

**Summary:** A detail-oriented chemical engineer with a strong background in computational modeling, data science and scientific software development, supported by research and professional work experience in process design and optimization.

## Education

**Doctor of Philosophy in Chemical Engineering** (May 2023)

**Master of Science in Chemical Engineering** (Oct 2021)

*University of Rochester, Rochester, NY*

*Thesis: "Physics-informed Machine Learning in Chemical Engineering"*

**Master of Science in Environmental Engineering** (May 2018)

*Missouri University of Science and Technology (UMR), Rolla, MO*

*Thesis: "Numerical Modeling of Capillary-driven Flow in Open Microchannels: An Implication of Optimized Wicking Fabric Design"*

**Bachelor of Science in Chemical Engineering** (July 2015)

*University of Tehran, Iran*

*Thesis: "Experimental Setup and Optimization for Electro-catalytical Generation of Hydroxyl Radicals in Wastewater Treatment"*

## Work Experience and Practical Training

**Research Assistant** (2019 - present)

*University of Rochester, Rochester, NY*

- Developing web-based deep learning [frameworks](#) for semi-supervised classification of the activity of antimicrobial peptides via positive-unlabeled learning
- Developed a [disease modeling framework](#) to predict future disease spreads and infer location of patient-zero
- Developed an automated [framework](#) in CFD modeling that reduces the number of simulations using active learning and generates a symbolic equation for the system of interest via symbolic regression
- Contributed to development of a [simulation-based inference framework](#) via maximum entropy re-weighting
- Contributed to development of a plugin with TensorFlow GPU-accelerated operations combined with HOOMD-Blue molecular dynamics simulation engine ([HOOMD-TF](#))
- Developed a [web-app](#) for peptide-based gelator transparency classification using Kernel ridge regression
- Developed an [automated module](#) on a Raspberry-Pi for real-time monitoring of HPC using Python, JS and HTML
- Implemented finite difference analysis in Python to study [2D shallow water dynamics](#)
- Implemented Monte Carlo simulations in MATLAB to study evolution of spin configurations of a ferromagnet using the Ising model

**Energy and Materials Research Intern** (May 2022 - present)

*Toyota Research Institute, Los Altos, CA*

- Developing deep learning framework to make inference on battery life cycle

**Teaching Assistant of "Advanced Transport Phenomena"** (Aug - Dec 2020)

*University of Rochester, Rochester, NY*

- Tutored students on homework related problems

**Teaching Assistant of "Fundamentals of Fluid Mechanics"** (Jan - May 2020)

*University of Rochester, Rochester, NY*

- Tutored students on homework related problems and organized laboratory experiments

**Lead CFD Analyst at Missouri S&T Solar Car Design Team** (2016 - 2018)

*Missouri University of Science and Technology, Rolla, MO*

- Developed validated [wind tunnel simulations](#) in STAR-CCM+ for aerodynamic optimization of the solar car
- Improved aerodynamic design efficiency prior to manufacturing

**Manufacturing Process Modeling Intern** (May-Dec 2017)

*The Goodyear Tire & Rubber Company, Akron, OH*

- Phase-change heat transfer modeling and optimization of tire vulcanization process in ANSYS
- Model verification based on plant data and analytical solution
- Utilized assets more efficiently through MATLAB post processing and automating the simulation process using OPTIMUS
- Provided faster simulation results using Adaptive Mesh Refinement and High-Performance Computing
- GUI development and coupling ANSYS with MATLAB for time-effective post processing

## Work Experience and Practical Training

### Research Assistant

(2016 - 2018)

Missouri University of Science and Technology, Rolla, MO

- Numerical modeling of multiphase flow in open microfluidics using ANSYS and STAR-CCM +
- Reduced simulation run-time by developing an algorithm for [Adaptive Mesh Refinement](#) (AMR)
- Increased solver's stability by developing an algorithm for Adaptive Time Step

### Teaching Assistant of "Applied Numerical Methods in CFD"

(Jan-May 2017)

Missouri University of Science and Technology, Rolla, MO

- Lectured on Finite Difference Analysis in fluid dynamics, heat and mass transfer using MATLAB
- Organized CFD and programming workshops for ANSYS and Star-CCM +

### Teaching Assistant of "Process Control"

(2014-2015)

University of Tehran, Iran

- Tutored undergraduate students in process control using MATLAB and VisSim

### Engineering Intern

(July-Sept 2014)

Emden-Leer University of Applied Sciences, Emden, Germany

- Design of experiments in advanced oxidation process (AOP) for wastewater treatment

### President of IAESTE Iran

(Apr 2013-July 2014)

(International Association for the Exchange of Students for Technical Experience)

- Led a team of college students that organized technical internships internationally

### MATLAB Programming Tutor

(July-Sept 2011)

University of Tehran, Iran

- Organized advanced programming workshops for engineering students

## Computer Skills

Scientific Softwares Developed:

- [MaxEnt](#)
- [PyQ](#)
- [HOOMD-TF](#)
- [AL-CFD](#)
- [Peptide.bio](#)
- [GTP](#)

**Other tools:** MATLAB, STAR-CCM+, ANSYS, OPTIMUS, CATIA

**Languages:** Python, JavaScript, HTML, CSS

## Honors and Awards

Kwang-Yu and Lee-Chien Wang Fellowship

(Nov 2021)

Department of Chemical Engineering, University of Rochester

Earl W. Costich Graduate Fellowship

(May 2020)

Department of Chemical Engineering, University of Rochester

First place winner: 2017 Mike Alizadeh Scholarship

(Aug 2017)

American Society of Civil Engineers (ASCE)

Recognized reviewer: *Journal of Environmental Chemical Engineering*

(May 2016)

MATLAB programming contest

(Mar 2014)

University of Sharif Computer-Aided Chemical Engineering Contest (SC<sub>3</sub>)

Sharif University of Technology, Iran

## Publications

1. [Serverless Prediction of Peptide Properties with Recurrent Neural Networks](#)  
Bioinformatics (Submitted June 2022)  
**M Ansari**, AD White.
2. [Book chapter: Hyper-parameter Optimization in Deep Learning](#)  
Deep Learning for Molecules and Materials. (May 2022)  
**M Ansari**, AD White.
3. [Inferring Spatial Source of Disease Outbreaks using Maximum Entropy](#)  
American Physical Society, Physical Review E. (Submitted 2021)  
**M Ansari**, D Soriano-Paños, G Ghoshal, AD White.
4. [Iterative Symbolic Regression for Learning Transport Equations](#)  
AIChE Journal, Special Edition for AI (March 2022)  
**M Ansari**, HA Gandhi, DG Foster, AD White.
5. [Simulation-based Inference with Approximately Correct Parameters via Maximum Entropy](#)  
Advances in Neural Information Processing Systems 33: Workshop on Machine Learning for Structural Biology. (2020)  
Machine Learning in Science and Technology (April 2022)  
R Barrett, **M Ansari**, G Ghoshal, AD White.