SCHOOL OF
CHEMICAL ENGINEERING
College of Engineering, Architecture and Technology

CHE-PETE SEMINAR SERIES

Optimizing Experiments: From Data-Driven to Intrusive Model-Based Methods

ALEXANDER DOWLING, PH.D.

ENGINEERING NORTH 450

APRIL 14 | 3-4PM

Laboratory and computational experiments are often time and resource-intensive, which motivates the fundamental question: how to optimally design an experimental campaign (e.g., sequence of experimental conditions) or an experimental apparatus (e.g., select sensors) to maximize the value of information gained under a constrained budget? In this seminar, I will share our recent experiences using data-driven Bayesian optimization, classical model-based experiment design, and hybrid approaches. This will include an overview of recent methodological advances in uncertainty quantification and optimal experiment design in the computational open-source Pyomo ecosystem. I will summarize the key benefits of each approach, offer recommendations on selecting the most suitable method for a specific problem, and provide best practices.

References

Alexander (Alex) Dowling is the Tony and Sarah Earley Collegiate Associate Professor of Energy and the Environment at the University of Notre Dame (Indiana, USA). He is in the Department of Chemical and Biomolecular Engineering, with a concurrent appointment in Applied and Computational Mathematics and Statistics.

Prof. Dowling's research combines chemical engineering, computational optimization, machine learning, and data science, organized in three research themes: (1) molecular-to-systems (multiscale) modeling and optimization, (2) optimal design of experiments and statistical inference, and (3) machine learning for bridging timescales. Application domains include energy markets and infrastructure, integrated energy systems, carbon sequestration, sustainable hydrogen, critical mineral recycling, advanced separations (membranes, ionic liquids), and systems biology. His research group contributes to several open-source scientific computing projects, including the Institute for the Design of Advanced Energy Systems (IDAES). Within the Pyomo project, Prof. Dowling's group leads the development of instructive uncertainty quantification and optimal experiment design capabilities.

Prof. Dowling has been recognized with an NSF CAREER award (2019), the CAST Outstanding Young Researcher Award from AIChE (2025), the Junior Sargent Medal from IChemE (2023), the university-wide Mentoring Award from the Graduate Student Government (2023), the James A. Burns, C.S.C., Award (2025), and two R&D 100 awards. He holds a B.S.E. from the University of Michigan - Ann Arbor and a Ph.D. from Carnegie Mellon University, all in chemical engineering.