



孙伟振

所属学院 化工学院  
学科领域 化学工程与技术  
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## 个人简介

### 【工作经历】

1999 至 2001 年，青岛钢铁集团公司润滑油厂任副厂长。  
2004 年至今，华东理工大学化学工程联合国家重点实验室工作，历任助教、讲师、副教授、教授。  
2012 至 2013 年，美国加州大学伯克利分校化工系，与 Berend Smit 教授合作从事分子模拟研究。

### 【所获荣誉】

上海市技术发明一等奖（2014）  
中国石油和化学工业联合会科技进步一等奖（2018）

### 【学术任职】

美国化学工程师学会（AIChE）高级会员  
中国化工学会会员

## 研究方向

- 1、化工过程强化  
通过研究多相反应（液 - 液、气 - 液、气 - 固、气 - 液 - 固）界面上小分子的溶解、扩散、自组织等表面现象，理解并指导反应过程的强化和催化剂设计。研究对象包括 C4 烷基化、烃类液相氧化、乙烷氧化、Deacon 反应等。
- 2、跨尺度模拟计算  
常规蒙特卡罗（MC）、分子动力学（MD）模拟以及基于反应力场的分子动力学（ReaxFF-MD）模拟（用于研究燃烧、裂解等快反应）；复杂反应体系的动力学建模；反应器模拟；化工流程模拟。
- 3、化工过程开发  
大型工业反应器开发、化工过程强化与优化等，研究内容包括（1）气 - 液反应体系如芳烃（PX、MX）氧化、均四甲苯氧化、萘二甲苯氧化、5-HMF 氧化等新型聚合物单体的制备与提纯；（2）液 - 液反应体系如离子液体 / 硫酸催化 C4 烷基化合成高品质清洁汽油等；（3）高值精细化学品（日化产品、食品添加剂）的连续化工艺改造等。
- 4、材料化学工程  
可控制备 MOF、ZIF、COF 等纳米多孔材料，研究其在化工分离、医学杀菌和载药、锂离子电池等方面的应用。合成各类新型离子液体（IL）用于催化反应和医学杀菌。

## 研究成果及主要发表文章

### 【代表性论文】（第一或通讯作者）

- （一）过程强化
  - 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.
- （二）反应动力学、催化剂、反应器
  - 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.
- （三）材料化学工程（多孔材料、锂离子电池）
  - 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.
- （四）燃烧与裂解反应
  - 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.

### 【代表性项目】

- 1) 离子液体催化烷基化反应液 - 液两相界面的介尺度机制及调控 - 国家自然科学基金
- 2) 全生物基聚对苯二甲酸乙二醇酯聚合工艺研究及示范 - 国家重点研发计划课题
- 3) 异山梨醇（IS）生产催化剂及工艺技术开发 - 中国石油
- 4) 硫酸烷基化与离子液体烷基化工艺适应性研究 - 中国石化
- 5) 大型精间苯二甲酸生产装置工艺开发 - 中国石油
- 6) 环己基苯过氧化工艺优化及反应动力学研究 - 中国石化
- 7) 非裂解法烷基化废酸再生利用技术开发 - 中国石化
- 8) 吡啶酮类香料工业装置连续化工艺开发 - 上海爱普香料集团
- 9) 6000 吨／年对（间、邻）甲基苯甲酸连续氧化生产工艺装置开发 - 山东敏德化工有限公司
- 10) 三氯蔗糖氯化反应器开发及氯化工艺优化 - 山东康宝生化科技有限公司