Weizhen Sun

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Profile

Weizhen Sun is a full professor of Chemical Engineering at East China University of Science & Technology (ECUST). He obtained his B.S. in Chemical Technology from ECUST (1999) and earned his Ph.D. in Chemical Engineering from ECUST (2009). He worked in the Lubricating Oil Factory of Qingdao Iron & Steel Co. Ltd as a deputy director (1999-2001). From 2004 after earning master's degree in Chemical Engineering, he started to work at ECUST as an assistant Professor, associate Professor and full professor in Chemical Engineering. He studied molecular simulation technology at UC Berkeley as a visiting scholar under the supervision of Prof. Berend Smit from 2012 to 2013. His current research interests include Chemical Reaction Engineering, Chemical Process Intensification, and Process Simulation on petrochemical, new energy, and new materials. He published more than 80 research papers.

Research Field

1. Chemical Process Intensification

By studying surface interface phenomena such as dissolution, diffusion, and self-organization of small molecules on the surface of multiphase reactions (liquid-liquid, gas-liquid, gas-solid, gas-liquid-solid), to understand and guide the enhancement of reaction processes and the design of catalysts. Research objects include C4 alkylation, liquid phase oxidation of hydrocarbons, ethane oxychlorination, Deacon reaction, etc.

2. Multiscale Simulations

Conventional Monte Carlo (MC), molecular dynamics (MD) simulation and reaction force field-based molecular dynamics (ReaxFF-MD) simulation (to study fast reactions such as combustion and cracking); kinetic modeling of complex reaction systems; Reactor simulation; Chemical process simulation.

3. Chemical Process Development

Development of industrial reactors, enhancement and optimization of chemical process, etc. Research contents include (1) Gas-liquid reaction systems such as aromatic hydrocarbon (PX, MX) oxidation, 1,2,4,5-Tetramethylbenzene oxidation, 2,6-Dimethylnaphthalene oxidation, 5-HMF oxidation and preparation and purification of monomers for new polymers; (2) Liquid-liquid reaction systems such as ionic liquid/sulfuric acid catalyzed C4 alkylation to synthesize high-quality clean gasoline, etc.; (3) The continuous process design of high-value fine chemicals, etc.

4. Chemical Engineering for Materials

The controllable preparation of nanoporous materials such as MOF, ZIF, and COF, and their applications in chemical separation, medical sterilization and drug loading, and lithium-ion batteries. The synthesis of various new ionic liquids (IL) for catalytic reactions and medical sterilization.

Research results and main published thesis

1、Process Intensification

1) Enhanced catalytic performance of H2SO4-catalyzed C4 alkylation by formyl functional [N1,1,1,1][C10SO4] additive. AIChE Journal, 2023, 69: e18179.
2) Molecular-level swelling behaviors of poly (ethylene terephthalate) glycolysis using ionic liquids as catalyst. Chemical Engineering Science, 2023, 267: 118329.
3) Target high-efficiency ionic liquids to promote H2SO4-catalyzed C4 alkylation by machine learning. AIChE Journal, 2022, 68: e17698.
4) Effects of deep eutectic solvents on H2SO4-catalyzed alkylation: Combining experiment and molecular dynamics simulation. AIChE Journal, 2022, 68: e17556.
5) H2SO4-catalyzed isobutane alkylation under low temperatures promoted by long-alkyl-chain surfactant additives. AIChE Journal, 2021, 67: e17349.
6) Unveiling the microenvironments between ionic liquids and methanol for alcoholysis of poly(ethylene terephthalate). Chemical Engineering Science, 2021, 247: 117024.
7) Promoting the Sulfuric Acid Catalyzed Isobutane Alkylation by Quaternary Ammonium Ionic Liquids. AIChE Journal, 2020, 66: e16979.
8) Towards an Understanding of the Microstructure and Interfacial Properties of the Ionic Liquid/Sulfuric Acid Catalyst in Liquid-Liquid Reactions. Chemical Engineering Science, 2019, 205: 287-298.
9) Probing Interfacial Behaviors of Brønsted Acidic Ionic Liquids Improved Isobutane Alkylation with C4 Olefin Catalyzed by Sulfuric Acid. Chemical Engineering Journal, 2019, 377: 119744.
10) Experimental and Modeling Study of Isobutane Alkylation with C4 Olefin Catalyzed by Brønsted Acidic Ionic Liquid/Sulfuric Acid. Chemical Engineering Journal, 2019, 377: 119578.
11) Understanding Structure-Property Relationship of SO3H-Functionalized Ionic Liquids together with Sulfuric Acid in Catalyzing Isobutane Alkylation with C4 Olefin. Industrial & Engineering Chemistry Research, 2018, 57: 15310-15318.
12) Microstructures of the Sulfonic Acid-Functionalized Ionic Liquid/Sulfuric Acid and Their Interactions: A Perspective from the Isobutane Alkylation. Journal of Physical Chemistry B, 2018, 122: 1460-1470.
13) Understanding Interfacial Behaviors of Isobutane Alkylation with C4 Olefin Catalyzed by Sulfuric Acid or Ionic Liquids. AIChE Journal, 2018, 64: 950-960.
14) Screening of Imidazolium Ionic Liquids for the Isobutane Alkylation Based on Molecular Dynamic Simulation. Chemical Engineering Science, 2018, 183: 115-122.
15) Modeling of the Interfacial Behaviors for the Isobutane Alkylation with C4 Olefin Using Ionic Liquid as Catalyst. Chemical Engineering Science, 2017, 166: 42-52.

2、Kinetics, Catalysts, and Reactors

1) Understanding the Co/Mn/Br Synergistic Catalysis in Liquid Phase Oxidation of 5-Hydroxymethyl Furfural to 2,5-Furandicarboxylic Acid Based on the Effective Collision Theory. Industrial & Engineering Chemistry Research, 2023, 62: 10973-10981.
2) Kinetic Modeling of Homogenous Catalytic Oxidation of 5-Hydroxymethylfurfural to 2,5-Furandicarboxylic Acid. Industrial & Engineering Chemistry Research, 2022, 61: 18352–18361.
3) Understanding the zeolites catalyzed isobutane alkylation based on their topology effects on the reactants adsorption. Chemical Engineering Science, 2022, 250: 117387.
4) Understanding the Catalytic Oxidation of Hydrogen Chloride to Chlorine from Thermodynamics and Reaction Kinetics. Industrial & Engineering Chemistry Research, 2022, 61: 13397–13407.
5) Thermodynamics and Reaction Kinetics of the Sorbitol Dehydration to Isosorbide Using NbOPO4 as the Catalyst. Industrial & Engineering Chemistry Research, 2022, 61: 7833-7841.
6) Experiments and Kinetic Modeling on the Co/Mn/Br Catalyzed Oxidation of Prehnitene to Mellophanic Acid in the Liquid Phase. Industrial & Engineering Chemistry Research, 2022, 59: 19226-19234.
7) The shape selectivity of zeolites in isobutane alkylation: An investigation using CBMC and MD simulations. Chemical Engineering Science, 2021, 245: 116966.
8) Modeling of the Co-Mn-Br catalyzed liquid phase oxidation of p-xylene to terephthalic acid and m-xylene to isophthalic acid. Chemical Engineering Science, 2021, 232: 116340.
9) Multiscale Modeling of Isobutane Alkylation with Mixed C4 Olefins Using Sulfuric Acid as Catalyst. Industrial & Engineering Chemistry Research, 2019, 58: 6340-6349.
10) Multi-Scale Modeling of Isobutane Alkylation with 2-Butene Using Composite Ionic Liquids as Catalyst. Chemical Engineering Science, 2018, 186: 209-218.

3、Chemical Engineering for Materials (Porous Materials, Lithium Metal Battery)

1) Accelerating the discovery of acid gas-selective MOFs for natural gas purification: A combination of machine learning and molecular fingerprint. Fuel. 2023, 350: 128757.
2) Computational evaluation of RHO-ZIFs for CO2 capture: From adsorption mechanism to swing adsorption separation. Separation and Purification Technology, 2023, 313: 123469
3) Understanding the Effective Capture of H2S/CO2 from Natural Gas Using Ionic Liquid@MOF Composites. Journal of Physical Chemistry C. 2022, 126: 19872-19882.
4) Unraveling the Role of Chemistry and Topology of MOFs in Psoralen Adsorption. Industrial & Engineering Chemistry Research, 2022, 61: 7172-7182.
5) Confined ionic liquids in covalent organic frameworks toward the rational design of high-safety lithium metal battery. Chemical Engineering Journal, 2022, 433: 133749.
6) One-step preparation of epoxy resin-based ionic gel electrolyte for quasi-solid-state lithium metal batteries. Journal of Power Sources, 2022, 524: 231070.
7) Screening of Biocompatible MOFs for the Clearance of Indoxyl Sulfate Using GCMC Simulations. Industrial & Engineering Chemistry Research, 2022, 61: 6618-6627.
8) Covalent Organic Frameworks-Enhanced Ionic Conductivity of Polymeric Ionic Liquid-Based Ionic Gel Electrolyte for Lithium Metal Battery. ACS Applied Energy Materials, 2022, 61: 6618-6627.
9) Synthesis of ZIF-8 and ZIF-67 Nanocrystals with Well-Controllable Size Distribution Through Reverse Microemulsions. Chemical Engineering Journal, 2016, 289: 59-64.
10) Computational Screening of Porous Metal-Organic Frameworks and Zeolites for the Removal of SO2 and NOx from Flue Gases. AIChE Journal, 2014, 60: 2314-2323.

4、Combustion

1) Combustion of Fuel JP8-1: Mechanism and Reaction Kinetics Based on ReaxFF MD. Industrial & Engineering Chemistry Research, 2021, 60: 14674-14684.
2) Initial Mechanism and Kinetics of Diesel Incomplete Combustion: ReaxFF Molecular Dynamics Based on a Multicomponent Fuel Model. Journal of Physical Chemistry C. 2019, 123: 8512-8521.
3) Combustion Mechanisms and Kinetics of Fuel Additives: A ReaxFF Molecular Simulation. Energy & Fuels. 2018, 32: 11852-11863.
4) Molecular Simulation of the Catalytic Cracking of Hexadecane on ZSM-5 Catalysts Based on Reactive Force Field (ReaxFF). Energy & Fuels. 2017, 31: 10515-10524.
5) High-Temperature and High-Pressure Pyrolysis of Hexadecane: Molecular Dynamic Simulation Based on Reactive Force Field (ReaxFF). Journal of Physical Chemistry A. 2017, 121: 2069-2078.