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 AI in process modelling, optimization and design, iii) biochemical/integrated energy system**. For more information, please visit Zixuan Zhang's website.

Education

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

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: **Assoc. Prof. Yujiao Zeng** & **Dr. Jie Li**

- Proposed a machine learning powered feasible path (MLFP) algorithm combined with adaptive sampling to solve general black-box optimization problems. This method only requires a small amount of sampling, avoiding the large number of intermediate variables and nonlinear terms imposed by the full-space formula of the surrogates, ensuring convergence to the KKT point of the surrogate model.
- Improved a spatial branch-and-bound (sBB) framework by integrating convex neural networks as data-driven convex underestimators. Lower bounds are solved via MLFP, 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.

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** & **Assoc. 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.
- MLFP is used to solve the surrogate-assisted optimization problem under three different scenarios.
- 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.

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.

Publication & Working paper

Machine Learning Powered Feasible Path Framework with Adaptive Sampling for Black-box Optimization. — **AIChE J.**, Major Revision
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**, Dec. 2025
Zixuan Zhang, Xiaowei Song, Yujiao Zeng*, Jianhua Chen, Limin Wang, Zhuiwu Zhou, Shaoxiu Xue, Songlin Liu, Jie Li, Xin Xiao*
Links:[DOI]

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]

Conference Presentation

LLM-Driven Multi-Agent System for Surrogate Optimization Workflow. — Boston, USA
2025 AIChE Annual Meeting (Poster, First Author, Accepted)
Links: [Abstract]

Spatial Branch-and-Bound Algorithm with Convex Neural Network Underestimators and Hyperplane Tree. — 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
- National Scholarship for Graduate Students — Oct. 2025
- 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