



Profile

Education

1999: PhD, Chemical Technology, East China University of Science and Technology.
1996: ME, Chemical Engineering, East China University of Science and Technology.
1989: BE, Chemical Engineering, East China University of Science and Technology.

Academic Experience

2008-present: ECUST, Professor.
2005-2008: University of Waterloo, Research Associate.
1999-2005: Max Planck Institute for Dynamics of Complex Technical Systems, Research Associate.

Non-academic Experience

1991 - 1993: Ezhou Chemical Company, Chemical Engineer, full time.

Research Field

1. Process intensification

Focusing on reactive distillation and solvent intensification, the technologies of bio-based vitamin E separation and deep desulfurization of diesel and gasoline based on low co-melting solvent, esterification based on ionic liquid, Olefin conversion reactive distillation, and solvent recovery technology in pharmaceutical process.

2. Molecular design

The design method of multi-scale simulation combining quantitative calculation and process optimization was developed, functional solvents, adsorbents and polymers were designed, and the structure-activity relationship between characteristic functional groups and process effects was studied. The process is enhanced by the polyphase evolution of the mixture of solvent and system and the regulation of operating conditions.

3. Simulation and optimization of complex process

The simulation and optimization platform for complex processes based on gProms is developed to study the dynamic and polymorphic characteristics of complex processes.

Research results and selected published papers

- (1) Zhen Song, Chenyue Zhang, Zhiwen Qi*, Teng Zhou*, Kai Sundmacher. Computer-aided design of ionic liquids as solvent for extractive desulfurization process. *AIChE Journal*. 2018, 64(3), 1013-1025.
- (2) Hongye Cheng, Jiangsheng Li, Jingwen Wang, Lifang Chen, Zhiwen Qi*. Enhanced vitamin E extraction selectivity from deodorizer distillate by a biphasic system: A COSMO-RS and experimental study. *ACS Sustainable Chemistry & Engineering*, 2018, 6:5547-5554.
- (3) Qian Zeng, Biao Hu, Hongye Cheng*, Lifang Chen, Junmei Huang, Zhiwen Qi*. Liquid-Liquid Equilibrium for the System of Ionic Liquid [BMIm][HSO₄] Catalyzed Isobutyl Isobutyrate Formation. *Journal of Chemical Thermodynamics*. 2018, 122:162-169.
- (4) Hongye Cheng, *Chongyang Liu, Jingjing Zhang, Lifang Chen, Bingjian Zhang, Zhiwen Qi*. Screening deep eutectic solvents for extractive desulfurization of fuel based on COSMO-RS model. *Chemical Engineering Processing: Process Intensification*. 2018, 125:246-252.
- (5) Hongye Cheng, Jinwei Zhang, Zhiwen Qi*. Effects of interaction with sulfur compounds and free volume in imidazolium-based ionic liquid on desulfurization: A Molecular dynamics study. *Molecular Simulation*, 2018, 44(1):55-62.
- (6) Qian Zeng, Jinwei Zhang, Hongye Cheng*, Lifang Chen, Zhiwen Qi. Corrosion properties of steel in 1-butyl-3-methylimidazolium hydrogen sulfate ionic liquid systems for desulfurization application. *RSC Advances*. 2017, 7:48526-48536.
- (7) Lei Qin, Jiangsheng Li, Hongye Cheng, Lifang Chen, Zhiwen Qi*, Weikang Yuan. Association extraction for vitamin E recovery from deodorizer distillate by in situ formation of deep eutectic solvent. *AIChE Journal*, 2017, 63(6):2212-2220.
- (8) Jianan Zhang, Daili Peng, Zhen Song, Hongye Cheng, Lifang Chen, and Zhiwen Qi*. COSMO-descriptor based computer-aided ionic liquid design for separation processes. Part I: Modified group contribution methodology for predicting surface charge density profile of ionic liquids. *Chemical Engineering Science*, 2017, 162:355-363.
- (9) Jianan Zhang, Lei Qin, Daili Peng, Hongye Cheng, Lifang Chen, and Zhiwen Qi*. COSMO-descriptor based computer-aided ionic liquid design for separation processes. Part II: Task-specific design for extraction process. *Chemical Engineering Science*, 2017, 162:364-374.
- (10) Daili Peng, Jianan Zhang, Hongye Cheng, Lifang Chen*, and Zhiwen Qi*. Computer-aided ionic liquid design for separation processes based on group contribution method and COSMO-SAC model. *Chemical Engineering Science*, 2017, 159:58-68.
- (11) Wenrong Cao, Zhenyou Gui, Lifang Chen*, and Zhiwen Qi. Facile synthesis of sulfate-doped Ag₃PO₄ with enhanced visible light photocatalytic activity. *Applied Catalysis B: Environmental*, 2017, 200:681-689.
- (12) Zhen Song, Teng Zhou*, Zhiwen Qi*, Kai Sundmacher, A systematic method for screening ionic liquids as extraction solvents exemplified by an extractive desulfurization process. *ACS Sustainable Chemistry & Engineering*, 2017, 5 (4), 3382-3389.
- (13) Xueqing Kang, Hongye Cheng, Liwei Tong, Lifang Chen, Zhiwen Qi*. Development of a bifurcation analysis approach based on gProms platform. *Chinese Journal of Chemical Engineering*, 2016, 24:1742-1749 (cover story).
- (14) Zhenyou Gui, Wenrong Cao, Shunmugavel Saravanamurugan, Anders Riisager, Lifang Chen, *Zhiwen Qi*. Efficient aerobic oxidation of 5-hydroxymethylfurfural in aqueous media with Au-Pd supported on zinc carbonate hydroxide. *ChemCatChem*, 2016, 8:3636-3642.
- (15) Zhen Song, Qian Zeng, Jinwei Zhang, Hongye Cheng, Lifang Chen, Zhiwen Qi*. Solubility of imidazolium-based ionic liquids in model fuel hydrocarbons: A COSMO-RS and experimental study. *Journal of Molecular Liquids*, 2016, 224(Part A): 544-550.
- (16) Zhen Song, Jingjing Zhang, Qian Zeng, Hongye Cheng, Lifang Chen, Zhiwen Qi*. Effect of cation alkyl chain length on liquid-liquid equilibria of {ionic liquids + thiophene + heptane}: COSMO-RS prediction and experimental verification. *Fluid Phase Equilibria*, 2016, 425:244-251.
- (17) Lifang Chen, Xin Xu, Jingjing Song, Xuedong Zhu, Zhiwen Qi*. Microwave assisted hydrothermal synthesis of MnO₂·0.5H₂O ion-sieve for lithium ion selective adsorption. *Separation Science and Technology*. 2016, 51(5):874-882.
- (18) Lei Qin, Jianan Zhang, Hongye Cheng, Lifang Chen, Zhiwen Qi*, Weikang Yuan, Selection of imidazolium-based ionic liquids for vitamin E extraction from deodorizer distillate. *ACS Sustainable Chemistry & Engineering*, 2016, 4 (2):583-590.
- (19) Jun Li, Zhongde Dai, Muhammad Usman, Zhiwen Qi*, Liyuan Deng*. CO₂/H₂ separation by amino-acid ionic liquids with polyethylene glycol as co-solvent, *International Journal of Greenhouse Gas Control*, 2016, 45:207-215.
- (20) Shaohua Zheng, Hongye Cheng, Lifang Chen, Zhiwen Qi*. Feasibility of bio-based lactate esters as extractant for biobutanol recovery: Liquid-liquid equilibria, *Journal of Chemical Thermodynamics*, 2016, 93:127-131.
- (21) Chenjia You, Chi Zhang, Lifang Chen*, and Zhiwen Qi*. Highly dispersed palladium nanoclusters incorporated in amino-functionalized silica spheres for selective hydrogenation of succinic acid to γ -butyrolactone, *Applied Organometallic Chemistry*, 2015, 29(7):653-660.
- (22) Teng Zhou, Zhaoxian Lyu, Zhiwen Qi, Kai Sundmacher*. Robust design of optimal solvents for chemical reactions - A combined experimental and computational strategy, *Chemical Engineering Science*, 2015, 137:613-625.
- (23) Jun Li, Chenjia You, Zhaoxian Lyu, Chi Zhang, Lifang Chen, Zhiwen Qi*. Fuel-based ethanol dehydration process directly extracted by gasoline additive, *Separation and Purification Technology*, 2015, 149:9-15.
- (24) Zhen Song, Teng Zhou, Jianan Zhang, Lifang Chen, and Zhiwen Qi*. Screening of ionic liquids for solvent-sensitive extraction - with deep desulfurization as an example. *Chemical Engineering Science*, 2015, 129:69-77.
- (25) Teng Zhou, Kevin McBride, Xiang Zhang, Zhiwen Qi, Kai Sundmacher*. Integrated solvent and process design exemplified for a Diels-Alder reaction. *AIChE Journal*, 2015, 61(1):147-158.
- (26) Liwei Tong, Lifang Chen, Yinmei Ye, Zhiwen Qi*. Kinetic studies on the dimerization of isobutene with Ni/Al₂O₃ as a catalyst for reactive distillation process. *Chinese Journal of Chemical Engineering*, 2015, 23:520-527.
- (27) Teng Zhou, Zhiwen Qi, Kai Sundmacher*. Model-based method for the screening of solvents for chemical reactions, *Chemical Engineering Science*, 2014, 115:177-185.
- (28) Zhaoxian Lyu, Teng Zhou, Lifang Chen, Yinmei Ye, Kai Sundmacher, Zhiwen Qi*. Ionic liquid screening for benzene-cyclohexane extractive separation by a multi-scale simulation approach. *Chemical Engineering Science*, 2014, 113:45-53.
- (29) Liwei Tong, Lifang Chen, Yinmei Ye, Zhiwen Qi*, Analysis of intensification mechanism of auxiliary reaction on reactive distillation: methyl acetate hydrolysis process as example, *Chemical Engineering Science*, 2014, 106:190-197.
- (30) Teng Zhou, Ziyun Wang, Yinmei Ye, Lifang Chen, Jing Xu, Zhiwen Qi*. Deep separation of benzene from cyclohexane by liquid extraction using ionic liquids as solvent. *Industrial & Engineering Chemistry Research*, 2012, 51(15), 5559-5564.
- (31) Teng Zhou, Lifang Chen, Yinmei Ye, Zhiwen Qi*, Hannsjörg Freund and Kai Sundmacher, An overview of mutual solubility of ionic liquids and water predicted by COSMO-RS model. *Industrial & Engineering Chemistry Research*, 2012, 51(17), 6256-6264.
- (32) Jun Li, Chenjia You, Lifang Chen, Yinmei Ye, Zhiwen Qi*, Kai Sundmacher. Dynamics of CO₂ absorption and desorption processes in alkanolamine with co-solvent polyethylene glycol, *Industrial & Engineering Chemistry Research*, 2012, 51, 12081-12088.
- (33) Chi Zhang, Lifang Chen*, Hongye Cheng, Xuedong Zhu, Zhiwen Qi*. Supported palladium single atom catalysts for the selective hydrogenation of succinic acid to γ -butyrolactone. *Catalysis Today*, 2016, 276:55-61.
- (34) Zhen Song, Qian Zeng, Jinwei Zhang, Hongye Cheng, Lifang Chen, Zhiwen Qi*. Mutual solubility of imidazolium-based ionic liquids and model hydrocarbons in fuel oils: an experimental and COSMO-RS study. *Journal of Molecular Liquids*, 2016, 224(Part A): 544-550.
- (35) Chi Zhang, Wenrong Cao, Hongye Cheng, Lifang Chen, * and Zhiwen Qi. Regenerable subnanometre Pd clusters on zirconia for highly selective hydrogenation of biomass-derived succinic acid in water. *Catalysts*, 2016, 6(7):100-108.
- (36) Zhen Song, Jingjing Zhang, Qian Zeng, Hongye Cheng, Lifang Chen, Zhiwen Qi*. Effect of cation alkyl chain length on liquid-liquid equilibria of {ionic liquids + thiophene + heptane}: COSMO-RS prediction and experimental verification. *Fluid Phase Equilibria*, 2016, 425:244-251.
- (37) Lifang Chen, Xin Xu, Jingjing Song, Xuedong Zhu, Zhiwen Qi*. Microwave assisted hydrothermal synthesis of MnO₂·0.5H₂O ion-sieve for lithium ion selective adsorption. *Separation Science and Technology*. 2016, 51(5):874-882.
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- (42) Jun Li, Chenjia You, Zhaoxian Lyu, Chi Zhang, Lifang Chen, Zhiwen Qi*. Fuel-based ethanol dehydration process directly extracted by gasoline additive, *Separation and Purification Technology*, 2015, 149:9-15.
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- (44) Wenrong Cao, Lifang Chen, * and Zhiwen Qi*. Microwave-assisted synthesis of Ag/Ag₂SO₄/ZnO nanostructures for enhanced visible-light-induced photocatalysis. *Journal of Molecular Catalysis. A, Chemical*, 2015, 401:81-89.
- (45) Zhenyou Gui, Wenrong Cao, Lifang Chen, and Zhiwen Qi*, Propene carbonate intensified cyclohexane oxidation over Au/SiO₂ catalyst, *Catalysis Communications*, 2015, 64:58-61.
- (46) Jun Li, Lifang Chen, Yinmei Ye, Zhiwen Qi*, Solubility of CO₂ in the mixed solvent system of alkanolamine and polyethylene glycol. *Journal of Chemical Engineering Data*. 2014, 59(6), 1781-1787.
- (47) Wenrong Cao, Lifang Chen, and Zhiwen Qi*, Highly dispersed Ag₂SO₄ nanoparticles deposited on ZnO nanoflakes as photocatalysts, *Catalysis Letters*, 2014, 144(4):598-606.