Process Systems Engineering, 1. Introduction

ULLMANN'S ENCYCLOPEDIA OF INDUSTRIAL CHEMISTRY

Rafiqul Gani, Technical University of Denmark, Department of Chemical and Biochemical Engineering, Lyngby, Denmark

Krist V. Gernaey, Technical University of Denmark, Department of Chemical and Biochemical Engineering, Lyngby, Denmark

Gürkan Sin, Technical University of Denmark, Department of Chemical and Biochemical Engineering, Lyngby, Denmark

Modern society increasingly relies on continuous development and supply of chemical-based products with new or significantly improved properties and functionalities in order to satisfy consumer needs. As chemical products, we consider bulk chemicals as well as low-volume specialty chemicals representing a wide range of industries, such as oil and gas, petrochemical, chemical, pharmaceutical, food, agrochemical, and biochemical sectors. For example, the bulk chemicals act as raw materials, solvents, process fluids, etc., needed in the manufacture of specialty chemicals that may become an active ingredient for a pharmaceutical (drug) and/or agrochemical (pesticide) product. Therefore, improved designs of continuous processes needed for the manufacture of bulk chemicals are as important as designs of batch operations needed for the manufacture of specialty chemicals. Globalization of the industry has opened new markets and with it new demands. However, how does one identify the chemicals and their synthesis routes that will help to meet these demands, taking into account also the questions of sustainability and protection of the environment? The sources for many of the raw materials used, especially those derived from oil, gas, and some plants and animals continue to be depleted and may soon become economically infeasible to use. Therefore, one increasingly needs to consider renewable replacements, and the processes to manufacture them. Methods and tools developed within process systems engineering (PSE) can help to address these and other process engineering problems in a systematic, structured, and efficient way.

PSE has been traditionally concerned with the understanding and development of systematic procedures for the design, control, and operation of chemical process systems [1, 2]. The core disciplines of PSE are listed below.

The oil and gas industry, the petrochemical industry, and to some extent, the chemical industry have been the traditional users of methods and tools, including software, from the PSE community. Problems related to process optimization, process integration, and process synthesis/design are currently routinely solved through knowledge-based techniques as well as mathematical programming techniques. Also, systematic methods and tools have been developed and applied to solve industrial problems in the areas of, e.g., planning and scheduling, online optimization, solvent selection/design and chemical product design. Examples of such methods and tools are the development of mixed integer nonlinear programming (MINLP) - based process synthesis, design, integration; computer-aided molecular design; generation of optimal heat and mass exchange networks; model-predictive control for optimizing plant operation, planning and scheduling optimization models.

Most of the above developments can be linked to chemical processes involved with the manufacture of high-volume bulk chemicals and their related industries, such as oil and gas, petrochemical, and chemical industries. To a lesser extent, these methods and tools have also been applied to the manufacture of low-volume specialty chemicals. The main issues that can be viewed as opportunities and challenges for

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PSE [3–6] include the areas of chemical based products, energy, sustainability, biosystems engineering, and enterprise-wide optimization. The objective of this article is to give the reader a good overview of PSE, its core disciplines, the emerging topics, and some examples of PSE methods and tools in practice. The further keywords dealing with PSE are summarized in the following list.

- Modeling and simulation → Process Systems Engineering, 2. Modeling and Simulation: process simulators need models of the process together with a set of constitutive models such as models for property prediction and reaction kinetics. Therefore, mathematical models and their solution through appropriate numerical methods play a very important role in understanding the behavior of the process and/or product during operation/application and based on these, their design and optimization. Since the methods and tools developed within the PSE community are mostly model-based, the solution accuracy and/or application range of the tools depend to a large extent on the accuracy/application range of the models used.
- Mathematical programming → Process Systems Engineering, 3. Mathematical Programming (Optimization): development and use of efficient mathematical programming techniques are very important in tackling problems (e.g., process optimization, product and process synthesis, enterprise-wide optimization). A large collection of numerical methods (solvers) are available to solve different types of optimization problems(e.g., linear programming, nonlinear programming, MINLP, dynamic and parametric optimization). Typically, tools from here are used in the other core disciplines of PSE. Large-scale and/or complex product and process optimization problems (e.g., synthesis of an olefin plant, synthesis/design of the optimal heat exchange networks) continue to be solved through appropriate mathematical programming tools.
- Product and process synthesis and design → Process Systems Engineering, 4. Process and Product Synthesis/Design/Analysis: even though the design approach for most chemical-based products and the processes to manufacture them is experiment-based, significant amounts of time and resources can be saved by using PSE methods and tools to first define a search space and then to identify within it, the potential candidates [7]. This model-based approach is not meant to eliminate experimentation in product and process development. Experimentation both at laboratory and pilot/demonstration-scales will remain important when developing new products and processes. The model-based approach advocated by the PSE community should result in improvements of the product and process development by (i) reducing the number of experiments needed, (ii) speeding up the development time for product and process as computer simulations for feasible product and process candidates can be analyzed faster at different spatial and temporal scales, and (iii) screening and evaluating different process monitoring and control strategies in a fast and efficient way especially suitable for implementation of process analytical technology (PAT) in pharmaceutical manufacturing.
- Process dynamics, control, and monitoring → Process Systems Engineering, 5. Process Dynamics, Control, Monitoring: producing products on specification and ability of the processes to reject disturbances are high on the priority list. Based on a good understanding of the process and its dynamics, schemes for monitoring and control are developed and implemented, resulting in control systems that contribute to achieve product specifications consistently. Due to the ever-increasing complexity of process plants, PSE methods for the design of plant-wide control systems become more and more important. For the future, it is expected that development in advanced control methods, and especially model-based predictive control (MPC), will further promote the general acceptance and usage of this technology, with development of an increasing number of MPC applications in domains such as pharmaceutical production and drug delivery. Automated systems have a big role to play, especially for complex – continuous or batch – production plants, but in order to be successful they rely on the ability of performing dynamic process simulation and optimization in real time.

- Cyberinfrastructure and intelligent systems → Process Systems Engineering, 6. Cyberinfrastructure, Informatics and Intelligent Systems: decision-making systems in all areas of chemical engineering are receiving increasing attention, use of cyberinfrastructure and informatics concepts, in conjunction with intelligent systems, therefore have a major role to play.
- Abnormal event management and safety → Process Systems Engineering, 7. Abnormal Event Management and Safety: abnormal event management is concerned with timely detection of an abnormal event, diagnosing its causal origins and then taking appropriate decisions and actions to bring the process back to a normal and safe operating state. Process safety analysis is, on the other hand, concerned with development of methods and tools to identify and analyze hazards and implement appropriate changes to process design (as in early stage analysis to obtain safety by design) and/or prevention, control, and mitigation barriers to the manufacturing processes such that one can manage the risks involved in manufacturing to a legally, socially, and environmentally acceptable level.
- Process operation → Process Systems Engineering, 8. Plant Operation, Integration, Planning/Scheduling and Supply Chain: process operations deal with the models, methods, and tools that support the technical decisions associated with the safe, efficient, and reliable execution of the manufacturing functions of a process industry enterprise. Here, one seeks, e.g., to employ the plant and other enterprise resources in the most effective manner while meeting market demands and constraints, or, to address and remedy disturbances beyond the scope of regulatory control and to conduct higher level functions such as updating of setpoints or target profiles, scheduling and planning of resource allocations and assignment, and coordination with supporting functions such as customer and supplier logistics.
- Domain engineering → Process Systems Engineering, 9. Domain Engineering: the areas of energy and sustainability clearly provide new challenges and opportunities to the PSE community. The shift towards renewable resources for energy, most notably through biomass, requires addressing processes that have quite different characteristics than the traditional petrochemical processes in that reactions are biochemical in nature, mildly exothermic and take place at relatively moderate temperatures. Of course the area of energy is closely tied to the area of sustainability in which the broader challenges include developing process systems that are sustainable in the long term. Furthermore, the other important aspect is the environmental one in which the effective use of resources like water is paramount, and the negative impact of production plants on the air quality is minimized. An area that has also been receiving increasing attention in recent years is the area of biochemical engineering systems, which range all the way from protein design to biomass feedstock processing going through metabolic networks. A major issue here for the PSE is how to provide meaningful and useful simulation and optimization tools for modeling these complex systems that in turn require integration with data-intensive experimentation. Then there is the added dimension of biomedical applications in which design of drug delivery or therapeutic treatment can in principle benefit from quantitative simulation and control models that the PSE community has been so successful in developing. The area of enterprise-wide optimization has also emerged as a new opportunity for the PSE community given the increasing need for integrating the functions of R&D, manufacturing, and supply in the chemical industry. This has in a large part been driven by advances in information technologies that allows the access of data across an entire supply chain. A major challenge here is the use of these data in models for the integration of planning, scheduling, and control activities across geographically distributed sites, which in turn gives rise to very large-scale optimization models, which presently are unsolvable.

From the above trends it is clear that current and future problems require a multidisciplinary approach because the model development (including data) comes from different sources and the performance criteria, factors, etc., involve other communities besides the PSE community. The advantage for the PSE community, however, is that it can play the role of the "integrator" or "glue". That is, develop systematic solution approaches that combine methods and tools from different sources into a single, flexible, reliable, and efficient system. However, for the PSE to meet the challenges for the future, computer-aided frameworks for generation and use of multiscale models, software platforms, and advances in computing sciences for enabling implementation of improved, more powerful and user-friendly software tools, methods for design of experiments to collect and analyze data, methods and tools for product and process monitoring systems (and their design), techniques for optimization of the enterprise and its supply chain, systematic methods for product discovery would need to be developed, and validated through convincing and industrially challenging case studies. These case studies will also need to highlight the scope and significance of the new methods and tools in terms of satisfying the technological, economic and social issues. Models need to be predictive under an increasingly wide range of application conditions and uncertainties related to their predictions due several sources (e.g., uncertainties in data, parameters, and constitutive equations [8]) so that first-time right, reliable, and truly innovative product and process development solutions can be ensured.

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