Yuxiang Chen

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EDUCATION

East China University of Science and Technology Shanghai, China

M.S. (2018-2021), **Ph.D.** (2021-2023), Chemical Process Sep 2018 - Dec 2023 (Expected)

GPA: 3.0/4.0 (84.5/100) *Advisor*: Hui Sun, Ph.D., Fahai Cao, Ph.D.

Relevant Coursework: Mathematical Modeling of Chemical Processes, Multiscale Simulation of Chemical Products, Advanced Reaction Engineering, Combinatorial Optimization

Changzhou University Jiangsu, China

B.S., Oil & Gas Storage and Transportation Engineering Sep 2014 - Jun 2018

GPA: 3.1/4.0 (85/100)

Relevant Coursework: Engineering Fluid Mechanics, Engineering Thermodynamics

RESEARCH EXPERIENCE

East China University of Science and Technology Sep 2018 - Dec 2023

Intelligent Design of Molecular Composition of Solvents for Natural Gas Desulfurization

• Expanded our custom-designed models and revealed chemical mechanisms to a total of 13 organosulfides.

• Developed an intelligent solvent composition design strategy that can dynamically respond to feedstock organosulfides, facilitating the removal of organosulfides from natural gas in one step.

Study on the Mechanism of Physical and Chemical Coupling Effect of Solvent-Solute Synergistic Competition

• Proposed a physical-chemical coupling ML approach that predicts solubilities of carbonyl sulfide (COS) in both reactive and non-reactive solvents well.

• Developed a descriptor-based molecule generation method that has identified potential solvents for COS capture.

Determining Reaction Mechanisms via Chemical Reaction Kinetics Models Constructed with Machine Learning Techniques

• Constructed random forest models to predict reaction kinetics of COS with solvents.

• Revealed that the charge distribution and steric hindrance of solvent molecules largely determine the reaction kinetics, and designed two molecular descriptors to improve the kinetics predication performance.

Development of Compound Solvent for Desulfurization of High Sulfur Content Natural Gas

• Developed a Molecular Active Selection Machine Learning (MASML) computational framework, MASML can accelerate the solvent screening process by integrating molecular similarity search and active learning methods.

• Identified three solvent molecules that show promising potential for capturing methyl mercaptan (MeSH), and one of them has reached the stage of industrial trial.

Changzhou University Jan 2018 - Jun 2018

• Designed and manufactured an automated adsorption removal device, equipped with electric valves to control the amount of gas inflow, a Raspberry Pi to regulate the electric valves, and sensors to record pressure within the device.

LEADERSHIP & TEACHING

Assistant Researcher, East China University of Science and Technology Jan 2019 - Dec 2023

• Led a team of 5 members to develop new high-performance solvents for desulfurization of high sulfur content natural gas.

• Provided training to newly enrolled graduate students on computational chemistry and mathematical modeling.

Assistant Class Supervisor, Changzhou University Sep 2016 - Jun 2018

• Assisted the class advisor in managing a cohort of 29 new college students, organized and facilitated group activities to enhance student engagement.

HONOR & COMPETITION

HONOR

• Outstanding student at the university, East China University of Science and Technology Dec 2022

• PetroChina Scholarship, China National Petroleum Co. Dec 2022

• Titan-Adamas Scholarship, Titan Shanghai Technology Co. Dec 2021

• Outstanding graduate, Changzhou University Jun 2018

COMPETITION

• National Third Prize, The 18th China post-graduate mathematical contest in modeling Dec 2021
• National Third Prize, The 17th China post-graduate mathematical contest in modeling Dec 2020
• National Second Prize, The 16th China post-graduate mathematical contest in modeling Dec 2019
• National Second Prize, The 1st Petroleum & Gas Storage and Transportation Engineering Design Competition Dec 2016

PUBLICATION & PRESENTATION

JOURNAL

Energy & Fuels (First Author, IF = 4.654, Under Review) Jun 2023
• "Intelligent Molecular Identification Approach to High-efficiency Solvent for Organosulfide Capture Using Active Machine Learning Framework"

Chemical Engineering Science (First Author, TOP, IF = 4.889, DOI: 10.1016/j.ces.2023.118984) Jun 2023
• "Physical–chemical Coupling Machine Learning Approach to Exploring Reactive Solvents for Absorption Capture of Carbonyl Sulfide"

Industrial & Engineering Chemistry Research (Co-first Author (2), IF = 4.326, DOI: 10.1021/acs.iecr.2c04559) Mar 2023
• "Interpretable Machine Learning Model for Predicting Interaction Energies between Dimethyl Sulfide and Potential Absorbing Solvents"

Chemical Engineering Journal (First Author, TOP, IF = 16.744, DOI: 10.1016/j.cej.2022.136662) Sep 2022
• "Machine-learning-guided Reaction Kinetics Prediction towards Solvent Identification for Chemical Absorption of Carbonyl Sulfide"

Industrial & Engineering Chemistry Research (Co-first Author (2), IF = 4.326, DOI: 10.1021/acs.iecr.2c00321) Apr 2022
• "Revealing the Structure–Interaction–Dissolubility Relationships through Computational Investigation Coupled with Solubility Measurement: Toward Solvent Design for Organosulfide Capture"

Industrial & Engineering Chemistry Research (First Author, IF = 4.326, DOI: 10.1021/acs.iecr.0c05483) Jan 2021
• "Structure–Property–Energetics Relationship of Organosulfide Capture Using Cu (I)/Cu (II)-BTC Edited by Valence Engineering"

CONFERENCE

Mathematics in (bio)Chemical Kinetics and Engineering (First Author, Oral Presentation) Oct 2021
• "Intelligent Molecule Design to Explore Potential Solvents for Carbonyl Sulfur (COS) Absorption Based on Reaction Kinetics Prediction"

PATENT

Chinese Patent Application

• A Compound of Alkoxylated Propylamine and Its Application in Organic Sulfur Absorption and Removal May 2023 (Third Inventor, Invention Patent Disclosed, CN202310106624.0)

• Etheramine Compounds for Efficient Absorption and Removal of Organosulfide and Their Design Methods Jul 2022 and Applications (Fourth Inventor, Invention Patent Disclosed, CN202210236109.X)

• The Application of An Amine Compound for Removal of Organosulfide (Third Inventor, Invention Patent Jul 2022 Granted, ZL202110640696.4)

• The Application of An Amine Compound in Enhancing the Solubility and Absorption of Organosulfide for Jul 2022 Removal Purposes (Third Inventor, Invention Patent Granted, ZL202110640678.6)

• A Catalytic Reaction Device (First Inventor, Invention Patent Granted, ZL201910583467.6) Sep 2021