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Editorial

Special Issue "Research on Process System Engineering"

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Process system engineering (PSE) is a multidisciplinary research field that aims to address engineering problems related to the design, operation, control, and management of process systems. PSE often integrates engineering principles, mathematics, computer science, control theory, etc., for process modelling, simulation, analysis, and optimization. The scope of PSE is wider than any single domain and covers all topics relating to the development of systematic techniques in these domains. Over recent decades, PSE has achieved notable accomplishments in academia and also provided solutions for process industries regarding energy and mass utilization [1,2], cost savings [3], and emissions reduction [4], among others. Although PSE emphasizes the system's unity, most PSE techniques are developed focusing on one or several subsystems of a real industrial system and usually rely on simplifications and assumptions of system's elements to avoid solving difficulties. It is a fact that PSE research is much broader and more popular than industrial applications. PSE techniques with high-fidelity models, low computational effort, and thoughtful consideration of the interactions between subsystems are required to realize the full potential of PSE [5].

This Special Issue of *Processes* entitled "Research on Process System Engineering" has attracted 12 research articles that are all within the scope of PSE. The contributions are listed below:

Accurate vapor–liquid equilibrium data are a basic requirement for PSE research and application [6]. Although these data can be obtained by means of experimental methods, such methods are labor-intensive and time-consuming and may be restricted by the experimental conditions, especially for complex fluids. Liu et al. (contribution 1) propose a generalized UNICAC (Universal Quasi-Chemical elements and chemical bonds Activity Coefficient) model to predict the activity coefficients of nonelectrolytes based on elements and chemical bonds. They consider equilibrium data of 1085 sets and 14,323 points for binary systems containing 14 types of compounds and regress the interaction energy parameters between 10 elements and 33 chemical bonds. The proposed model can handle binary and multicomponent systems with little or no experimental information and can provide good predictions for a large variety of systems.

Process modelling and analysis can not only show insights into chemical and physical changes within processes, but also provide quantitative relations between parameters and results. Through process modelling and analysis, engineers can obtain a better understanding of processes regarding product quality, raw material and energy consumption, economy, environmental impacts, etc. [7]. Moreover, it facilitates the optimal design and operation of processes. Three contributions within this Special Issue concentrate on the selected topic of "Process modeling, analysis, simulation, and optimization".

Wang et al. (contribution 2) propose and simulate a chemical looping enhanced oil shale-to-liquid fuel process. The retorting gas from oil shale retorting is used to produce hydrogen, which is then used for shale oil hydrogenation. The technical analysis shows that the shale oil yield and the light fraction yield can increase from 65% to 95.7% and from 20% to 64–83%, respectively. Moreover, the proposed process with light fraction hydrogenation has the highest return on investment.

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Sun et al. (contribution 3) apply process simulation and optimization to the rich gas compression system and the absorption stabilization system of a fluid catalytic cracking (FCC) unit. The key operating parameters including the compressor outlet pressure, absorbent flowrate, and supplementary absorbent are considered for optimization. The medium-pressure steam consumption can be reduced by 2.4% compared to the base case, resulting in a notable utility cost reduction. The optimization strategy can provide insightful guidance for the practical operation of the FCC unit.

The life cycle performance regarding energy consumption and GHG (greenhouse gas) emissions of copper production between 2004 and 2017 in China is comprehensively analyzed by Liu et al. (contribution 4). The energy consumption is in the range of 31.72 to 101.78 GJ/t copper, and the GHG emissions are between 3.09 and 9.96 t CO_2-eq/t copper. Both indexes show decreasing trends from 2004 to 2017, with an exception in 2011. This publication also analyses the influence of electricity source, auxiliary material consumption, and copper ore grade on life cycle performance. The electricity source is identified as the most important factor and optimization of the electricity structure should be given priority to mitigate energy consumption and GHG emissions.

Dynamic simulation is useful to analyze and optimize processes with time-varying behaviors [8]. Three publications are related to the selected topic of "Process dynamics, control, and monitoring" in this Special Issue.

Dang et al. (contribution 5) present a comparative study of the phase-field model and the cellular automaton model for the simulation of solidification processes. The crystallization process of water is taken as an example for illustration. These two approaches describe the problem in different ways with different model parameters, but the snowflake patterns in some cases can be reproduced in both methods. The qualitative relationship between the parameters of the cellular automaton model and the phase-field model is found by means of systematic analysis. The dendrite formation process can be better understood by combining the two methods to explain the dendrite growth process. This research is expected to be applied to other solidification processes.

Deng et al. (contribution 6) study the transition state process of green ammonia to guarantee the device's stable operation through dynamic simulation and optimization. They analyze the change in system energy consumption in the transition state process and identify the reactor's outlet heat exchanger and the ammonia separation tower's heat exchanger as the main points for optimization. The process control parameters are adjusted to shorten the fluctuation time and reduce energy consumption, which unfortunately sacrifices the product output.

Wang et al. (contribution 7) propose an adaptive-noise-bound-based set-membership identification method to fully capture the dynamics of a linear ordinary dynamic process without introducing incremental components. This method estimates noise bound through optimization algorithms, while current methods mostly rely on simplistic assumptions. The proposed method is applied to build dynamic mechanistic models for key variables in the catalytic cracking unit, catering to demands of operating variable analysis, advanced control, and online optimization. The experimental results show that compared to traditional collective identification methods, the proposed method can enhance the modeling accuracy and exhibit better robustness.

Process synthesis emphasizes the unity of the process and considers the interactions between different unit operations, more than optimizing them separately [9]. In this Special Issue, there are two publications related to the selected topic of "Product and process synthesis/design".

Duan et al. (contribution 8) present an insightful analysis of the integration of distillation into the overall process considering the change in operating pressure using pinch technology. The effects of changing the operating pressure of a distillation column are graphically represented and incorporated into the grand composite curve (GCC) to determine the change tendencies of the GCC, pinch temperature, and total utility consumption.

With insights gained from analysis, rules are proposed to identify the best operating pressure that minimizes the overall energy consumption.

Yang et al. (contribution 9) study the integration of a refinery and a chemical synthetic plant that are complementary in hydrogen and carbon oxide utilization. A superstructure is developed that couples a syngas network and a hydrogen network, which results in a non-linear programming model. The case study shows that H_2, CO, and CO_2 can be completely consumed, and thus 19.1% and 21.2% of coal and natural gas can be conserved. This publication offers suggestions for future developments in the chemical industry.

Artificial intelligence drives significant innovations across products, systems, services, and management in various industries. Intelligent manufacturing is promising to revolutionize the process industries, such as product/process design, process monitoring and control, process optimization, plant management, etc. [10]. Three publications within this Special Issue shed light on the selected topic of "Intelligent process systems and manufacturing".

Zheng et al. (contribution 10) propose a method that incorporates data-driven machine learning techniques into process optimization. The proposed method is illustrated by a chemical absorption-based postcombustion CO_2 capture process. The extreme gradient boosting and support vector regression algorithms are employed to build models to predict carbon capture rate and specific reboiler duty. The results show that computations with the data-driven models incorporated in the optimization technique are faster than first-principle modeling approaches. The advantages of fast model predictions can be extended in the application of advanced online control and optimization methods.

Shao and Zhang (contribution 11) propose a gas emission prediction method based on feature selection and improved machine learning. Different optimization algorithms are employed to optimize the hybrid kernel extreme learning machine (HKELM), the least squares support vector machine (LSSVM), and the input variables, which shows that HKELM outperforms LSSVM in prediction accuracy, stability, and running speed. The results show that the proposed model has a high prediction accuracy and widespread applications. Moreover, it is more practical and easier to operate than models in previous research.

Borisut and Nuchitprasittichai (contribution 12) propose an adaptive Latin hypercube sampling (LHS) method that generates additional sample points from areas with the highest output deviations to optimize the required number of samples. Artificial neural networks are employed as the surrogate model for the optimization problem. The findings indicate that for all case studies, the proposed LHS optimization algorithm requires fewer sample points than random sampling to achieve optimal solutions of similar quality.

Based on the publications gathered in this Special Issue, the following future directions are identified.

Industrial applications, especially digital and intelligent manufacturing, require accurate and reliable schemes and results. Thus, models should contain information across multiple scales, from molecules, to fluids and devices, and to unit operations. The interactions between the studied system and the associated systems should also be taken into account. There are growing research and application demands for multi-scale and multi-system modelling strategies and techniques.

High-fidelity models usually lead to solving challenges regarding computational efforts, convergences, and optima. Effective solution strategies and algorithms are necessary to obtain optimal results. The need to solve challenges also compels PSE researchers to improve modelling strategies and techniques.

Digitalization and intelligence are the transformation directions of process industries. With digital technology, the operation, management, and optimization of processes can be handled in a more holistic manner. However, industrial processes always pursue stable operation, which leads to the main challenge relating to a lack of sufficiently different data. Another issue is that a digital model has too many characteristics of the observed process, so it may have limited extensions even for similar processes. Digitalization and intelligence are also a venture for process industries. The return on investment, safety, and risks should be analyzed carefully.

Conflicts of Interest: The authors declare no conflicts of interest.

List of Contributions

1. Liu, H.; Li, X.; Wang, Y.; Sun, X.; Zhao, W.; Xia, L.; Xiang, S. Elements and Chemical Bonds Contribution Estimation of Activity Coefficients in Nonideal Liquid Mixtures.
2. Wang, Q.; Yang, Y.; Zhou, H. Chemical Looping Enhanced Oil Shale-to-Liquid Fuels Process: Modeling, Parameter Optimization, and Performance Analysis.
3. Sun, J.; Yu, H.; Yin, Z.; Jiang, L.; Wang, L.; Hu, S.; Zhou, R. P Process Simulation and Optimization of Fluid Catalytic Cracking Unit's Rich Gas Compression System and Absorption Stabilization System.
4. Liu, L.; Xiang, D.; Cao, H.; Li, P. Life Cycle Energy Consumption and GHG Emissions of the Copper Production in China and the Influence of Main Factors on the above Performance.
5. Dang, Y.; Ai, J.; Dai, J.; Zhai, C.; Sun, W. Comparative Study on Snowflake Dendrite Solidification Modeling Using a Phase-Field Model and by Cellular Automaton.
6. Deng, W.; Huang, C.; Li, X.; Zhang, H.; Dai, Y. Dynamic Simulation Analysis and Optimization of Green Ammonia Production Process under Transition State.
7. Wang, Z.; Wang, Q.; Zhang, S. An Adaptive-Noise-Bound-Based Set-Membership Method for Process Identification of Industrial Control Loops.
8. Duan, W.; Yang, M.; Feng, X. Comprehensive Analysis and Targeting of Distillation Integrated into Overall Process Considering Operating Pressure Change.
9. Yang, S.; Zhang, Q.; Feng, X. Integrated Optimization for the Coupling Network of Refinery and Synthetic Plant of Chemicals.
10. Zheng, H.; Mirlekar, G.; Nord, L. O. Agent-Based and Stochastic Optimization Incorporated with Machine Learning for Simulation of Postcombustion CO_2 Capture Process.
11. Shao, L.; Zhang, K. A Gas Emission Prediction Model Based on Feature Selection and Improved Machine Learning.
12. Borisut, P.; Nuchitprasittichai, A. Adaptive Latin Hypercube Sampling for a Surrogate-Based Optimization with Artificial Neural Network.

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