Angan Mukherjee

Department of Chemical and Biological Engineering, University of Wisconsin-Madison
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EDUCATION

West Virginia University 2019–2024
Ph.D. in Chemical Engineering
Minor: Process Controls, Statistics
Advisor: Prof. Debangsu Bhattacharyya
Research Area: Process Systems Engineering, Machine Learning, Optimization
GPA: 4.00/4.00

Jadavpur University, Kolkata, India 2015–2019
B.E./B.S. in Chemical Engineering
GPA: 9.23/10.00
1^{st} rank in a class of 86 students

EXPERIENCE

University of Wisconsin-Madison Aug 2024-present
Postdoctoral Research Associate
Advisor: Prof. Victor M. Zavala
- Research focus on developing new scalable paradigms for uncertainty-aware data-driven modeling, optimization, and decision making, including digital twins.
- Developed novel approaches for data analytics using topology for applications in process monitoring, control, and visualization of proteins, polymers, and metallic glasses.

West Virginia University Aug 2019-Aug 2024
Graduate Research Assistant
- Developed innovative sparse AI/ML tools for efficient data-driven modeling of complex process systems.
- Developed mass, energy, and thermodynamics constrained machine learning models and training algorithms for transient chemical processes under uncertainty.
- Developed open-source software for formulating physics constrained ML models in chemical engineering.
- Developed hybrid first principles - artificial intelligence models for accurate and affordable modeling of clean energy systems.

Indian Institute of Technology, Kharagpur, India May 2018-Jul 2018
Indian Academy of Sciences (IAS) Summer Research Fellow (Supervisor: Prof. Indranil Manna)
- Developed approaches for preparation and isothermal oxidation of HVOF and APS coated samples.

Indian Institute of Technology, Kharagpur, India May 2017-Jul 2017
Summer Research Intern (Supervisor: Prof. Rabibrata Mukherjee)
- Worked on evaporation and condensation on slippery surfaces.

CSIR–Central Glass & Ceramic Research Institute, Kolkata, India Dec 2016-Jan 2017
Winter Research Intern (Supervisor: Dr. Sourja Ghosh)
- Worked on treatment of dye-containing wastewater using ceramic membrane-based filtration and adsorption.

PRODUCTS

Journal Publications

[1] **Mukherjee, A.**, Kung, P., Annamareddy, A., Morgan, D., Voyles, P., and Zavala, V. 2026. Topological Data Analysis for Complex Correlation Spectroscopy Data. *(under preparation)*

[2] Barajas-Villarruel, L.R., **Mukherjee, A.**, Buzhardt, J., Graham, M., Rico-Ramírez, V., and Zavala, V. 2026. A Latent Space Approach for High-Dimensional Optimal Control. *Computers & Chemical Engineering* [under review]

[3] **Mukherjee, A.**, Giridhar, N., and Bhattacharyya, D. 2026. On the Automatic Discovery of Optimal Hybrid First Principles-Machine Learning Models for Process Systems. *Computers & Chemical Engineering* [under review]

[4] **Mukherjee, A.**, Park, B., Malmstrom, A., Cisewski-Kehe, J., Van Lehn, R., and Zavala, V. 2026. Scalable Extraction of Information on Protein-Protein Interactions using Topological Data Analysis. *bioRxiv preprint bioRxiv:2026.08.06.743405.* [link]

[5] Das, P., **Mukherjee, A.**, and Bhattacharyya, D. 2026. VIBES – A Two-Stage Scalable Bayesian Uncertainty Quantification Framework: Application to a Biomass Valorization Process. *arXiv preprint arXiv:2607.06743.* [link]

[6] **Mukherjee, A.**, Soderstrom, T., Kurtz, M., and Zavala, V. 2026. Topological Data Analysis for High Dimensional Dynamic Process Monitoring. *Computers & Chemical Engineering*, 216: 109883. [link]

[7] Flory, J., **Mukherjee, A.**, Dauenhauer, P., and Zavala, V. 2026. Computing Optimal Programs for Programmable Catalysts using Bayesian Optimization. *Computers & Chemical Engineering*, 216: 109919. [link]

[8] **Mukherjee, A.** and Zavala, V. 2026. Physics-Constrained Machine Learning for Chemical Engineering. *Current Opinion in Chemical Engineering*, 51: 101228. [link]

[9] Saini, V., Purdy, D., **Mukherjee, A.**, Adeyemo, S., Bhattacharyya, D., Parker, J., Lolla, T., and Boohaker, C. 2026. Development of a Hybrid First Principles - Machine Learning Adaptive Modeling Framework for Health Monitoring of Power Plant Boiler Superheaters. *Fuel*, 406: 136795. [link]

[10] González, L., Pulsipher, J., Jiang, S., **Mukherjee, A.**, Soderstrom, T., and Zavala, V. 2025. A digital twin simulator of a pastillation process with applications to automatic control based on computer vision. *Computers & Chemical Engineering*, 201: 109205. [link]

[11] **Mukherjee, A.** and Bhattacharyya, D. 2025. Development of Mass, Energy, and Thermodynamics Constrained Steady-State and Dynamic Neural Networks for Interconnected Chemical Systems. *Chemical Engineering Science*, 309: 121506. [link]

[12] **Mukherjee, A.**, Gupta, D., and Bhattacharyya, D. 2025. Mass-Constrained hybrid Gaussian radial basis neural networks: Development, training, and applications to modeling nonlinear dynamic noisy chemical processes. *Computers & Chemical Engineering*, 197: 109080. [link]

[13] **Mukherjee, A.**, Saini, V., Adeyemo, S., Bhattacharyya, D., Purdy, D., Parker, J., and Boohaker, C. 2025. Development of hybrid first principles – artificial intelligence models for transient modeling of power plant superheaters under load-following operation. *Applied Thermal Engineering*, 262: 124795. [link]

[14] **Mukherjee, A.**, Adeyemo, S., and Bhattacharyya, D. 2025. All-nonlinear static-dynamic neural networks versus Bayesian machine learning for data-driven modelling of chemical processes. *The Canadian Journal of Chemical Engineering*, 103(3): 1139-1154. [link]

[15] **Mukherjee, A.** and Bhattacharyya, D. 2024. Development of Steady-State and Dynamic Mass and Energy Constrained Neural Networks for Distributed Chemical Systems Using Noisy Transient Data. *Industrial & Engineering Chemistry Research*, 63(32): 14211-14239. [link]

[16] **Mukherjee, A.** and Bhattacharyya, D. 2024. On the Development of Steady-State and Dynamic Mass-Constrained Neural Networks Using Noisy Transient Data. *Computers & Chemical Engineering*, 187: 108722. [link]

[17] **Mukherjee, A.** and Bhattacharyya, D. 2023. Hybrid Series/Parallel All-Nonlinear Dynamic-Static Neural Networks: Development, Training, and Application to Chemical Processes. *Industrial & Engineering Chemistry Research*, 62(7): 3221-3237. [link]

Conference Publications (Peer-Reviewed)

[1] **Mukherjee, A.**, Soderstrom, T., Kurtz, M., and Zavala, V. 2026. Recent Advances in Real-Time Process Monitoring and Event Detection. *Systems & Control Transactions (Proceedings of 2027 FOCAPO-CPC Conference)*, 10-14 January, 2027, Tucson, AZ.

[2] Das, P., **Mukherjee, A.**, and Bhattacharyya, D. 2026. Development of a Scalable Bayesian Uncertainty Quantification Framework for Biomass Valorization. *Systems & Control Transactions (Proceedings of 2027 FOCAPO-CPC Conference)*, 10-14 January, 2027, Tucson, AZ.

[3] **Mukherjee, A.** and Bhattacharyya, D. 2024. Development of Steady-State and Dynamic Mass-Energy Constrained Neural Networks using Noisy Transient Data. *Systems & Control Transactions (Proceedings of 2024 FOCAPD Conference)*, 3: 330-337, 14-18 July, 2024, Breckenridge, CO. [link]

Oral Presentations (only as presenting author)

[1] **Mukherjee, A.**, Soderstrom, T., Kurtz, M., and Zavala, V. Anomaly Detection for High-Dimensional Dynamic Systems Using Topology. *2026 AIChE Annual Meeting*, 8-12 November, 2026, Minneapolis, MN. [link]

[2] **Mukherjee, A.**, Giridhar, N., and Bhattacharyya, D. ADOPT-FPML: Automatic Discovery of Optimal Hybrid First Principles - Machine Learning Models. *2026 AIChE Annual Meeting*, 8-12 November, 2026, Minneapolis, MN. [link]

[3] **Mukherjee, A.** and Zavala, V. Scalable Parameter Estimation and Uncertainty Quantification for Physics-Constrained Machine Learning using Variational Inference. *2026 AIChE Annual Meeting*, 8-12 November, 2026, Minneapolis, MN. [link]

[4] (*Invited*) **Mukherjee, A.** Seeing Data through the Lens of Topology: Applications to Chemical and Biomolecular Systems. *Purdue PSE Fall Seminar Series*, 9 October, 2026 (virtual).

[5] **Mukherjee, A.** and Zavala, V. Uncertainty Quantification in Physics-Constrained Machine Learning. *Texas-Wisconsin-California Control Consortium, Spring 2026 Meeting*, 23-24 February, 2026, Austin, TX.

[6] **Mukherjee, A.**, Thompson, J., and Zavala, V. Data-Driven Dynamic Modeling and Uncertainty Quantification Using Variational Inference: Applications to Microkinetic Modeling. *2025 AIChE Annual Meeting*, 2-6 November, 2025, Boston, MA. [link]

[7] **Mukherjee, A.**, Soderstrom, T., Kurtz, M., and Zavala, V. Event Detection in Multivariate Time-Series Data Using Topology. *2025 AIChE Annual Meeting*, 2-6 November, 2025, Boston, MA. [link]

[8] **Mukherjee, A.**, Giridhar, N., and Bhattacharyya, D. Development of a Framework for Automatic Discovery of Optimal Hybrid First Principles - Machine Learning Models. *2025 AIChE Annual Meeting*, 2-6 November, 2025, Boston, MA. [link]

[9] **Mukherjee, A.** and Zavala, V. Approaches to Physics-Constrained Machine Learning. *Texas-Wisconsin-California Control Consortium, Fall 2025 Meeting*, 8-9 Sep, 2025, Madison, WI.

[10] **Mukherjee, A.** and Bhattacharyya, D. Development of Steady-State and Dynamic Mass-Energy-Thermodynamics Constrained Neural Network (MET-CNN) Models for Interconnected Systems Using Noisy Transient Data. *2024 AIChE Annual Meeting*, 27-31 October, 2024, San Diego, CA. [link]

[11] **Mukherjee, A.** and Bhattacharyya, D. Development of Steady-State and Dynamic Mass-Energy Constrained Neural Network Models Using Noisy Temporal Data for Dynamic Optimization of Distributed Chemical Systems. *2024 AIChE Annual Meeting*, 27-31 October, 2024, San Diego, CA. [link]

[12] **Mukherjee, A.** and Bhattacharyya, D. Hybrid Gaussian Radial Basis Neural Networks (GRAB-NN): Development, Training, and Applications to Modeling Nonlinear Dynamic Noisy Chemical Processes. *2024 AIChE Annual Meeting*, 27-31 October, 2024, San Diego, CA. [link]

[13] **Mukherjee, A.**, Saini, V., Adeyemo, S., and Bhattacharyya, D. Development of Hybrid First Principles – Artificial Intelligence Models: Applications to an Industrial Steam Superheater System. *2023 AIChE Annual Meeting*, 5-10 November, 2023, Orlando, FL. [link]

[14] **Mukherjee, A.** and Bhattacharyya, D. Hybrid Series and Parallel All-Nonlinear Dynamic-Static Neural Networks: Development, Training, and Application to Chemical Processes. *15th AIChE Midwest Regional Conference*, 11-12 April, 2023, Chicago, IL. [link]

[15] **Mukherjee, A.** and Bhattacharyya, D. Development of Mass and Energy Constrained Neural Networks. *2022 AIChE Annual Meeting*, 13-18 November, 2022, Phoenix, AZ. [link]

[16] **Mukherjee, A.** and Bhattacharyya, D. Data-Driven Modeling of Complex Nonlinear Systems Using Hybrid Series and Parallel Nonlinear Static-Nonlinear Dynamic Neural Networks. *AIChE Advanced Manufacturing and Processing Conference*, 1-3 June, 2022, Bethesda, MD. [link]

[17] **Mukherjee, A.** and Bhattacharyya, D. Modeling Complex Nonlinear Systems Using Concatenated Static-Dynamic Neural Networks. *2021 AIChE Annual Meeting*, 7-19 November, 2021, Boston, MA. [link]

[18] **Mukherjee, A.** and Bhattacharyya, D. Development of a Hybrid First Principles – Artificial Intelligence Approach for Dynamic Modeling of Complex Systems. *2020 Virtual AIChE Annual Meeting*, 16-20 November, 2020. [link]

Poster Presentations (only as presenting author)

[1] **Mukherjee, A.** New Scalable Paradigms for Data-Driven Modeling, Optimization, and Decision-Making. *2026 AIChE Annual Meeting*, 8-12 November, 2026, Minneapolis, MN. [link]

[2] **Mukherjee, A.**, Soderstrom, T., Kurtz, M., and Zavala, V. Topological Data Analysis for High-Dimensional Dynamic Multivariate Process Monitoring. *Texas-Wisconsin-California Control Consortium, Fall 2026 Meeting*, 14-15 September, 2026, Madison, WI.

[3] **Mukherjee, A.** and Zavala, V. Scalable Parameter Estimation and Uncertainty Quantification in Physics-Constrained Machine Learning. *Hougen PSE Symposium*, 11-12 May, 2026, Madison, WI.

[4] **Mukherjee, A.** and Zavala, V. Data-Driven Modeling and Uncertainty Quantification using Variational Inference. *Texas-Wisconsin-California Control Consortium, Spring 2026 Meeting*, 23-24 February, 2026, Austin, TX.

[5] **Mukherjee, A.** and Zavala, V. Data-Driven Dynamic Modeling and Uncertainty Quantification using Variational Inference. *Optimal Control & Decision Making under Uncertainty for Digital Twins, Institute for Mathematical & Statistical Innovation (IMSI)*, 27-31 October, 2025, Chicago, IL. [link]

[6] **Mukherjee, A.**, Soderstrom, T., Kurtz, M., and Zavala, V. Topological Data Analysis for Multivariate Process Monitoring. *Texas-Wisconsin-California Control Consortium, Fall 2025 Meeting*, 8-9 September, 2025, Madison, WI.

[7] **Mukherjee, A.**, Kung, P., Voyles, P., and Zavala, V. Detection of Relaxation Events in Supercooled Liquids using Topological Data Analysis. *Midwest Thermodynamics and Statistical Mechanics (MTSM) Conference*, 1-3 June, 2025, Madison, WI. [link]

[8] **Mukherjee, A.** and Bhattacharyya, D. Physics-Constrained Machine Learning. *Texas-Wisconsin-California Control Consortium, Fall 2024 Meeting*, 23-24 September, 2024, Madison, WI.

[9] **Mukherjee, A.** and Bhattacharyya, D. Development of Steady-State and Dynamic Mass-Energy Constrained Neural Networks using Noisy Transient Data. *Foundations of Computer-Aided Process Design (FOCAPD) Conference*, 14-18 July, 2024, Breckenridge, CO. [link]

[10] **Mukherjee, A.** and Bhattacharyya, D. Hybrid Series/Parallel All-Nonlinear Dynamic-Static Stochastic Neural Networks: Development, Training and Application to Chemical Processes. *2023 AIChE Annual Meeting*, 5-10 November, 2023, Orlando, FL. [link]

[11] **Mukherjee, A.** and Bhattacharyya, D. Development of Algorithms for Mass and Energy Constrained Dynamic Neural Network Models. *2023 AIChE Annual Meeting*, 5-10 November, 2023, Orlando, FL. [link]

[12] **Mukherjee, A.** New Data-Driven Modeling Paradigms in Systems Engineering Using Novel Neural Network Structures. *2023 AIChE Annual Meeting*, 5-10 November, 2023, Orlando, FL. [link]

[13] **Mukherjee, A.** and Bhattacharyya, D. Development of Algorithms for Mass-Constrained Dynamic Neural Networks. *Foundations of Process/Product Analytics and Machine Learning (FOPAM) Conference*, July 30-Aug 3, 2023, UC Davis, CA. [link]

[14] **Mukherjee, A.** and Bhattacharyya, D. Data-Driven Modeling of Complex Nonlinear Systems Using Hybrid Series and Parallel Nonlinear Static – Dynamic Stochastic Neural Networks. *2022 AIChE Annual Meeting*, 13-18 November, 2022, Phoenix, AZ. [link]

Open-Source Software

[1] ADOPT-FPML: Automatic Discovery of OPTimal First Principles-Machine Learning models [GitHub]

[2] Hybrid All-Nonlinear Static-Dynamic Neural Networks [GitHub]

[3] MCNN: Steady-State and Dynamic Mass Constrained Neural Networks [GitHub]

[4] MECNN: Steady-State and Dynamic Energy Constrained Neural Networks [GitHub]

[5] GRAB-NN: Mass-Constrained Hybrid Gaussian Radial Basis Neural Networks [GitHub]

[6] TDA for Multivariate Process Monitoring [GitHub]

[7] TDA for Protein-Protein Interface Prediction [GitHub]

MENTORING EXPERIENCE

Co-advised Students

- Luis R. Barajas-Villarruel (co-advised with Prof. Victor M. Zavala, Jan 2026 - Present) - Project: Optimal control on latent spaces
- Kang Qiu (co-advised with Prof. Victor M. Zavala, Feb 2026 - Sep 2026) - Project: Dual model predictive control for closed-loop learning
- Joseph Flory (co-advised with Prof. Victor M. Zavala, Jan 2026 - Present) - Project: Data-driven control and uncertainty quantification

- Adam Malmstrom (co-advised with Prof. Victor M. Zavala, Jan 2025 - Aug 2025) - Project: Topological feature extraction for predicting protein-protein interaction sites
- Md Abdur Rakib (co-advised with Prof. Debangsu Bhattacharyya, Aug 2024 - Present) - Project: Physics constrained machine learning for solid oxide cells
- Dipendu Gupta (co-advised with Prof. Debangsu Bhattacharyya, Aug 2023 - Apr 2024) - Project: Process modeling using Gaussian radial basis function networks

SKILLS

- **Analytical Skills:** Optimization, Machine Learning, Data Science, Systems Engineering, Process Control, Topological Data Analysis, Uncertainty Quantification, Applied Statistics
- **Software Skills:** MATLAB, Python, Pyomo, TensorFlow, PyTorch, Julia, R, C++, Aspen One
- **Grant Writing:** Research proposal development and writing for the National Sciences Foundation (NSF) and U.S. Department of Energy (DOE) funding opportunities

RELEVANT COURSEWORK

- Human-Centered Teaching & AI (Spring 2025)
- CHE 693A (Advanced Process Control)
- MATH 593A (Advanced Linear Algebra)
- CHE 620 (Advanced Thermodynamics)
- CHE 615 (Transport Phenomena)
- CHE 625 (Chemical Reaction Engineering)
- Research Mentor Training (Spring 2025)
- CHE 693A (Advanced Optimization)
- EE 515 (Linear Control Systems)
- EE 517 (Optimal Control)
- STAT 512 (Statistical Methods 2)
- STAT 561 (Theory of Statistics 1)
- STAT 562 (Theory of Statistics 2)

AWARDS, HONORS, AND SERVICES

Services

- Served as a reviewer for the American Chemical Society (*Industrial & Engineering Chemistry Research*), IEEE (*Conference on Decision and Control*, *American Control Conference*), Elsevier (*Digital Chemical Engineering*, *Chemical Engineering Research and Design*), and Wiley (*Optimal Control Applications and Methods*) journals.
- Session Co-Chair: "Data-Driven and Hybrid Modeling for Decision Making I", 10E Computing and Systems Technology (CAST) Division, *2026 AIChE Annual Meeting*, 8-12 November, 2026, Minneapolis, MN.
- Session Co-Chair: "Operations under Uncertainty", 10C Computing and Systems Technology (CAST) Division, *2026 AIChE Annual Meeting*, 8-12 November, 2026, Minneapolis, MN.
- Session Co-Chair: "Advances in Machine Learning and Intelligent Systems I", 10E Computing and Systems Technology (CAST) Division, *2026 AIChE Annual Meeting*, 8-12 November, 2026, Minneapolis, MN.
- Session Co-Chair: "Design Under Uncertainty", 10A Computing and Systems Technology (CAST) Division, *2025 AIChE Annual Meeting*, 2-6 November, 2025, Boston, MA.
- Session Co-Chair: "Process Synthesis & Design for Sustainability II", 10A Computing and Systems Technology (CAST) Division, *2025 AIChE Annual Meeting*, 2-6 November, 2025, Boston, MA.

- Session Co-Chair: "AI/ML and Data-Driven Estimation and Optimization for Control", 10B Computing and Systems Technology (CAST) Division, *2025 AIChE Annual Meeting*, 2-6 November, 2025, Boston, MA.
- Served as a judge for the graduate student poster session for the Computing and Systems Technology (CAST) Poster Session, *2025 AIChE Annual Meeting*, 2-6 November, 2025, Boston, MA.
- Session Moderator, *Midwest Thermodynamics and Statistical Mechanics (MTSM) Conference*, 1-3 June, 2025, Madison, WI.
- Served as a judge for the graduate student poster session for Computing and Systems Technology (CAST) Poster Session, *2024 AIChE Annual Meeting*, 27-31 October, 2024, San Diego, CA.
- Served as a judge for the undergraduate student poster session for Computing and Systems Technology (CAST) Poster Session, *2023 AIChE Annual Meeting*, 5-10 November, 2023, Orlando, FL.

Awards and Honors

- University Medal, *Jadavpur University, India*, 2019 (1^{st} rank in batch).
- Jatindra Krishna Memorial Bronze Medal, *Jadavpur University, India*, 2019.
- Chemical Engineering Diamond Jubilee Gold Centered Silver Medal, *Jadavpur University, India*, 2019.
- Bandana Ghosh Memorial Silver Medal, *Jadavpur University, India*, 2019.
- Chittaranjan Khastagir Memorial Gold Medal, *Jadavpur University, India*, 2019.

Outreach and Engagement

- Volunteered in outreach activities through the Department of Chemical and Biological Engineering and the Wisconsin MRSEC, *UW-Madison*, including the Wisconsin Science Festival, Science Expeditions, and Engineering Expo School Day.
- Co-taught a remote short course on physics-constrained machine learning with Prof. Victor M. Zavala, *PEQ Colloquium 2026*, COPPE, Federal University of Rio de Janeiro, Brazil, 3 November, 2026.

PROFESSIONAL MEMBERSHIPS

Member: American Institute of Chemical Engineers (AIChE) Jan 2020-Present
Member: American Chemical Society (ACS) May 2025-Present
Selected Member: Phi Kappa Phi Honor Society Apr 2023-Present