ASHFAQ IFTAKHER

Graduate Research Assistant
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RESEARCH INTERESTS

Mathematical Optimization; Mixed-integer Quantum Optimization; Machine Learning; Data Science; Process Systems Engineering; Computer-aided Molecular and Process Design; Reinforcement Learning and Control

EDUCATION

Texas A&M University (TAMU), College Station, TX

Ph.D. in Chemical Engineering — January 2021 – Present
Thesis Area: *Theoretical, Algorithmic, and Quantum Approaches for Multiscale Process Systems Engineering*
Advisor: M. M. Faruque Hasan

Bangladesh University of Engineering and Technology (BUET), Dhaka, Bangladesh

M.Sc. in Chemical Engineering — 2018 – 2020
Thesis: *Integrated Process Design and Control of Reactive Distillation Systems*
Advisors: Rafiqul Gani and M. A. A. Shoukat Choudhury

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

HONORS AND AWARDS

Academy for Future Faculty Fellowship Program — Fall 2024 – Summer 2025
- Selected by the Center for Teaching Excellence, TAMU to prepare outstanding future faculty in STEM.

74th Lindau Nobel Laureate Meeting, Germany — June 2025
- Selected to participate in this '*outstanding convention*' in recognition of '***demonstrated research excellence, leadership and innovation in chemistry or a closely related field***'. All expenses covered.

Global Young Scientists Summit, GYSS 2025, Singapore — January 2025
- Selected to participate in the premier event that brings together ***Nobel Laureates***, ***Field Medalists***, ***Turing Fellows,*** and the '***brightest emerging minds in science from around the world***'. All expenses covered.

Phillips 66 Technical Fellowship, Texas A&M University — 2023 – 2024
- This fellowship is awarded to the top student from a pool of 135 graduate students in the department as recognition of '***excellence in research capabilities and productivity'***.

FOCAPD 2024 Travel Award, AIChE — July 2024
- Awarded to present at the Foundations of Computer Aided Process Design (FOCAPD) Conference.

Graduate Mentoring Academy Fellowship Program — Fall 2024 – present
- Seven evidence-based mentorship competencies organized by Graduate Mentoring Academy, TAMU.

BUET Abrar Memorial Scholarship — 2020
- Selected from a pool of ~150 students for M.Sc. thesis at the Dept. of Chemical Engineering, BUET.

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 (Top **2.3**%: 23rd out of 985 teams).

Champion of Regional Bangladesh Mathematical Olympiad 2012, 2011

Regional winner of Bangladesh Physics and Informatics Olympiad 2012

RESEARCH EXPERIENCE

Research Assistant (Ph.D.) 2021 – Present

Department of Chemical Engineering, Texas A&M University
Advisor: M. M. Faruque Hasan

Multiscale 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.
- Discovered new ionic liquids and process configurations by high-throughput screening of over 340,000 molecules and rigorous process optimization, resulting in 48% reduction in energy consumption and 27% reduction in CO_2 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.

Surrogate optimization and data science

- Proposed a hybrid optimization algorithm with local optimality guarantee 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.

Research Assistant (M.Sc.) 2019 – 2020

Department of Chemical Engineering, BUET
Advisors: M. A. A. Shoukat Choudhury and Rafiqul Gani

Integrated Design and Control of Reactive Distillation Processes

- Established near-optimal controllability of driving-force-based 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 from PSEforSpeed: https://youtu.be/VqxWVOXlxMw?si=2Hrcr1suavgsiQR2).

Molecular Property Prediction using Sigma Profiles

- Generated sigma profiles of 800+ organic chemicals through molecular simulation.
- Regressed sigma-profiles for property prediction, demonstrated good agreement with experimental data for the pure component property prediction of ionic liquids.

PROPOSAL WRITING EXPERIENCE

EPA 2024

- Budget: USD 1.5 million for "*SMART-RECLAIM: Scalable, Modular and Adaptable Reclamation Technology for Hydrofluorocarbon Refrigerant Enhancement, Circular Logistics, and Intelligent Manufacturing*". **Awarded**. LPI: Assoc. Prof. M. M. Faruque Hasan
- Contributed to writing several sections, and building groundwork from ongoing Ph.D. research

NSF 2022

- Budget: USD 50,000 for "*Quantum computing for solving mixed integer optimization*". **Awarded**. LPI: Assoc. Prof. M. M. Faruque Hasan
- Contributed to writing section on methodology, and building groundwork from ongoing Ph.D. research

JOURNAL PUBLICATIONS

J1. **Iftakher, A.**; Monjur, M. S.; Leonard, T.; Gani, R.; Hasan, M. M. F. Multiscale High-Throughput Screening of Ionic Liquid Solvents for Mixed-Refrigerant Separation. *Computers. & Chemical Engineering*, 2025, Accepted.

J2. **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. *Computers. & Chemical Engineering*, 2024, 192, 108890. DOI: https://doi.org/10.1016/j.compchemeng.2024.108890.

J3. **Iftakher, A.**; Hasan, M. M. F. Exploring Quantum Optimization for Computer-aided Molecular and Process Design. *Systems & Control Transactions,* 2024, 3, 292-299. DOI: https://doi.org/10.69997/sct.143809.

J4. Helmer, R.; Borkar, S.S.; Li. A.; Mahnaz, F.; Vito, J.; Bishop, M.; **Iftakher, A.**; Hasan, M. M. F.; Rangarajan, S.; Shetty, M. Tandem Methanolysis and Catalytic Transfer Hydrogenolysis of Polyethylene Terephthalate to p-xylene over Cu/$ZnZrO_x$ Catalysts. *Angewandte Chemie*, 2024, e202416384. DOI: https://doi.org/10.1002/anie.202416384.

J5. Aras, C. M.; **Iftakher, A.**; Hasan, M. M. F. Guaranteed Error-bounded Surrogate Framework for Solving Process Simulation Problems. *Systems & Control Transactions*, 2024, 3, 105-112. DOI: https://doi.org/10.69997/sct.182073.

J6. **Iftakher, A.**; Monjur, M. S.; Hasan, M. M. F. An Overview of Computer-aided Molecular and Process Design. *Chemie. Ingenieur. Technik*, 2023, 95, 3, 315–333. DOI: https://doi.org/10.1002/cite.202200172.

J7. **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. *Computers. & Chemical Engineering*, 2022, 164, 107869. DOI: https://doi.org/10.1016/j.compchemeng.2022.107869.

J8. **Iftakher, A.**; Aras, C. M.; Monjur, M. S.; Hasan, M. M. F. Data-Driven Approximation of Thermodynamic Phase Equilibria. *AIChE Journal*, 2022, 68, 6, e17624. DOI: https://doi.org/10.1002/aic.17624.

J9. Monjur, M. S.; **Iftakher, A.**; Hasan, M. M. F. Separation Process Synthesis for High-GWP Refrigerant Mixtures: Extractive Distillation using Ionic Liquids. *Industrial & Engineering Chemistry Research*, 2022, 61, 12, 4390–4406. DOI: https://doi.org/10.1021/acs.iecr.2c00136.

J10. **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 Journal*, 2021, 67, e17227. DOI: https://doi.org/10.1002/aic.17227.

J11. Nahid, A.; **Iftakher, A.**; Choudhury, M.A.A.S. Control Valve Stiction Compensation – Part II: Performance Analysis of Different Stiction Compensation Methods. *Industrial & Engineering Chemistry Research*, 2019, 58 (26), 11326 – 11337. DOI: https://doi.org/10.1021/acs.iecr.9b00335.

J12. Nahid, A.; **Iftakher, A.**; Choudhury, M.A.A.S. Control Valve Stiction Compensation - Part I: A New Method for Compensating Control Valve Stiction. *Industrial & Engineering Chemistry Research*, 2019, 58 (26), 11316-11325. DOI: https://doi.org/10.1021/acs.iecr.9b00334.

Journal Articles Currently Under Review

J13. **Iftakher, A.**; Hasan, M. M. F. Encodings and Reformulations of Mixed-Integer Linear, Quadratic and Signomial Programs for Direct Quantum Optimization. Under Review at *IEEE Transactions on Quantum Engineering*.

J14. **Iftakher, A.**; Monjur, M. S.; Nahid, A.; Dukissis, M.; Hasan, M. M. F. Combined Molecular Screening and Process Design Reveals Hundreds of New Ionic Liquids as Superior Solvents for HFC Separation. Under Review at *Chemical Engineering Journal*.

Peer-Reviewed Conference Publications

C1. **Iftakher, A.**; Gani, R.; Hasan, M. M. F. Computer-aided Molecular and Process Design (CAMPD) for Ionic Liquid Assisted Extractive Distillation of Refrigerant Mixtures. *Computer Aided Chemical Engineering*, 2024, 53, 1303-1308. DOI: https://doi.org/10.1016/B978-0-443-28824-1.50218-0.

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 / Chemical Process Control Conference (FOCAPO/CPC)*. 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. DOI: https://doi.org/10.23919/ACC53348.2022.9867870.

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. DOI: https://doi.org/10.1016/B978-0-323-85159-6.50305-5.

C5. Monjur, M. S.; **Iftakher, A.**; Hasan, M. M. F. Sustainable Process Intensification of Refrigerant Mixture Separation and Management: A Multiscale Material Screening and Process Design Approach. *Computer Aided Chemical Engineering*, 2022, 49, 661-666. DOI: https://doi.org/10.1016/B978-0-323-85159-6.50110-X.

C6. **Iftakher, A.**; Mansouri, S.S.; Nahid, A.; Tula, A.K.; Choudhury, M.A.A.S.; Lee, J.H.; Gani, R. Driving Force Based Design and Control Performance Analysis of Reactive Distillation Columns. *Computer Aided Chemical Engineering*, 2021, 50, 1209-1214. DOI: https://doi.org/10.1016/B978-0-323-88506-5.50186-8

C7. **Iftakher, A.**, Nahid, A., Choudhury, M. S., Mansouri, S. S., Gani, R. Application and Performance Evaluation of Model Predictive Controllers on Driving Force Based Reactive Distillation Processes. *Chemical Engineering Research Bulletin*, 2021. 22(1), 49–53. DOI: http://dx.doi.org/10.3329/cerb.v22i1.54299.

C8. Nahid, A.; **Iftakher, A.**; Choudhury, M.A.A.S. An Efficient Approach to Compensate Control Valve Stiction. *In Proceedings of the 10th International Conference on Electrical and Computer Engineering*, 2018, 161-164. DOI: https://doi.org/10.1109/ICECE.2018.8636727.

CONFERENCE PRESENTATIONS

T1. **Iftakher, A.**, Leonard, T., Hasan, M. M. F. Combining Machine Learning and Optimization for the Inverse Design of Ionic Liquids for Refrigerant Separation. *AIChE Annual Meeting*, San Diego, CA, 2024.

T2. **Iftakher, A.**, Hasan, M. M. F. Direct Quantum Optimization of a Class of MINLP involving Quadratic and Signomial Terms. *AIChE Annual Meeting*, San Diego, CA, 2024.

T3. **Iftakher, A.**, Gani, R., Hasan, M. M. F. Computer-aided Molecular and Process Design (CAMPD) for Ionic Liquid Assisted Extractive Distillation of Refrigerant Mixtures. *ESCAPE34-PSE24*, Florence, Italy, 2024.

T4. **Iftakher, A.**, Kazi, M., Hasan, M. M. F. Solving Mixed-Integer Linear and Quadratic Programs using Quantum Computing. *AIChE Annual Meeting*, Orlando, FL, 2023.

T5. **Iftakher, A.**, Kongcharoenkitkul, J., Gani, R., Hasan, M. M. F. A Generic Decomposition-Based Framework for Computer-Aided Molecular and Process Design. *AIChE Annual Meeting*, Orlando, FL, 2023.

T6. **Iftakher, A.**, Kazi, M., Hasan, M. M. F., Mixed-Integer Optimization using Quantum Computing for Process Systems Engineering. Proceedings of the 11th World Congress of Chemical Engineering, *WCCE11*, Buenos Aires, Argentina, 2023.

T7. **Iftakher, A.**, Kazi, M., Hasan, M. M. F., Mixed-Integer Quadratic Optimization using Quantum Computing for Process Applications. Proceedings of the Foundations of Computer-Aided Process Operations and Chemical Process Control, *FOCAPO/CPC*, San Antonio, TX, 2023.

T8. **Iftakher, A.**, Monjur, M. S., Aras, C. M., Hasan, M. M. F. GEMS: A Framework for Surrogate Modeling and Optimization with Guaranteed Error Bounds. *AIChE Annual Meeting*, Phoenix, AZ, 2022.

T9. **Iftakher A.**, Chinmay, M. A., Monjur, M. S., Hasan, M. M. F. A Framework for Guaranteed Error-bounded Surrogate Modeling. *American Control Conference*, Atlanta, GA, 2022.

T10. **Iftakher, A.**, Aras, C. M, Monjur, M. S., Hasan, M. M. F. Guaranteed Error-bounded Surrogate Modeling and Application to Thermodynamics. Proceedings of the 14th International Symposium on Process Systems Engineering, *PSE 2021+*, Virtual, 2022.

T11. Monjur, M. S., **Iftakher, A.**, Hasan, M. M. F. Multiscale Inverse Design of High-Performance Ionic Liquid Solvents for High-GWP Refrigerant Separation. *AIChE Annual Meeting*, Phoenix, AZ, 2022.

T12. Monjur, M. S., **Iftakher, A.**, Hasan, M. M. F. Combining Solvent Screening with Process Synthesis for Separating Refrigerant Mixtures using Ionic Liquids. *AIChE Annual Meeting*, Phoenix, AZ, 2022.

T13. Monjur, M. S., **Iftakher A.**, Hasan, M. M. F. Sustainable Process Intensification of Refrigerant Mixture Separation and Management: A Multiscale Material Screening and Process Design Approach. Proceedings of the 14th International Symposium on Process Systems Engineering, *PSE 2021+*, Virtual, 2022.

T14. **Iftakher, A.**, Monjur, M. S., Aras, C. M., Hasan, M. M. F. Surrogate Thermodynamics for Process Synthesis: A Computational Study on Model Selection, Accuracy and Performance. *AIChE Annual Meeting*, Boston, MA. 2021.

T15. Monjur, M. S., **Iftakher, A.**, Hasan, M. M. F. SPICE ED: A Framework for Simultaneous Materials Screening and Process Synthesis for Extractive Distillation. *AIChE Annual Meeting*, Boston, MA, 2021.

T16. Monjur, M. S., **Iftakher, A.**, Hasan, M. M. F. Material Selection and Design of Ionic Liquid-based Extractive Distillation for Hydrofluorocarbons Separation. *AIChE Annual Meeting*, Boston, MA, 2021.

T17. **Iftakher, A.**, Nahid, A., Mansouri, S.S., Gani, R., Choudhury, M.A.A.S. Model Predictive Control Performance Analysis to Driving Force Based Reactive Distillation Columns. *AIChE Annual Meeting*, Virtual, 2020.

LEADERSHIP, TEACHING, MENTORING AND SERVICE

Conference Director at 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.
- Assigning accepted abstracts to appropriate oral tracks, and effective communication with oral presentation session chairs to ensure smooth functioning of the sessions.

Primary Teaching Assistant for a Core Graduate Course, Chemical Engineering, TAMU Fall 2023

- *CHEN 604: Chemical Engineering Process Analysis 1* - taken by **61 PhD and MS students**.
- Effectively addressed student questions, graded homework, held weekly office hours.
- Delivered a 45-minute lecture on '*Divergence of a vector field in spherical coordinates*'.

Research Mentorship 2022 – Present

- Currently mentoring three PhD students from TAMU.
    - *Toufik Ahmed*: Delivering in-depth training in mathematical modeling using GAMS, aiding in their research on **optimizing reaction systems involving tandem catalysts**.
    - *Ahaduzzaman Nahid*: Providing training on molecular property and thermodynamic modeling, and process optimization for **discovering mixtures of ionic liquids for refrigerant separation**.
    - *Deepshika Dutta*: Supervising project on **decomposition techniques for solving large-scale QUBO problems**.
- Mentored two international undergraduate exchange students from TAMU Qatar.
    - *Hiba Namany*: Provided hands-on training on group-contribution-based representation of Ionic Liquids and the development of regression models for their properties.
    - *Amna Cassim*: Directly mentored and supervised their project on simulating extractive-distillation processes to separate refrigerant mixtures using Ionic Liquids.
- Actively mentoring two undergraduate students from TAMU.
    - *Ty Leonard*: Providing training on ASPEN Plus simulations using Ionic Liquid property definitions and property modeling using multivariable linear regression. Resulted in co-authored publications.
    - *Michael Dukissis:* Supervising their project on developing thermal conductivity models for ionic liquids. Providing training on mathematical modeling in GAMS.

Journal Reviewer 2024 – Present

- Industrial & Engineering Chemistry Research, IECR.

Author of a Supplementary Physics Book for High School Students of Bangladesh 2017

- Book Name: "***Shoishob Koishore Podarthobigganer Mukhomukhi***"
- Publisher: **Anindya Prokash**, Bangla Academy Book Fair, 2017, 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**.

Academic Instructor at the Bangladesh Mathematical Olympiad 2014 – 2016

- Instructed middle-school and high-school students on Euclidean geometry and number theory.
- Prepared problem sets and graded answer sheets at regional Olympiads.

SOFTWARE DEVELOPMENT

RD-Toolbox (Lead developer)

- Integrated Design-Control Toolbox for Reactive Distillation (RD) Systems. Automatically designs RD systems at the maximum driving force.
- Reduces expert knowledge needed to design and control complex systems by guiding a user to set up steady-state and dynamic simulations as well as perform controllability analysis.
- Written in C# (back-end) and Windows Forms Applications (front-end), interfaces with Aspen Plus and MATLAB.

GEMS (Contributor)

- Guaranteed Error-bounded Modeling of Surrogates.
- Computes bounds on Hessian and Jacobian of C^2 continuous functions using automatic differentiation and interval arithmetic.
- Performs sampling, parameter estimation with embedded edge-concavity-based constraints, and generation of the surrogate forms with guaranteed error-bounds. Written in Python.

SKILLS AND SOFTWARE PROFICIENCIES

- **Programming Language:** C, C++, C#, Python, Object Oriented Programming
- **Algebraic Modeling, Solvers and Operating Systems:** GAMS, Pyomo, Gurobi, Baron, Linux, Git
- **Simulation Tools:** Aspen Plus, Aspen HYSYS, Aspen Dynamics, MATLAB, Simulink, Mathematica
- **Quantum Chemistry and Optimization:** COSMO-RS, COSMO-SAC, IBM Qiskit, D-Wave Ocean

REFERENCES

M. M. Faruque Hasan (Ph.D. Supervisor)

Associate Professor, Chemical Engineering

Kim Tompkins McDivitt ’88 and Phillip McDivitt ’87 Faculty Fellow

Assistant Director of Decarbonization, Texas A&M Energy Institute

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Rafiqul Gani (M.Sc. Supervisor)

Distinguished Professor, Hong Kong University of Science & Technology

Distinguished Professor at Széchenyi István University

Ex-president of the European Federation of Chemical Engineering, EFCE, (2015-2018)

Member of the Danish Academy of Science, Fellow of AIChE, IChemE, AIAA, AIIA

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