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Editorial

Smart Process Manufacturing toward Carbon Neutrality: Digital Transformation in Process Manufacturing for Achieving the Goals of Carbon Peak and Carbon Neutrality

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At present, the energy-supply and process-manufacturing industries suffer from the outstanding problems of heavy industrial structure, high energy consumption, and high carbonization of the energy supply, with the global demand and consumption of energy continuing to grow. Pollution emissions from high-carbon energy systems are significantly accelerating the global climate crisis. Therefore, there is urgent need for an energy revolution and industrial transformation in these industries. The digitalization of process manufacturing by relying on big data and artificial intelligence can effectively help process-manufacturing companies improve their efficiency and energy conservation. To achieve the goals of a carbon peak and carbon neutrality, innovative digital technology and its application in the fields of pharmaceuticals, chemicals, energy sources, metals, and polymeric materials should be promoted.

To help the process-manufacturing industry more effectively achieve green and low-carbon production, improve energy efficiency, reduce environmental pollution, and achieve the goal of collaborative digital and low-carbon development, this special issue focuses on how to solve bottleneck problems in operating management, production operations, efficiency, security, and information integration. This issue aims to promote the digital transformation of all phases of the production process, including modeling, optimization, intelligent perception, mechanism traceability, autonomous control, and efficiency analysis.

It has been our great pleasure to welcome academicians and prominent researchers from several nations, including Belgium, the United Kingdom, and China, to report on ideas, theories, and technologies related to digital transformation in process manufacturing, with significant support from the Chinese Academy of Engineering. We have chosen six papers for publication after a rigorous and thorough peer review procedure. A brief summary of these articles is provided below.

Drug research and development (R&D) has a huge impact on human health, making the pharmaceutical industry one of the most important manufacturing industries. However, developing new medications is a time-consuming and costly procedure. Thus, the application of artificial intelligence is critical in driving the development process of new medications, as it can effectively enhance productivity and break down technical analytical bottlenecks by combining large amounts of accessible data. In this issue, Lu et al. present an overview of common artificial intelligence models used in drug discovery and discuss the specific applications of these models in various stages of drug R&D, including target discovery, drug design, preclinical research, automated drug synthesis, and market influences. The scholars also investigate the possible benefits of artificial intelligence technologies in reducing researchers' workload and shortening the drug R&D cycle.

Many of the important chemical processes used in industry are long and complex. Appropriately designing experiments to develop new chemical processes and optimize established ones allows maximal information to be obtained with a minimum of effort, ensuring the efficient use of time and resources. Thus, applying machine learning to high-dimensional and nonlinear data helps speed up the experimentation and development of new technology by automating the entire experimental cycle. Shi et al. highlight some important achievements that have been made in the field of chemistry through the use of machine learning techniques; their article discusses the data available for use, typical machine learning algorithms and their application scenarios, and the prospective future of machine learning applications in this field. In addition, Ureel et al. focus on the application of active machine learning in chemical experiments ranging from molecule and catalyst design to reaction and reactor design. Their article introduces the principles of active learning and its application in chemical engineering, explores the advantages of machine learning, and suggests directions for future improvement.

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Polymeric materials are the foundation for developing high-tech and advanced manufacturing. To accelerate materials research and reduce the cost, algorithms and large amounts of data are utilized to guide virtual synthesis, property prediction, and screening of polymeric materials. This revolutionary paradigm has received a great deal of attention and has proven to be effective and valuable. Gao et al. outline current research and accomplishments in polymeric materials genome engineering, propose the use of machine learning for extracting underlying rules from data, and highlight obstacles and opportunities in the field.

With the growing scale of industrial engineering, it is necessary to optimize decision-making processes and control strategies to ensure closed-loop stability and high-precision performance in process manufacturing. Wei et al. propose a multi-objective adaptive optimization model predictive control (MAO-MPC) method to deal with challenges in the zinc smelting industry in achieving green production and resource efficiency. The researchers introduce a dynamical computational fluid dynamics (DCFD) model of a zinc oxide rotary kiln based on energy conservation laws with a sparse identification-based model reduction method to overcome the high computational complexity of traditional DCFD models. Moreover, Chai et al. propose an intelligent control method for the low-carbon operation of energy-intensive equipment based on end–edge–cloud collaboration. Their proposed method combines mechanism analysis with deep learning and consists of three parts: setpoint control, self-optimized tuning, and tracking control.

In summary, this special issue of *Engineering* presents six essential papers that report on cutting-edge advances in the digital transformation of process manufacturing in various arenas, including the pharmaceutical, chemical, polymeric materials, and energy-source industries. We hope that this special issue will assist researchers and practitioners in both academia and industry to better grasp the significance of the digital transformation of process manufacturing for achieving China's goals of carbon peak and carbon neutrality. Finally, we sincerely thank the authors, reviewers, editorial staff, and guest editors for their great efforts and hard works.