NUPUR MEHRA

PhD Student, Chemical Biomolecular Engineering, Cornell Unversity

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EDUCATION

- **Bachelor of Technology** — **Indian Institute of Technology, Kanpur**
  Major: Chemical Engineering, GPA: ***8.9/10*** — *2021*
- **High School- CBSE** — **Subodh Public School, Jaipur**
  Science and Mathematics, Percentage: ***94.6%*** — *2017*
- **Class 10- CBSE** — **Subodh Public School, Jaipur**
  Common Subjects, GPA: ***9.6/10*** — *2015*

ACHIEVEMENTS AND ACCOLADES

- Secured **perfect GPA** of **10** in the Fall Semester, Academic Year 2020-21.
- Received **Pre-Placement Offer** from Vedanta Resources for exceptional internship performance.
- Conferred with **Academic Excellence Award** based on the academic performance for the year 2019-20, given to **top 10%** students among the institute.
- Selected for **Student Undergraduate Research Graduate Excellence** (**SURGE**) by IIT Kanpur, given to top 150 applicants from all the colleges **across the country**

ONGOING PROJECT

- **Identifying best Metal-Organic Framework for Xylene Isomers separation** — **Jan'21-Dec'21**
  Mentor: Prof. Jayant K. Singh (*IIT Kanpur*)
  - Performed machine learning (ML) aided high throughput screening to identify top performing Metal-Organic Frameworks (MOFs) for adsorptive separation of Xylene mixture.
  - Determined the structural and chemical descriptors for 163,401 hypothetical MOFs using Zeo++.
  - Tested TraPPE, TraPPE with charges and OPLS force fields for Xylene and Universal Force Field for MOFs.
  - Determined partial charges for 10% of MOFs employing PACMOF after examining various methods.
  - Performed GCMC molecular simulations on the 10% MOFs at industrial feed composition of Xylene mixture obtaining their adsorption capacities and selectivities.
  - Trained ML model on the 10% of MOFs to predict the Xylene isomer selectivity for rest 90% of MOFs.

OTHER RELEVANT PROJECTS

- **Low Salinity Waterflooding for Enhanced Oil Recovery** — **Sep'20-Dec'20**
  Undergraduate Project, Prof. Himanshu Sharma (*IIT Kanpur*)
  - Conducted a comprehensive literature study of sedimentary rocks, crude oil formation and recovery methods.
  - Learned basics of fluid flow in porous media including relative permeability curves, capillary pressure curves and effect of wettability on fluid flow.
  - Examined mathematical models for single-phase and multiphase flow in porous media and attempted simulations of waterflooding using MATLAB reservoir simulation toolbox (MRST).
  - Modelled two-phase flow experiments of low salinity water flooding in carbonate rocks on in-house simulator.
  - Model included key geochemical reactions occurring at the oil-water and water-rock interfaces resulting in wettability alteration from oil-wet to water-wet state.
  - Achieved high accuracy upon comparing simulation results, including oil recovery and effluent ions, with single-phase and oil recovery results reported in the literature and the experimental data.
  - Performed sensitivity study to understand the effect of brine composition and relative permeability parameters on oil recovery.

- **Phase Diagrams of Salt Hydrates** **Aug'19-Dec'19**
  Undergraduate Project, Prof. Jayant K. Singh (IIT Kanpur)
  - Examined different models to plot the Salt Hydrate phase diagrams and coded them in MatLab.
  - Simplified the Pitzer-Simonson-Clegg (PSC) model for plotting phase diagrams of monovalent salts.
  - Plotted the phase diagram for the system of Lithium Chloride and water by implementing the PSC model.
  - Plotted the phase diagram for Calcium Dichloride and water using Brunauer–Emmet–Teller (BET) model.
- **Enhancing the wetting ability of surfaces using Surfactant and Nanoparticles** **May'19-Jul'19**
  SURGE'19, Mentor: Prof. Jayant K. Singh (IIT Kanpur)
  - Experimentally evaluated the effectiveness of Triton X-100 (TX-100) surfactant at varying concentrations to alter Glass weattability and adhesion by Sessile Drop Method.
  - Examined the interaction of TX-100 and Silicon Dioxide (SiO_2) nanoparticles at varying compositions for the colloid on Glass and Aluminum surfaces.
  - Partitioned the surface energy of colloids in polar and dispersive components by a reverse protocol to Owens-Wendt method using experimentally determined energy components of Glass, Aluminum and Teflon surfaces.
  - Concluded that surfactants can be effectively used to enhance wetting and the increasing trend of polar surface energy component with increasing nanoparticles in the colloid.
  - Prepared and presented a research poster summarizing the project.

INDUSTRIAL EXPERIENCE

- **Vedanta Aluminium, Vedanta Resources Ltd.** **Jul'21 – May'22**
  Process Analyst
  - Tuned the parameters of 15 Hall Heroult electrolysis pots to operate them at 1% increased excess AlF_3 to improve current efficiency by 1+% without impacting the pot health.
  - Enhanced the thermal balance of 15 Hall Heroult electrolysis pots to diminish the pot leakages.
  - Tracked the daily noise, temperature, metal height, current efficiency and specific power consumption of the 12 Potline rooms to analyze their performance.
- **Chanderiya Lead Zinc Smelter, Hindustan Zinc Ltd.** **Jul'20 – Sep'20**
  Summer Intern
  - Formulated the mass balance for a 35,000 MTPA Raw Zinc-Oxide treatment plant project employing the reaction conversions and final pH levels deduced by performing 4+ steps lab-scale reactions.
  - Created utility balance for total water, air and steam requirements by heat balance for 7 unit processes.
  - Achieved the cost saving of $ 0.26 million by evaluating new equipment sizes and quantities for the project utilising the calculated capacities and considering the market availability .
  - Completed the process flow diagram with the flow balance table for 26 slurry streams.

RELEVANT COURSEWORK & TECHNICAL SKILLS

Chemical Engineering	Process Design | Colloids and Interface Science | Process Control | Unit Operations Lab | Electronic, Polymeric & Ceramic Materials | Process Industries
Maths & Computing	Numerical Methods | Algorithmic Toolbox | Probability & Statistics | Data Structures & Algorithms
Languages	Python, C/C++, MATLAB
Simulation	Aspen Plus, MATLAB Simulink, MRST toolbox, Zeo++

EXTRACURRICULARS

Leadership	*Overall Coordinator*, Photography Club, IIT Kanpur
Mentorship	*Student Guide*, Counseling Service, IIT Kanpur
	Academic Mentor, Counseling Service, IIT Kanpur
Sports	*Player of the Camp*, Table Tennis Summer Camp, IIT Kanpur
Photography	*First Position* in Street Photography, Inter-IIT Cultural Meet-2019