



# Editorial Special Issue "Progress in Thermal Process Engineering"

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**Abstract:** The Special Issue "Progress in Thermal Process Engineering" contains a total of eight articles, seven research papers and a review article. The topics of the individual articles reflect the variety of current research in the field of thermal process engineering. The contributions address important issues such as modularization, digitization, new equipment and simulation techniques. It becomes clear that efficiency efforts are an essential feature of current research in the mentioned field. Efficiency in the sense of energy efficiency as well as in the sense of more efficient, i.e., more flexible, production. The authors of the articles originate from the USA, Russia, Switzerland and Germany.

**Keywords:** modularization; process intensification; flexibilization; multiple Dividing-Wall-Column; CFD Simulation; parameter estimation

## 1. Introduction

Thermal process engineering is a mature discipline and thermal separation operations as distillation or extraction have been applied for thousands of years. However, thermal separation processes are most widespread in the chemical industry and account, to a large extent, for the energy demand of chemical production. In the past few years, the chemical industry has been struggling with stricter regulations, increased global competition, higher market volatilities and changing supply chains. To react to these burdens and maintain competitiveness, it is mandatory for the chemical industry to develop more flexible and efficient processes. The fast evolution in the field of intensified processes, for instance, reactive distillation or the dividing wall column, reflects this trend very well. In recent years, the focus has moved towards the flexibility of equipment and entire production plants. The idea is to reduce CAPEX by utilization of standardized equipment that can be applied in a wide operation window. Flexible container-based or skid-mounted production units are also discussed in this context. These plants can easily be adapted to changing production volumes by a simple numbering-up, which reduces the risk of large investments in a volatile market.

The mentioned concepts also make new methods for modelling and simulation necessary. Significant progress has been made, for instance, in the field of CFD-simulations or mathematical optimization of mixed integer non-linear problems in the past few years.

Even though thermal process engineering is old, it still holds plenty of opportunities for improvements, optimization and new concepts. This Special Issue reflects the abovementioned trends.

## 2. Brief Overview of the Contributions to this Special Issue

Many authors underline the fact that chemical industry is facing severe challenges driven by increasing market uncertainties. In order to maintain competitiveness, the industry has to answer these issues by improving process efficiency, improving process flexibility as well as improving process understanding by modeling. Two contributions highlight the modularization of separation units for chemical production in order to establish an increased flexibility for chemical productions [1,2].

Seyfang et al. [1] describe the use of extraction centrifuges using practical examples from industry. In these centrifuges, the separation of the two phases does not take place in the earth's gravity field but by high g-forces due to the rotation of the apparatus. This allows the separation of systems whose material properties are unsuitable for classical extraction processes. Furthermore, the residence times are very short and the volume of the apparatus is small. Due to the rotation speed as an additional degree of freedom, these apparatuses can also be flexibly adapted to the respective process conditions and allow the use for different separation tasks. It is also possible to superimpose a reaction. Riese et al. [2] contribute a review paper regarding flexibility options of absorption and distillation to better cope with material supply and product demand uncertainties. They discuss current research and development activities in the field of micro distillation and absorption as flexible large-sale units. Although there are a number of different approaches, these are generally not sufficiently developed and understood to be robustly applied in production. There is still a lot of research work to be done in this area in the future.

Regarding new and intensified unit operations, Preißinger et al. [3] discuss the technical design of the first multiple dividing-wall-column for a pilot plant. A simplified version of the fully thermally coupled four-product dividing wall column is described, with only two instead of three dividing walls. Moreover, the authors proved that this simplification is feasible to separate quaternary mixtures without an energy penalty. However, the proof of concept by experiments is still missing.

The modeling of processes is a key to generate process understanding and to quickly evaluate different process variants without experimental effort. Here, different modeling depths are used from short cut to fully rigorous models. In this context, the provision of reliable thermodynamic data as parameters for the models is also of great importance. Three articles in this special issue deal with these issues. Höller et al. [4] discuss parameter estimation strategies in thermodynamics. The contribution covers standard approaches such as least-square. However, the authors conclude that measurement errors in the input data lead to constrained least-squares problems, where the number of equality constraints grows with the number of measurement points. In this situation, the Patino-Leal formulation is a valuable alternative, since it transforms the constrained least-squares problem to a non-restricted optimization problem. Paluch et al. discuss in their paper the thermodynamic assessment of the suitability of the limiting selectivity to screen ionic liquid entrainers for homogeneous extractive distillation processes [5]. A method is described to quickly identify the ability of an ionic liquid to break an azeotrope. This is important since already small amounts of ionic liquid added to an azeotropic solution might break the azeotrope and outperform conventional entrainers, leading to more efficient and slim processes. In their contribution Tsirlin et al. [6] suggest a technique for the selection distillation sequences for which the total energy consumption of the distillation train reaches a minimum. This is a nice example for the benefitial application of thermodynamic modeling in the context of conceptual process design. The high potential of CFD simulation to gain deep process insight is showed by Renze and Akermann [7]. Using an open-access CDF package, the conjugate heat transfer of complex geometries was simulated and compared to theory. The application of the proposed methods to plant-scale units (e.g., heat exchanger) was demonstrated.

Last but not least, a major topic is addressed by Maiwald [8]. The author states that digitalization of the chemical industry is a key factor toward more efficient chemical production. At the same time, the application of intelligent production networks is progressing hesitantly in industry. This gap represents a major threat to future competitiveness. The potential of "Industry 4.0" application within the process industry are described in the contribution. The author concludes that, besides the technical skills of digitalization, changes in structures and management of companies are also necessary. This makes the transformation highly demanding.

## 3. Conclusions

The chemical industry is facing great challenges caused by rapidly changing conditions in the supply of raw materials and product qualities. At the same time, the life cycles of the products are shortening. A whole package of measures is required to meet these challenges. This Special Issue gives a good overview of current research, especially in thermal separation technology as a sub-discipline of process technology. It becomes clear that many promising ideas exist but at the same time only a few approaches are understood and established to the point where they can be applied industrially. There is still a lot of research work to be done in the future to close this gap.

Conflicts of Interest: The author declares no conflict of interest.

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