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Editorial

Special Issue on "Chemical Process Design, Simulation and Optimization"

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Since humanity has been able to transform materials, such as raw minerals, and produce food or beverages, a central question was the type of operation and how and where it should be performed. Thus, furnaces, ovens and simple distillation stills were operated, to cite a few. Thermodynamics already started as a new science with the development of vapor engines, from Denis Papin in the seventeenth century to James Watt in the eighteenth. The nineteenth century saw the huge development of industries devoted to large productions and the arrival of electricity. New methods started to be available to engineers for the design of workshops in factories. However, chemical engineering started as a real science with the concept of unit operations first taught by G. Davis at the University of Manchester in 1887 and quickly spread to MIT. At the beginning of the twentieth century, the development of the petroleum industry and the building of refineries strengthened the need for new and more efficient calculation procedures; thus, new concepts were invented. Transport phenomena, heat and mass transfer and chemical reaction engineering became new fields of research and found important applications. After the Second World War, the arrival of computers modified the landscape for engineers as, for the first time, it allowed them to perform extremely complex calculations and no frontiers seemed impossible to reach. First, custom computing codes were developed, then commercial codes, often created in research labs before industrial development, were largely available to design engineers for their simulation needs. Simultaneously, it seemed that chemical engineering was too restrictive and its methods could be applied in other domains, such as metallurgy and biotechnology, hence the broader denomination of chemical process engineering. Batch as well as continuous processes are considered, and dynamic simulation as well as steady-state simulation is a usual practice. Furthermore, with more and more powerful computers, it was possible to aggregate the optimization with respect to parameters and even unit operations together with the design. Nowadays, even process control seems possible at early stages of the design. It is also usual to use dedicated codes of computational fluid dynamics integrating heat transfer and possibly chemical reactions, in industries as well as in research departments.

In this context, it is natural that this Special Issue of "Chemical Process Design, Simulation and Optimization" was likely to attract a large number of proposals for authors of many different countries. It must be underlined that these proposals are very different from what they would have been forty or twenty years before with the availability of computing codes.

General Methods

Some articles deal with general methods which belong to the methodology of chemical process engineering. The article by Furda et al. [1] proposes a general approach, coupling two commercial codes, Aspen Plus® and MATLAB®, for optimal design, with a special focus on energy saving, particularly with regard to steam use, such as in turbines, compressors, pumps and fans. They describe a coupled steam- and process-side modeling approach, taking into account the varying inlet steam parameters or shaft work requirements and implementing fix turbine and driven equipment efficiencies. They even show the influence on the balances. They apply this method to an industrial case of the heat-pump-assisted distillation of a liquid propane–propylene mixture, where the energy for separation is provided by a condensing steam turbine. They propose a serious change due to the increase in high-pressure steam. The impact on the gas emissions is also studied and the economic gains are assessed. Zecevic et al. [2] are also concerned by energy savings applied to a real industrial steam methane reformer unit used for ammonia production. They develop an integrated detailed model which takes into account the production parameters. This enables them to exchange data between the distributed control system and the model to continuously monitor and optimize the steam methane reformer catalyst and tubes. Thus, the overall energy saving is 3% in the real plant. Dizabar et al. [3] compare the exergy and advanced exergy analysis in three different organic Rankine cycles. Exergy is the extent of energy to the second law of thermodynamics by considering entropy and it allows to take into account the irreversibilities in a process. Thus, again, this study focuses on energy saving and process optimization. By advanced exergy analysis, they can separate the exergy loss between unavoidable and avoidable and endogenous and exogenous contributions for each component. This allows them to improve the design by concentrating on the most important components from an energy point of view. Wang et al. [4] propose an efficient numerical method to solve the calculation of a set of nonlinear equations applied to a reactive distillation column and to a distillation column. Their method, called inside-out, divides the calculation into two loop iterations. Sun et al. [5] study the problem of model-based fault diagnosis for a distillation column and, again, this study is strongly related to a numerical and algorithmic point of view. Although it might seem a particular case, their approach is general and can be used for different applications. It consists in adopting a hybrid inverse problem approach using partial least squares to fit and forecast trajectories of the fault parameters generated by least squares. It is applied to the classical Tennessee Eastman process. Skorych et al. [6] study the solution of population balance equations. This type of equation occurs in the description of the distributions of sizes of granular materials, such as polymers and crystals. This is an important problem which often poses numerical difficulties, particularly when it is met in flowsheets and in dynamic problems, resulting in partial differential equations. The authors propose a new model based on transformation matrices. They also use finite volumes to describe the phenomena of agglomeration and breakage. They are able to implement their method in the specially designed Dyssol simulator, which uses a sequential-modular approach. Simulation examples are taken from the pharmaceutical industry. This sufficiently general approach allows the users to apply this method to their own population balance models. Mukhtar et al. [7] study a problem very close to the previous one as it deals with the numerical study of a batch crystallization. They include fines dissolution, which is critical in the industrial practice. Their numerical method is based on a quadrature method of moments. The application refers to test problems, not real problems.

Coupling with Fluid Mechanics

As previously mentioned, due to the progress of computer efficiency, memory and rapidity and the availability of both commercial and open-source codes of fluid mechanics, these advanced numerical techniques are more and more frequently applied to traditional processes, which are, thus, revisited and improved. Zeng et al. [8] study a particular unit, the turbo air classifier, which is used to separate powders into coarse and fine. Based on the governing equations and using a commercially available software, they study the influence of operation parameters, such as rotation speed and

air volume. Studies are performed for multiple particles. Simulation and experimental results are favorably compared. Cheng et al. [9] also use a computational fluid dynamics code to better understand bubble columns, which are frequently used in process industries and whose behaviour is complex and not totally predictable. They use the Euler–Euler approach, consisting in obtaining mean local properties to describe the bubble plume, and compare their simulation results to laboratory experiments. They reveal the correlation of operating conditions with the gas mixing and plume oscillation period. The commercial code of CFD is the same as used by [8].

Studies of Given Processes

It is natural and usual that some given processes are studied by researchers who either try to promote specialized models or improve their behavior by examining operation parameters. Many studies can be gathered in this category. Yang et al. [10] study an in-situ combustion method that can be used for bitumen sands or heavy oil production. Their numerical study deals with a given block of a Chinese oil field. They analyze the influence of production (huff and puff rounds, air injection speed and air injection temperature) and geological parameters (bottom water thickness, stratigraphic layering, permeability ratio and formation thickness). They are thus able to extract the main operation parameters. Shakeel et al. [11] compare the industrial production of formaldehyde using two different catalysts. They use a commercial steady-state process simulator to simulate the process and deduce the advantages and drawbacks of these configurations. Chinh et al. [12] study a nitrogen gas separator. This is a fixed bed operated by pressure swing adsorption. Thus, it is an appropriate subject for modeling and simulation with its dynamic and sequential operation, but the authors also compare their results to a laboratory pilot plant. The model, composed of partial differential and algebraic equations, is fully described together with its operating parameters. Chen et al. [13] study the production of butyric anhydride by means of a single reactive distillation column. Although this process has already been described in the literature, its applications are not numerous due to many operation difficulties and lack of generality. Moreover, the authors have replaced a two-column process with a single one by using the internal circulation of acetic anhydride. They show that this can be extended to similar reactive distillation two-column processes. The simulation is performed by a commercially available steady-state process simulator by which they optimize the process. Finally, they perform an economic analysis of the novel process. Marecka-Migacz et al. [14] study a membrane process—more specifically, ceramic nanofiltration for the separation of succinic acid aqueous solutions. They provide a detailed model of nanofiltration for ion transport, taking into account convection, diffusion and electromigration. They compare the results obtained by their elaborate model to those issued from more standard approaches. In their case, all species are considered, as well as solutes, ions and solvent, pH-regulating solutions and water. The conditions of use of their more complete model are emphasized. Experiments are also performed for comparison. Nguyen et al. [15], again, study a membrane process of ultrafiltration of protein. The model is simpler than in [14]. Their objective is to perform an economic assessment of the process and, for this purpose, their focus is related to the design parameters. With the latter being numerous, they perform the optimization by means of a genetic algorithm in a black-box manner, although they rely on their analytical model.

Original Processes

By original process, we mean processes that are rarely studied from a process point of view and/or that recently emerged. Among these, the process synthesis of carbon dots studied by Pudza et al. [16] can be ranked. A part of the article deals with the chemical synthesis of these carbon dots and has little connection with process engineering. However, the latter is concerned when the authors apply a surface response methodology using design of experiments to optimize their process. This strategy is often used when researchers or engineers meet great difficulties in modeling the process. From that angle, it could also mean that such a process presents interest for modeling based on first principles.

Nevertheless, the authors are able to propose conditions for efficient and sustainable synthesis of carbon dots.

Safety Studies

Finally, one article deals with safety. This is an extremely important aspect of any practical operation, especially at the industrial level. Often, safety studies are published in dedicated journals and less in more general journals, such as *Processes*. Wang et al. [17] study the process of natural gas explosion in the case of linked vessels with three structures. They perform a numerical simulation by means of an available and efficient software designed for predicting the consequences of gas explosions in three dimensions. They also build an apparatus to infer some parameters. Simulations deal with the influence of parameters such as pipe length, ignition position, length of connection pipes and sizes of vessels. This article demonstrates how a very elaborate code can be useful in performing a safety study.

Conclusions

A large variety of manuscripts were proposed. Without aiming at a particular classification chosen a priori, it appears that the accepted articles are mainly divided in two categories. The first one deals with general methods applicable to many processes and pursuing the goal of improving the methods of process engineering, either from an analytical or from a numerical point of view. General simulation codes are regularly used and sometimes coupled between themselves, even with advanced computational fluid dynamics, to provide new insights. The second category deals with dedicated processes, often related to an experimental laboratory or industrial process unit. In this case, the objective is rather to show how a refined model can improve the simulation or simply how a process can be optimized. Economic aspects are treated in several articles, revealing an important purpose of process engineering. Even if only one article dealing with safety was retained, it shows how process studies are interlinked, as it also makes use of computational fluid dynamics. In general, when possible, the authors try to compare their simulation results with experimental results obtained at the laboratory or plant level.

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