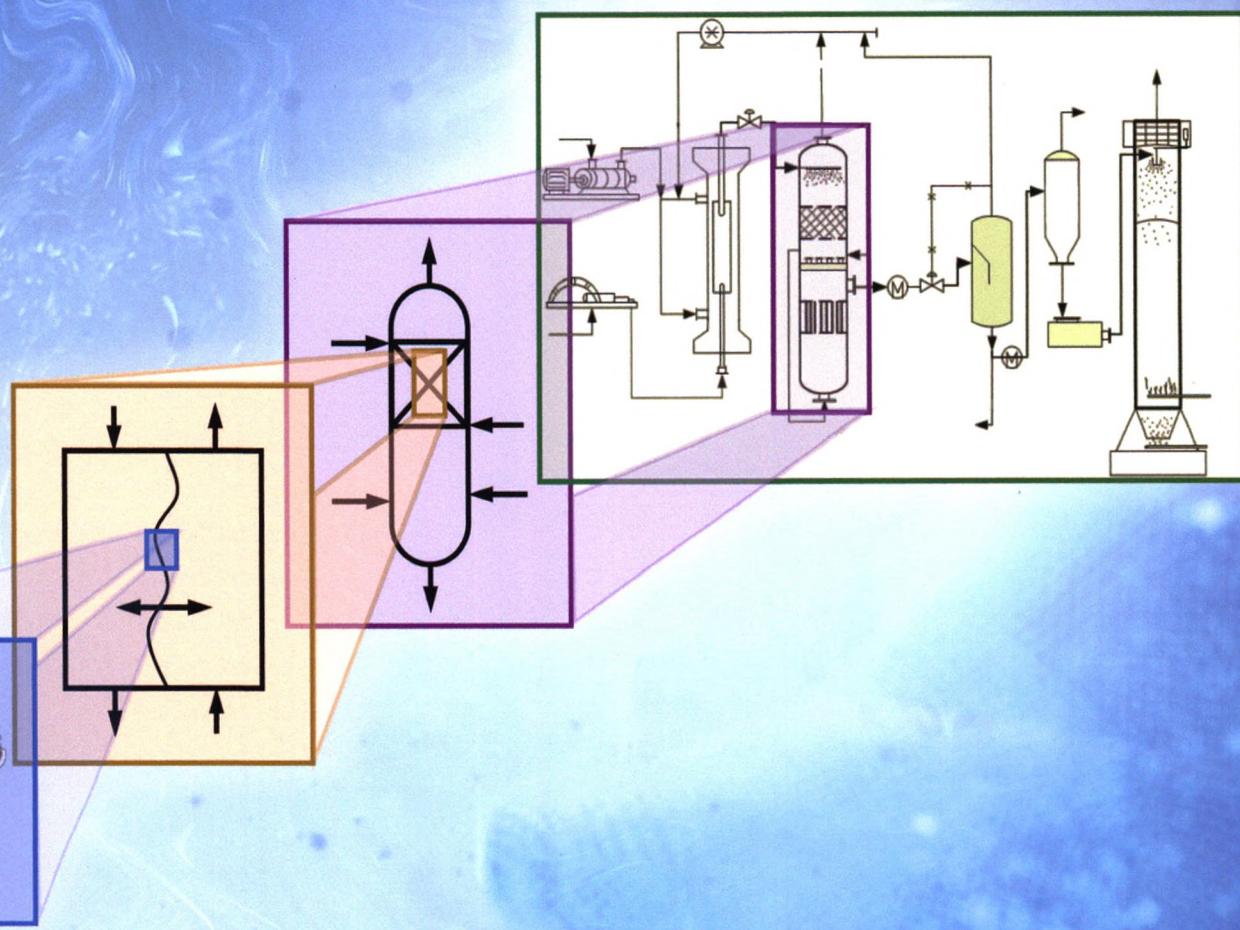




Frontiers of Chemical Science and Engineering

化学科学与工程前沿



Higher Education Press

万方数据



Springer

EDITORIAL

- 137 Multiscale process systems engineering—analysis and design of chemical and energy systems from molecular design up to process optimization

Teng Zhou, Kai Sundmacher

RESEARCH ARTICLE

- 141 Molecular level understanding of CO₂ capture in ionic liquid/polyimide composite membrane

Linlin You, Yandong Guo, Yanjing He, Feng Huo, Shaojuan Zeng, Chunshan Li, Xiangping Zhang, Xiaochun Zhang

- 152 A computational toolbox for molecular property prediction based on quantum mechanics and quantitative structure-property relationship

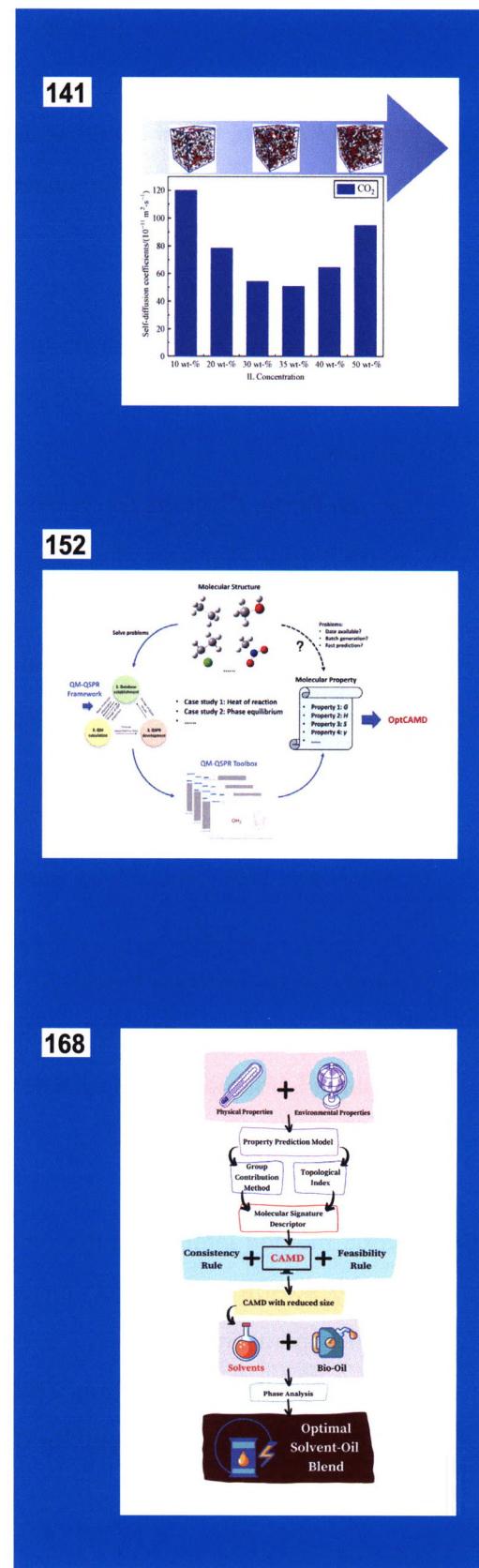
Qilei Liu, Yinke Jiang, Lei Zhang, Jian Du

- 168 Design of bio-oil additives via molecular signature descriptors using a multi-stage computer-aided molecular design framework

Jia Wen Chong,
Suchithra Thangalazhy-Gopakumar,
Kasturi Muthoosamy,
Nishanth G. Chemmangattuvalappil

- 183 Using machine learning models to explore the solution space of large nonlinear systems underlying flowsheet simulations with constraints

Patrick Otto Lidl, Raoul Heese, Johannes Höller, Norbert Asprion, Michael Bortz



- 198 Dynamic modelling and simulation of a post-combustion CO₂ capture process for coal-fired power plants
Jianlin Li, Ti Wang, Pei Liu, Zheng Li

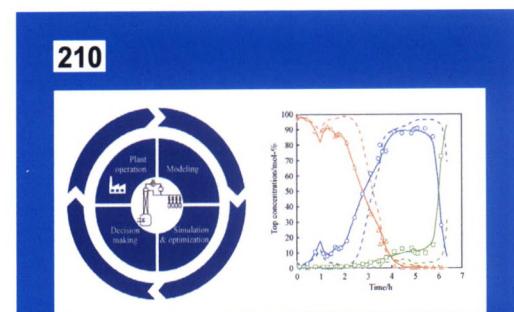
- 210 Decision support for the development, simulation and optimization of dynamic process models
Norbert Asprion, Roger Böttcher, Jan Schwientek, Johannes Höller, Patrick Schwartz, Charlie Vanaret, Michael Bortz

- 221 Dynamic response surface methodology using Lasso regression for organic pharmaceutical synthesis
Yachao Dong, Christos Georgakis, Jacob Santos-Marques, Jian Du

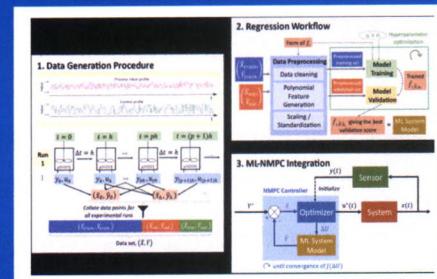
- 237 An integrated approach for machine-learning-based system identification of dynamical systems under control: application towards the model predictive control of a highly nonlinear reactor system
Ewan Chee, Wee Chin Wong, Xiaonan Wang

- 251 Synergistic optimization framework for the process synthesis and design of biorefineries
Nikolaus I. Vollmer, Resul Al, Krist V. Gernaey, Gürkan Sin

- 274 Hybrid method integrating machine learning and particle swarm optimization for smart chemical process operations
Haoqin Fang, Jianzhao Zhou, Zhenyu Wang, Ziqi Qiu, Yihua Sun, Yue Lin, Ke Chen, Xiantai Zhou, Ming Pan



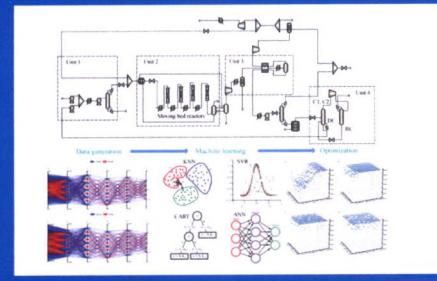
237



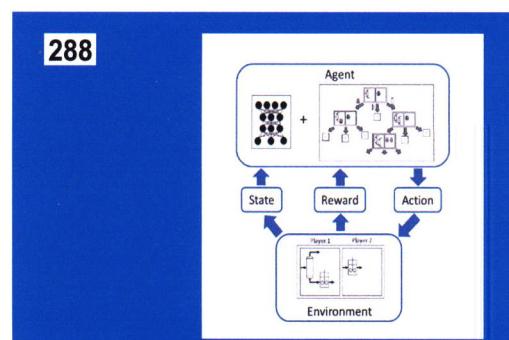
251



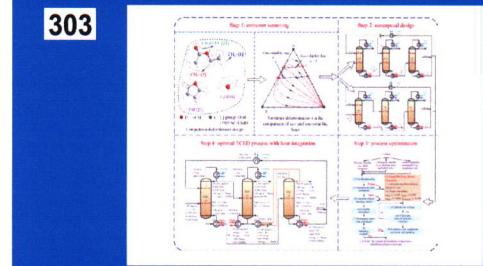
274



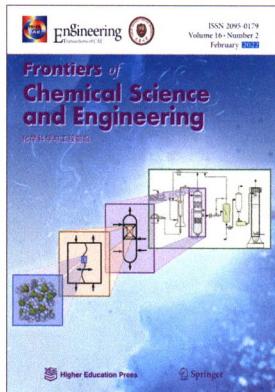
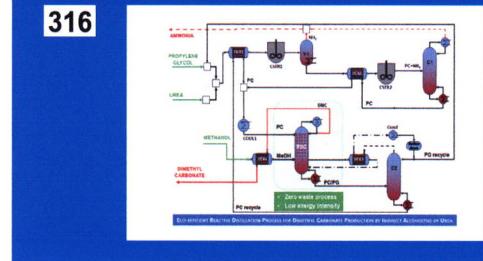
- 288** Automated synthesis of steady-state continuous processes using reinforcement learning
Quirin Göttl, Dominik G. Grimm, Jakob Burger



- 303** Energy-efficient recovery of tetrahydrofuran and ethyl acetate by triple-column extractive distillation: entrainer design and process optimization
Ao Yang, Yang Su, Tao Shi, Jingzheng Ren, Weifeng Shen, Teng Zhou



- 316** Novel eco-efficient reactive distillation process for dimethyl carbonate production by indirect alcoholysis of urea
Iulian Patrăscu, Costin S. Bîldea, Anton A. Kiss



COVER

A process system can be generally decomposed into hierarchical levels or scales at which different physical and/or chemical phenomena take place.
(Teng Zhou, Kai Sundmacher, pp. 137–140)

Frontiers of
Chemical Science
and Engineering

Vol. 16 No. 2 February 2022

Available online
<http://www.springerlink.com>

CN 11-5981/TQ
邮发代号: **80-969**

ISSN 2095-0179

