Rajasi Shukre

PhD Candidate, Chemical Engineering
Texas Tech University

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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, LaTeX
  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] **Rajasi Shukre**, Thomas Ericson, Daniel Unruh, Hannah Harbin, Sheima Khatib, Anthony Cozzolino, Siva Vanapalli and Chau-Chyun Chen. "Continuous Synthesis of HKUST−1 in a millifluidic reactor". In: *(In preparation)* (2021).

[2] **Rajasi Shukre**, Rajesh Khare and Chau-Chyun Chen. "Estimation of binary interaction parameters of the aNRTL model using molecular simulations". In: *(In preparation)* (2021).

[3] 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.

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.*