



## Summary:

A detail-oriented chemical engineer with a strong background in **computational modeling**, **machine learning** and **scientific software development**, supported by academic research and professional work experience.



## Education



### Doctor of Philosophy in Chemical Engineering

(May 2023)

### Master of Science in Chemical Engineering

(Oct 2021)

University of Rochester, Rochester, NY

Thesis: "Applications of Physics-informed Machine Learning in Chemical Engineering". Advisor: [Andrew D White](#)

### 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



### Postdoctoral Research Fellow

(June 2023 - present)

Acceleration Consortium, Toronto, ON

- Developing [agent-based chemistry plugins](#) via large language models to accelerate design of materials for CO<sub>2</sub> reduction

### Research Assistant

(2019 - 2023)

University of Rochester, Rochester, NY

- Developed a HuggingFace [app](#) that answers questions from scientific papers using OpenAI's large language models
- Developed a [edge-computing cheminformatics tool](#) for semi-supervised classification of the activity of antimicrobial peptides via positive-unlabeled learning using recurrent neural networks
- Developed a [disease modeling tool](#) to predict future disease spreads and infer location of patient-zero
- Developed an [automated tool](#) 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 tool](#) via maximum entropy reweighting
- 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 tool](#) 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 & Materials Intern and Research Engineer

(May 2022 - Mar 2023)

Toyota Research Institute, Los Altos, CA

- Developed deep learning tools to predict degradation of used batteries with unknown cycling histories. **US Patent pending**

### Teaching Assistant of "Advanced Transport Phenomena"

(Jan - Dec 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

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

(Jan-May 2017)

Missouri University of Science and Technology, Rolla, MO

- Organized CFD and programming workshops for ANSYS and Star-CCM +



## 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

### Engineering Intern

(July-Sept 2014)

Emden-Leer University of Applied Sciences, Emden, Germany

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



## Computer Skills



#### Scientific Softwares Developed:

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

Other tools: AWS, TensorFlow, PyTorch, Scikit-learn, JAX, Pandas

Languages: Python, JavaScript, HTML, CSS



## Honors and Awards



Acceleration Consortium Research Fellowship

(May 2023)

University of Toronto, Toronto

 1<sup>st</sup> place winner at [Battery Informatics & ML Kaggle Competition](#)

(Dec 2022)

Materials Research Society, Boston, MA

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

 1<sup>st</sup> 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)

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


## Publications and Patents ([Google Scholar](#))



1. [Learning Peptide Properties with Positive Examples Only](#) (June 2023)  
M Ansari, AD White
2. [History-agnostic Battery Degradation Inference](#) and **US Patent Pending** (Mar 2023)  
*Journal of Applied Energy*  
M Ansari, S Torrisi, A Trewartha, S Sun
3. [Serverless Prediction of Peptide Properties with Recurrent Neural Networks](#) (Apr 2023)  
*Journal of Chemical Information and Modeling*  
M Ansari, AD White
4. [Assessment of Chemistry Knowledge in Large Language Models that Generate Code](#) (Jan 2023)  
*Digital Discovery*  
AD White, GM Hocky, HA Gandhi, M Ansari, S Cox, GP Wellawatte, S Sasmal, Z Yang, K Liu, Y Singh, WJ Peña Ccoa
5. [Book chapter: Hyper-parameter Optimization in Deep Learning](#) (July 2022)  
*Deep Learning for Molecules and Materials, Living Journal of Computational Molecular Science*  
M Ansari, AD White
6. [Inferring Spatial Source of Disease Outbreaks using Maximum Entropy](#) (July 2022)  
*American Physical Society, Physical Review E*  
M Ansari, D Soriano-Paños, G Ghoshal, AD White
7. [Iterative Symbolic Regression for Learning Transport Equations](#) (Mar 2022)  
*AIChE Journal, Special Edition for AI*  
M Ansari, HA Gandhi, DG Foster, AD White
8. [Simulation-based Inference with Approximately Correct Parameters via Maximum Entropy](#) (Apr 2022)  
*Machine Learning in Science and Technology*  
R Barrett, M Ansari, G Ghoshal, AD White



## Presentations and Talks



1. Maximum Entropy Inference in Chemical Reaction Networks with Unknown Kinetic Parameters (Nov 2022)  
*AIChE, Phoenix, AZ*
2. Rescuing Physics-based Models with Maximum Entropy Reweighting (Sept 2022)  
*Wang Lecture, University of Rochester, NY*
3. Positive Unlabeled Learning of Peptide Properties (July 2022)  
*Fundamentals of Molecular Modeling and Simulation, Delavan, WI*
4. Serverless Prediction of Peptide Properties with Recurrent Neural Networks (June 2022)  
*Middle Atlantic Regional Meeting of the American Chemical Society, Ewing Township, NJ*
5. [Simulation-based Inference with Approximately Correct Parameters via Maximum Entropy](#) (Dec 2020)  
*Advances in Neural Information Processing Systems 33: Workshop on Machine Learning for Structural Biology*