Zixuan Zhang

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Profile

I am looking for a **PhD position starting Fall 2026**. My research interests include: **i) data-driven global optimization, ii) application of ML & LLM in process modeling, optimization and design , iii) renewable energy/biochemical process system**. For more detailed information, please visit Zixuan Zhang's personal website.

Education

Institute of Process Engineering, Chinese Academy of Science *Sept. 2023 – July 2026*
GPA: 3.88/4 *(Expected)*
M.S. in Chemical Engineering

School of Chemical Engineering, Xi'an Jiaotong University *Sept. 2019 – July 2023*
GPA:3.39/4.3 , Rank: 5/48
B.S. in Chemical Engineering and Technology

Research Experience

Multi-Objective optimization and software development for heat exchanger networks in methanol synthesis plants. Undergraduate thesis
Corporate-sponsored
Funded by **Yingde Gas Group Co., Ltd** Nov. 2022 - June 2023
Supervisor: **Prof. Guilian Liu**

- Analyzed and quantified fluctuation propagation in heat exchanger networks (HENs) with graph theory and identified the trade-off between structural complexity and heat exchange load.
- Developed a feasibility-driven structure-load optimization algorithm based on NSGA-II for multi-objective optimization improvement.
- Designed and implemented analysis software for industrial application and published 1 journal article.

Development of simulation and optimization technology for phosphoric acid preparation process. Corporate-sponsored
Jan. 2024 - June 2025
Funded by **Guizhou Phosphate Chemical Group**
Supervisor: **Prof. Xin Xiao** & **Prof. Yujiao Zeng**

- Developed a Fortran subroutine for modeling the apparent reaction kinetics of ore acidulation in Aspen Plus , achieving less than 3% relative error under nominal conditions.
- Constructed a hybrid dataset using simulation and plant data and built a surrogate model using the W&D model with transfer learning, enabling model adaptation across scenarios with less than 2% relative error.
- Proposed a machine-learning-surrogated feasible path SQP algorithm (MLSQP), ensuring rapid convergence to KKT points.
- Validated the optimization in both mechanistic models and real-world plants, reducing non-water-soluble phosphorus content in gypsum by 8.2% through feed ratio adjustment.

A data-driven framework for global optimization of chemical processes and intelligent implementation via LLM agents. Graduate thesis
In preparation
Primary advisor: **Prof. Xin Xiao**
Co-advisor: **Prof. Yujiao Zeng** & **Dr. Jie Li**

- Improved a spatial branch-and-bound (sBB) framework by integrating convex neural networks as data-driven convex underestimators. Lower bounds are solved via MLSQP, and branching with hyperplanes which is determined based on both fitting performance and convexity analysis.
- Developed a multi-agent system leveraging large language model (LLM) to automate process modeling and optimization. The platform enables using natural-language to implement Aspen simulation, sampling, surrogate training, optimization problem modeling and executing optimization algorithms.

Publication & Working paper

Multi-objective optimization of heat exchanger network with disturbances based on graph theory and decoupling. **Chem. Eng. Sci.** Feb. 2024

Zixuan Zhang,Liwen Zhao, Ibrahim Tera, Guilian Liu*

Links:[DOI]

Machine Learning Powered Feasible Path Framework with Adaptive Sampling for Black-box Optimization. **AIChE J.** Under Review

Zixuan Zhang, Xiaowei Song, Jiaming Li, Yujiao Zeng, Yaling Nie, Min Zhu, Dongyun Lu, Yibo Zhang, Xin Xiao*, Jie Li*

Links: [ArXiv] [GitHub]

Surrogate-assisted optimization for real-world wet-process phosphoric acid production. **I&ECR** Minor Revision

Zixuan Zhang, Xiaowei Song, Yujiao Zeng*, Jianhua Chen, Limin Wang, Zhuiwu Zhou, Shaoxiu Xue, Songlin Liu, Jie Li, Xin Xiao*

Conference Presentation

An automatic platform for process modeling and optimization leveraging large language models. Boston, USA

2025 AIChE Annual Meeting (Poster, First Author, Accepted)

Links: [Abstract]

Convex neural network tree for black-box or expensive global optimization. Boston, USA

2025 AIChE Annual Meeting (Poster, First Author, Accepted)

Links: [Abstract]

Application of explicit algebraic formulation of multilayer perceptron in process system optimization. Yulin, China

2024 Process Systems Engineering Annual Meeting (Oral, First Author)

Global optimization of heat exchange network based on ReLU neural network approximation. Dalian, China

2024 Process Big Data and Intelligence Frontier Forum (Poster, First Author)

Awards & Honors

Scholarship

- Jizhi First Prize Scholarship — Dec. 2021
- Third Prize Scholarship of Xi'an Jiaotong University (XJTU) — Dec. 2020

Awards

- Excellent Award of XJTU in National College Student Energy Conservation and Emission Reduction Competition — Sep. 2022
- Third Prize in Northwest Division in National College Student Chemical Design Competition — Aug. 2022
- Second Prize of Shaanxi Province in National College Student Mathematical Modeling Competition — Dec. 2021

Honors

- Merit Student of University of Chinese Academy of Sciences — May. 2025
- Outstanding volunteer of the 14th 2021 National Games of China — Jan. 2022
- Outstanding Student Cadres of Xi'an Jjiaotong University — Dec. 2020, Dec. 2021

Skills

Languages: English, Mandarin Chinese
Programming: Python, C++, Matlab, Fortran
Software: Aspen Plus, GAMS