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

Teng Zhou (✉)^{1,2}, Kai Sundmacher^{1,2}

¹ Process Systems Engineering, Max Planck Institute for Dynamics of Complex Technical Systems, D-39106 Magdeburg, Germany

² Process Systems Engineering, Otto-von-Guericke University Magdeburg, D-39106 Magdeburg, Germany

© Higher Education Press 2021

As indicated by Grossmann and Westerberg [1], a process system can be generally decomposed into hierarchical levels or scales at which different physical and/or chemical phenomena take place (see Fig. 1). The first step of multiscale process modeling is to connect the molecular level with the phase level, where the main task is to model and predict the properties of fluid mixtures based on the atomic- or molecular-level information. Typically, quantum chemical (QC) computation, molecular simulation, and equations of state are used to provide such predictions. Recently, due to the ever-increasing number of available data and fast development of cheminformatics and machine learning tools, data-driven descriptor models have been developed and widely used for property predictions [2]. With the properties of the system, it is then possible to derive the constitutive relations (e.g., kinetics and phase equilibria) and implement them into the mass, energy, and momentum conservations of each process unit. Taking into account the connections between different units, one can finally scale the system up toward the process level where process modeling, intensification, and optimization are performed to maximize the economic and environmental performances of the process. It is clear that domain knowledge (e.g., chemical engineering) as well as data science and systems engineering methods are essential for an adequate description or modeling of a

Fig. 1 Multiscale structure of process systems.

complex multiscale process system.

The special issue “Multiscale process systems engineering” in collaboration with *Frontiers of Chemical Science and Engineering* comprises 13 article contributions. Research topics cover molecular simulation and computer-aided molecular design (CAMD), steady-state and dynamic process modeling, process synthesis and optimization, as well as process intensification and integration. The employed modeling methods include mechanistic or first-principle modeling, data-driven or machine learning modeling, and their hybrid modeling [3].

As indicated in the multiscale figure, functional molecules or materials (e.g., solvent and adsorbent) with tailored properties represent the heart of the process systems [4]. Since the experimental trial-and-error method is slow and inefficient, the CAMD method has been developed and widely used for systematic molecular discovery. One of the key steps of CAMD is to build reliable structure-based property prediction models. You et al. [5] studied the microscopic mechanism of CO₂ adsorption in ionic liquid/polyimide composites by molecular simulation. This molecular-level understanding of material properties is crucial for designing new efficient CO₂ capture sorbents. Liu et al. [6] established a framework combining QC computation and structure-property relationship modeling for fast molecular property predictions. Next, Chong et al. [7] used the CAMD method to design blending solvents to upgrade biofuel properties toward high heating value, low viscosity, and low toxicity.

To build an accurate process model is one of the most critical steps for process analysis, design, and control. The next five articles are focused on steady-state or dynamic process modeling. Ludl et al. [8] developed a machine learning method based on an improved adaptive sampling technique for the modeling and simulation of continuous chemical processes with complex and nonlinear constraints. Li et al. [9] built and validated a dynamic model for a solvent-based post-combustion CO₂ capture process. Based on the established model, dynamic process simulation and analysis was performed to identify key operating parameters. Asprien et al. [10] extended an existing BASF steady-state modeling tool to dynamic modeling. Through two applications on a distillation and reaction processes, the authors proved that the extended tool could be efficiently used for dynamic process modeling. Dong et al. [11] developed a data-driven dynamic response surface (DRS) method and proposed a new regression approach for the estimation of model parameters. Through two cases studies, the authors demonstrated that the DRS method combined with the new regression strategy could quickly generate reliable dynamic models for simulating complex pharmaceutical processes. Chee et al. [12] used data-driven machine learning methods to derive nonlinear black-box models and performed model predictive control based on the obtained model. It was demonstrated that process control across a wide operating range can be efficiently performed without any prior knowledge of system dynamics.

The next three contributions deal with the synthesis and optimization of energy conversion systems and industrial chemical processes. Vollmer et al. [13] proposed a novel framework that incorporates data-driven surrogate modeling and superstructure optimization for the optimal synthesis of biorefinery processes. It was found that in order to ensure the consistency and quality of the optimal solution, the type of surrogate, sampling strategy, and size of the training and validation sets must be carefully selected. Fang et al. [14] presented another hybrid framework that integrates machine learning modeling and particle swarm optimization for complex industrial process optimization. A propane dehydrogenation process was studied to demonstrate the validity and efficiency of the method. As indicated by the above-mentioned works, supervised machine learning is now widely used to build data-driven models for process design and optimization. Göttl et al. [15] demonstrated how reinforcement learning (RL), an important type of unsupervised machine learning method, could support automated process synthesis. In the RL, the environment consists of a steady-state process simulator incorporating all physical knowledge and an agent is trained to take discrete actions and sequentially build the process flowsheet that achieves a given task.

The final two articles are dedicated to process intensification and integration. Yang et al. [16] developed an energy-efficient triple-column extractive distillation process to recover tetrahydrofuran and ethyl acetate from wastewater. The process development followed a multiscale design procedure that involves computer-aided solvent design, thermodynamic analysis, process optimization, and heat integration. Patraşcu et al. [17] developed another heat-integrated reactive distillation process for dimethyl carbonate production. It was proved that less equipment was required and the overall energy consumption was also reduced through the process intensification and heat integration.

This special issue is a collection of current representative researches in the broad area of multiscale process systems engineering. While it is certainly impossible to cover the whole field in a single special issue, we feel that the collections can properly capture the dynamic development of this area. Besides, some important methods or tools, such as CAMD, advanced sampling and surrogate modeling, superstructure optimization, machine learning and reinforcement learning, have been highlighted. We hope that this special issue can incite and promote the development and implementation of these methods or tools for solving more challenging problems.

The special issue would not have been possible without the effort and support of many people. First, we would like to thank all the authors for their great contributions. Second, we thank all the reviewers for their insightful and timely

reviews. Finally, we would like to thank the Editor-in-Chief Prof. Jing-Kang Wang, who has been supporting the idea of this special issue from the beginning to the end.

References

1. Grossmann I E, Westerberg A W. Research challenges in process systems engineering. *AIChE Journal*, 2000, 46(9): 1700–1703
2. Zhou T, Song Z, Sundmacher K. Big data creates new opportunities for materials research: a review on methods and applications of machine learning for materials design. *Engineering*, 2019, 5(6): 1017–1026
3. Zhou T, Gani R, Sundmacher K. Hybrid data-driven and mechanistic modeling approaches for multiscale material and process design. *Engineering*, 2021, 7(9): 1231–1238
4. Shi H, Zhou T. Computational design of heterogeneous catalysts and gas separation materials for advanced chemical processing. *Frontiers of Chemical Science and Engineering*, 2021, 15(1): 49–59
5. You L, Guo Y, He Y, Huo F, Zeng S, Li C, Zhang X, Zhang X. Molecular level understanding of CO₂ capture in ionic liquid/polyimide composite membrane. *Frontiers of Chemical Science and Engineering*, 2022, 16(2): 141–151
6. Liu Q, Jiang Y, Zhang L, Du J. A computational toolbox for molecular property prediction based on quantum mechanics and quantitative structure-property relationship. *Frontiers of Chemical Science and Engineering*, 2022, 16(2): 152–167
7. Chong J W, Thangalazhy-Gopakumar S, Muthoosamy K, Chemmangattuvalappil N G. Design of bio-oil additives via molecular signature descriptors using a multi-stage computer-aided molecular design framework. *Frontiers of Chemical Science and Engineering*, 2022, 16(2): 168–182
8. Ludl P O, Heese R, Höller J, Asprien N, Bortz M. Using machine learning models to explore the solution space of large nonlinear systems underlying flowsheet simulations with constraints. *Frontiers of Chemical Science and Engineering*, 2022, 16(2): 183–197
9. Li J, Wang T, Liu P, Li Z. Dynamic modelling and simulation of a post-combustion CO₂ capture process for coal-fired power plants. *Frontiers of Chemical Science and Engineering*, 2022, 16(2): 198–209
10. Asprien N, Böttcher R, Schwientek J, Höller J, Schwartz P, Vanaret C, Bortz M. Decision support for the development, simulation and optimization of dynamic process models. *Frontiers of Chemical Science and Engineering*, 2022, 16(2): 210–220
11. Dong Y, Georgakis C, Santos-Marques J, Du J. Dynamic response surface methodology using Lasso regression for organic pharmaceutical synthesis. *Frontiers of Chemical Science and Engineering*, 2022, 16(2): 221–236
12. Chee E, Wong W C, Wang X. 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. *Frontiers of Chemical Science and Engineering*, 2022, 16(2): 237–250
13. Vollmer N I, Al R, Gernaey K V, Sin G. Synergistic optimization framework for the process synthesis and design of biorefineries. *Frontiers of Chemical Science and Engineering*, 2022, 16(2): 251–273
14. Fang H, Zhou J, Wang Z, Qiu Z, Sun Y, Lin Y, Chen K, Zhou X, Pan M. Hybrid method integrating machine learning and particle swarm optimization for smart chemical process operations. *Frontiers of Chemical Science and Engineering*, 2022, 16(2): 274–287
15. Göttl Q, Grimm D G, Burger J. Automated synthesis of steady-state continuous processes using reinforcement learning. *Frontiers of Chemical Science and Engineering*, 2022, 16(2): 288–302
16. Yang A, Su Y, Shi T, Ren J, Shen W, Zhou T. Energy-efficient recovery of tetrahydrofuran and ethyl acetate by triple-column extractive distillation: entrainer design and process optimization. *Frontiers of Chemical Science and Engineering*, 2022, 16(2): 303–315
17. Patraşcu I, Bîldea C S, Kiss A A. Novel eco-efficient reactive distillation process for dimethyl carbonate production by indirect alcoholysis of urea. *Frontiers of Chemical Science and Engineering*, 2022, 16(2): 316–331

Guest Editors

Jun.-Prof. Dr. Teng Zhou is currently a Junior Professor at the Max Planck Institute (MPI) for Dynamics of Complex Technical Systems, Magdeburg and Otto-von-Guericke University (OvGU) Magdeburg, Germany. He received his bachelor and master degrees in Chemical Engineering from China. In 2016, he obtained his doctoral degree with the highest distinction in Process Systems Engineering from OvGU Magdeburg. Afterwards, he worked as a Postdoctoral Scientist at MPI Magdeburg and TU Denmark before he got appointed as a Junior Professor in 2019. Dr. Zhou's research lies at the intersection of Chemical Engineering, Molecular Engineering, and Data and Systems Engineering. He is currently interested in data-driven functional molecule/material design and multiscale process modeling and optimization. He has published more than 40 journal articles and his work has received > 1300 citations. Dr. Zhou earned several important honors and awards, including the CAST Directors Award granted by the American Institute of Chemical Engineers (AIChE) and Future Chemical Engineering Scholar granted by the Global Academy of Chinese

Chemical Engineers (GACCE). He is currently a founding Associate Editor of two international journals and an Editorial Board Member of several SCI-indexed journals.

Prof. Dr. Kai Sundmacher has been Director of the Department of Process Systems Engineering at the Max Planck Institute for Dynamics of Complex Technical Systems in Magdeburg since 2001. At the same time, he holds a full professorship for Process Systems Engineering at Otto von Guericke University Magdeburg. Kai Sundmacher graduated from the Clausthal University of Technology as Diplom-Ingenieur and Doktor-Ingenieur (summa cum laude). In 2007/2008, he was a postdoctoral fellow at the Department for Chemical and Process Engineering at the University of Newcastle, UK. His current research interests include modeling, simulation, analysis, and synthesis of complex process systems with applications in sustainable chemical production, renewable energy conversion and storage, and advanced biotechnology processes and systems. Prof. Sundmacher has published more than 400 articles in peer-reviewed journals and edited 5 books. He has received several awards for his research, including the Carl

Zerbe Prize (DGMK), the Arnold Eucken Prize (GVC/VDI), the Dr. Meyer-Struckmann Science Prize (BTU Cottbus), and the Einstein Professorship of the Chinese Academy of Sciences (CAS). In 2021, Prof. Sundmacher was elected as a member of the Berlin-Brandenburg Academy of Sciences.