



## Perspectives for process systems engineering—Personal views from academia and industry

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### ABSTRACT

Process systems engineering (PSE) has been an active research field for almost 50 years. Its major achievements include methodologies and tools to support process modeling, simulation and optimization (MSO). Mature, commercially available technologies have been penetrating all fields of chemical engineering in academia as well as in industrial practice. MSO technologies have become a commodity, they are not a distinguishing feature of the PSE field any more. Consequently, PSE has to reassess and to reposition its future research agenda. Emphasis should be put on model-based applications in all PSE domains including product and process design, control and operations. Furthermore, systems thinking and systems problem solving have to be prioritized rather than the mere application of computational problem solving methods. This essay reflects on the past, present and future of PSE from an academic and industrial point of view. It redefines PSE as an active and future-proof research field which can play an active role in providing enabling technologies for product and process innovations in the chemical industries and beyond.

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## 1. Introduction

Process systems engineering (PSE) is a largely mature and well-established discipline of chemical engineering with roots dating back to the 1950s (Anonymous, 1963). The systems approach (e.g. van Bertalanffy (1950, 1968), van Gigch (1991), Klir (1985), Simon (1981)) has been successfully adapted and refined to address the needs of designing, controlling and operating chemical process systems in a holistic manner. PSE has been evolving into a specialized field at the interface between chemical engineering, applied mathematics and computer science with specific model-based methods and tools as its core competencies to deal with the inherent complexity of chemical processes and the multi-objective nature of decision-making during the lifecycle of the manufacturing process of chemical products. PSE has been successfully implemented as a discipline in its own right in research, industrial practice as well as in chemical engineering education.

This paper assesses the status and the future perspectives of PSE from an academic as well as from an industrial point of view. It cannot and will not aim at a comprehensive review of the numerous scientific achievements. Its objective is to rather assess: (i) the overall progress made with respect to the formation of a self-contained and independent scientific discipline and (ii) the concrete contributions and impact in industrial problem solving. Furthermore, it will reflect on the future perspectives and the potential impact of PSE on research and industrial practice.

The paper is organized as follows. Section 2 gives an introduction into the nature of PSE emphasizing its roots in general systems engineering. The academic achievements and their impact on industrial practice are discussed in Section 3 to prepare for a look into the future. Clearly visible emerging trends are identified in Section 4. Furthermore, desirable extensions of the scope of PSE and a route for further development of the field are given in Section 5, before we summarize and conclude in Section 6.

## 2. The nature of process systems engineering

The nature of PSE can be only fully appreciated if it is put into the context of related lines of research. We therefore briefly review

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the foundations of general systems theory and systems engineering before we address PSE.

### 2.1. General systems theory

General systems theory has been created as a scientific discipline in the 1930s by L. v. Bertalanffy, a biologist, aiming at a set of generic problem solving methods and tools to represent, analyze and synthesize complex systems comprising many interacting parts in general, regardless of the context they occur in. van Bertalanffy (1950) gives the following definition:

... a new basic scientific discipline which we call General Systems Theory. It is a logico-mathematical discipline, the subject matter of which is the formulation and deduction of those principles which are valid for systems in general.

The creation of such a meta-science was intended to overcome the progressing segmentation of the sciences on the one and to efficiently deal with systems complexity on the other hand (Simon, 1981). Obviously, this motivation is of even higher relevance today given the explosion of the scientific literature, the continuously progressing specialization in science and engineering, and the increasing complexity of socio-technical systems.

A large number of monographs have been published in the last 50 years including those of van Bertalanffy (1968), Klir (1985) or van Gigch (1991) to elaborate on the basic concepts of general systems theory. These authors characterize a system to constitute “an assembly or a set of related objects” (van Gigch, 1991) that “interact in a non-simple way” (Simon, 1981). A system is any material or abstract entity which is distinguished by its boundary to delimit it from its environment. Its properties are defined by a set of attributes. These attributes are chosen to characterize the entity under consideration such that all information which is of interest to the observer is captured. Hence, the representation of a system is a model in the sense of Minsky (1965)—it does not capture reality but is confined to a certain perspective of reality which is considered relevant in the context the model is supposed to be used in. A system interacts with its environment by means of inputs and outputs. The inputs represent the influences of the environment on the system while the outputs reveal information on the properties and the state of the system to reflect its behavior. Systems can be decomposed or aggregated to form smaller or larger systems. In such complex systems “the whole is more than the parts, not in an ultimate metaphysical sense, but in the important pragmatic sense that, given the properties of the parts and the laws of their interaction, it is not a trivial matter to infer the properties of the whole” (Simon, 1981).

The aggregation and decomposition of a system across a hierarchy of appropriately chosen levels as shown in Fig. 1 is a key concept of general systems theory to deal with complexity: it facilitates and guides systems problem solving, namely: (i) systems analysis aiming at an understanding of the behavior and function of a (natural or artificial) system and (ii) systems synthesis comprising the design and implementation of an (artificial) system according to given requirements.

The basis for systems problem solving is a system representation of an adequate degree of formality which may range from natural language to semi-formal information models or ontologies (Bunge, 1979; Gomez-Perez, Fernandez-Lopez, & Corcho, 2003; Uschold & Grüninger, 1996) and ultimately to mathematical process models (Hangos & Cameron, 2001).

### 2.2. Systems engineering

While general systems theory established the systems paradigm conceptually on an abstract level (van Gigch, 1991), systems engi-

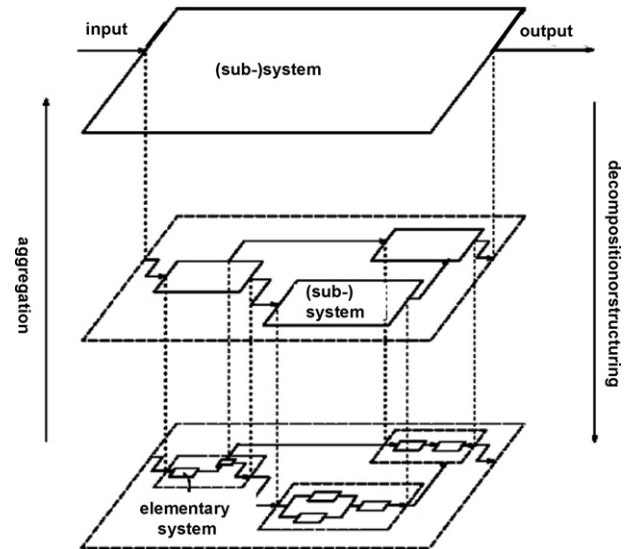


Fig. 1. Decomposition and aggregation of systems.

neering addresses all practical aspects of a multi-disciplinary structured development process that proceeds from concept to realization to operation (Bahill & Gissing, 1998). Wymore (1993) gives the following formal definition:

Systems engineering is the intellectual, academic and professional discipline, the principal concern of which is the responsibility to ensure that all requirements for a bioware, hardware or software system are satisfied throughout the life-cycle of the system.

It is worth emphasizing that this definition interprets a technical system as being composed of hardware (i.e. the process plant and its equipment), of software (i.e. the operation support systems), and bioware (i.e. the plant operators and management). Only a proper design of these three interacting subsystem will implement the desired function of the system according to the specified requirements (Schuler, 1998). Multiple business and technical objectives have to be considered to generate alternative solutions, to assess their performance and to finally provide a quality product which meets the users' requirements. Systems engineering is in the first place a methodology to solve systems design problems in a coordinated and well-understood systematic design process (Braha & Maimon, 1997; van Gigch, 1991). Bahill and Gissing (1998), for example, have developed the SIMILAR process which is widely accepted in the systems engineering community. It comprises seven coarse-granular tasks which refer to the letters in SIMILAR:

- (1) **State the problem:** identify the requirements the system must satisfy.
- (2) **Investigate alternatives:** generate alternatives which meet the requirements and define a multi-criteria decision-making process to identify the most promising alternative.
- (3) **Model the system:** analyse promising alternatives and find the *as is* and determine the *to be* by any kind of system model which can be processed and interpreted.
- (4) **Integrate:** connect the designed system to its environment to optimize the function of the overall system the designed system is embedded in.
- (5) **Launch the system:** implement the system, run it and produce output.
- (6) **Assess performance:** measure the systems performance against the requirements in the design problem statement.

- (7) **Re-evaluate:** continuously monitor and improve the performance of the system during its whole lifecycle.

General systems theory and systems engineering methodologies such as the SIMILAR design process are powerful instruments to deal with complexity on a conceptual level but are necessarily weak when it comes to concrete problem solving in a specific domain. The generic principles and design tasks have to be refined and enriched by specific domain knowledge to be successful, covering the scientific foundation and the engineering paradigms of a given technological field.

The rapidly evolving computing technology has initiated a radical change in the way systems engineers have thought about their problem solving capabilities shifting from manual to automated design by means of computers. This expectation has been built on the working hypothesis that an algorithmic procedure can be found, implemented in software and executed by a computer, if the problem statement can be cast into a sound formal representation (Hill, 1967). Such formal problem representations and algorithmic problem solving approaches have not really resulted in design automation but have rather contributed to effectively support at least part of human problem solving. Any computer-aided support is built on formal systems representations building on logic expressions or on mathematical equations. Such a mathematical formalization has been pioneered in the field of control engineering where a theory of linear dynamic systems in continuous and discrete time can be traced back to the 1950s (Gertler, 2006). A formal mathematical treatment of more general systems problems has been centred around the theory of discrete-event systems. Wymore (1993) presents a very general formal framework for systems representation and design with an exemplification for discrete systems which is based on set and function theory. Formal methods have a long tradition in software engineering (Clarke & Wing, 1996). Their objective is the design and implementation (or more precisely the *specification and verification*) of a piece of software, a special kind of artificial system.

### 2.3. Process systems engineering

PSE follows the systems engineering paradigm and targets at the analysis and synthesis of (chemical) process systems. Its objectives have been defined by Takamatsu (1983) as follows:

PSE is an academic and technological field related to methodologies for chemical engineering decisions. Such methodologies should be responsible for indicating how to plan, how to design, how to operate, how to control any kind of unit operation, chemical and other production process or chemical industry itself.

Hence, PSE is all about the systematic and model-based solution of systems problems in chemical engineering (Ponton, 1995). The outreaching definition of Takamatsu (1983) is emphasized by Fig. 2, which is reprinted here from his original paper. It already has a multi-scale flavour including physical phenomena on the meso-scale, unit operations, whole processes and the socio-economic system they are embedded in. Furthermore, the scope is explicitly not restricted to chemical process systems but also mentions energy systems and biomedical systems, two systems problem classes which have received significant interest in recent years. The multi-scale perspective already proposed by Takamatsu (1983) has been emphasized more recently by Grossmann and Westerberg (2000). They interpret the role of PSE as a set of methods and tools to support decision-making for the creation and operation of the chemical supply chain constituting of the discovery, design, manufacturing and distribution of chemical products. Hence, PSE is more than *computer-aided process engineering* (CAPE) since its

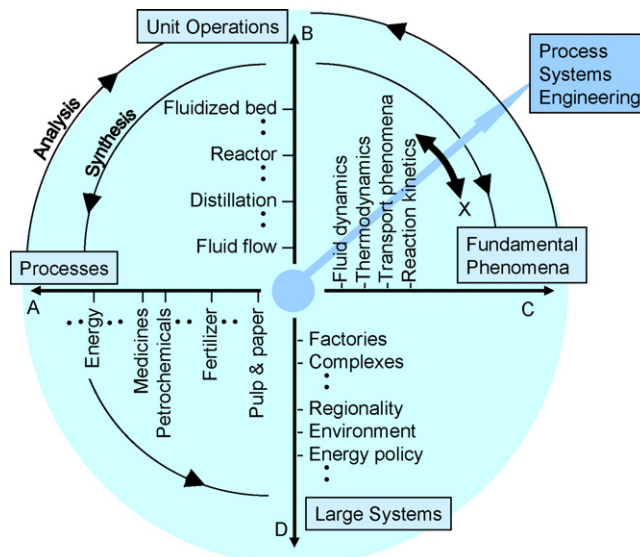


Fig. 2. The nature of process systems engineering, reprinted from Takamatsu (1983).

core business is not merely the use of computers to assist problem solving – or more specifically engineering design processes – which has been the original scope of CAPE (Motard, 1989; Winter, 1990). PSE rather addresses the inherent complexity in process systems by means of systems engineering principles and tools in a holistic approach and establishes systems thinking in the chemical engineering profession. Mathematical methods and systems engineering tools constitute the major backbone of PSE. However, it has to be mentioned that there is some terminological confusion in the scientific community, since some authors, e.g. Kraslawski (2006), have used CAPE and PSE synonymously in the recent literature.

The field of PSE has been rapidly developing since the 1950s reflecting the tremendous growth of the oil, gas and petrochemical industries and their increasing economical and societal impact. Though, the roots of this field can be traced back to the UK and to the US (Anonymous, 1963; Sargent, 1967, 1972), it has also been picked up very early on in the eastern part of Germany with a first book publication in German language in 1976 (Gruhn et al., 1976). The PSE series of conferences has been established in 1982 with a first event in Tokyo (Japan) and follow-up conferences in Cambridge (United Kingdom, 1985), Sydney (Australia, 1988), Montebello (Canada, 1991), Kyong-ju (Korea, 1994), Trondheim (Norway, 1997), Keystone (USA, 2000), Kunming (China, 2003) and Garmisch-Partenkirchen (Germany, 2006). Related conference series are the European Symposia of Computer-Aided Process Engineering (ESCAPE) with general emphasis on computer-applications in process engineering and the International Conferences on Foundations of Computer-Aided Process Design (FOCAPD), Foundations of Computer-Aided Process Operations (FOCAPO) and on Chemical Process Control (CPC) focusing on design, operations and control, respectively.

The appreciation of PSE as an independent scientific discipline also becomes apparent in the dedicated centres of excellence which have been established at universities and in industry. For example, the Centre for Process Systems Engineering has been established at Imperial College, London, in 1990 to promote and focus research in PSE in one central location in the United Kingdom, while the Lehrstuhl für Prozesstechnik has been founded at RWTH Aachen University in 1992 by a joint initiative of industry and academia to broaden the scientific base of this field in Germany. Many chemical companies started their own R&D activities focusing on process flowsheeting software during the late 1970s and the

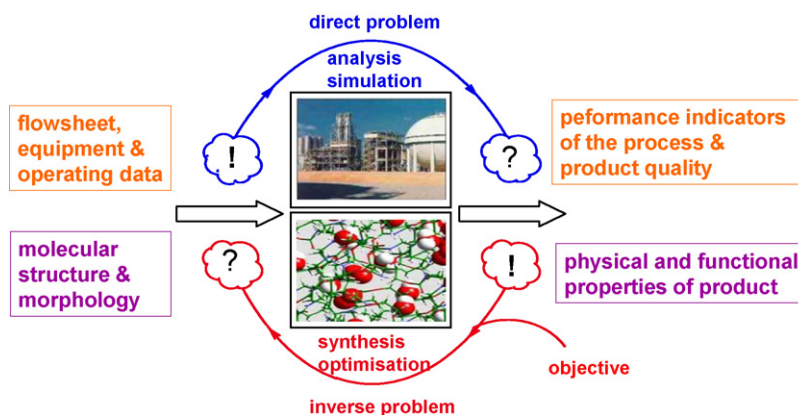


Fig. 3. Model-based product or process design.

1980s (Marquardt, 1999) and extended their attention later to more general PSE topics. For example, a department “Systemverfahrenstechnik” (Process Systems Engineering) has been established at Bayer AG in 1992.

There are two major paradigms in PSE – analysis and synthesis – which are schematically depicted and illustrated from a product as well as from a process perspective in Fig. 3. Both paradigms assume the availability of a suitable process or product model (cf. centre of Fig. 3) which describes either the behaviour of the process or the properties of the product. The *direct* or *analysis problem* assumes that the process flowsheet, the equipment and operating data (or the molecular structure and morphology) are given. The model is then used to predict the performance indicators of the process and the structural, morphological and functional properties of the product by means of simulation studies. If – in contrast – the specifications are given as process performance indicators (or as physical properties of the products) the *inverse* or *synthesis problem* has to be solved either by a search in the space of the decision variables by means of repetitive simulation or by rigorous numerical optimization algorithms which automate the search for the best alternative.

Modeling, simulation and optimization (MSO) of large-scale (product or process) systems is a core technology to deal with the complexity and connectivity of chemical processes and their products on multiple scales (Grossmann & Westerberg, 2000; Pantelides, 2001). These technologies have to be implemented into easy-to-use software systems to render them accessible to problem solving practitioners. The systematic (explicit or implicit) generation and evaluation of a comprehensive set of design alternatives is considered to be a key to success. Integration of different problem formulations in the lifecycle and across multiple scales of chemical, spatial and temporal resolution is desirable to drive a design to a true optimum (Marquardt, von Wedel, & Bayer, 2000). This attempt for integration links PSE tightly with its traditional focus on complete plants to both, *process intensification* (Moulijn, Stankiewicz, Grievink, & Gorak, 2008) and to *chemical product design* (Gani, 2004). While the meso-scale kinetic phenomena are systematically exploited to develop compact, highly efficient and multi-functional equipment, product design aims at a quantitative understanding of the micro-scale molecular phenomena to tailor chemicals, materials, fuels and the like to display desired properties in some context of application. Model-based process control and operations (Edgar, 2004; Ydstie, 2002) as well as supply chain and enterprise-wide optimization (Grossmann, 2004; Varma, Reklaitis, Blau, & Pekny, 2007) together with their links to information technology, to operations research and management sciences complement the various research tracks of PSE. PSE is obviously a cross-sectional topic form-

ing the interface of chemical engineering to mathematics, computer science, management science and economics.

### 3. The past and present

This section will give a short and selective overview on the past and present of PSE. We distinguish the achievements in the research community on the one and in industrial practice on the other hand. It is not possible to adequately acknowledge the contributions of the many successful PSE researchers but limit ourselves to a few representative publications.

#### 3.1. Early research efforts

The early years of academic research in the 1950s and 1960s have been largely focused on mathematical modeling, simulation and optimization to design selected unit operations. These early works have been exemplarily exploring the potential of mathematical analysis and numerical algorithms implemented on a computer to deal with the mathematical complexity of the nonlinear and fairly large process models. Emphasis has been on individual unit operations like adsorption (Acrivos, 1956; Amundson, 1948), distillation (Acrivos & Amundson, 1953; Amundson & Pontinen, 1958; Mah, Michaelson, & Sargent, 1962) or chemical reactors (Aris, 1960; Blakemore & Aris, 1962; Davidson & Shah, 1965; Gilles & Hofmann, 1961; Youle, 1961) but also on complete processes (Brambilla, Diforino, Celati, Kardasz, & Nardini, 1971; Frank & Lapidus, 1966). The models were surprisingly sophisticated and covered spatially (Gilles, Lubeck, & Zeitz, 1970) as well as substantially (Valentas & Amundson, 1968; Zeman & Amundson, 1965) distributed systems. These and other early results on modeling, mathematical and simulation-based analysis and optimization not only revealed a more profound understanding of these processes but also demonstrated the opportunities of employing mathematical concepts and algorithms in chemical engineering problem solving. These new methods have been recognized to help substituting crude design heuristics and avoiding time-consuming manual calculation procedures. Considering the very limited capabilities of analogue or digital computers at the time, the lack of understanding of process modeling and the non-existence of modeling languages and simulation tools, those early applications were extremely ambitious and in many cases far ahead of time.

#### 3.2. Recent progress in academic research and development

Research has been developing along many lines. A very recent and quite comprehensive monograph edited by Puigjaner



and Heyen (2006) documents important research areas and the progress made.

Most importantly, methods at the interface to mathematics and computer science have been (further) developed and tailored to satisfy the needs of process systems problem solving. Mathematical modeling, numerical algorithms and a variety of software tools have been emerging. Scalability of all these methods, algorithms and tools to large-scale process systems has always been an important issue since the quality of a design crucially depends on the choice of the system boundary. This choice has to be controlled by the degree of interaction between subsystems rather than by the capabilities of methods and tools in dealing with problem complexity. In the first phase of research, the scope of a unit operation has been widened to whole processes; later the site and even the supply chain have been covered in addition.

The scope has not only been widened to cover larger spatial and coarser temporal scales, but also to cover an increasingly higher phenomenological resolution which opens up the spatial and temporal scales towards meso-scale and molecular micro-scale phenomena. Initially only mass and energy balances were considered with the assumption of thermodynamic equilibrium between co-existing phases. Reaction and transport kinetics, particle population dynamics, fluid dynamics and more complicated transport phenomena in complex geometries even with simultaneous chemical reactions and transport across phase interfaces have been gradually added to render the mathematical models more sophisticated. These models have always been used to formulate problems in design, control and operations which rely on these models.

Furthermore, the type of problems studied has been steadily evolving from steady-state and spatially lumped to dynamic and spatially distributed modeling and simulation, from an analysis of some design to systematic methods for process synthesis, from simple monitoring and control to model-based control and real-time optimization, from production planning to supply chain and logistics management. Accordingly, problem formulations have been getting more and more integrated to overcome the potential loss of profit by breaking a system into parts and necessarily neglecting the interactions and interdependencies between the (sub-)systems of the integrated whole—the plant, the Verbund at a site, the whole enterprise or the supply chain spanning several companies and geographical regions. Examples include control-integrated design, integrated product-process design, green designs accounting for all aspects of sustainability, the integration of process, supply chain and market, and last but not least complete life-cycle assessment.

These attempts towards an increased scope of integration also opened up the interfaces of PSE:

- To the natural sciences to extend the scope of phenomena considered from the flowsheet to the molecular level.
- To economics and management sciences to shift the attention from the operation of a single process in isolation to the process as part of its supply chain and even of the global market, and last but not least.
- To mathematics and computer science to keep track of the latest developments in new methodologies, concepts, algorithms and software.

### 3.3. Modeling, simulation and optimization for synthesis and design

The research of the last roughly 50 years has led to a number of areas where a very high level of expertise is available. This is particularly true for steady-state and dynamic modeling of fluid-

phase unit operations and single- as well as multi-phase reactors, of flowsheets of large continuous or batch plants, the Verbund at a site or even the supply chain at varying degree of detail determined by the target application.

Simulations with models comprising some 100,000 to even 1,000,000 algebraic or even differential-algebraic equations, some 10 partial differential-algebraic equations in two space dimensions or a few such equations in three space dimensions are routinely solved today not only by expert users. Though fairly large optimization models can be solved with high-performance numerical algorithms, this technology is not yet widely used by non-experts in chemical engineering research and development.

Expert users solve nonlinear programs with some 100,000 equality constraints, some 100 inequality constraints and some 1000 decision variables, optimal control problems with about 10,000 differential-algebraic constraints, some 10 inequality path or end-point constraints and 10 control variables or even optimization problems with a few PDE constraints in two space dimensions possibly with state constraints with a fairly large number of decision variables. While very large mixed-integer problems with linear constraints and objectives are solved routinely, the solution of nonlinear problems or even of mixed-integer dynamic optimization problems is still a challenge if reasonable sized models need to be tackled. These rough estimates assume deterministic mathematical programming algorithms which only lead to local results. Though there has been significant progress in deterministic algorithms for global optimization in recent years, practically relevant problems can only be solved by means of stochastic methods requiring massive computational resources.

The most important achievements of the PSE research community are related to the development and deployment of mature and reliable methods and tools for steady-state and dynamic modeling, simulation and optimization of processes described by strongly nonlinear large-scale process models. Those methods and tools provide support for design and analysis. They are indispensable in today's industrial practice and have proven to be profitable and reliable in a very broad range of applications (Bausa & Dünnebier, 2006).

Nowadays, in the area of large-scale (petro-)chemical processes, there is no serious process design and development activity in industry not heavily relying on modeling and simulation technology. While the direct model-based solution of the (inverse) process design problem by means of optimization methods (cf. Fig. 3) is more rigorous and exact from a systems engineering point of view, today's industrial practice mainly features a pragmatic solution of the design problem by educated guesses, supported by an iterative solution of the process simulation and an experience-based analysis of the respective simulation results. Process synthesis methodologies relying on rigorous optimization (Grossmann, Caballero, & Yeomans, 2000) are rarely used in industrial practice. This statement even holds for special cases such as heat exchanger network design or distillation column sequencing and design but even more for the treatment of integrated processes.

Despite significant achievements and numerous success stories in the field of model-based process design and development, some limitations still exist from the practitioner's point of view. For example, we still have no adequate modeling and simulation methods and tools to deal with solids and biotechnological processes, to efficiently formulate very large-scale models and design problems, or to document, maintain and reuse models across the lifecycle of the plant in an efficient and economical way. A further challenge in the area of modeling and simulation is to properly and efficiently match models and their parameters to lab- or pilot-scale experiments and to existing production plants, accordingly.

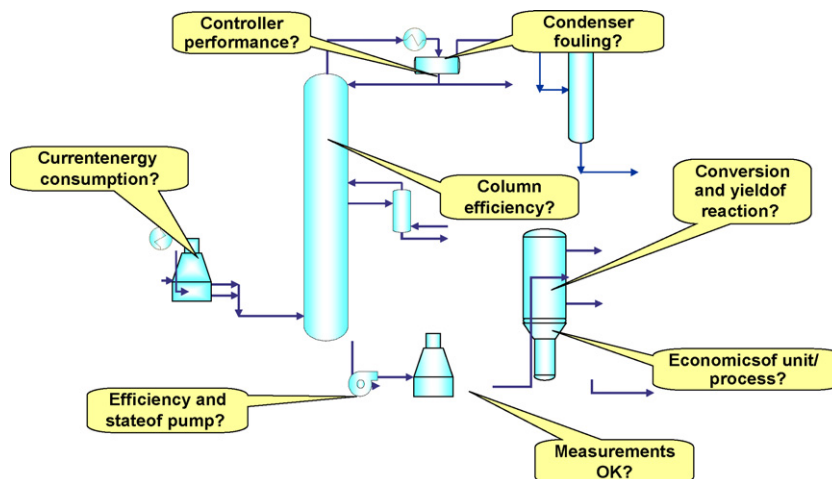


Fig. 4. Typical key performance indicators of a process.

### 3.4. Process control and operations

A very successful application of PSE methods and tools in industrial practice is the implementation and utilization of performance monitoring systems (see e.g. Bamberg et al., 2002; Dünnebier & vom Felde, 2003; Qin, 1998; Soderstrom, Edgar, Russo, & Young, 2000). Here, on-line process data, process models and engineering knowledge are combined to assess the actual process status by calculation, visualization, and monitoring of so-called key performance indicators (KPI). A selection of typical process KPI is shown in Fig. 4.

The methods and tools for the calculation of the respective KPI range from purely data driven approaches to completely rigorous modeling based on first principles (cf. Fig. 5). In this context, so-called hybrid models (Agarwal, 1997; Mogk, Mrziglod, & Schuppert, 2002; Schuppert, 2000) got increasing attention in recent years. Regardless of the utilized approach, the crucial factors for successful performance monitoring applications are the identification of the economically relevant KPI and tailor-made monitoring concepts for the specific process and plant. PSE methods and insights are indispensable to address these problems.

Significant progress has also been made in control and operations. Model-based predictive control (Qin & Badgwell, 2003) and real-time optimization (Marlin & Hrymak, 1997) have reached a reasonable level of maturity. Commercial linear model predictive control packages forged ahead and resulted in numerous practical applications. These methods are nowadays more or less standard

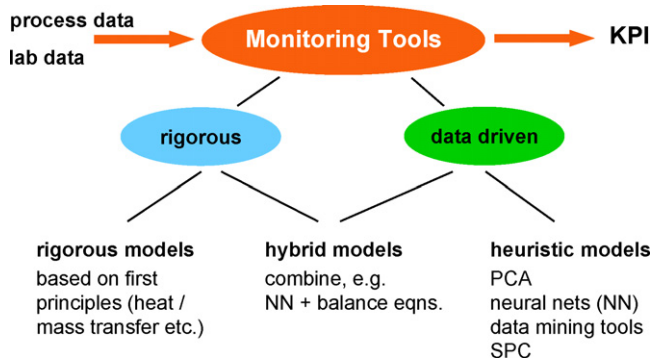


Fig. 5. Performance monitoring methods and tools (KPI = key performance indicator; NN = neural nets; PCA = principal component analysis; SPC = statistical process control).

for advanced control in the petrochemical industries. In contrast, nonlinear model predictive control and real-time dynamic optimization (Binder et al., 2001) has indeed been a very active area in academic research but still is on the fringes in industrial practice.

There are numerous examples for the successful application of modern control techniques in industrial practice and a comprehensive review of those would go far beyond the scope of this contribution. A very impressive and economically very attractive example is the combination of model-based control with modern online analytics (Dünnebier & Bamberg, 2004). Fig. 6 sketches the application of such a concept to the concentration control of a distillation column, separating an isomeric mixture. Here, the close boiling points require inline concentration measurements by near infrared spectroscopy, because the temperature sensitivity is not sufficient for the realization of a properly working advanced control system. The proposed combination results in a very reliable and robust control system for this application on the one hand and short payback times and a high economic impact on the other hand.

The consistent improvement in the area of dynamic process simulation and the steadily increasing computational power gave rise to the increasing use of *operator training simulators* (OTS) in the chemical and petrochemical industry in recent years (Schaich & Friedrich, 2004). A detailed dynamic simulation model of the plant, covering not only the standard operational regime but also start-up and shut-down as well as other extreme operating situations (e.g. caused by equipment malfunctions and/or operating errors), is connected to an emulation of the original process control system and a trainer station. Beyond its use as a training tool, an OTS is the ideal platform for testing and improving the control system, developing and assessing advanced control strategies, and analyzing any malfunctions of the process response. Furthermore, the optimization of the process design and its operation can be significantly supported by an OTS. The integration of an OTS system and an advanced process control system has proven to be extremely beneficial for the commissioning and start-up of new plants. Several successful projects show that both start-up time and start-up errors can thus be reduced significantly. Similar industrial experience has been recently reported by Cox, Smith, and Dimitratos (2006).

While on the one hand production units often become more integrated but on the other hand the whole production process including the supply chain becomes more and more complex and networked due to today's dynamic business environment, production planning and management including the coverage of complex logistics is a matter of particular interest and in an advanced state of

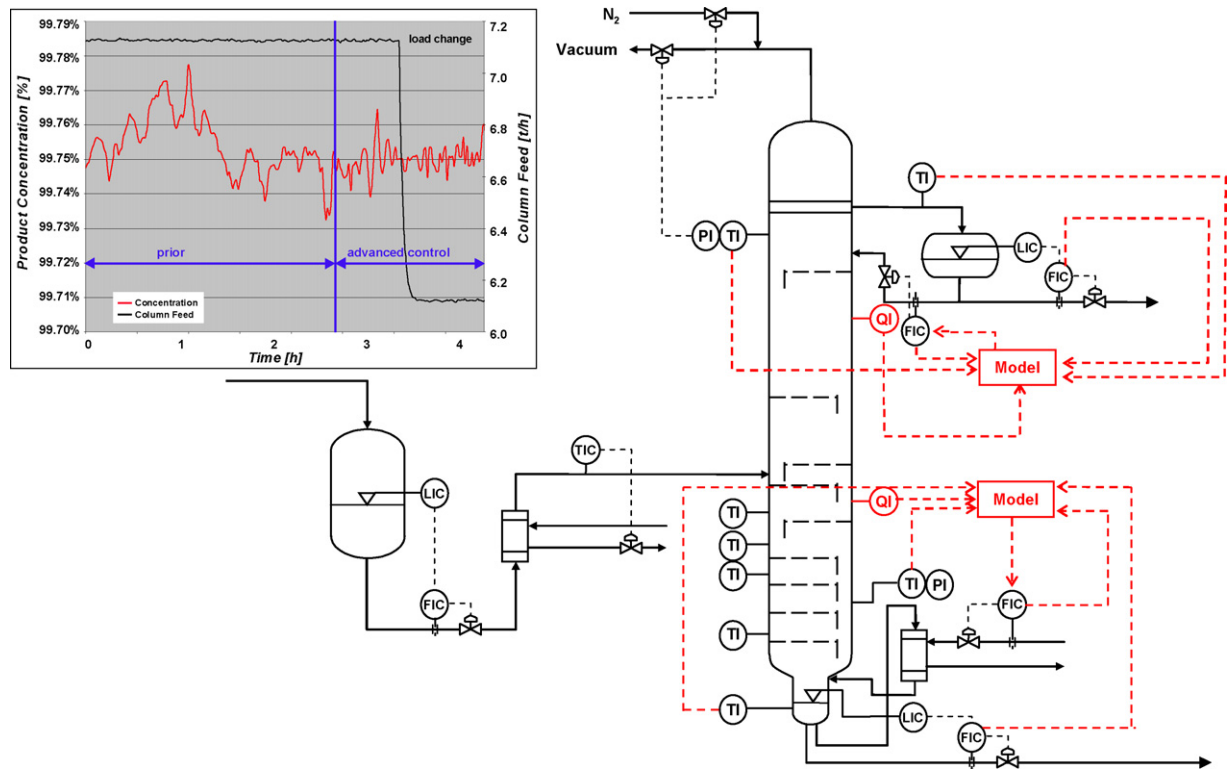


Fig. 6. Advanced concentration control for a distillation column.

development. However, there are many more open issues in control and operations than in design from an industrial perspective.

### 3.5. Actual shortcomings and open issues

Most of the PSE methodologies and computational methods have not been developed without a concrete application-oriented objective. A variety of sophisticated methodologies have been suggested which link problem formulation, modeling and computational methods to a problem solving strategy which results in high quality solutions at limited engineering effort. However, these PSE methodologies have unfortunately not penetrated industrial practice to the extent possible. This is largely due to a lack of commercial software which packages these methodologies into user-friendly tools which are easily accessible to the industrial practitioner on a steep learning curve. For example, the integration of design and control is a crucial issue for process development and operation, both from a technical and an economic perspective. State of the art approaches either employ controllability measures or rigorous model-based optimization techniques (see Sakizlis, Perkins, & Pistikopoulos, 2004 for a survey or Chawankul, Sandoval, Budman, and Douglas, 2007; Gerhard, Marquardt, and Mönnigmann, 2008; Grosch, Mönnigmann, and Marquardt, 2008 for more recent approaches). None of them has actually penetrated into industrial practice to a reasonable extent, because they are either limited to a specific problem class (e.g. continuous processes, linear models), or because the available methodologies result in complex problems the solution of which requires excessive computational effort. In any case, though limited in coverage, the proper application of the methods proposed in the literature requires a systems engineering skill level which is typically not prevalent among industrial practitioners.

Despite the numerous successful applications of PSE methods and tools in industrial practice, it is still a challenge in many cases

to realize economically attractive projects with model-based applications using currently available methods and tools, which have to offer short pay-out times to successfully compete with other projects. PSE applications in the process industry are often unique. Thus, they are like a tailor-made suit and costs usually cannot be cut down by quantity. Obviously, the main driver for industrial application is not only the mere existence of a certain problem solving method in academia, but also the availability of these technologies in robust software tools and more importantly its profitability in routine industrial problem solving. Unfortunately, PSE methods and solutions often are considered to be just “nice-to-have” and not to be essential for stable and economic production. In addition, the benefit of their application is usually difficult to quantify in exact numbers. The systems thinking and holistic problem treatment of PSE is clearly one of its greatest advantages. Thus, PSE experts often integrate many disciplines and solution approaches within a certain process optimization project and contribute significantly to the feasibility and economics of a plant design, but it is quite difficult to allocate, e.g. exact cost savings to the application of a certain PSE methodology or tool.

Maintenance and sustainability of PSE applications is not for free and often a problematic issue. This aspect has rarely been addressed so far both in academic development and in industrial practice, but is of utmost importance in order to guarantee the economic efficiency of the implementation in the longer range.

Current research and development concentrates on application areas with high profitability, in particular on large-scale, continuous production processes. The extension to small-scale and often multi-purpose production facilities has yet not been successfully established, but is absolutely essential for ensuring reasonable development and payback times and for tapping the full potential of PSE in the life science area. For example, the paradigm shift initiated by the PAT initiative of the US Food and Drug Administration (FDA) forces the pharmaceutical manufacturers to ensure

final product quality by timely measurement and control of critical quality and performance parameters. Dünnebiel and Tups (2007) have shown that industry has accepted this challenge and that PSE methods and solutions can make a substantial contribution.

#### 4. The future

There are a number of emerging fields in PSE which are already under investigation and which are considered to be of high future industrial relevance, though the fundamental problem of transferring research results into industrial work processes and computing infrastructure will remain. We first focus on new PSE methodologies and then move on to challenging and rewarding fields of application which currently are emerging. Obviously, the covered topics represent the background and experience of the authors and should not be considered a comprehensive set.

##### 4.1. PSE methodologies

###### 4.1.1. Multi-scale modeling in the design lifecycle

While MSO technology has been focusing traditionally on the scale of the unit and above, the integration of process, equipment and product design requires a unifying modeling approach spanning all the scales from the molecular micro-scale to the mega-scale of a site during all phases of the design lifecycle (Marquardt et al., 2000). A straightforward approach to multi-scale modeling (Vlachos, 2005) is the computation of some desired information on a finer scale to pass it to a coarser scale or vice versa. More sophisticated settings integrate multi-scale models to resolve the level of detail where needed and at the same time limiting the computational effort (Pantelides, 2001). By traversing the scales, not only the number and type of degrees of freedom typically change but also a switch in the modeling paradigm – most notably from the continuum to some particle paradigm – is typically involved. The ultimate objective of multi-scale modeling is the development of the skills for predictive “ab initio” modeling in combination with a set of systematic methods for model reduction. This way, information obtained on small scales can be systematically transferred to coarser scales to bridge the scales in a single multi-scale model or in a sequence of single-scale models employed in different tasks during the design lifecycle. Obviously, the documentation and reuse of models along the design lifecycle is a closely related issue (Eggersmann, von Wedel, & Marquardt, 2004). Such techniques have to be incorporated in computer-aided modeling tools which are tailored to the requirements of multi-scale modeling (Yang, Morbach, & Marquardt, 2004).

###### 4.1.2. Linking experiments to models

Modeling does not only involve the formulation and solution of the set of model equations but also the identification of the model structure and the model parameters from experiments either on the plant-, pilot- or lab-scale. Such models are typically of a hybrid nature since ab initio modeling is hardly possible. Though desirable, the true physical mechanisms are only captured in part depending on the requirements resulting from the scope of model application on the one and the availability of experimental data for model fitting and validation on the other hand. The modeling of the measuring instrument for improved calibration to transform the measured data into physically meaningful quantities has to be addressed in particular in the context of high-resolution measurements (such as focused beam reflectance measurement (FBRM) probes for monitoring of particulate systems, nuclear magnetic resonance (NMR) imaging or near infrared and Raman spectroscopy

on a line) aiming at the discovery and discrimination of competing mechanistic models. Systems engineering methods including the model-based design of experiments can be favorably applied to obtain valid models at minimum experimental effort (Marquardt, 2005).

###### 4.1.3. Sustainable process synthesis

Optimization-based process synthesis (Grossmann et al., 2000), though a classical topic of PSE, has not received sufficient attention in an industrial environment. Educated guesses and intensive simulation studies still dominate industrial practice. Easy to use model-based process synthesis methodologies, not only for large-scale continuous plants but also for small-scale batch plants and even for continuous micro-plants, could make a tremendous difference in lifecycle cost. Such methods not only have to support the generation and evaluation of an enormous number of alternative process structures but should also facilitate the integration of engineering experience, the support of multi-objective decision-making to reconcile the conflicting objectives of sustainability (Bakshi & Fiksel, 2003), and the systematic management of risk and uncertainty. The synthesis problem formulation has to cover all the significant steps including the market-driven specification of desired product properties (and thus links process to product design and vice versa), the identification of favourable (catalytic) reaction pathways, the invention of possible process alternatives, the screening for attractive process alternatives, conceptual equipment design, equipment sizing and the decision on favourable operational strategies. Such a framework has to explicitly cover continuous, macro- and micro-scale, dedicated and multi-purpose plants as well as batch plants which require very different synthesis strategies in order to respond to the trend towards a large variety of specialized low volume products and more and more complex chemistries. It is very unlikely that a single integrated problem formulation can be found which on the one hand covers all possible alternatives in a superstructure and is still computationally tractable on the other hand. Rather a systematic work process with a gradual refinement of the design specifications in combination with an increasing level of detail in the model used to reflect the increasing level of confidence in the prior knowledge is expected to be more promising. Such a work process can be designed to facilitate a step-wise construction of a superstructure and a systematic initialization of rigorous optimization-based synthesis methods (see Marquardt, Kossack, & Krämer, 2008, for a related attempt).

###### 4.1.4. Equipment synthesis and design

Multi-functional units, micro-reactors and plants can benefit from MSO technologies applied to the meso-scale to achieve process intensification (Keil, 2007). Partial differential equation models dominate these scales and contribute to complexity. A prominent example is the analysis of mixing processes by means of computational fluid dynamics. While modeling and repetitive simulation studies are currently used to support the invention process (the direct approach to design, cf. Fig. 3), there is significant scope for the development of optimization-based methods which solve the inverse design problem directly. This approach to the design of multi-functional units leads to demanding optimization problems with PDE constraints. Besides the usual operational degrees of freedom the arrangement of subunits and their geometric design are subject to optimization adding a combinatorial component to the problem formulation. Obviously, such an approach will give rise to extremely challenging mathematical problems. An active research community has already formed addressing related so-called “shape optimization” (e.g. Bendsoe & Sigmund, 2003) and “topology optimization” (e.g. Haslinger & Mäkinen, 2003) problems



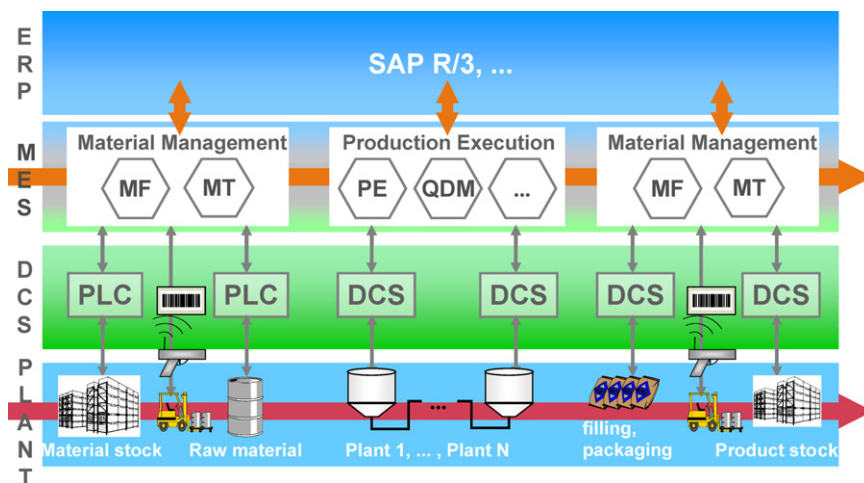


Fig. 7. Horizontally and vertically integrated production management (ERP = enterprise resource planning; MES = manufacturing execution system; DCS = distributed control system; PLC = programmable logic controller; MF = material flow; MT = material tracking; PE = production execution; QDM = quality data management).

in computational mechanics with applications in fluid dynamics, acoustics and materials processing.

#### 4.1.5. Process operations and management

In industry, there is a distinct shift in focus from controlling a process plant in isolation towards an agile management of a process plant as an integral part of the global supply chain comprising a number of enterprises in different geographical locations. While classical process control aims at attenuating disturbances and maintaining the plant at its desired steady-state, future process operations will have to exploit the dynamics of the environment – most notably caused by changing market conditions – by means of model-based optimization techniques (Backx et al., 1998). They have to integrate vertically across the automation hierarchy of a single process plant and horizontally along the supply chain (Ydstie, 2002) connecting various plants by material and information flows (Fig. 7). The objective of plant operation is hence moving from controlling the plant at its set-point to maximizing its economics in real-time subject to equipment, safety and product related constraints (Engell, 2007; Helbig, Abel, & Marquardt, 2000; Kadam & Marquardt, 2007). Obviously, such a forward looking understanding of process operations sheds new light on the integration of designing the process and its associated operational support system including control, optimization and scheduling functionalities (Shobrys & White, 2002). Only such an integrative approach – even accounting for the role of the operating personnel – can guarantee a fully functional and economically optimally operated process plant operated at its economical optimum in nominal as well as exceptional operating regimes (Schuler, 1998). This definitely has to be taken into account when prospectively setting up practicable methods and tools for optimal integration of process design and process operation. A mere optimization of (linear) controller structure and parameters will by no means be sufficient. Asset management and maintenance are as well emerging topics of high industrial relevance which have not yet gained sufficient attention in academic research.

#### 4.1.6. Information technology (IT) support of engineering design and development processes

Understanding and managing design processes is at the heart of systems engineering research and practice (Braha & Maimon, 1997). Despite the fact that this topic has been brought up in PSE quite some time ago (Westerberg et al., 1997), only little activity

has been observed in academia despite the tremendous opportunities and enormous potential for cost reduction and quality improvement in industrial design processes. An integrated view on the design process in the various lifecycle phases together with IT methods and tools for its support have been the focus of the IMPROVE project at RWTH Aachen University (Marquardt & Nagl, 2004; Nagl & Marquardt, 2008). The focus of this research has been on the modeling of creative, multi-disciplinary, organizationally and geographically distributed work processes in chemical engineering and the development of novel, work-process centered support functionality which integrates existing engineering design tools in a posteriori fashion. The better understanding, structuring and even modeling of design processes is not only a prerequisite for the conceptual design and implementation of design support software, but also helps to identify the gaps between industrial practice and research efforts on PSE methodologies. A new generation of cost-effective and tailor-made supporting software solutions is suggested which reflect the culture and the specific work processes of an enterprise. Semantic technologies seem to offer an attractive platform for knowledge capturing, information management and work process guidance (Brandt et al., 2008) in the design processes including their associated control and operating support systems. They also support a smooth integration of information modeling and mathematical modeling in a single modeling framework. Such technologies have to be integrated with existing PSE tools and with the IT environment of an enterprise to have a chance to be adopted by industrial practice. Such support functionality is not only restricted to process design but can also be adopted to product design and manufacturing (cf. Venkatasubramanian et al., 2006).

#### 4.1.7. Numerical algorithms and computing paradigms

The solution of complex models will remain one of the major areas of activity in PSE. The size of models for simulation as well as optimization applications will steadily grow without seeing any saturation. Particularly challenging are the requirements on numerical algorithms if multi-scale behavior is displayed by the model. Local mesh refinement and suitable adaptation strategies are indispensable in such cases. There is still much room for improvement, in particular, with respect to optimization algorithms, to effectively deal with nonlinearity, integer variables and (partial) differential equation constraints (Grossmann & Biegler, 2004). It remains an interesting question whether the currently favored simultane-

ous approach will be complemented by suitable modular methods (Grund, Ehrhardt, Borchardt, & Horn, 2003) which even take advantage of distributed and parallel computing architectures. Such a strategy would also support the use of multiple numerical methods tailored to the requirements of a partial model which may comprise a special structure of a selection of algebraic, differential, partial differential or integro-differential equations. Run-time integration platforms like Cheops (Schopfer, Yang, von Wedel, & Marquardt, 2004) or agent-based technologies (Sirola, Hauan, & Westerberg, 2004) are promising directions.

#### 4.2. Emerging application domains

While the research in PSE has been focusing on novel methods and tools, there are challenging emerging fields of application. Reaching out into new application domains is rewarding in two ways. Firstly, PSE offers a powerful set of methods and tools for systems problem solving in all those domains which share a lot in common with chemical engineering though they are not considered to be part of this field. Such domains are characterized by interacting transport phenomena in complex systems constituting of non-trivially interacting subsystems. Secondly, the transfer of methods and tools from one domain to another typically reveals new requirements which have not been faced yet. Hence, the migration of PSE methods and tools to another domain requires at least the tailoring of existing or even the development of completely new methods and tools to address the specific problems of the new domain in an effective way. Hence, reaching out to novel areas of application can be considered a necessity in order to avoid getting trapped in marginal improvements of existing PSE methods and tools. We will point out a few of those emerging application domains for the sake of illustration.

##### 4.2.1. Small-scale production

PSE has been largely focusing on methods and tools for design, control and operation of large-scale chemical processes operated in continuous mode. The scale of operation and consequently the potential economical benefit of optimized designs and operational strategies justify demanding modeling projects and costly implementations of model-based applications. PSE methods and tools have largely been focusing on this problem class in the past. However, there is a well-known trend towards small-scale, flexible production in multi-purpose plants in particular in the highly developed countries. Often, the mini-plant used for product development serves as the production plant. Even disposable units for batch processing are under investigation in the pharmaceutical industries to reduce cost and to avoid costly cleaning procedures. The variety of chemistries and the low volumes do not allow for expensive modeling studies. Model development and exploitation has to accompany process development and manufacturing following an incremental model refinement and process improvement strategy. Novel modeling strategies and tailored model-based methodologies and applications – possibly radically different from existing problem solving techniques – seem to be indispensable for this class of problems to facilitate economically attractive model-based methodologies.

##### 4.2.2. Integrated micro-plants

Micro-reaction technologies have been steadily maturing in recent years (Ehrfeld, Hessel, & Lehr, 2000). A tremendous effort is being spent to develop industrial strength solutions for continuous multi-product or dedicated micro-plants not only aiming at the production of low-volume and high-price specialty chemicals but also of bulk intermediate chemicals with interesting market perspectives (Pieters, Andrieux, & Eloy, 2007). The dis-

tributed nature of the required process models, physico-chemical phenomena only emerging or becoming dominant in micro-plants as well as numbering-up rather than scaling-up of production facilities to larger capacity will call for extended modeling capabilities and for novel methods and tools for design as well as operation (Kano, Fujioka, Tonomura, Hasebe, & Noda, 2007). Furthermore, microchemical systems are interesting discovery tools (Jensen, 2006) which offer completely new possibilities of data acquisition. Together with high throughput strategies new paradigms for reaction pathway synthesis and product design are possible. PSE methods can contribute in the management and model-based processing of the immense amounts of data.

##### 4.2.3. Processing of renewable feed stocks

There is a common understanding that the chemical and petroleum industries will have to switch from oil and gas carbon and hydrogen sources to alternative raw materials sooner or later. Most likely, the processing of coal to synthesis gas will see a revival in the near future at least in some parts of the world. However, in the longer run, the exploitation of renewable resources will face increasing interest. Solar powered thermochemical or electrical water decomposition is a potential green hydrogen source. The processing of lignocelluloses from biomass feed stocks into platform chemicals (Corma, Iborra, & Velty, 2007) or automotive fuels (Huber, Iborra, & Corma, 2006) – preferably without competing with the food chain – is another challenge which will come up in the next decades. Novel large-scale processes will have to be developed. They will have to deal with an enormous variety of bio-renewable feedstock, new classes of chemical substances with multi-functional molecular structure, new chemical and bio-chemical pathways and with new intensified processing technologies. PSE is expected to significantly contribute to efficient development processes resulting in environmentally benign, economically attractive, and sustainable manufacturing processes.

##### 4.2.4. Infrastructure systems

Infrastructure systems comprise water and energy supply networks, waste processing including the recycling of valuable materials, transportation systems for people and goods and telecommunication systems. Infrastructure systems link the industrial with the domestic sector. The complexity of such systems, in particular in urban centers has reached a critical level which calls for systematic analysis and synthesis methods to establish proper functioning even in anomalous situations such as the recent collapses of a part of the electrical network in Europe and the US. The design and the management of active grids of interconnected infrastructure components of different kinds which adapt to supply and demand is a rewarding problem for process systems engineers (Herder, Turk, Subramanian, & Westerberg, 2000). Though infrastructure system improvement and design has a lot in common with the design of agile supply chains and their embedded process plants, there is the socio-economical dimension in addition to the technical dimension which calls for tailored methods and tools.

##### 4.2.5. Particulate and nano-structured products

Particulate or nano-structured products such as carbon nanotubes, nano-particle additives, catalysts, nano-scale functionalized surfaces or nano-composite materials – although completely different in nature – also require the tailoring of PSE methods and tools (see e.g. Fung and Ng, 2003 for an attempt in pharmaceutical product-process engineering). A first challenge is the modeling of the product and its properties which has to go well beyond chemical composition, but must also cover shape and morphology.

Structure–property relations, though useful to describe the function of the product in an application, should be enhanced to incorporate a priori knowledge in the sense of hybrid modeling. The relation between the characteristic product properties and the processing conditions need to be understood. Multi-scale modeling – with particular emphasis on the molecular level – and novel PSE methods and tools employing such multi-scale models are still missing to a large extent.

#### 4.2.6. Functional products

The chemical industries have been largely focusing on fluidic or particulate intermediate products. In recent years, a number of chemical companies have been reshaping the product portfolio to cover functional end-products often showing a high level of complexity in the systems engineering sense. Examples include lab-on-the-chip technologies for medical diagnosis, the electronic book, fuel cells, or battery systems. The design and development of such functional products resemble to some extent the design and development of manufacturing plants. However, conceptual and equipment design including geometry and layout have to be often considered at the same time. PSE methods and tools can be favorably migrated and adapted to effectively address these kinds of design problems (Mitsos, Hencke, & Barton, 2005; Pfeiffer, Mukherjee, & Huan, 2004).

#### 4.2.7. Systems biology

The complexity of living systems can only be understood if experimental research is complemented by modeling and simulation (Tomita, 2001). Furthermore, similar to a model of a chemical process system, a model of the cell (or any part of a living system) can become the repository for the shared knowledge to make it widely accessible and easy to interpret. An excellent review from a control systems engineering perspective on the modeling and control opportunities and challenges has been given recently by Wellstead (2007). The skills of PSE in modeling, analysis and design can play an instrumental role in all areas of systems biology including protein design, metabolism, cell signaling, physiology and systems medicine. The latter is particularly interesting from an industrial perspective. The business of the pharmaceutical companies has been changing in recent times. Rather than discovering and manufacturing an active agent which is part of a relatively simple tablet or capsule, the market calls for complete diagnostic and therapeutic, personalized solutions. Diagnostic systems include sophisticated devices including array, biochip, biomarker and enzyme technologies to assess the status of the patient in an impressive level of detail. Modeling and simulation of the human body on multiple scales provides the information necessary to develop highly efficient therapy strategies which aim at providing the active agent in the desired level of concentration right at the biological target such as a tumor by appropriate dosing strategies. A further advantage of these models is the potential reduction of the expense for clinical trials as well as minimization of their risks. Successful therapeutic strategies require multi-scale modeling of the metabolism on the level of cell, the organs and the complete human body on the one hand and the drug delivery and dosing systems on the other. The design of such therapeutic and diagnostic systems shares all the interesting features of process systems problem solving. It offers a plethora of interesting systems problems which should be amenable to PSE methods and tools after appropriate tailoring.

#### 4.3. Industrial expectations

The topics discussed in the previous subsection are of vital interest to the chemical industries not only to improve competitive-

ness and increase profitability of their core businesses, but also to reshape their product portfolio and to facilitate product and process innovations in new markets.

Regardless the particular processes and products, it is of utmost importance for the further industrial success of PSE and its methodologies and tools that the economic impact and advantages become obvious at first glance. Most plant and production managers are only willing to support long-term projects if they get at least some benefit rather quickly. Thus, we need more modern, easy to apply computer-based methods and tools to pick the low hanging fruits. This would also be helpful to establish the PSE methodologies and tools in areas which are today dominated by “barebone-engineering” (e.g. 1st generation biofuel plants).

The PSE community has to pay more attention to the industrial end user’s common opinion. From this point of view, too much incremental improvement with no or little practical impact has been published. Even if this may not really apply, it is alarming that this impression occurs. Furthermore, one should be careful to promise too much too early, e.g. in the field of mixed-integer non-linear programming (MINLP), many companies tried early (say in the late 1980) and failed, which gave a bad reputation for the whole field.

The model-based PSE methodologies both have to be enhanced further and made available to a larger number of users. Especially the new fields of application require at least in parts a fundamental adaptation of the methods and tools. We do not expect that the methods and tools established in the area of large-scale continuous production of bulk chemicals and commodities can simply be transferred to the life science area. Here, customized solutions for batch processes, small-scale productions and multi-purpose plants are needed, which result in reasonable payback times. Undoubtedly, no quick success will be possible but long-term research is necessary. The history shows that many PSE results take more than 30 years to be adopted by industry, if at all. This is definitely much too long in view of the brevity of today’s economic cycles and the constant pressure to reduce time to market. To be successful on this way, industry has to be kept interested in research on the one hand, but has to show a certain degree of patience and confidence on the other. During this process, academic researchers have to shape their focus in close cooperation with industry, try to shorten the development times, and, of particular importance, aim at establishing computer-based PSE tools which are easy to apply in industrial practice. So far, no clear trend can be seen whether fully integrated tool suites or specialized solutions are more beneficial, and if a more generic solution approach is preferable over a more specific one. This strongly depends on the problem characteristics and the application area as well. In any case, the time and effort spent until economic benefits are visible have to be kept as small as possible for the development of new PSE methods and tools because we expect that the pressure to succeed on the industrial users and sponsors will even increase in the foreseeable future.

### 5. Towards a sustainable strategy for the future of PSE

The reflection on PSE subject areas has shown that the scope has widened since the early days and that it will continue to widen in the future. There is the obvious risk that a widening scope ultimately results in a diffuse profile of the discipline. Hence, it might get more and more difficult to define the boundaries and the essential core of expertise of PSE. Consequently, a reassessment of the essential core and the boundaries is mandatory if PSE does not want to risk losing its appeal (Sargent, 2004). The necessity of such a reassessment does not come as a surprise, has it been progressing for quite some time in chemical engineering itself (Denn, 1991).

### 5.1. Where are we?

The core competence of PSE has been undoubtedly related to modeling, simulation and optimization (MSO) methods and tools and their application to the analysis and design as well as to automation and control of single pieces of equipment as well as of largely continuous complete processes. However, we still have to admit serious limitations of the latest research results on PSE technologies, when it comes to a routine industrial application of model-based problem solving in the design lifecycle.

The further development and the application of PSE technologies are not anymore restricted to PSE experts. In particular, the application of modeling and simulation methods and tools has not only become an integral part of problem solving in all segments of the process industries, but it is also considered to be one of the indispensable tools to routinely assist and accelerate the research process in all chemical engineering disciplines. Undoubtedly, there is a marked difference in the level of professional competence in MSO of both industrial practitioners and academic researchers on the one and PSE experts on the other hand. However, it is often not easy for the PSE experts to convince their colleagues on the value their expertise can bring to the problem solving process. Rather, than solving a given problem cheaper and faster, PSE experts have to show their competencies in enabling radically different innovative products and processes.

Furthermore, research on novel MSO methodologies and tools is not restricted to the PSE community anymore. For example, research on multi-scale modeling, molecular modeling, computational fluid dynamics or logistics and supply chain modeling is carried out by experts who would not consider themselves as process systems engineers. Even worse, most of these researchers would not even know about the core ideas of PSE and the relevance to their research.

### 5.2. Facing the risk

For these reasons, the PSE community is at risk to loose attention and influence in its core area of activity and hence its impact on research and industrial practice. A loss of reputation resulting in a loss of attractiveness to students and young scientists, a loss of interest in industry and last but not least a loss of sources of funding could become consequences if no appropriate action is taken. Such a development seems to be inevitable to the authors, if the PSE community will only focus on the migration of its knowledge into non-traditional application domains which are not yet fully exploited. The following measures are suggested to diminish this risk.

### 5.3. Back to the roots

We need to refocus on the classic PSE topics, most notably modeling and numerical algorithms implemented in robust software tools, integrated product and process design, and last but not least manufacturing process management. The research should concentrate on the foundations of model-based methods. Since models are at the core of any PSE technology, research on modeling methodologies should be of primary interest to our discipline. There are still lots of problems which have been identified in recent years, but where no good solutions are yet available. Examples include lifecycle and multi-scale modeling, product modeling, dealing with complexity, uncertainty and risk, linking experiments to models, sustainable process and supply chain synthesis, supply-chain conscious control and operations, work-process centered IT support of design processes, etc. However, the quality and possible impact of any further development of existing PSE methods or improve-

ment of known methods have to be assessed and implemented in prototypical software tools as part of the research process in academia in order to be credible from an industrial perspective. Unfortunately, this research objective is not well rewarded by the current measures of academic performance, because the building of prototypes requires a lot of resources and does not result in many journal publications.

Systems thinking and the holistic treatment of problems is a sustainable value in itself, well beyond the use of computers on simulation-assisted problem solving employing off-the-shelf commercial tools. The extension of the system boundaries – towards coarser scales to the supply chain and beyond and towards finer scales to the molecular level – is rewarding from the academics' as well as the practitioners' point of view. Such extensions naturally lead to task integration across the product and process lifecycles with new problem formulations and solution methods to successfully address for example the integration of process and control system design, of process and equipment design or product and process design to name just a few examples.

A note of caution seems to be appropriate: the remaining methodological problems are quite tough and need quite long-term engagement, academics have to take up this challenge without aiming at short-term successes and industrialists have to be patient and open-minded towards long-term research efforts oriented to the fundamentals of PSE.

### 5.4. Reaching out

PSE has a strong culture in cross- and trans-disciplinary communication and collaboration. Method development requires PSE to team up with experts in the fundamental scientific disciplines, in particular with experts in mathematics and computer science but also in physics, chemistry and biology, to adopt their latest research results and tailor them to the peculiar requirements in process systems problem solving. On the other hand, PSE experts have to absorb and integrate MSO technologies developed in neighbouring fields (such as computational fluid dynamics, molecular simulation, high-resolution measurement techniques and the like) in the systems tradition to provide the domain experts the tools to address systems problems. PSE should also bridge the gap to established disciplines in engineering and science dealing with systems problems and offer the sensible application of the powerful PSE toolbox to solve the problems of those disciplines. Promising target disciplines can be identified in energy, materials, production and automotive engineering.

There are lot of emerging areas where systems thinking and systems engineering methods and tools are most likely a key to success. The PSE community has to identify such emerging systems problems and exploit its set of skills to make mission critical contributions. Examples include (i) systems biology with applications not only in medicine but also in white biotechnology, (ii) structured and particulate products, (iii) functional (end) products such as e-books, diagnostics, or electronic components and (iv) infrastructure systems including energy, water and waste networks.

Obviously, PSE first has to take the initiative, and next has to raise confidence of the collaborators in its skill set. Often a natural reluctance has to be overcome, until a win-win situation can be proven in a concrete collaborative project. This interaction should also lead to an improved split of work between systems engineers and domain experts to exploit the available expertise in a synergistic manner towards high quality solutions to complex problems of a systems nature. Some of the scientific target areas have been discussed in the last subsection. In all these cases, PSE should not content itself to the role of a scientific service provider but should consider itself a partner to the domain experts who has to offer



a self-contained contribution which is a crucial stepping stone to solve the scientific problem of the domain.

### 5.5. Interaction with industry

The main reason for the commonly addressed gap between industrial practice and academic research seems to be the different scope: while industry mainly focuses on sustainability and profitability, academia aims at scientific progress. It is a challenging task not to let this gap grow but to benefit from this complement. A too large displacement between the industrial and academic perspectives may result in a loss of interest in industry in the research and development activities in PSE and a loss of correspondence to industrial reality in academia. In order to guarantee a sustainable success of PSE in industrial practice, we thus need consistent co-operations between academia and industry.

An important aspect of this co-operation is benchmarking. A new method has to be benchmarked against state-of-the-art best practice both from an economic and technical point of view. Benchmarking of new methods and prototyping of new tools should be done in two stages. First, a few demanding literature problems have to be chosen to demonstrate the advantages of the suggested method compared to the best existing technologies. If this test is successful, an industrial problem should be picked in close collaboration with an industrial partner to demonstrate the value of the method in an industrial setting.

### 5.6. Towards a new paradigm

The future challenges in chemical engineering (Charpentier & McKenna, 2004) are essentially systems problems. PSE can contribute to their solution if it reshapes its profile and readjusts its target of research.

In the first place, we should not any longer afford to have two terms for the same chemical engineering discipline and consequently give up to use either CAPE or PSE depending on the preferences and the personal background of the user. The authors are favouring PSE rather than CAPE and suggest not using the term computer-aided process engineering and the acronym CAPE any longer but completely replace them by process systems engineering and PSE. This choice is not a matter of personal taste. Rather, it is motivated by the more expressive power of the term which clearly emphasizes the systems approach and points explicitly and unambiguously beyond the mere use of computers to solve chemical engineering problems.

The scope of process systems engineering has to be further developed from a systems engineering discipline with a focus on process systems problems on the granularity of a unit, a plant, a site and beyond, grossly simplifying the meso- and micro-scale phenomena, to *multi-scale product and process systems engineering (MPPSE)*, a chemical engineering discipline which bridges the scales and addresses product design, reaction pathway synthesis as well as equipment and process design in an integrated manner linking users' requirements to engineering solutions. Equipment and process design are not restricted to process engineering technology but include all control and operational support systems and even care for the interface to the operator to implement the desired functionality. Such a shift requires a recalibration of the interfaces of PSE to the other sciences; in particular, the interfaces to the natural sciences and to the core disciplines of chemical engineering – probably neglected in the past in favour to the interfaces to mathematics and computer science – have to be re-emphasized.

Functionally integrated process units combining at least two functional objectives in one piece of equipment (e.g. reactive distillation) and intensified process units systematically exploit-

ing meso-scale phenomena (e.g. intensified energy supply by microwaves or ultrasound) are naturally incorporated as subsystems in the complete plant in the spirit of systems engineering. Hence, PSE and *process intensification* (PI) under the roof of MPPSE are faced with a very natural way to establish not only a friendly symbiosis (Moulijn et al., 2008) but also a strong partnership with an increasing impact on the chemical engineering profession. Obviously, this partnership has to be built on the specific strength of the partners, i.e. systems engineering and computational methods for PSE and experimental methods, product orientation and the systematization of invention for radically new processes (like for example TRIZ, cf. Altshuller, 1994 and related methods) for PI.

Furthermore, product design has to rely on the molecular sciences, in particular chemistry, physics and biology, to tailor product properties via a profound understanding on the molecular level. The PSE community should be aware of the fact that product design is a field which is actively pursued and “owned” by other disciplines, most notably by materials sciences with strong participation of physics and chemistry. Again, PSE has to collaborate and convince these disciplines that its problem-oriented approach combined with systems thinking brings value to the research process. The integration of product systems engineering with the process plant scale comes again naturally because the processing conditions will ultimately determine the product properties.

## 6. Summary and concluding remarks

We have sketched the past and present of PSE and have reflected on the future of PSE. Our field has significantly contributed to the chemical engineering profession in the last decades by providing MSO technology to routinely address demanding and large-scale process problems in academia and industrial practice. Systems thinking and systems problem solving are considered to be an indispensable ingredient in the academic education of chemical engineers and in industrial practice. Consequently, the objective of PSE is the penetration of other chemical engineering disciplines with systems thinking.

The risk of losing its identity can only be diminished by long-term research on the core expertise with a focus on model-based systems engineering methods and tools to assist problem solving in order to establish high quality solutions. A plethora of interesting and challenging problems will show up if this research on the core MSO technologies is positioned in the broader perspective of MPPSE. Nevertheless, PSE has to also reach out and contribute to the solution of “non-traditional” systems problems in related engineering and science disciplines. PSE has the competence and the skills to even drive the research process not in competition but in close collaboration with the domain experts. PSE has to strengthen its position in chemical engineering by cooperation within and outside its community.

The PSE community has to further emphasize its efforts to further develop and integrate methodological advances into industrial work processes by means of a combination of technology push and market pull. Specific technology transfer agencies such as AixCAPE e.V. (AixCAPE, 2007) may act as an enabler of the interaction between academia and industry.

Since PSE is a relatively small community in between the disciplines with many interfaces and with a lot of commons grounds with systems engineering communities in other fields of science and engineering, one may think of joining forces to form a larger community spanning different engineering and scientific fields. There is scope for such a concentration of forces, since model-based and computational approaches to systems problem solving will rely on the same principles, conceptual and algorithmic methods and tools regardless of the type of engineering discipline.

Process systems engineering has definitely a bright future with sustainable impact on the chemical engineering sciences as well as on the whole industrial manufacturing process, if we – the PSE community – actively shape it by implementing the transformation process described in this essay and by presenting ourselves as an enabler for process and product innovation rather than a service provider to our “customers” in research and industrial application.

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