/acs.iecr.4c03805) offers chemical engineers practical tools for implementing FL, with examples covering manufacturing optimization, multimodal data integration, and drug discovery. Comparative studies indicate that FL can match or surpass centralized methods, especially when datasets are heterogeneous.
Building on this foundation, we introduce QUAFFLE (Quantum U-Net Assisted Federated Flood Learning and Estimation), which merges quantum-enhanced U-Net layers into an FL pipeline for multimodal (SAR + optical) flood mapping. QUAFFLE tackles computational and communication bottlenecks by combining (1) FL to minimize data transfer, (2) quantum-enhanced layers based on gate-based and photonic computing paradigms to decrease parameter counts while maintaining expressivity, and (3) heterogeneous data fusion for more robust segmentation. QUAFFLE was named a finalist in NASA's Beyond the Algorithm Challenge (https://www.nasa-beyond-challenge.org/project-gallery/secquoia), demonstrating its potential for large-scale geoscience applications.

These efforts connect with wider advances at the intersection of FL and quantum computing, including tensor-network-based frameworks for healthcare (https://doi.org/10.1088/2632-2153/ad8c11) and the integration of quantum computing with fully homomorphic encryption for privacy-preserving ML (https://openreview.net/forum?id=Is6AZWd0g5). Together, the tutorial and QUAFFLE demonstrate how combining FL, quantum computing, and multimodal learning can unlock scalable, privacy-preserving intelligence for industrial and environmental systems, while outlining open challenges in communication efficiency, robustness, and hardware-software co-design that are central to process systems engineering.

David E. Bernal Neira is an Assistant Professor in the Davidson School of Chemical Engineering at Purdue University. His research centers on mathematical optimization, artificial intelligence, and computational methods for solving scientific and engineering problems, with applications in process systems, energy, and chemical engineering. His core expertise is in nonlinear discrete optimization, encompassing theory, algorithms, and software. He also leads research in quantum computing, with emphasis on quantum algorithms for optimization, computational chemistry, and machine learning. He has co-authored peer-reviewed publications, developed open-source tools, and delivered invited talks across academia, government, and industry. He has taught several courses, including one he co-designed on optimization, quantum computing, and machine learning. He collaborates broadly with researchers in academia, national laboratories, government agencies, and industry. At Purdue, he leads the SECQUOIA lab (Systems Engineering via Classical and QUantum Optimization for Industrial Applications).

Multiscale Design Strategies for Process and Product Design. Energy and Consumer Product Applications

Mariano Martín
Professor, Department of Chemical Engineering
Universidad de Salamanca

This work presents a multiscale design methodology that combines hybrid phenomenological and machine learning modelling, modular design and economies of numbers, together with simultaneous process, selecting technologies, and product design, for its application to the deployment of a more sustainable chemical industry. The methodology is tested in two cases of study. The first one deals with energy storage and management, designing the fluid that will be the energy or heat transfer fluid and the power plant. At process scale economic, safety, and environmental criteria are considered. Metrics are proposed and used for the systematic prescreening of alternatives at an early stage. Then, a detailed process analysis and optimization are considered for the most promising candidates. The units involved in the process are modelled first at a higher detailed level and then surrogate models are developed using machine learning techniques. The processes are optimized for different capacities. Process scale up/down strategies play an essential role for the facility to adapt to the availability of local resources towards strategic decision making. In addition, the methodology is applied to the design of novel ingredients for formulated products and their production out of renewable resources is also addressed. The product design step comes up with the ingredient, where machine learning is required for property prediction to be integrated within the molecular design formulation. Next, an integrated process and product design approach is formulated to obtain such a product selecting the most interesting biomass residue. The case of biosurfactant design is depicted.

Prof. Martín is full Professor of Chemical engineering at the University of Salamanca and member of the Royal Academy of Sciences of Spain. Mariano Martin graduated with honors in the integrated BSc and MSc in Chemical engineering at USAL in 2003. Prof. Martín completed his PhD on the analysis of multiphase reactors and received the Outstanding Thesis award in 2008 also at USAL. He joined Procter & Gamble as a postdoctoral Engineer at their technical center of Newcastle Upon Tyne where he led the last challenge in the laundry business for which he obtained the P&G award for its outstanding contribution to modelling and simulation. He was Fulbright Postdoc at Carnegie Mellon University working on the systematic design of renewable based processes before accepting the challenge of building a process systems laboratory in the oldest university in Spain. Prof. Martín's research interests focus on the systematic optimal design of processes and products using renewable based resources towards a more sustainable power, chemical and process industry. Prof Martin has been visiting prof. at CMU (US), UWM (US), Univ. Texas A&M (US), Univ Leeds (UK), Univ Birmingham (UK), Plapiqui (Argentina), UNC-Bogotá (Colombia), U. Guanajuato (Mexico), Udelar (Uruguay) or Univ Maribor (Slovenia) among others. Prof. Martín has been included within the 1% Top researchers in chemical engineering in the ranking by Univ. Stanford, he has authored over 200 papers in peer reviewed journals (h=45 SCOPUS), 65 book chapters, 2 monographic books and 3 textbooks for Elsevier, Springer in CRC Press. Prof. Martín has graduated 12 PhD's and over 70 Master students. He is executive editor of Chem. Eng. Sci, associate editor of J. Clean Production, LAAR and sits in the editorial board of Com. Chem Eng., Int. J Green Energy, PIOS among others.

A General Optimization-Based Framework for Designing Flexible Chemical & Energy Systems

Christos Maravelias
Anderson Family Professor in Energy and the Environment, Professor of Chemical and Biological Engineering
Princeton University

We present a general optimization framework for designing chemical and energy systems that experience variability at multiple timescales, motivated by an environmental need to decarbonize manufacturing, we seek to understand the viability of chemical and energy systems subject to temporal variability in physical and economic conditions. The proposed framework includes (1) a set of unit models, (2) a system specific superstructure, (3) a representative time structure, and (4) the corresponding mathematical program for operation-informed design. The framework can be applied to determine the basic configuration and size of unit operations, associated material and energy flows, and relevant state variables (like temperature and pressure). It is also possible to study optimal design between different cases and identify how optimal design evolves over time. Understanding these behaviors is key to designing processes that successfully operate under multi-scale variability. We apply our framework to study green ammonia synthesis and identify optimal process designs with distinct operational behavior at hourly, seasonal, and (multi-)yearly timescales.

Christos Maravelias is the Chair of the Department of Chemical and Biological Engineering, and the Anderson Family Professor in Energy and the Environment at Princeton University. His research interests lie in the general area of process and energy systems engineering and optimization. Specifically, he is studying production planning and scheduling, supply chain optimization, and energy systems synthesis and analysis with emphasis on renewable energy technologies. He has authored a research monograph on Chemical Production Scheduling and co-authored more than 200 journal articles. He is the recipient of numerous awards including the Computing in Chemical Engineering Award and the Sustainable Engineering Forum Research Award, both from AIChE; the Applied Research Challenge Award from the Production and Operations Management Society; and the Horizon Prize from the Royal Society of Chemistry.

Group website: https://cbe.princeton.edu/people/christos-maravelias

Optimizing Processes with Hybrid Models: Energy and Biomedical Case Studies

Selen Cremaschi
B. Redd & Susan W. Redd Eminent Scholar Chair Professor and Department Chair
Auburn University

Leveraging the growing capabilities of artificial intelligence (AI) and machine learning (ML) holds great potential to advance the fundamental understanding of the underlying phenomena for processing and biomanufacturing systems and to optimally design and operate them. These systems, unlike many of the native application domains of AI/ML algorithms, typically produce relatively structured data sets that may have poor information content and may not be abundant. Additionally, there is a wealth of accumulated knowledge about some of these systems. Therefore, the application of AI/ML techniques requires careful selection and customization to incorporate existing knowledge for processing and biomanufacturing systems.

Hybrid modeling, which combines first-principles models with data-driven models based on AI/ML algorithms, offers a promising approach. In this framework, the first-principles model captures known process knowledge, while the data-driven model addresses discrepancies due to incomplete understanding of the process mechanisms, thereby enhancing model accuracy. This talk will explore the strengths and challenges of building hybrid models for engineering applications using three seemingly disparate examples from energy and biomedical domains.

Dr. Cremaschi is the Chair, B. Redd & Susan W. Redd Endowed Eminent Scholar Chair Professor, and Head of the Cremaschi group in the Department of Chemical Engineering, Auburn University. Her research focuses on optimization, process synthesis, machine learning, and planning under uncertainty. Her group develops systems analysis and decision support tools for complex systems, mainly focusing on the biomanufacturing, pharmaceutical, and energy industries. She is a recipient of the NSF CAREER award (2011), the Zelimir Schmidt Award for Outstanding Researcher (2013), and the Senior Research Award for Excellence (2021), among others. She is a member of the 2018 Class of Influential Researchers selected by the Industrial and Engineering Chemistry Research journal. Her research work has been consistently supported by industrial collaborations in addition to federal agencies. She also serves on the Dow Chemical Company Digital Technology Advisory Board. She earned a Ph.D. from Purdue University and an M.S. and B.S. from Bogazici University (Turkey), all in chemical engineering.

Advances in Process Scheduling and Control for Chemical and Energy Systems using Deep Reinforcement Learning Strategies

Luis Ricardez-Sandoval
Professor, Department of Chemical Engineering
University of Waterloo

Optimal integration of scheduling and control decisions in chemical systems has gained interest as it provides economic advantages and promotes long-term sustainability. Recently, the use of Deep Reinforcement Learning (DRL) algorithms has emerged as an attractive option to generate policies for decision-making processes. Despite the novel applications of machine learning in chemical engineering and advanced energy systems, the application of such tools to address problems in process scheduling, process control and optimal process integration is limited but it is gaining traction. This talk will cover the latest DRL frameworks developed in our group to address problems emerging in process scheduling of batch plants, process control for emerging energy systems such as Chemical Looping Combustion (CLC), and the integration of scheduling and control decisions for a chemical manufacturing plant. The set of methods presented in this talk will illustrate the advantages and limitations of the incorporation of DRL as an alternative strategy to design online policies that can aid in the decision-making process during the operation of chemical plants and advanced energy systems.

Dr. L. Ricardez-Sandoval is a Professor in the Department of Chemical Engineering at the University of Waterloo (UW). Dr. Ricardez-Sandoval holds a Canada Research Chair (Tier II) in Multiscale Modelling and Process Systems and leads the development of methods for optimal design and operations management under uncertainty, the development of novel CO2 capture and conversion technologies aimed at reducing the carbon footprint, and computer-aided design of novel catalyst materials. Dr. Ricardez-Sandoval has published more than 235 journal articles, 80 full-length peer-reviewed conference papers, 5 book chapters and 1 book. Dr. Ricardez-Sandoval (h-index: 51) has 15 publications that each have been cited more than 100 times and has published numerous publications on optimal process integration, modelling and optimization of conventional and emerging CO2 capture technologies, atomistic and molecular design of novel catalyst materials for CO2 conversion, chemical looping combustion (CLC) technologies, and the implementation of machine learning (ML) methods for the optimal design and manufacture of nano-scale and macro-scale systems and materials. Dr. Ricardez-Sandoval's novel contributions in optimal process integration, multiscale modelling, process systems and CO2 capture and conversion technologies have been widely recognized by delivering multiple plenary and keynote talks at international conferences, leading the organization of top-tier conferences (e.g. International Program Chair: 2022 DYCOPS-CAB IFAC Symposium) and receiving multiple research-related awards, e.g., the 2024 D.G. Fisher Award sponsored by the Chemical Institute of Canada (CIC), the NSERC Discovery Accelerator Supplement (2017), and Ontario's Early Researchers Award (2015). Dr. Ricardez-Sandoval serves as editor of Computers and Chemical Engineering, Digital Chemical Engineering and the Canadian Journal of Chemical Engineering. More information about Dr. Ricardez-Sandoval's research activities can be found at the following links:
https://www.linkedin.com/in/luis-ricardez-sandoval-182b72298/
https://uwaterloo.ca/chemical-process-optimization-multiscale-modelling-process-systems/

AI for Science and the Science of AI

Venkat Venkatasubramanian
Samuel Ruben-Peter G.Viele Professor, Department of Chemical Engineering
Columbia University

The dramatic success of generative AI models in natural language processing and image synthesis has sparked great interest among researchers in science and engineering. However, there is a crucial difference between these applications and those in scientific research. Scientific applications are governed by fundamental laws of physics, chemistry, and biology, as well as constitutive relations and highly specialized knowledge of materials, processes, and systems. Although data-driven machine learning has immediate uses, the long-term success of AI in scientific fields will depend on effectively combining first principles with specialized knowledge. We need to transition from large language models (LLMs) to large knowledge models (LKMs) using hybrid AI.

Furthermore, an even more exciting opportunity lies in advancing the science of AI. The current state of LLMs resembles that of steam engines at the dawn of the Industrial Revolution in the 18th century. Engineers discovered steam power and used it in many ways before fully understanding its mechanics. It took around 80 years for the science of steam engines to evolve into statistical thermodynamics. Similarly, at the start of the automated cognition (i.e., AI) revolution, we find ourselves in a comparable situation– developing numerous applications while having a limited understanding of LLMs.

The key questions are: What is the science of LLMs? What new concepts and laws remain to be discovered? Consider this rather surprising and sobering historical fact: the innovators who developed steam engine technology were not the ones who developed its science. It was achieved by an entirely different group of pioneers– Carnot, Clausius, Kelvin, Maxwell, Gibbs, Helmholtz, and Boltzmann–who possessed very different skill sets. Is there a lesson for us in the LLM revolution? In this talk, I will discuss the challenges and opportunities in AI for science and the science of AI.

Professor Venkat Venkatasubramanian is the Samuel Ruben-Peter G. Viele Professor of Engineering at Columbia University. He earned his Ph.D. in chemical engineering from Cornell, M.S. in physics from Vanderbilt, and his B.Tech. from the University of Madras. He taught at Purdue University for 23 years. Venkat considers himself an artist in science, with a natural tendency to conduct curiosity-driven research in an impressionistic style, emphasizing conceptual issues over mere techniques. Venkat's research interests are diverse, spanning AI, systems engineering, theoretical physics, and economics, but with a focus on understanding complexity and emergent behavior across various domains.

Venkat is an elected member of the U. S. National Academy of Engineering. AIChE recognized him with the William H. Walker Award (2024), the Computing in Chemical Engineering Award (2009), and the designation of Fellow (2011). He received Doctor Honoris Causa from the Széchenyi István University, Hungary, in 2024. Venkat received the Norris Shreve Award for Outstanding Teaching in Chemical Engineering three times at Purdue University, as well as the Research Excellence Award. Three of his papers are among the ten most-cited papers in the 46-year history of Computers & Chemical Engineering. His 2019 paper on AI in chemical engineering is the most-cited paper in the AIChE Journal in the last 20 years. His first book, How Much Inequality is Fair?, was published in 2017. His second book, Emergence as Harmony: Mathematical Principles of Self-organization, Complexity, and Collective Behavior, is scheduled for publication in 2026 by Columbia University Press. Venkat's other interests include comparative theology, classical music, and cricket.

AI for Science and Sustainability: A Journey from Process Systems Engineering

Fengqi You
Roxanne E. and Michael J. Zak Professor in Energy Systems Engineering
Cornell University

Artificial Intelligence (AI) is rapidly transforming scientific discovery and sustainability research. While AI has advanced across many disciplines, key challenges in AI for Science and Sustainability (AI4S) remain closely aligned with the core methodologies of Process Systems Engineering (PSE). This talk traces a journey from rigorous systems theory and computational methods to the frontier of AI-driven innovation across materials, energy, agri-food, and climate systems.

We begin by highlighting recent theoretical and algorithmic advances in PSE and automation that offer a valuable bridge to modern AI paradigms. We then explore how PSE approaches can complement and enrich emerging AI techniques for building intelligent, data-driven systems. Through illustrative case studies, we examine the role of AI in sustainable energy systems, perovskite photovoltaic materials, biomass valorization, carbon capture, climate-smart food production, and quantum-enhanced materials discovery.

The presentation will also introduce the Cornell AI4S Initiative (CAISI) – a dynamic and collaborative ecosystem advancing research, education, and innovation in AI4S. With a focus on decarbonizing energy and agri-food systems, CAISI brings together interdisciplinary expertise to address sustainability challenges across scales. Attendees will see how foundational PSE principles can enable scalable, impactful AI solutions and will be invited to engage with this growing community at the intersection of systems engineering, AI, and sustainability.

Fengqi You is the Roxanne E. and Michael J. Zak Professor in Energy Systems Engineering at Cornell University. He serves as Co-Director of the Cornell University AI for Science Institute (CUAISci), Co-Director of the Cornell Institute for Digital Agriculture (CIDA), and Director of the Cornell AI for Sustainability Initiative (CAISI). He is a graduate field faculty member in Chemical Engineering, Computer Science, Electrical and Computer Engineering, Operations Research and Information Engineering, and several other programs. His research focuses on systems engineering theory and computational methods, with applications in materials informatics, energy systems, digital agriculture, and sustainability. He has published over 300 journal articles in journals such as Nature, Science, PNAS, Nature Sustainability, Nature Computational Science, Nature Food, Nature Communications, and Science Advances. His work has been featured in Science and Nature editorials, highlighted on dozens of journal covers (e.g., Energy & Environmental Science), and , and widely covered by major media outlets including The New York Times, BBC, Reuters, Forbes, The Guardian, Scientific American, National Geographic, and CNN. He has received over 30 major national and international awards and is a Fellow of AAAS, AIChE, and RSC.

Digital Twins for Production/Distribution Systems: A Process Systems Engineering Perspective

Metin Türkay
Professor, Department of Industrial Engineering
Koç University

The escalating complexity of global commerce necessitates a transition from traditional linear modeling to integrated, cyber-physical architectures. This presentation delineates a formal framework for the deployment of Digital Twins (DT) within the domain of Process Systems Engineering (PSE), focusing specifically on the end-to-end synchronization of production facilities and multi-echelon distribution networks. By leveraging real-time data streams and advanced optimization heuristics, the Digital Twin serves as a high-fidelity decision-support tool capable of managing the inherent stochasticity of modern supply chains.

In the context of PSE, a Digital Twin is defined not merely as a static simulation, but as a dynamic virtual mirror that maintains a bi-directional data exchange with physical assets. This architecture facilitates a "System-of-Systems" approach, where individual production nodes are digitally linked to logistics hubs and transportation corridors. The integration of Internet of Things (IoT) sensors and enterprise resource planning (ERP) data allows the twin to reflect the current state of inventory levels, transit delays, and manufacturing throughput, enabling proactive rather than reactive management. The core utility of a supply chain DT lies in its ability to solve large-scale, multi-period optimization problems.

The application of Digital Twins extends to the strategic mitigation of the bullwhip effect. By providing granular visibility across the distribution network, the DT allows for inventory management, transportation planning and sustainability accounting.

The convergence of PSE methodologies and Digital Twin technology represents a paradigm shift toward autonomous supply chain operations. By establishing a robust "Digital Thread" that connects production scheduling with downstream logistics, organizations can achieve unprecedented levels of agility and resilience. This talk concludes by addressing the computational challenges of scaling these twins across global networks with examples.

Metin Turkay is a Professor of Industrial Engineering at Koc University, Istanbul, Türkiye. He holds a PhD from Carnegie Mellon University (1996) and MS (1991) and BS degrees (1989) from Middle East Technical University. His research focuses on optimizations theory, mixed-integer programming, and development of novel solution algorithms for mixed-integer programming problems and machine learning. He is applying these theoretical developments on energy planning, sustainable energy, sustainable supply chain management and logistics, design of transportation system with special emphasis on sustainable supply chain and logistics and systems biology. Before joining Koc University in 2000 where he set up Systems Lab, he was principal consultant on optimization technologies at Mitsubishi Corporation Mizushima Research Center. His doctoral work and publications on generalized disjunctive programming was recognized with the 1997 Ted Peterson Student Paper Award by Computing and Systems Technology Division of AIChE. He is also the recipient of the Scientific and Technological Research Council of Turkey (TÜBİTAK) Career Award (2005), the TÜBİTAK Young Researcher Incentive Award (2006), Turkey's first IBM Shared University Research Award (2007), the IBM Faculty Award (2009) and the Open Collaborative Research Award by IBM Haifa Research (2012). He set up the Koc-IBM Supply Chain Research Center with funds from the IBM Shared University Research Award. In 2006, he was elected as the Chair of the EURO Working Group on Computational Biology, Bioinformatics and Medicine. Metin Türkay published over 150 papers and is the recipient of 14 international patents.

Leveraging LLMs in PSE Applications: from Prompt Design to Iterative Generation

Xi Chen
College of Control Science and Engineering
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Large Language Models (LLMs) have become valuable partners for engineers in fields such as software engineering and data science. In Process Systems Engineering (PSE), LLMs open new opportunities for addressing industrial challenges by providing automated, scalable, and tailored solutions. However, their application in PSE remains limited due to several practical challenges, such as ambiguous and underspecified prompts, managing tasks with intricate logical dependencies, and uncertainties in task complexity. A systematic framework consisting of three key strategies is proposed in this paper to deal with these challenges. The strategies, standardized prompt structure, task decomposition, and iterative generation can help engineers improve the precision and relevance of LLM's responses for PSE tasks. The framework is illustrated through practical applications including system decomposition, flowsheet ordering, process flowsheet visualization, process simulation and HEN synthesis. The results demonstrate how LLMs, when guided with structured methodologies, can enhance problem-solving in PSE, ultimately streamlining engineering workflows and decision-making processes.

Xi Chen is a professor in the College of Control Science and Engineering, Zhejiang University, China. He also serves as the director of the Institute of Industrial Intelligence and Systems Engineering and the deputy director of National Center for International Research on Quality-targeted Process Optimization and Control. His research interests include complex process modeling and optimization, parallel computation, symbolic computation, and industrial applications. He has published about 200 peer-reviewed international journal/proceedings articles. He also serves as an editor for IET Digital Twins and Applications, an associate editor for Journal of Process Control and an editorial board member of Computers & Chemical Engineering. He was enlisted in the Program for New Century Excellent Talents of the Ministry of Education, China in 2013 and the Program for Outstanding Talents of Zhejiang Province, China, in 2025. He received the Natural Science Award and the Science and Technology Progress Award of Ministry of Education in China in 2013 and 2005, respectively.

Agent-based AI Augmented PSE Software Tools with Problem Solving and Learning Options

Rafiqul Gani
CEO, PSE for Speed

The presentation will highlight two software tools in the areas of modelling, and separation operations. The tools offer one of the fundamental objectives of PSE, namely, problem solving options. Additionally, the tools include an educational module, which is designed as a complement to learning from courses, textbooks and research publications. The presentation will highlight several illustrative examples.

RAFIQUL GANI, PhD, is currently the CEO of PSE for SPEED, a company he co-founded in 2018 and is also a distinguished adjunct professor at HKUST (Hong Kong University of Science & Technology) in Guangzhou, and at ECUST (East China University of Science & Technology) in Shanghai, and a distinguished research professor at Széchenyi István University at Győr (Hungary). For 32 years, starting from 1985, Prof Gani worked at the Department of Chemical & Biochemical Engineering, Technical University of Denmark as professor in systems design, where he also founded the Computer Aided Process-Product Engineering Center in 1996. Prof Gani served as an editor-in-chief of Computers and Chemical Engineering journal (2009-2015) and currently serves as editor for the Sustainable Production & Consumption journal. He is also a member of the editorial advisory boards of several international journals, including Computers and Chemical Engineering and Current Opinion in Chemical Engineering. Prof Gani has been awarded five Doctor Honoris Causa degrees (University Politehnica Bucharest, University of Pannonia, Babes-Bolyai University, University of Maribor & Universidad Autonoma Metropolitana). Prof Gani served as the president of the European Federation of Chemical Engineering (EFCE) from 2015 to 2018, he is a member of the Danish Academy of Science, Fellow of two chemical engineering related associations (AIChE and IChemE), and also Fellow of two Artificial Intelligence related associations (AIAA and AIIA). He received numerous awards, for example, the AIChE Computers in Chemical Engineering award in 2015, the EFCE Jacques Villermaux Medal in 2019, the AIChE Sustainability Engineering Forum award in 2020, the IChemE Sargent Medal in 2021 and the Thomas and Donna Edgar CACHE Award for Excellence in Computing in Chemical Engineering Education given by American Society of Engineering Education in 2022. At PSE for SPEED Company, Prof Gani helps to develop, implement, and employ state of the art PSE methods and tools to solve a wide range of problems of industrial and research significance, reliably, efficiently, and very rapidly. He has published 570 articles in peer reviewed international journals and proceedings plus 5 edited books and 1 textbook. His publications have given him a H-index of 84 in Google Scholar, 69 in SCOPUS and 62 in Web of Science (January 2025). Prof Gani's current research interests continue with the development and application of AI based computer aided methods and tools for modelling; property estimation; process-product synthesis, design & intensification; and process-product-tools integration with emphasis on energy, sustainability, and application of a systems approach.

Protocol for Safety-Intelligent Cyber-Physical Monitoring and Control System in Energy Management Applications

Stratos Pistikopoulos
University Distinguished Professor
Dow Chemical Chair
Director, Texas A&M Institute
Editor-in-Chief, Computers & Chemical Engineering
Artie McFerrin Department of Chemical Engineering
Texas A&M University

Current safety systems typically create conflicts between safety objectives and operational performance, resulting in unnecessary shutdowns that may cost industries billions annually. The global process safety systems market reached $4.2 billion in 2024 and is expected to reach $6.5 billion by 2033, driven by increasing regulatory requirements and industrial safety concerns. Here, we address critical safety challenges in energy management systems through an integrated safety-aware monitoring and control framework that has the potential to transform how industrial processes manage safety and operational decision-making and optimization. We describe a protocol for the design of safety-intelligent cyber-physical real-time control systems by integrating dynamic risk assessment with advanced multiparametric model predictive control (mp-MPC) to enable proactive hazard prevention. This represents a paradigm shift by embedding safety barriers directly within real-time decision making, eliminating the separation between safety and control functions. We demonstrate the capabilities of the proposed framework in an integrated energy system involving a Proton Exchange Membrane (PEM) Electrolysis unit, a Metal Hydride Storage (MHS) device and a Proton Exchange Membrane Fuel Cell (PEMFC), and a Battery Safety Management System (BSMS), where operational risks such as thermal runaway, fuel starvation, and overcharging are considered. These risks compromise system reliability and efficiency while also posing significant safety hazards, particularly under dynamic operating conditions. It is shown that the proposed protocol simultaneously achieves safety assurance and operational optimization through real-time risk evaluation, automatic mode switching and overall intelligent, predictive and proactive decision-making capability.

Professor Pistikopoulos is the Director of the Texas A&M Energy Institute and holds the Dow Chemical Chair Professorship in the Artie McFerrin Department of Chemical Engineering at Texas A&M University. He was a Professor of Chemical Engineering at Imperial College London, UK (1991-2015) and a former Director of its Centre for Process Systems Engineering. He holds a Ph.D. degree from Carnegie Mellon University, and he worked with Shell Chemicals in Amsterdam before joining Imperial. He has authored or co-authored over 600 major research publications in the areas of modelling, data analysis, control and optimization of energy, process and systems engineering & automation applications, 15 books and 5 patents. A co-founder of Process Systems Enterprise (PSE) Ltd (now part of Siemens), he is a Fellow of AIChE and IChemE and the Editor-in-Chief of Computers & Chemical Engineering. Prof. Pistikopoulos was a co-recipient of the prestigious Mac Robert Award from the Royal Academy of Engineering in 2007, the recipient of the Computing in Chemical Engineering Award of CAST/AIChE in 2013, the IChemE's Sargent Medal in 2020, and the AIChE's Sustainable Engineering Forum Award in 2021. At Texas A&M, he received The Association of Former Students Distinguished Achievement Award for Research in 2021 and was named a University Distinguished Professor in 2023. He is a Fellow of the Royal Academy of Engineering in the UK, and a Member of the Texas Academy of Medicine, Engineering, Science and Technology.

Bridging Process Models and Practice: Model Based Design of Experiments Enabled Digital Twins for Biomanufacturing

Marianthi Ierapetrito
Bob and Jane Gore Centennial Chair of Chemical & Biomolecular Engineering
University of Delaware

Digital transformation is reshaping biopharmaceutical manufacturing, with Process Analytical Technology (PAT) and Digital Twins (DTs) enabling new opportunities for real-time monitoring, predictive modeling, and decision support. This work highlights advances in DT development for upstream processes, emphasizing metabolic, glycosylation, and fluid dynamics models as critical enablers of predictive capability. We present a Model-Based Design of Experiments (MBDoE) framework applied to a dynamic metabolic flux analysis (DMFA) model of Chinese Hamster Ovary (CHO) cells. Through identifiability and sensitivity analyses, we reduced a highly parameterized kinetic model to a simplified version with stronger predictive power and lower data demands. The refined model was validated across pseudo-perfusion and perfusion systems, demonstrating robust applicability at different scales. Using MBDoE guided by the Fisher Information Matrix, we iteratively designed informative experiments to reduce parameter uncertainty and improve model reliability. This approach enables more efficient experimental planning, conserves resources, and accelerates process development. Beyond methodological advances, we discuss challenges in DT implementation, tradeoffs between model complexity and predictability, and practical pathways for leveraging DTs to deliver original, impactful solutions for biopharmaceutical manufacturing.

Marianthi Ierapetritou is the Bob and Jane Gore Centennial Chair Professor of Chemical and Biomolecular Engineering at the University of Delaware. Previously a Distinguished Professor at Rutgers University, she also served as Associate Vice President spearheading initiatives that advanced women's STEM careers.

Her research spans process operations; design of flexible pharmaceutical production systems; energy-sustainability modeling, including biomass conversion and plastics recycling; and biopharmaceutical manufacturing. Her innovative optimization frameworks and digital twin methodologies greatly influence industrial practice and regulatory guidance worldwide today, significantly. Funding comes from FDA, NIH, NSF, DOE, ONR, NASA, and industrial partners such as Bristol Myers Squibb, Johnson & Johnson, GSK, Bosch, Eli Lilly, and PSE.
She has authored over 350 publications and numerous invited seminars worldwide. Honors include the 2025 Sargent Medal; the 2025 AIChE Margaret Hutchinson Rousseau Pioneer Award for Lifetime Achievement by a Woman Chemical Engineer, the AIChE's 2024 Excellence in Pharmaceutical Process Development and 2022 Excellence in Process Development Research Awards; the 2016 CAST Division Award in Computing in Chemical Engineering; the Society of Powder Technology Japan's PPD Award; the 2024 Rutgers College of Engineering Award for Service and Community Engagement; Rutgers' Outstanding Faculty Award and Board of Trustees Research Award; and the NSF CAREER Award. She became University of Delaware's Gore Centennial Chair in 2019, was promoted to Distinguished Professor at Rutgers University in 2017, and is an elected AIChE Fellow and former Board Director. She has also advised the FDA's Advisory Committee for Pharmaceutical Science and Clinical Pharmacology.
Dr. Ierapetritou earned her BS from the National Technical University of Athens, her PhD from Imperial College London, and completed postdoctoral research at Princeton University.

Optimal Design and Operation of Renewable-Energy-Integrated Microgrids under Uncertainty

Erdal Aydın
Asst. Prof., Department of Chemical and Biological Engineering
Koç University

Multi-energy microgrids integrate diverse energy carriers and technologies, including solar, wind, hydro, biomass, and conventional fossil-based units, to enable efficient, reliable, and low-carbon energy supply. The increasing penetration of renewable energy technologies and electrification-based transitions has intensified the need for systematic design and operational strategies that explicitly account for environmental, economic, and policy-driven challenges. In particular, uncertainty associated with renewable intermittency, energy demand, and carbon regulatory mechanisms plays a critical role in microgrid planning and operation.
In this talk, deterministic and stochastic optimization frameworks are presented for the optimal design and operation of renewable-energy-integrated multi-energy microgrids. The proposed decision-making models are formulated as mixed-integer linear and nonlinear programming (MILP and MINLP) problems and simultaneously address long-term investment planning and short-term operational scheduling. Uncertainties in hourly electricity demand, wind speed, solar irradiance, ambient temperature, carbon emission trading prices, carbon caps, and CO_2 emission limits are explicitly considered. The models aim to identify optimal technology portfolios and their hourly operating strategies that minimize the net present cost over a finite planning horizon while complying with emission and policy constraints. Case studies illustrate the impact of uncertainty modeling on technology selection, system flexibility, and cost-emission trade-offs.

Erdal Aydın received his BSc in Chemical Engineering from Middle East Technical University (METU), his MSc in Chemical and Biological Engineering from Koç University, and his PhD in Process Systems Engineering from the Max Planck Institute for Dynamics of Complex Technical Systems. He subsequently worked as a postdoctoral researcher at the Massachusetts Institute of Technology (MIT). He is currently a faculty member at Koç University, where his research focuses on optimization and design of energy systems, stochastic and dynamic optimization, artificial intelligence for process systems engineering, and optimal control.

Toward Scalable Lithium Extraction from Unconventional Feedstocks: A Process Systems Engineering Perspective

Burcu Beykal
Assistant Professor, Department of Chemical & Biomolecular Engineering
University of Connecticut

Lithium is the elemental backbone of modern energy storage systems, serving as the key functional material in the cathode and electrolyte of lithium-ion batteries. However, conventional mining and processing methods cannot keep pace with rapidly growing demand, creating severe constraints on the global lithium supply chains and necessitating new sourcing strategies. While salt lake brines remain the dominant source of lithium, the economic and environmental viability of alternative brines (e.g., geothermal) with moderate lithium concentrations is still underexplored at scale. A key barrier is the lack of sufficient data on pre- and post-recovery brine processing, including unit operations, operating conditions, and key process parameters. Moreover, a systems engineering perspective is required to identify process integration opportunities that can reduce energy and water consumption while producing high-purity Li_2CO_3–the preferred lithium product for batteries. In this talk, we will demonstrate a new process model for lithium recovery from geothermal brines using chemical precipitation. We will further discuss its techno-economic feasibility and environmental impacts through cradle-to-gate life cycle assessment, showing that low-concentration brines (<200 mg/L) are economically viable only under high product selling prices. Finally, we will discuss future pathways and supply chain considerations for enhancing resource recovery through direct lithium extraction.

Dr. Burcu Beykal is an Assistant Professor in the Department of Chemical & Biomolecular Engineering at University of Connecticut (UConn). She earned her B.S. in Chemical and Biological Engineering from Koç University, her M.S. in Chemical Engineering from Carnegie Mellon University, and her Ph.D. in Chemical Engineering from Texas A&M University. Her research focuses on process design for large-scale lithium extraction from marginal sources and on developing computational frameworks for data-driven optimization and reinforcement learning of complex simulation-based problems. She also works broadly on machine learning methods for chemical, environmental, and biological systems. Dr. Beykal's honors include the ACS Petroleum Research Fund Doctoral New Investigator Award, the 2020 AIChE CAST Directors' Award, and recognition as a Rising Star in Chemical Engineering by MIT. In May 2025, she was appointed the Eversource Energy Assistant Professor in Environmental and Sustainability Education by the UConn College of Engineering, in recognition of her achievements in research, education, and service.

Process Systems Engineering Approaches for Sustainable Apparel Manufacturing

Mohidus Samad Khan
Professor, Department of Chemical Engineering
Bangladesh University of Engineering and Technology

The apparel sector extends over the entire fiber-to-fabric value chain, which is rapidly growing to be a USD 4 trillion-dollar market by 2033. The apparel supply chain has grown into one of the most resource-intensive industrial systems, consuming over 79 billion m3 of water annually and contributing nearly 10 percent of global greenhouse gas emissions. In response, conventional sustainability initiatives have largely concentrated on end-of-pipe downstream treatment after production. Process Systems Engineering (PSE) approaches this challenge from a different decision level, reframing the problem at the system level. Through multiscale modeling, process intensification, numerical process synthesis, and supply-chain optimization, PSE improves sustainability through process redesign. This study demonstrates that Process Intensification efforts across apparel manufacturing can bring quantifiable sustainability benefits. Process intensification targets, methods, and performance improvements across the apparel sectors are defined through network-level analyses of tasks, operations, phenomena, and processes involved in yarn production, yarn preparation, weaving, and wet processing. Intensified yarn spinning technologies, such as compact spinning, reduce sizing chemical requirements by up to 50 percent and improve productivity by approximately 3-5 percent. In yarn preparation, ultrasound-assisted sizing and CO2-based sizing can reduce energy demand by nearly 35 percent and eliminate chemical consumption in selected applications. Further improvements can be made to the fabric formation stage. Process intensification through 3-D weaving and multiphase loom technologies reduces greenhouse gas emissions by up to 53 percent and energy demand by about 50 percent, while simultaneously increasing machine efficiency.
The largest sustainability gains occur in wet processing, which is the most water and energy-intensive stage of apparel manufacturing. Intensified dyeing and finishing technologies, including supercritical CO_2 dyeing, foam dyeing, and air dyeing, significantly reduce water and chemical consumption while maintaining uniform color distribution. These technologies also shift the viewpoint towards a regenerative operation, enabling recovery of water, solvents, and dyes. Complementary recovery strategies, such as caustic recovery, dye recovery, Zero Liquid Discharge, and waste heat recovery, further elevate resource and energy savings across the system. The results demonstrate that PSE integrated intensification has the potential to transform the current sustainability landscape of the apparel supply chain from unit operations to system-level impact.

Prof. Dr. Mohidus Samad Khan is a sustainability and biotechnology expert, researcher, and academician working as the Director of the Institute of Appropriate Technology (IAT) and a Professor of the Chemical Engineering Department at Bangladesh University of Engineering and Technology (BUET) (www.buet.ac.bd). His research interests include biotechnology and industrial sustainability. He also worked in the industry and development sectors. To date, Dr. Khan has authored and co-authored over 100 technical articles, including peer-reviewed journal and conference articles, international patents, industrial reports, books and book chapters. He also serves as a reviewer of several reputed international journals.
Dr. Khan completed his B.Sc. in Chemical Engineering (2004) from BUET in 2004. He completed his PhD in Bio-surface and Biotechnology (2006-2010) from Monash University, Australia. Dr. Khan worked as a Post-Doctoral Fellow at McGill University, Canada, to continue his research work (2010-13) on Bio-surface Engineering and Biomolecular Simulation. For his research in biotechnology, Dr. Khan received several prestigious awards. Since 2013, Dr. Khan has been working as a full-time faculty member in the Department of Chemical Engineering, BUET.
He served as a Visiting Professor (2015) at McGill University, Canada, and as a Visiting Research Scholar (2016-17) at Texas A&M University, USA. Dr. Khan also served as a Member of the Technical Advisory Group (2020-2021), Access to Medicines and Health Products Division, WHO Geneva (HQ).
Dr. Khan also has wide experience working in the industry and development sectors. He started his professional career working (2004-2006) in an international research project on Cleaner Production options, led by DFID and USAid. He is a certified trainer (CSP-US Department of State) for chemical inventory, management, and accountability. Dr. Khan works with local industries and international associations on sustainability and cleaner production issues. He worked as the Executive Director and the Chief Sustainability Officer (CSO) (2021-2023) of a multi-billion-dollar business conglomerate in Bangladesh. He has been featured in the 'Victorian Alumni Leaders of Industry' calendar 2024 by the Government of Victoria, Australia. Dr. Khan is also a Lien Environmental Fellow (2025-2026) awarded by the Nanyang Environment and Water Research Institute, Singapore.

AI-Driven Multi-Scale Frameworks for Net-Positive Housing and WEFE Nexus Governance in the Global South

Iqbal M. Mujtaba
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University of Bradford

Communities in the Global South face overlapping crises of climate stress, displacement, and resource scarcity, where housing and Water-Energy-Food-Environment (WEFE) systems interact in complex ways. Conventional interventions often treat these domains in isolation, underscoring the need for process systems engineering approaches that integrate optimization, machine learning, and participatory knowledge.

The SIAH-NP[1] project addresses challenges at the household and housing-system level in Jordan and South Africa through a net-positive design framework. More than 160 household datasets were processed using clustering and classification to identify socio-technical variability and climate-sensitive dependencies. Machine learning outputs informed digital twin environments coupling parametric 3D housing models with energy simulations. Multi-objective optimization quantified trade-offs among affordability, resilience, and net energy generation, while scenario analyses under stochastic inputs enabled identification of robust design candidates. Validation through stakeholder workshops linked computational outcomes with practical implementation, ensuring designs were technically optimized and socially grounded.

At the community scale, the CoMAP[2] project applies participatory digital mapping in refugee camps in Jordan. Youth-led data collection with Kobo Toolbox and OpenStreetMap was combined with qualitative interviews, structured through data science methods to transform narratives into actionable variables for decision-support frameworks. Integration of geospatial and social data enhanced understanding of infrastructure gaps and resource inequalities, supporting WEFE nexus governance under conditions of uncertainty.

Machine learning and data science act as unifying drivers, converting raw socio-technical and spatial data into predictive models, optimization routines, and decision-support systems. Embedding these methods within participatory frameworks establishes a paradigm where resilient housing and resource governance are designed as adaptive, data-informed systems.

[1]SIAH project contributors:
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Iqbal M. Mujtaba is Professor of Chemical Engineering, a Fellow of the Royal Academy of Engineering, and a Fellow of the IChemE. He was Associate Dean for Learning & Teaching from 2018-2025 and was Head of School of Engineering from 2016-2018. He was the Chair of the European Committee for Computers in Chemical Engineering Education from 2010-2013 and the Chair of the IChemE's Computer Aided Process Engineering Special Interest Group from 2012-2019. Professor Mujtaba leads research in distillation, energy, desalination and wastewater treatment. He has supervised 44 PhD students to completion and is currently supervising 10 PhD students. He has published over 420 technical papers including several books. He has organised and chaired several symposiums linked to Energy, Food and Water (Qatar, 2015; India, 2015; South Africa, 2016; Jordan, 2024). He has authored/co-authored textbooks (1) 'Batch Distillation: Design & Operation' (textbook) published by the Imperial College Press, London, 2004 (2) 'Wastewater treatment by Reverse Osmosis' published by CRC Press, 2020 (3) 'Desalination technologies: Design & Operation', Elsevier, 2022. He is one of the co-editors of the books (1) 'Application of Neural Networks and Other Learning Technologies in Process Engineering', Imperial College Press, London, 2001 (2) 'Composite Materials Technology: Neural Network Applications' CRC Press, 2009, (3) 'The Water-Food-Energy Nexus', CRC Press, 2017, (4) 'Water Management: Social & Technological Perspective', CRC Press, 2018.

Physics Constrained Machine Learning for PSE Applications

Faruque Hasan
Kim Tompkins McDivitt '88 and Phillip McDivitt '87 Faculty Fellow Professor of Chemical Engineering
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In process systems, the relationship between inputs and outputs is governed by mass and energy conservation laws, inter-variable dependencies, and operational constraints, often expressed as linear or nonlinear equalities and inequalities. Unlike purely data-driven models, physics-informed neural networks (PINNs) incorporate such laws into the training process, typically by adding penalty terms to the loss function. However, this soft-constraint approach does not guarantee exact constraint satisfaction. To address this limitation, we propose KKT-HardNet [1], a neural network framework that enforces exact satisfaction of nonlinear equality and inequality constraints during both training and inference. The method integrates a differentiable projection layer, based on the Karush-Kuhn-Tucker (KKT) conditions of a distance-minimization problem, directly into the network. A Newton-type iterative scheme is used to perform the projection efficiently. In this architecture, the multilayer perceptron serves as the feature extractor, while the projection layer ensures feasibility, thereby improving prediction reliability. We also provide an open-source, fully automated implementation of KKT-HardNet (https://github.com/SOULS-TAMU/kkt-hardnet). In this talk, we will describe KKT-HardNet with several applications related to process simulation, thermodynamically consistent hybrid modeling of molecular properties, and optimal control. We will also discuss data-driven discovery of governing equations [2] that can be embedded in KKT-HardNet as hard constraints towards a novel hybrid data-driven/mechanistic approach for modeling complex process systems.

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[2] Golder, R.; Hasan, M. M. F. Discovering Interpretable Ordinary Differential Equations from Noisy Data. arXiv:2507.21841.

Faruque Hasan is a Professor of Chemical Engineering at Texas A&M University and an Associate Director of the Texas A&M Energy Institute. He received his B.Sc. in Chemical Engineering from Bangladesh University of Engineering & Technology in 2005 and a Ph.D. from National University of Singapore in 2010. After a postdoctoral training at Princeton University, he joined Texas A&M University in 2014. His research interests include nonlinear optimization and machine learning with applications to integrated molecular and process design, computer-aided process intensification, design of carbon capture, utilization and storage, sustainable hydrogen economy, energy storage, and circular economy. Hasan is the recipient of a CAREER award from the U.S. National Science Foundation, Outstanding Young Researcher Award from the American Institute of Chemical Engineers (AIChE) Computing and Systems Technology (CAST) Division, I&EC Research 2019 Class of Influential Researchers Award, New Directions Award from the American Chemical Society (ACS) Petroleum Research Fund, Ralph E. Powe Junior Faculty Enhancement Award, and Best Paper Awards from Computers & Chemical Engineering (2015) and Journal of Global Optimization (2017). His research has been externally funded by the U.S. National Science Foundation, U.S. Department of Energy, American Chemical Society Petroleum Research Fund, Oak Ridge Associated Universities, and several industries. He served as a Director of AIChE CAST Division and was a member of the U.S. National Academies of Science, Engineering and Medicine (NASEM) Committee on 'Atmospheric methane removal: Development of a research agenda'.

Digital Twins for Health: A Process Systems Engineering Perspective with Applications in Drug Delivery

Luke Achenie
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Virginia Polytechnic Institute and State University

Digital twins (virtual, data-driven representations of physical systems that evolve in real time) are increasingly recognized as a transformative paradigm for health and biomedical engineering. While the concept originated in manufacturing and aerospace, many of the foundational ideas underpinning digital twins in health draw directly from process systems engineering (PSE), including system-level modeling, multiscale integration, dynamic simulation, data reconciliation, optimization, and uncertainty quantification. This workshop presentation provides a focused review of digital twins for health through a PSE lens, highlighting how established systems methodologies can be adapted to address the complexity, variability, and uncertainty inherent in biological and clinical systems.

The review surveys major application areas such as physiological and organ-level digital twins, patient-specific disease modeling, and healthcare system twins. Emphasis is placed on the integration of first-principles mechanistic models (e.g., transport phenomena, reaction kinetics, and pharmacokinetics/pharmacodynamics) with data-driven and AI-based models, mirroring long-standing hybrid modeling strategies in PSE. Core PSE concepts–including model reduction, parameter estimation, feedback and control, optimization, and verification, validation, and uncertainty quantification (VVUQ)–are discussed as essential enablers for building trustworthy and deployable digital twins in health.

Building on this review, the presentation will highlight the author's ongoing research on digital twins for drug delivery as a unifying and high-impact application area. This work explicitly leverages PSE methodologies to couple molecular-scale modeling, transport and distribution models, and patient-specific physiological data into

predictive, multiscale digital twins of drug delivery in complex biological systems. These frameworks aim to support rational therapeutic design, individualized dosing strategies, and improved prediction of efficacy and toxicity, extending classical PSE ideas of process design and optimization into the domain of personalized medicine.

The presentation concludes by outlining open research challenges and opportunities, including scalable multiscale coupling, hybrid physics-AI modeling, regulatory considerations, and workforce development. Overall, this contribution positions digital twins for health as a natural extension of process systems engineering into the biomedical domain, with drug-delivery digital twins serving as a compelling exemplar of how PSE principles can drive innovation in next-generation healthcare.

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Dr. Luke Achenie has B.S. (Chemical Engineering at MIT), M.S. (Engineering Science at Northwestern University), an MS in Applied Mathematics and Ph.D. in Chemical Engineering at Carnegie Mellon University. After three years at Shell Development Company in Houston, he joined the University of Connecticut in 1991 in the Chemical Engineering department. He was the Director of the School of Engineering Computing Services. He is currently at Virginia Tech as a Professor in Chemical Engineering. He served as the Program Director of the Reaction and Engineering Program at NSF in 2012.

Dr. Achenie's work is in several different interdisciplinary fields including process design, molecular modeling, AI/Machine Learning, multi-scale modeling and uncertainty analysis. He is a pioneer in molecular design, a subset of computer aided product design. This is an advanced simulation model that addresses the systematic design of chemical compounds with desired physical and chemical properties, with the goal of producing computer based "designer" compounds. He has also worked to develop entirely new formulations for flexibility analysis that considers accuracy of uncertain parameters in physical models.

Artificial Intelligence-Assisted Small Molecule Drug Ddesign

Lei Zhang
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Dalian University of Technology

Drug research and development is a protracted and systematic challenge. It is estimated that the chemical space of drug-like molecules exceeds 1060. How to screen or design a batch of lead drug molecules with high druggability potential from this enormous chemical space constitutes the primary issue to be addressed in small-molecule drug discovery. In recent years, the rapid advancement of artificial intelligence (AI) technology has dramatically transformed the paradigm of drug discovery. In particular, the remarkable success of AlphaFold in both academic and industrial sectors has brought brand-new opportunities and challenges to drug discovery. Taking the open-sourcing of AlphaFold 3 as a historical milestone, this report divides the research related to AI-assisted small-molecule drug design into the pre-AlphaFold and post-AlphaFold eras. It presents a complete workflow framework for lead drug discovery, spanning from the prediction of protein target binding sites and drug-target binding affinity to virtual screening and de novo drug design, thereby offering a novel AI-driven alternative to the traditional experimentally trial-and-error-based model of drug R&D. Meanwhile, the report deliberates on key questions in the post-AlphaFold era: what can protein models do for us? What unresolved problems persist in the field of AI for Science? And most importantly, how can we effectively tackle the challenges of new drug discovery amid the booming development of artificial intelligence?

Lei Zhang is a Professor of School of Chemical Engineering, Dalian University of Technology since 2024. He was an Associate Professor during 2017-2023 at Dalian University of Technology. He was a Postdoctoral research fellow at Hong Kong University of Science and Technology and Technical University of Denmark (2014-2017), and a visiting scholar at Carnegie Mellon University (2013-2014). He received BS and PhD degrees from Tsinghua University in China (2009-2014). His current research interests include development of methods and tools for chemical product and process design integrated with information and computing technologies, AI for Science, computational chemistry and molecular simulation. He received the best paper award (2017) from the Computers and Chemical Engineering journal, the PSE Young Researcher Award (2019) issued by PSE – Systems Engineering Society of China, RINENG Young Investigator Award of Results in Engineering Journal (2023), Future Chemical Engineer Scholars (2025) issued by Global Academy of Chinese Chemical Engineering Scholars, Hou Debang Chemical Engineering Science and Technology Youth Award (2025) issued by CIESC.

Refinery-Wide Diesel Network Optimization

Ahmet Can Serfidan
Data Science Manager
Socar Tech Türkiye

This study presents a comprehensive “Refinery-Wide Diesel Network Optimization” framework implemented at the refinery to bridge the gap between individual unit operations and final product blending. The project initially focused on the major diesel-producing units, utilizing a novel, in-house developed soft sensor modeling technique to predict T95 of diesel product. The continuous, real-time predictions were integrated directly into the plant operations, enabling operators to execute immediate manual interventions based on inferential data rather than waiting for delayed laboratory results. Moving beyond unit-level control, the scope was expanded to the refinery macro-level by using these real-time T95 and Density inputs to model the dynamics of the diesel blending tanks. This end-to-end digitalization creates a holistic view of the diesel network, allowing for precise tracking of quality properties from the distillation columns to the storage tank, thereby significantly reducing quality giveaway and optimizing the final blend composition through enhanced operational visibility.

I am driven by the power of applying data solutions to address complex, real-world challenges. I firmly believe that deep domain knowledge is the cornerstone of this pursuit. By continuously aligning technical capability with business context, I ensure that project objectives are clear and constraints are well-defined. As a result-oriented professional, I excel in breaking down intricate problems into manageable tasks to deliver high-impact outcomes.

From MILP to Learned Policy Constraint Aware Imitation Learning for Industrial Scheduling

Mert Can Özcan
Chief Technology Officer
SmartOpt

Mixed-integer linear programming (MILP) is widely used for scheduling and planning because it can solve complex, constrained problems to optimality, but it requires significant compute time and commercial solvers with high cost, and each new instance must be solved from scratch. This makes repeated daily optimization expensive and slow. In this work we leverage the fact that near-optimal MILP solutions can serve as high-quality labeled data. We have collected over a year of optimization runs from a global washing-machine factory and develop a constraint-aware imitation learning framework that learns to mimic the expert behavior of the MILP solutions. The model maps plant state (inventory, demand look-ahead, lead-time effects, and sequence history) to the next action, using a temporal transformer to encode full-horizon dynamics and a graph attention network to capture relationships among feasible actions; hard feasibility rules are enforced via action masks. The aim is to train a policy that can be used either as a warm-start to accelerate MILP or as a standalone scheduler, reducing time, cost, and computation.

Mert Can Özcan is the Chief Technology Officer and a founding engineer at SmartOpt. He completed his undergraduate studies at Koç University, Turkey, with a double major in Computer Science and Business Administration and earned an M.S. in Computational Science and Engineering. His thesis, conducted under Prof. Dr. Metin Türkay, focused on solving planning optimization problems with reinforcement learning. He began his career as a founding engineer and full-stack systems/software engineer, building servers and software architectures for SaaS supply-chain optimization applications. He later shifted his research focus toward optimization and machine learning.

Application of Artificial Intelligence for Quality Prediction in Refineries

Gizem Kuşoğlu
Head of Digitalization
Tüpraş

Petroleum refineries handle a diverse range of crude oil types to produce high-value products, including liquefied petroleum gas (LPG), diesel, gasoline, and jet fuel. Production starts with crude oil units (CDU) and continues through cracking and treatments processes. Integrating artificial intelligence into all process units in the refinery is essential for supporting operational decision-making. In these settings, AI applications primarily focus on predicting product quality, thereby enhancing efficiency and ensuring consistent output standards. Prediction models can be integrated in process control systems or utilized as monitoring dashboards via AI-based digital twins to prevent some processing costs. In this study, prediction models were created and then used for the optimization of reactor temperature. Machine learning models are embedded for optimization and chemometric models are used for increasing number of laboratory measurements. All these models provide predictions with high accuracy.

Gizem Kuşoğlu Kaya is Head of Digitalization at Turkish Petroleum Refineries Corporation (TÜPRAŞ), where she leads a multidisciplinary team working on data-driven and AI-based solutions for refinery operations. She holds a PhD in Chemical and Biological Engineering from Koç University, with a thesis on modeling of the Delayed Coker Unit. Her professional experience spans process modeling, advanced process control, real-time optimization, and the development of machine learning and deep learning applications for industrial processes. She also manages international research projects and supports the implementation of agile practices and emerging technologies such as robotics, edge computing, and quantum computing in refinery digital transformation initiatives.

Process Simulation and Sustainability Assessment of Biohydrogen Production Integrated into an Istanbul Wastewater Treatment Plant: An Aspen Plus Study

Sevim Özgül
Asst.Prof., Energy Systems Engineering
Bahçeşehir University

This study presents a comprehensive process simulation and sustainability assessment for hydrogen production from biogas generated at a municipal wastewater treatment plant (WWTP) in Istanbul. The proposed system aligns with circular economy principles by valorizing organic waste. The process model, developed in Aspen Plus V11, encompasses the key stages of biogas purification, hydrogen production via steam methane reforming, and subsequent purification. For the final hydrogen purification step, a Pressure Swing Adsorption (PSA) model was implemented using the Cyclic Steady State methodology to accurately predict product purity and recovery. The overall model employs the Peng-Robinson equation of state for accurate thermodynamic property predictions.

The simulation investigates the effects of critical operating parameters, such as reformer temperature (750-950°C) and steam-to-methane ratio (2.0-4.0), on hydrogen yield, purity, and overall process efficiency. Simulation results, benchmarked against the reported hydrogen production efficiency of 65.8% for a similar biogas-to-hydrogen pathway, demonstrate that the integrated WWTP case can produce high-purity hydrogen (>99.9%) with a competitive energy efficiency ranging between 65% and 70%. The sustainability assessment combines the simulation output with a preliminary life-cycle thinking approach to evaluate the system's carbon footprint reduction potential and its role in enhancing the resource efficiency of the urban water-energy nexus. This work provides a validated techno-environmental model that can serve as a decision-support tool for integrating renewable hydrogen production into existing urban infrastructure, contributing to Türkiye's sustainable energy goals.

Sevim Özgül is Asst.Prof., Energy Systems Engineering at Bahçeşehir University

Next Generation Process Simulators: Hybrid and Agent-oriented Systems

Seyed Mansouri
Assoc. Prof, Department of Chemical and Biochemical Engineering
Technical University of Denmark

The challenges in orchestrating complex industrial processes—whether in biomanufacturing, supply chains, or sustainable fuel production—stem from their inherently nonlinear dynamics, the opacity of real-time measurements in harsh environments, and the escalating demands for resilience amid global disruptions and decarbonization mandates. Traditional centralized control architectures, reliant on exhaustive sensor arrays and rigid optimization routines, falter under these uncertainties, leading to suboptimal yields, safety vulnerabilities, and inefficient resource use. As articulated in seminal perspectives on agentic AI in process systems engineering, these limitations underscore the urgent need for paradigms that harness emergent intelligence from distributed, adaptive entities to bridge sensing gaps, infer hidden patterns, and enact proactive decisions. In this perspective, we have revitalized the foundational Adaptive Agent-Oriented Software Architecture, the very blueprint that powered early distributed AI innovations like Apple's Siri—and evolved it into the Adaptive AgentOriented System Control (AAOSC) framework. By integrating MQTT-brokered publish-subscribe communication, redundant servers, hybrid physics-informed ML/SML models, digital twins, and a hierarchy of specialized AI agents (Sensor, Simulator, Executive, and domain-specific Control Agents), AAOSC operationalizes agentic autonomy at an industrial scale. The four case studies presented herein—spanning supply chain security, closed-loop biomanufacturing control, quantumenhanced anomaly detection, and prospective optimization of digital twin for biomass-derived sustainable aviation and maritime fuels—collectively demonstrate AAOSC's prowess: reducing deviation durations, averting shutdowns in severe fault scenarios, and boosting efficiency through virtual sensing and decentralized reasoning, all while aligning with regulatory imperatives for safety and sustainability. Looking ahead, AAOSC charts a pathway toward fully autonomous, regulator-ready cyber-physical ecosystems that not only minimize human fatigue-related risks– a leading cause of incidents in manufacturing—but also democratize advanced control for decentralized operations worldwide. Future implementations must prioritize hybrid edge-cloud deployments for low-latency actuation, robust cryptographic protocols for agent authentication in multi-stakeholder networks, and qualification frameworks compliant with FDA/EMA standards for biopharma and food production. Extensions could incorporate multi-logic decision ensembles within agents, quantum-accelerated reasoning for ultra-fast inference, and seamless integration with emerging generative models for predictive scenario generation. By thus extending agentic principles from consumer interfaces to mission-critical sustainability challenges, AAOSC promises to catalyze a new era of resilient, equitable industrial intelligence, where computational agents tirelessly safeguard and optimize the physical world.

Soheil Mansouri is an Associate Professor in the Department of Chemical and Biochemical Engineering at the Technical University of Denmark (DTU) since 2018. He was formerly an affiliate faculty member at the Sino-Danish Center for Education and Research in Beijing, China. He earned his PhD (2016) and MSc (2013) in Process Systems Engineering, both from DTU.

His research focuses on Process Systems Engineering (PSE), System Dynamics, Computational Agility (including AI and Quantum Computing), and Socio-Economic-Technological Analysis of Complex Dynamic Systems. He specializes in Process Synthesis, Design, Control, and Intensification, with applications in the chemical, pharmaceutical, and bio-manufacturing sectors.

Dr Mansouri is a senior member of the American Institute of Chemical Engineers (AIChE) and serves as the Danish representative to the Computer Aided Process Engineering (CAPE) Working Party of the European Federation of Chemical Engineers (EFCE). He is also current president of the European Committee for the Use of Computers in Chemical Engineering Education (EURECHA). Additionally, he acts as the international exchange coordinator for the AIM-Bio Program, a $27 million initiative between DTU and NC State University, funded by the Novo Nordisk Foundation. Furthermore, he contributes to the Biosolutions Zealand project, a major partnership aimed at developing a biomanufacturing hub in Denmark's Zealand Region, with total funding of approximately $12 million from the European Regional Development Fund. Since 2024, he is coordinating a 10 million EUR project funded by EU Commission to bring forward mobile and modular manufacturing of biofuels for decarbonizing the shipping industry, where they are heavily involved in developing a continent-wide integrated value chain digital twin from molecular and reaction dynamics all the way to enterprise and supply chain.

Within the domain of PSE - an interdisciplinary field in chemical and biochemical engineering - Dr Mansouri develops systematic methods and tools based on mathematical models and computational techniques for the analysis, design, operation, control, and optimisation of process systems. Recently, his work in the Biosolutions Zealand project has addressed the economics of scale in biomolecule production systems, integrating PSE with pilot-scale validation. He maintains strategic partnerships with international companies, and is a co-founder of SiC Systems Inc., Ensemble Biosystems Inc., Anaeco Inc. and Sqale ApS.

Impact of Modeling Research on Pharmaceutical Process Development

Hirokazu Sugiyama
Professor, Department of Chemical Systems Engineering
The University of Tokyo

The speaker and his team in UTokyo have been conducting PSE research on pharmaceutical processes covering a wide range of drug types and leveraging various modeling techniques. For small molecules (or synthetic molecules), flow synthesis of drug substances has been the main focus. Novel models on various reaction systems (e.g., Grignard reaction, amination, hydrogenation) have been proposed which were applied to determining design spaces and optimal conditions (e.g., Chem Eng Sci, 2025). For biopharmaceuticals, hybrid modeling (Ind Eng Chem Res, 2022) and data-driven (Comput Chem Eng, 2024) approaches have elucidated critical changes in cell metabolic behavior (Biotechnol Prog, 2024) and enhanced mechanistic process understanding. Data-driven approaches have enabled transfer learning of anomaly detection models across different industrial freeze-dryers (Comput Chem Eng, 2025). For stem cell / regenerative medicine, models for cell cultivation and cryopreservation have been developed (AIChE J, 2024; Chem Eng Red Des, 2024), and the model-based design space / optimal conditions have been experimentally validated (Commun Biolog, 2025; Cryobiology, 2024). Social-scale research is also the interest of the team. Most recently, an indicator-based assessment was performed regarding potential supply risks for pharmaceutical excipients, which identified critical compounds that would need mitigation actions (Int J Pharm, 2024). All these studies illustrated the power of model-based process development with actual cases, and also the importance of interactions between experimental and simulation researchers. Being conscious of the "cost of modeling" would help effectively determine the target of model-based development (Curr Opin Chem Eng, 2025).

Hirokazu Sugiyama studied chemical engineering at The University of Tokyo (BEng in 2001, MEng in 2003), and earned PhD from ETH Zurich (2007). Subsequently he joined F. Hoffmann-La Roche in Switzerland, and held different positions in a start-up facility of biological drug product manufacturing with increasing responsibilities. His last position was Head of Prefilled Syringe Production. In 2013 Dr. Sugiyama was appointed as an associate professor at Department of Chemical System Engineering, Graduate School of Engineering, The University of Tokyo, and started his academic career. He became a full professor in 2021, and is currently the head of the department.

Probabilistic Deep Learning–based Modeling for Thermal and Exergy Prediction in Organic Rankine Cycles

A. Mauricio Sales-Cruz
Professor, Departament of Process and Technology
Universidad Autónoma Metropolitana

Energy recovery from waste and residual energy streams is regarded as a key factor in reducing carbon emissions and improving sustainability metrics. However, a major challenge in the analysis of complex process systems exists, which lies in the construction of accurate and reliable process models that are required for simulation, optimization, design, and control. When first-principles physics-based models are found to be computationally intensive, or when the governing mechanisms are only partially known, data-driven surrogate modeling is adopted as a practical alternative. In this talk, fully connected feedforward deep learning architectures are described as nonlinear surrogate models to capture process behavior and to predict thermal and exergy efficiencies from noisy measurement data. The surrogate models are trained to represent high-dimensional, nonlinear process dynamics while accounting for the uncertainty inherent in measured data. Overall, this study is positioned as a contribution to process intensification methodologies by enabling efficient, data-driven modeling frameworks for energy recovery systems based on industrial exhaust and waste-energy sources.

Dr. Mauricio Sales-Cruz, PhD in Chemical Engineering by the Technical University of Denmark, is a professor and researcher at the Process and Technology Department, Universidad Autónoma Metropolitana campus Cuajimalpa (UAM-C), Mexico, since 2006. He has held various leadership roles including Head of the Process and Technology Department (UAM-C, 2009-2013), Director of the Natural Science and Engineering Division (UAM-C, 2017 - 2021), Secretary of the UAM campus Cuajimalpa (2016-2017),General Coordinator of Institutional Information at the Universidad Autónoma Metropolitana (2021-2025), and presently, he is rector of UAM, Campus Cuajimalpa (2025-2029)
During his career, Dr. Sales-Cruz has also been a guest professor at the CAPEC, Technical University of Denmark (2014-2015), and has contributed significantly to various research and academic institutions. Notable among his previous roles are his contributions to the National Development Support for Handicrafts (FONART) in Mexico (1995-2000), and as a researcher at the Mexican Petroleum Institute (2000-2001), and as a professor at Universidad Autónoma Metropolitana, Mexico (1994-1995) and Universidad del Valle de Mexico (1993-1996). He has also served as a guest researcher at the Department of Chemical Engineering and Materials, University of Cagliari, Italy (1992).
His areas of research interest lie in the domains of heat, momentum, and mass transfer, along with modeling, analysis, design, and simulation of chemical and biochemical processes, aided by computers. He has been recognized for his academic contributions, receiving awards such as the recognition of academic merit for the master's degree awarded by the UAM-Iztapalapa (2001), the Who's Who in Science and Engineering award by the Editorial Marquis (2006), and the "Most cited author 2006 -2009" award for Chemical Engineering Research and Design. A member of the National System of Researchers (SNI) at Level 1 from 2008-2022, and at Level 2 for the period 2023-2027, Dr. Sales-Cruz has a prolific publication record, including 12 book chapters, 65 papers in indexed journals with international arbitration, and numerous full-length reports. He has also shared his expertise through presentations at several national and international conferences, as well as through invited lectures.

Symbolic Regression and its Applications in Chemical Engineering

Lakshminarayanan Samavedham
Assoc. Prof., Department of Chemical Engineering
National University of Singapore

The process of constructing models from data is at the heart of many scientific fields including chemical engineering. Our field has been characterized as difficult to model but easy to control due to the complicated chemistry, physics and biological mechanisms involved and the relatively slow dynamics exhibited by chemical and environmental systems. Elucidating models using process/experimental data has been an extremely well-researched field – starting from classical system identification to the more recent machine learning approaches. While these methods result in models that provide a good mapping from input variables to output variables, engineers are more comfortable with deploying solutions that are based on transparent/explainable models. Symbolic Regression is a powerful method (enacted through genetic programming, neural networks etc.) optimizes both the structure and parameters of the chosen model class and results in transparent and often interpretable equations. This talk will present the origins and recent advances in this field along with some real-world applications covering static and dynamic systems. Lakshminarayanan Samavedham is an Associate Professor at the Department of Chemical and Biomolecular Engineering, National University of Singapore. His interests lie in Process Data Analytics, System Identification and Dynamic Optimization of Chemical and Biomedical Systems.

On the Techno-Economics of Three Emerging Desalination Technologies: Adsorption, Hydrate-Based, and Membrane Distillation Systems

Hassan Baaqeel
Dean, College of Chemicals and Materials
King Fahd University of Petroleum & Minerals

Emerging desalination technologies are increasingly being explored to address freshwater scarcity while reducing energy consumption, operational costs, and environmental impacts associated with conventional thermal and membrane-based processes. This presentation provides techno-economic assessments of three emerging desalination technologies: adsorption desalination, hydrate-based desalination, and membrane distillation (MD) systems. In addition, hybridized configurations are evaluated to examine their potential for improved economic performance.

Adsorption desalination is evaluated both as a standalone technology and in hybrid configurations, highlighting its ability to operate using low-grade heat and to simultaneously produce cooling. The integration of adsorption desalination with direct contact membrane distillation is shown to significantly enhance freshwater production, gain output ratio, and economic performance through effective waste-heat recovery.

Hydrate-based desalination, employing refrigerant hydrates such as R-152a, is examined as a salinity-independent alternative with reduced specific energy consumption. Further integration with a dual-effect absorption refrigeration cycle enables the utilization of exothermic hydrate formation heat, substantially lowering electricity demand, operating costs, and carbon dioxide emissions.

Hassan Baaqeel is the Dean of the College of Chemicals and Materials at King Fahd University of Petroleum & Minerals (KFUPM), where he leads academic and research initiatives across chemical engineering, materials science, chemistry, and bioengineering.

His work focuses on developing sustainable process systems that address critical challenges in water, energy, and resource management, with particular emphasis on advanced desalination technologies, low-carbon hydrogen production, and gas monetization. Dr. Baaqeel holds a PhD in Chemical Engineering from Texas A&M University and has extensive academic, industrial, and leadership experience spanning KFUPM, Saudi Aramco, and international research collaborations. He also serves as a Steering Committee Member of the Hydrogen Future Consortium (H2FC), a collaborative platform dedicated to accelerating the development and deployment of hydrogen technologies.

Mechanistic and Machine Learning Combined Examples from Health, Energy and Formulations

Joan Cordiner
Professor, School of Chemical, Materials and Biological Engineering
University of Sheffield

There are benefits of using the strengths of mechanistic modelling along with machine learning methods. Example will be presented in speeding up development of mRNA, optimising energy and heat provision for chemical production sites and predicting stable formulations for agrochemicals. The different techniques that are best for each type of modelling will be discussed along with challenges for future endeavours.

Professor Joan Cordiner
Head of the School of Chemical, Materials and Biological Engineering