

# Process systems engineering

## Editorial overview

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Though the term *process systems engineering* appeared explicitly first in 1961 in one of the volumes of the AIChE Symposium Series, its origin dates back to the 1940s as far as it has been stated by Roger Sargent [1]. Initially, the tools for process systems engineering (PSE) were developed for individual chemical processes or their specific parts; nowadays, highly complex systems of processes are successfully examined by the available apparatus. The scope of PSE is continuously widening from the beginnings. This tendency will continue in the future. Since certain components of the globalized world behave as an engineering system, PSE is to be extended to these areas. Current issues of the environment, natural world, global security, and weather require appropriate tools. PSE may play a key role in these developments verifying the long-term investment in its research.

PSE has been developing steadily in parallel to the development of computers, numerical tools, and mathematical programming. Several key centres and research institutes have contributed to the area during the last decades, and it has been a challenging task to select among them. The first part of this section includes four papers on PSE representing four major centres in four different countries.

The contribution delivered by Peter Glavič is dedicated to the history of PSE starting from the pioneering Process Systems Engineering Conference held in Kyoto thirty years ago. The evolution of the definition of the discipline has also been given covering from the general systems theory to the current opinion on process systems engineering. The major contribution of the eleven PSE symposia has been analysed together with other conferences in the area including the European Symposia on Computer Aided Process Engineering (ESCAPE), International Conferences on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction (PRES), Foundations of Computer Aided Process Design (FOCAPD), Foundations of Computer Aided Process Operations (FOCAPO), Chemical Process Control (CPC), and Process Systems Engineering Asia (PSE Asia). On the basis of the recent PSE conferences in Europe, Asia and the US, Glavič made an attempt to forecast the future developments and trends of process systems engineering.

Two contributions deal with one of the key problems tackled by the PSE, it is the supply chain management. José Miguel Laínez and Luis Puigjaner presented the paper Prospective and Perspective Review in Integrated Supply Chain Modelling for the Chemical Process Industry. This paper offers a comprehensive review for the most important topics of supply chain management in the process industries. It shows that the integrated supply

chain modelling is crucial for a competitive enterprise where the integration is considered in different dimensions. The extension of supply chains has also been taken into account in emerging areas including green energy resources and water cycle control. It has been shown that ontologies can be exploited to integrate analytical and transactional systems.

The paper by Ana Paula F.D. Barbosa-Póvoa entitled Progresses and Challenges in Process Industry Supply Chains Optimisation cites the European Chemical Industry Council's statement that the EU's chemical industry is the third largest manufacturing sector in terms of added value in Europe. Regarding the supply chain optimization, it has been shown that the research challenges are going to result in more complex problems. To satisfy the industry's ever increasing needs, a continuous investment is required in the development of effective solution methods. Naturally, process systems engineering provides the theoretical basis to these developments. The importance of sustainability in supply chain management is continuously increasing; it is expected to become a key issue in the future. Therefore, environmental and social values are also to be considered in the modelling of supply chains.

The paper on Recent Developments in Process Systems Engineering as Applied to Medicine by David L. Bogle is offering a novel approach to an important area. It has been shown that the methodologies of process systems engineering can successfully be applied to physiological systems. It is interesting to recognize that diagnosis, prognosis, and therapy correspond to the terms analysis, simulation, and design, respectively. Therefore, the analysis of systems relates to diagnosis of a condition, the model simulation provides predictions resulting in a potential use for prognosis, the design for an optimal action or set of actions based on a model and set of objectives which corresponds to devising a therapy. Examples show the evidence of the usefulness of the proposed approach; nevertheless, so far there is little evidence of clinical use of the results. In the future, greater interaction is required with clinicians to gain experience and confidence. This paper well illustrates that PSE tools are not just for processing industries.

Even this limited selection of PSE-related topics demonstrates that it is an important, fast developing, and growing discipline that has direct affect on the current industry and the future of our world. I strongly believe that this journal that provides condensed and target current opinions will revisit this topic in the near future with more options from a large available menu of forefront research results.

The second part of the section is dedicated to *product design*. Product design was identified as an important

yet undeveloped subject over a decade ago. It offered a new research direction to the process systems engineering community — the attainment of product attributes in an optimal manner through processing of the wide variety of chemical products. The progress in developing a coherent body of knowledge for applications in industry and for adoption in teaching has been steady but relatively slow. There are many hurdles, some of which are covered in the articles of this section.

One is the absence of basic scientific understanding of a large number of issues related to product design. This may seem odd after decades of effort on engineering sciences with major advances in thermodynamics, reaction kinetics, and so on. Indeed, the pursuit of product design has exposed what is missing in chemical engineering principles. Products in many industrial sectors ranging from skincare products to foods are often complex mixtures with microstructures, characterized by product attributes such as form, colour, touch and feel, ease of use, and so on. The fundamental understanding of these hard-to-quantify product attributes is in its infancy. In thermodynamics, the extensive database of relatively simple molecules is not adequate for the prediction of the behaviour of a multicomponent mixture with complex molecules such as surfactants and ligands. Similarly, it is challenging to predict the formation of various nanoparticles with different shapes and internal structures because the understanding of the interplay between reaction and crystallization kinetics is incomplete. The review by Picchioni and Broekhuis sheds light on what is referred to as the system composition-processing technology-product function triangle, which is the key to unlock the door to rational design of formulated and configured products.

A product does not exist in isolation. Its impact on the environment depends on the choice of raw materials, the manufacturing process, and the way in which the product is consumed. The coupling of life-cycle assessment and product design represents a huge challenge and an opportunity to achieve high-level optimality in the chemical processing industry. The assessment of environmental impact still carries a great deal of uncertainty and the tradeoff between product attributes and product sustainability is hard to quantify. The review by Villeda *et al.* examines these issues using novel biofuels as an example.

If all the advanced techniques in chemical engineering do not provide a ready solution to the product design problem, what do we teach to the students who will enter the workforce with a Bachelor's degree? These relatively large numbers of practicing chemical engineers arguably represent the profession more so than those with higher degrees. Can the chemical engineering educators provide

them with the necessary tool kit to penetrate and expand this job market? The review by Seider and Widagdo summarizes what has been achieved so far and discusses the necessary future developments.

The latter three reviews will not be the last as the profession inches forward in the direction of product design. Further development is expected to be an iterative process. The experience and understanding gained in

designing the myriad chemical products in practice should be captured and distilled for teaching.

Finally, the authors', reviewers', and publisher's effort is appreciated.

## References

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