Mehul Bapat

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Material design and mechanics engineer. PhD candidate with 5+ years of experience developing physics-based, reduced-order, and CFD models for reactors, absorbers, and transport-dominated unit operations. Expertise in reactor-scale CFD, mixing analysis, model validation, and computationally efficient digital representations to support process design, optimization, and scale-up. Strong background in translating complex simulations into actionable insights for experimentalists and engineers using COMSOL, Python, MATLAB, and commercial multiphysics tools.

EDUCATION

Carnegie Mellon University (CMU) — Pittsburgh, PA
Doctor of Philosophy in Mechanics, Chemistry and Materials — (Anticipated) February 2026
Master of Science in Mechanics, Chemistry and Materials — May 2025
Master of Science in Chemical Engineering — December 2020
Overall GPA: 3.78/4.0
Honors: Dean's Fellowship, Dr. Elio D'Appolonia Fellowship, Neil and Jo Bushnell Fellowship

Indian Institute of Technology (IIT) — Varanasi, India
Bachelor of Technology in Chemical Engineering — May 2019

SKILLS

- Physics-based and data-driven multi-scale modeling
- Multiphysics CFD simulations (COMSOL, FEniCS)
- Molecular and quantum chemistry simulations (LAMMPS, ORCA)
- In-silico synthesis and design (Avogadro, Ovito, FreeCAD, Solidworks)
- High-throughput computing and data analysis (Python, Bash, MATLAB, Visual-Basic)

PH.D. AND MASTERS THESIS RESEARCH

Improving design of fluid-repelling surfaces/interfaces — February 2021 - Present

- Published cover article in Royal Society of Chemistry and presented at 3 international conferences
- Modeled fluid-solid interfaces to design water-repelling materials and surfaces using LAMMPS
- Developed physics-based models to predict hydrophobicity with high accuracy (>99%)
- Created data-driven models to improve computational efficiency by $> 80\%$
- Mentored undergraduate researcher to study hydrophobic graphene-oxide membranes
- Developed a high-throughput pipeline (Python + MS Excel) to perform 25,000+ simulations
- Automated analysis of high-volume (500+ GB) simulation data (Python + MATLAB)

Optimizing absorber column for carbon capture
Collaboration with Lawrence Livermore National Laboratory — May 2022 - May 2023

- Simulated absorber column for carbon capture using CFD in COMSOL
- Optimized column topology and design for energy-efficient carbon adsorption
- Developed a novel method that maximized catalyst exposure while minimizing pumping costs
- Automated CAD geometry building, CFD simulations and data analysis using MATLAB

Eco-friendly plastic packaging via self-healing polymers — October 2023 - Present

- Collaborated with experimental researchers to design sustainable plastic polymers
- Developed molecular models of packaging plastic using LAMMPS, OVITO, Avogadro
- Modeled plastic stiffness and crystallinity by analyzing microstructural properties
- Validated experimental trends using computational techniques
- Synthesized 200+ polymers in-silico using (Python + Bash) automation

Gas transport and mixing inside a microreactor
Masters Research Project — January 2020 - March 2021

- Modeled experimental apparatus using CFD simulations in COMSOL
- Created 3D and 2D models of microreactor using CAD, parametrized geometry via MATLAB
- Identified bottlenecks in reactor performance for product mixing and conversion
- Derived flow conditions for optimal mixing and minimal reactant loss
- Received poster award among 60 posters in Chemical Engineering Research Symposium

Modeling transport of aqueous catalyst Fe-TAML for water treatment January 2025 - Present

- Collaborated with chemists at Sudoc LLC to improve catalyst design for water treatment
- Performed quantum chemistry simulations of Fe-TAML to model interactions with water
- Analyzed effect of surface chemistry on molecular orientations of Fe-TAML
- Created 25+ unique geometries using (Avogadro + CAD) to conduct 500+ simulations in LAMMPS

Additional Research

Assessing water permeability of Graphene-Oxide (GO) polymer composites January 2024 - December 2024

- Assisted experimental collaborators with improving membrane design using molecular models
- Performed simulations of water transport through GO membranes in LAMMPS
- Created atomistic models of GO membranes with different geometries and oxidation levels

Identifying body-parts of unicellular organisms through image processing and machine learning
Research at Computational Biology Department in CMU January 2020 - May 2020

- Contributed to a collaborative effort in detecting microbe body-parts from microscopic images
- Developed an image masking technique and improved body-part detection by 90%
- Programmed 2 MATLAB functions to automate processing of bio-format images

Publications

M. Bapat, G.J. Wang. "Revealing nanoscale slip within Taylor-Aris dispersion", Nanoscale, Royal Society of Chemistry, 2025, 17, 14157-14163. Published as cover article. https://doi.org/10.1039/D4NR03468F

J. Vinskus, **M. Bapat**, G.J. Wang, K. Noonan. "Synthesis and mechanical properties of degradable disulfide polymer nanocomposites" [under preparation]

M. Bapat, G.J. Wang. "Correlation between parameters of kinetic theory scaling for slip flow" [under preparation]

M. Bapat, R. Sullivan, M. Mills, G. J. Wang. "Orientational mechanics of Iron(III) Tetra-amido macrocyclic ligands in water" [under preparation]

Conference Presentations

Bapat, Mehul. "Understanding nanoscale slip velocity through the lens of Taylor-Aris dispersion". American Institute of Chemical Engineers (AIChE), San Diego, CA, October 2024. Conference Poster.

Bapat, Mehul. "Modeling nanoscale slip velocity through Taylor-Aris dispersion". American Physics Society, Division of Fluid Dynamics, Washington D.C., November 2023. Conference Talk.

Bapat, Mehul. "Microscopic insights into onset of slip in Lennard-Jones fluids". American Physics Society, Division of Fluid Dynamics, Indianapolis IN, November 2022. Conference Talk

Bapat, Mehul. "Slip in nanoscale Couette flow". Molecular Simulators Meet, Pittsburgh PA, May 2022. Conference Talk

Course Projects

Effect of Reynolds number on drag coefficient of a sphere
Advanced Transport Phenomena August 2024 - December 2024

- Performed CFD simulations in COMSOL to study drag on a sphere in a moving viscous fluid
- Computed drag coefficient of the sphere at different flow velocities to investigate the effect of Reynolds number

Fluid flow through porous media
Finite Element Method January 2023 - April 2023

- Derived weak form of porous-media flow equations and solved modified Navier-Stokes equations in FEniCS

Teaching Assistant Experience

Molecular Simulation of Materials, CMU Pittsburgh PA
Graduate Teaching Assistant Fall 2022, Fall 2023, Fall 2024

- Conducted 2 class lectures and 10+ recitation sessions to teach fundamentals of molecular dynamics
- Designed course content used in class lectures and recitation sessions
- Mentored 10+ student project teams, providing detailed feedback on modeling, code implementation, and interpretation of simulation results.
- Led coding workshops on parallel programming in Python & MATLAB, debugging student code & explaining best practices.