Akash Kumar Ball

Ph.D. in Chemical Engineering, MIT | akashball1998@gmail.com | LinkedIn | Google Scholar

SUMMARY

I have almost five years of extensive research experience in wide areas of Chemical Engineering e.g., molecular simulation, machine learning, delignification and enzymatic hydrolysis of biomass, nanoparticle-based sensing, Cahn-Hilliard flows, pyrolysis with several internships both in academia and industry. Till now, I have coauthored five internationally peer-reviewed journal papers. Publication statistics: Citations: 33, h-index: 3

EDUCATIONAL QUALIFICATION

Massachusetts Institute of Technology   Cambridge, MA, USA

Doctor of Philosophy (Ph.D.) in Chemical Engineering   Aug 2022 - Present

Indian Institute of Technology, Bombay   Mumbai, India

Master of Technology (M.Tech) in Chemical Engineering   Aug 2020 – July 2022

- CPI: **9.91/10**, **1st rank** holder in the class of **43** students.
- Relevant courses: Statistics, Computational Methods, Optimization, Advanced Reaction Engineering

Jadavpur University   Kolkata, India

Bachelor of Engineering (B.E) in Chemical Engineering   Aug 2016 – July 2020

- CGPA: **9.39/10**, **1st rank** holder in the class of **89** students.
- Relevant courses: CFD, Advanced Heat Transfer, Mass Transfer, Chemical Thermodynamics

PUBLICATIONS

- **Ball, A.K.**, Haque, S., Chatterjee, A. Relaxation dynamics in reverse Monte Carlo. (**Molecular Simulation**: in review).
- **Ball, A.K.**, Rana, S., Agrahari, G., Chatterjee, A. Accelerated calculation of configurational free energy using a combination of reverse Monte Carlo and neural network models: Adsorption isotherm for 2D square and triangular lattices. (**Computer Physics Communications**: In review)
- Ghosh, D., Basu, S., **Ball, A.K.**, Lal, S. and Sarkar, U., 2019. Spatio-temporal variability of CO over the Eastern Indo-Gangetic Plain (IGP) and in parts of South-East Asia: a MERRA-2-based study. *Air Quality, Atmosphere & Health, 12(10)*, pp.1153-1167. DOI
- Baksi, S., Sarkar, U., Saha, S., **Ball, A.K.**, Kuniyal, J.C., Wentzel, A., Birgen, C., Preisig, H.A., Wittgens, B. and Markussen, S., 2019. Studies on delignification and inhibitory enzyme kinetics of alkaline peroxide pre-treated pine and deodar saw dust. *Chemical Engineering and Processing-Process Intensification, 143*, p.107607. DOI
- Baksi, S., **Ball, A.K.**, Sarkar, U., Banerjee, D., Wentzel, A., Preisig, H.A., Kuniyal, J.C., Birgen, C., Saha, S., Wittgens, B. and Markussen, S., 2019. Efficacy of a novel sequential enzymatic hydrolysis of lignocellulosic biomass and inhibition characteristics of monosugars. *International journal of biological macromolecules, 129*, pp.634-644. DOI

RESEARCH EXPERIENCE

Thermodynamic calculations for adsorption on 2D lattices using reverse Monte-Carlo and ML   IIT Bombay

Master's thesis | Guide: Prof. Abhijit Chatterjee | Department of Chemical Engineering   *Jan 2021 – ongoing*

- Calculated the local environment of both 2D square and hexagonal lattice in terms of probability distributions using **reverse Monte-Carlo** (RMC) method for **1st nearest-neighbor** pair interactions.
- Trained **neural networks** to the probability distributions to predict surface arrangement.
- Calculated chemical potential for given bulk composition using the **RMC/ML** approach along with **detailed balance equation** (DBE). Isotherms at different interaction strengths were generated.
- Validated the isotherms generated from RMC/ML using **grand canonical Monte-Carlo** simulation.

Study of delignification and enzyme inhibition by monosugars during enzymatic hydrolysis of lignocellulosic biomass
<div align="right">Jadavpur University</div>

*Indo-Norwegian collaborative project | Funded by: **DST** (India) and **RCN** (Norway)*

Undergraduate Researcher| Guide: Prof. Ujjaini Sarkar| Department of Chemical Engineering   July '17 – Dec '19

- Developed a novel pretreatment method (**combined pretreatment**) which is **16.22 %** more efficient in **delignification** of lignocellulosic biomass than conventional **alkaline pretreatment**.
- **1st order** pseudo-kinetic model was found to be suitable for studying delignification kinetics of different pretreatment methods using various feedstocks.
- From **HPLC**, **glucose** and **xylose** were found to be the products of biomass enzymatic hydrolysis.
- Studied enzyme **inhibition kinetics** in **MATLAB**. **Competitive** inhibition by **glucose** was observed. The inhibition decreased with increased substrate concentration for particular enzyme loading.

Phase-separated flow described by Cahn-Hilliard equation
<div align="right">IIT Kharagpur</div>

Winter Intern |Guide: Prof. Sourav Mondal | Department of Chemical Engineering   Dec 2018 – Jan 2019

- Studied the **steady-state** patterns of **spinodal decomposition** using **COMSOL** and **MATLAB**.
- **Initial conditions**: Random and Strips of different thickness; **Boundary conditions**: Wetted wall with different contact angel; **Geometries**: Rectangular with different aspect ratio, circular.
- 2D **Cahn-Hilliard Navier-Stokes** equation was used to simulate velocity-imposed phase separation.

Electrochemical detection of As (III) using nanoparticle-based sensor and Molybdenum Blue test for detection of As (V) in Water
<div align="right">IIT Bombay</div>

Summer Intern |Guide: Prof. Rajdip Bandyopadhyaya| Department of Chemical Engineering   May '18 – July '18

- Prepared **citrate-stabilized 10 nm Au** nanoparticles (NP) and **Au-Fe₃O₄** nanocomposites (NC). Performed different characterizations of NP and NC like **UV-Vis**, **DLS**, **TEM-EdX**.
- Coated the NP and NC on **Glassy Carbon Electrode** (GCE) using drop-cast method. Performed **Anode Stripping Voltammetry** of As (III) solutions with GCE as working electrode.
- Prepared a calibration curve of maximum current vs As (III) concentration.
- Performed **Molybdenum blue** test of As (V) solutions of different concentration. The RGB values were determined using **ImageJ** and a calibration curve of intensity vs concentration was prepared.

Pyrolysis of soapnut cake residue (SCR) and soapnut seed (SS)
<div align="right">IIT Guwahati</div>

Winter Intern | Guide: Prof. Pankaj Tiwari | Department of Chemical Engineering   Dec 2017 – Jan 2018

- Performed **proximate analysis** (moisture, volatile matter, ash and fixed carbon) of SCR and SS. The volatile matter content was found to be very high (**88.5 %** for SCR and **87 %** for SS).
- Carried out pyrolysis of SCR in a batch reactor at 300 ℃ and 400 ℃. The liquid yield increased from **20.68 %** at 300 ℃ to **24.12 %** at 400 ℃. The gas yield decreased from **49 %** to **43.32 %**.

INDUSTRIAL EXPERIENCE

Reduction of 6,6-dichlorofulvene (DCF) degradation (collaborative project with Deccan FC)
<div align="right">IIT Bombay</div>

Industrial project| Guide: [Prof. Sanjay Mahajani](#)| Department of Chemical Engineering   *June 2021-ongoing*

- Reaction intermediate DCF is a temperature sensitive material with storage temperature $\leq -20\ ^\circ C$. 2-stage batch extraction at -2 to 0 $^\circ C$ for 3-4 hours causes significant DCF degradation.
- Proposed **continuous counter-current** extraction to reduce extraction time to **1 hour**.
- Performed simulation in **Aspen Plus** with **ELECNRTL** thermodynamic package to determine no of stages.
- Carried out extraction in a small-scale **Rotating Disk Contactor** column to validate simulation results.
- Determined the composition of extract using **Gas Chromatography** with **Flame Ionization Detector**.

Preparation of equipment design specifications (for costing purpose) and material selection diagram of sweet-mode renewable layout   Haldor Topsoe

R &D Intern | Guide: [Dr. Rajarshi Bandyopadhyay](#) | Principal Engineer, [Haldor Topsoe](#)   *May 2019 – July 2019*

- Accomplished basic engineering design of 3-phase separators, flash vessels, knock-out drums, stripper and stabilizer column, fractionator, centrifugal pumps of renewable **Ultra Low Sulfur Diesel** layout.
- Performed design of fired heaters, different shell and tube heat exchangers and air coolers using **HTRI**.
- Prepared **Material Selection Diagram** by determining the equipment design pressure, temperature and material of construction.

TEACHING EXPERIENCE

CL 255: Chemical Engineering Thermodynamics-I   IIT Bombay

Teaching Assistant| Instructor: [Prof. Rajdip Bandyopadhyaya](#)| Department of Chemical Engineering   *Fall 2021*

- Evaluation and grading answer sheets for examinations and quizzes of almost 80 students.
- Performing video proctoring of students in examinations during the online semester.

TECHNICAL SKILLS

Programming Languages: *MATLAB, Python, C*   Process Simulation: *Aspen Plus, HYSYS, DWSIM*

Applied Math: *Optimization, Statistics, Deep Learning*   Others: *HTRI, Origin Pro, ImageJ, AutoCad, MS Office*

Statistical Mechanics: *Grand-canonical Monte-Carlo, Reverse Monte-Carlo*

Laboratory Equipment: *UV-vis, DLS, Gas Chromatography, High Performance Liquid Chromatography (HPLC)*

AWARDS

Institute Silver Medal, IIT Bombay, 2022

- For being the 1st rank holder in Master of Technology (M.Tech) in Chemical Engineering.

University Medal, Jadavpur University, 2020

- For standing 1st at the Bachelor of Engineering in Chemical Engineering Final Examination.

Chemical Engineering Diamond Jubilee Gold Centered Silver Medal, Jadavpur University, 2020

- For standing 1st at the Bachelor of Engineering in Chemical Engineering Final Examination.

Chittaranjan Khastagir Memorial Gold Medal, Jadavpur University, 2020

- For standing 1st at the Bachelor of Engineering in Chemical Engineering.

Jatindra Krishna Memorial Bronze Medal, Jadavpur University, 2020

- For standing 1st at the Bachelor of Engineering in Chemical Engineering.

Bandana Ghosh Memorial Gold Centered Silver Medal, Jadavpur University, 2020

- For securing highest aggregate of marks at the B.E in Chemical Engineering Final Examination.

Sudhakar Burman Smriti Bronze Medal, Jadavpur University, 2020

- For standing 1st in the courses 'Chemical Technology - I' and 'Chemical Technology - II' taken together at the Bachelor of Engineering in Chemical Engineering final Examination.