

Rajasi Shukre

PhD Candidate, Chemical Engineering
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To develop intensified process technologies for the design and synthesis of novel materials with applications in chemical separations, catalysis and drug delivery via molecular simulations and high-throughput experiments.

Research Summary

- Molecular Simulation
- Gas Storage
- Metal Organic Frameworks
- Biomass Pyrolysis
- Thermodynamic modeling
- Liquid Adsorption
- Continuous Crystallization
- Physical Characterization

Professional Summary

- Process design and simulation
- HAZOP study

Education

2017– Present **Ph.D. (Chemical Engineering).**
Maddox Engineering Research Centre, Texas Tech University

2010–2014 **B.Tech (Chemical Engineering).**
Laxminarayan Institute of Technology, India.

Professional Positions

2017 – Present **Ph.D. Candidate, Texas Tech University,**
Advisor: [Dr. Chau-Chyun Chen](#),
Co-Advisors: [Dr. Siva Vanapalli](#) and [Dr. Rajesh Khare](#)
Thesis: *Adsorption: Synthesis, molecular simulation and thermodynamic modeling .*

- Designed a **novel, reusable continuous flow reactor** (droplet millifluidic) for the synthesis of the metal-organic framework (MOF) **HKUST-1** at a ultra-low residence time of 13 minutes
- Screened a **multidimensional reaction space** using batch synthesis on the basis of **crystallinity, yield and instantaneous precipitation**
- **Grand canonical Monte Carlo simulation** for computing pure and binary gas adsorption isotherms in non-porous and porous adsorbents such as **carbon black, exfoliated graphite, zeolites and metal-organic frameworks**
- Developed a **mathematical model** for computing binary interaction parameter of the **aNRTL model** using **molecular dynamics** simulations
- Developed a **thermodynamic framework** for the correlation of **adsorption of binary liquid mixtures** on silica gel using the **real adsorbed solution theory** and **generalized Langmuir isotherm**

- June – Aug 2021 **AIChE Remote Engineering intern**, *RAPID Manufacturing Institute*.
- Developed an **optimized force field** for molecular simulation of **gas adsorption on graphite**
 - **Modular Chemical Process Intensification** coursework
- 2014 – 2016 **Process Engineer**, *Fluor Corporation, India*.
- **Process Design** of **Fuel Gas Caustic Scrubber Unit** in “**Rotterdam Advanced Hydrocracker Project**” of Exxon Mobil (Esso Nederland, B.V.)
 - Development of Piping and Instrumentation Diagrams (**PID**)
 - **HAZOP Study** and **Pressure Relief Valve Contingency Analysis**
 - Prepared **vendor data sheets** of equipments, control valves and relief valves
- June – Aug 2013 **Summer Intern**, *Techint Corporation, India*.
- Heat Exchanger Design and pipeline insulation

Technical Skills

- **Computational**
Languages: C, C++, MATLAB, Python, L^AT_EX
Softwares: Aspen Properties, Aspen Plus, Aspen Hysys
Packages: RASPA, LAMMPS
- **Experimental**
Material Characterization: SEM, BET, FTIR, PXRD
Material Synthesis: Millifluidics, Batch Synthesis
- **Other Tools**
Visualization: VMD, OVITO, iRASPA
Others: Fusion 360, 3D Printing

Publications

To access the updated list of my work, please visit [my google scholar page](#).

- [1] **Shukre, Rajasi**, Bhaiya, Shikha, Hamid, Usman, Tun, Hla, and Chen, Chau-Chyun. “Thermodynamic modeling of adsorption at the liquid-solid interface”. In: *ChemRxiv* (2022).
- [2] **Shukre, Rajasi**, Ericson, Thomas, Unruh, Daniel, Harbin, Hannah, Cozzolino, Anthony, Chen, Chau-Chyun, and Vanapalli, Siva. “Batch-Screening Guided Continuous Flow Synthesis of the Metal-organic Framework HKUST-1 in a Millifluidic Droplet Reactor”. In: *ChemRxiv* (2022).
- [3] **Rajasi Shukre**, Rajesh Khare and Chau-Chyun Chen. “Adsorption on 3D porous materials : Modeling aNRTL theory using Molecular Simulation”. In: (*In preparation*) (2021).
- [4] **Rajasi Shukre**, Rajesh Khare and Chau-Chyun Chen. “Adsorption on non-porous and mesoporous materials : Modeling aNRTL theory using Molecular Simulation”. In: (*In preparation*) (2021).
- [5] Gorensek, Maximilian B, **Shukre, Rajasi**, and Chen, Chau-Chyun. “Development of a thermophysical properties model for flowsheet simulation of biomass pyrolysis processes”. In: *ACS Sustainable Chemistry & Engineering* 7.9 (2019), pp. 9017–9027.

Presentations

- [1] **Rajasi Shukre**, Rajesh Khare and Chau-Chyun Chen. “Estimation of binary interaction parameters of the aNRTL model using molecular simulations”. In: *AICHE Spring Meeting* (2022).

- [2] **Rajasi Shukre**, Thomas Ericson, Daniel Unruh, Hannah Harbin, Sheima Khatib, Anthony Cozzolino, Siva Vanapalli and Chau-Chyun Chen. “Continuous flow synthesis of metal organic framework in a millifluidic reactor”. In: *AIChE Fall Annual Meeting* (2021).
- [3] **Rajasi Shukre**, Rajesh Khare and Chau-Chyun Chen. “Estimation of binary interaction parameters of the aNRTL model using molecular simulations (*Poster*)”. In: *AIChE Fall Annual Meeting* (2021).
- [4] Ban Caudle, **Rajasi Shukre** and Chau-Chyun Chen. “Modeling and Metrics Development for Biomass Pyrolysis Intensification Via Autothermal Operation”. In: *AIChE Spring Meeting and 15th Global Congress on Process Safety* (2019).
- [5] **Rajasi Shukre** and Chau-Chyun Chen. “Thermodynamic Modeling of CO₂ Absorption in Aqueous Amino Acid Salt Solutions with Symmetric Electrolyte NRTL Model”. In: *AIChE Annual Meeting* (2018).

Teaching Experience

- Spring 2019 **Transport Lab**, ChE 3232, *Hosted Lab Sessions, graded performance of students during the sessions.*
- Fall 2018 **Introduction to Chemical Processes and Engineering**, ChE 2410, *Graded assignments, hosted discussion sessions and office hours.*

Student Advising and Mentorship

- Spring 2019 **Research Mentor**, Shikha Bhaiya, *Supervised Master’s student at Texas Tech University for MS thesis projects.*

Awards

- 2021 **Graduate School Travel Fund Scholarship**, Texas Tech University.
- 2020 **Society of Plastics Engineers Scholarship**, Texas Tech University Chapter.
- 2020-2021 **Study Abroad Competitive Scholarship**, Texas Tech University.
- 2015 **Recognition certificate for Front-End Engineering Deliverables**, Exxon Mobil.

References

Chau-Chyun Chen, Professor, Texas Tech University
Siva Vanapalli, Professor, Texas Tech University
Rajesh Khare, Professor, Texas Tech University

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