
ASHFAQ IFTAKHER

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SUMMARY

Fourth-year Ph.D. candidate in Chemical Engineering with over 7 years of research experience specializing in process systems engineering. Core expertise includes mathematical modeling, mixed-integer classical-quantum optimization algorithms, process design and optimization, machine learning, cheminformatics, and computer-aided design for discovering *optimal*, *efficient*, and *sustainable* novel molecules and chemical separation processes, thereby contributing to the decarbonization of the chemical industry. Highly experienced in collaborative research. Capable of delivering results in challenging, high-pressure environments.

EDUCATION

Texas A&M University

Ph.D. in Chemical Engineering; Advisor: M. M. Faruque Hasan 2021 – Present

Thesis Area: *Theoretical, Algorithmic, and Quantum Optimization Approaches for Multiscale Process Systems Engineering*

Bangladesh University of Engineering and Technology (BUET)

M.Sc. in Chemical Engineering; Advisor: M. A. A. Shoukat Choudhury and Rafiqul Gani 2018 – 2020

B.Sc. in Chemical Engineering; Advisor: M. A. A. Shoukat Choudhury 2014 – 2018

RESEARCH EXPERIENCE

Graduate Research Assistant (Ph.D.), Department of Chemical Engineering, Texas A&M University 2021 – Present

Multiscale mathematical modeling, machine learning, high-throughput screening, and process optimization

- Performing computer-aided molecular and process design for ionic liquid-based selective separation of azeotropic refrigerant mixtures. Developed neural net models for regression and classification of complex ionic-liquid properties.
- High-throughput screening over 340000 molecules and rigorous process optimization yielded discovery of novel ionic liquids and process configuration achieving 48% reduction in energy consumption and 27% reduction in CO₂ emissions.

Optimization theory and algorithms

- Proposed new reformulations and encodings of constrained mixed-integer nonlinear programs into equivalent quadratic unconstrained binary optimization (QUBO) programs, thereby allowing direct solutions using quantum annealing.
- Lead developer of interval arithmetic embedded automatic differentiation package that computes minima and Hessian bounds of arbitrary second-order continuous functions, thereby providing tight convex and edge-concave relaxations.

Data-driven surrogate optimization and data science

- Proposed a hybrid optimization algorithm that integrates multiple fidelity models for efficient process optimization. Demonstrated computational tractability of the algorithm in a case study where Bayesian optimization was performed on the equilibrium model (low fidelity) while the rate-based model (high fidelity) was used for sampling and validation.
- Topological analysis of high dimensional space using Euler Characteristic, Wasserstein distance, and Cosine similarity.

Graduate Researcher (M.S.), Department of Chemical Engineering, BUET

2019 – 2020

Integrated Design and Control of Reactive Distillation Processes

- Established near optimal controllability of driving-force-based process design of reactive distillation systems.
- Lead developer of RD-DCT, a driving-force-based design-control toolbox that interfaces with Aspen Plus and MATLAB for performing steady state and dynamic simulation as well as model predictive control analysis (Overview published from the PSEforSpeed YouTube Channel: <https://youtu.be/VqxWVOXlxMw?si=2Hrcr1suavgisQR2>)

SELECTED JOURNAL AND CONFERENCE PUBLICATIONS

- J1. **Iftakher, A.**; Leonard, T.; Hasan, M. M. F. Integrating Different Fidelity Models for Process Optimization: A Case of Equilibrium and Rate-based Extractive Distillation using Ionic Liquids. *Comput. Chem. Eng.*, 2024, Accepted.
- J2. **Iftakher, A.**; Monjur, M. S.; Hasan, M. M. F. An Overview of Computer-aided Molecular and Process Design. *Chem. Ing. Tech.*, 2023, 95, 3, 315–333.

- J3. **Iftakher, A.**; Liñán, D. A.; Mansouri, S. S.; Nahid, A.; Hasan, M. M. F.; Choudhury, M. A. A. S.; Ricardez Sandoval, L. A.; Lee, J. H. RD-toolbox: A computer aided toolbox for integrated design and control of reactive distillation processes. *Comput. Chem. Eng.*, 2022, 164, 107869.
- J4. **Iftakher, A.**; Aras, C. M.; Monjur, M. S.; Hasan, M. M. F. Data-Driven Approximation of Thermodynamic Phase Equilibria. *AIChE J.*, 2022, 68, 6, e17624.
- J5. Monjur, M. S.; **Iftakher, A.**; Hasan, M. M. F. Separation Process Synthesis for High-GWP Refrigerant Mixtures: Extractive Distillation using Ionic Liquids. *Ind. Eng. Chem. Res.*, 2022, 61, 12, 4390–4406.
- J6. **Iftakher, A.**; Mansouri, S.S.; Nahid, A.; Tula, A.K.; Choudhury, M.A.A.S.; Lee, J.H.; Gani, R. Integrated Design and Control of Reactive Distillation Processes Using the Driving Force Approach. *AIChE J.*, 2021, 67, e17227.
- J7. Nahid, A.; **Iftakher, A.**; Choudhury, M.A.A.S. Control Valve Stiction Compensation – Part II: Performance Analysis of Different Stiction Compensation Methods. *Ind. Eng. Chem. Res.*, 2019, 58 (26), 11326 – 11337.
- J8. Nahid, A.; **Iftakher, A.**; Choudhury, M.A.A.S. Control Valve Stiction Compensation - Part I: A New Method for Compensating Control Valve Stiction. *Ind. Eng. Chem. Res.*, 2019, 58 (26), 11316-11325.
- C1. **Iftakher, A.**; Hasan, M. M. F. Exploring Quantum Optimization for Computer-aided Molecular and Process Design. *In Proceedings of the Foundations of Computer Aided Process Design (FOCAPD 2024)*, 2024, Accepted.
- C2. **Iftakher, A.**; Kazi, M.; Hasan, M. M. F. Mixed-integer Quadratic Optimization using Quantum Computing for Process Applications. *In Proceedings of the Foundations of Computer Aided Process Operations Conference*. 2023, 1-6.
- C3. **Iftakher, A.**; Aras, C. M.; Monjur, M. S.; Hasan, M. M. F. A Framework for Guaranteed Error-bounded Surrogate Modeling. *In Proceedings of the 2022 American Control Conference (ACC)*, 2022, 4814-4819.
- C4. **Iftakher, A.**; Aras, C. M.; Monjur, M. S.; Hasan, M. M. F. Guaranteed Error-bounded Surrogate Modeling and Application to Thermodynamics. *Computer Aided Chemical Engineering*, 2022, 49, 1831-1836.

SKILLS AND SOFTWARE PROFICIENCIES

- **Programming Language:** C, C++, Python (Pandas, Numpy, PyTorch, Scikit-Learn), Object Oriented Programming
- **Algebraic Modeling, Solvers and Operating Systems:** GAMS, Pyomo, Gurobi, CPLEX, Baron, Linux, Git
- **Simulation Tools:** Aspen Plus, Aspen HYSYS, Aspen Dynamics, MATLAB, Simulink, Mathematica
- **Quantum Chemistry and Optimization:** COSMOtherm, COSMO-RS, IBM Qiskit, D-Wave Ocean

HONORS AND AWARDS

Phillips 66 Technical Fellowship, Texas A&M University	2023 – 2024
• USD \$5000 awarded as recognition of excellence in research capabilities and productivity	
FOCAPD 2024 Travel Grant, AIChE	July 2024
BUET Abrar Memorial Scholarship (BDT 120,000 awarded by BUET for M.Sc. thesis)	2020
BUET Technical Scholarship (recognizes academic excellence)	2014 – 2018
ACM-International Collegiate Programming Contest (ICPC)	2015
• Represented BUET at the 2015 ACM-ICPC Asia Regional Dhaka (Rank: 23rd out of 985 teams (Top 2.3%))	

LEADERSHIP, TEACHING, MENTORING, AND SERVICE

Conference Director Texas A&M Energy Research Society	2023 – 2024
• Responsible for the planning and effective execution of the 2024 TAMU Energy Research Conference, one of the largest student-led energy conferences in the USA.	
Primary Teaching Assistant for a Graduate Course, Chemical Engineering, TAMU	Fall 2023
• <i>CHEN 604: Chemical Engineering Process Analysis I</i> - a core graduate course taken by 61 PhD and MS students .	
Research Mentorship	2022 – Present
• Actively mentoring one PhD student (<i>Toufik Ahmed</i>) and one undergraduate student (<i>Ty Leonard</i>) from TAMU; previously mentored two undergraduate students from TAMU Qatar (<i>Hiba Namany, Amna Cassim</i>).	
Author of a Physics Book for High School Students in Bangladesh	2017
• Book Name: “ <i>Shoishob Koishore Podarthobigganer Mukhomukhi</i> ” (ISSN 9789845260213)	
• Written in Bengali language – spoken by more than 230 million people. Contributed ‘ Modern Physics ’ section, using an intuitive approach to make high school physics concepts more accessible to less privileged high school students .	