Computer Aided Process and Product Engineering
Luis Puigianer and Georges Heyen

Introduction

Since 1991 the working party (WP) of the European Federation of Chemical Engineering with the title "The Use of Computers in Chemical Engineering" adopted new term of reference and a new title-the Working Party on Computer Aided Process Engineering.

This decision followed an internal debate on issues involving concepts like computer integrated manufacturing (CIM), computer-aided process operations (CAPE) and computer-aided process design (CAPD). The consensus reached in the new title naturally embraced computer-aided process operations as a subset of CIM, which is focused on the application of computing technology to integrate and facilitate the key technical decision processes which arise in chemical manufacture. Thus, CAPE focuses on algorithms, procedures and frameworks, which automate the operating/design decisions for those functions which are automatable and support those operating decisions for which human intervention is necessary or desirable (Pekny et al. 1991).

This re-structuring of the WP reflected the actual trends in the process industries. Never before had the enterprises so much invested in information processing. Computer-controlled production proved in many cases that it was capable of reducing the costs and increasing the flexibility far more greatly then any other technology in the past decades. Information and communication technology offered plenty of standardized but also specific possibilities of applications and solutions as never before. Therefore, a management strategy aiming at the strengthening of the competitiveness of production should obviously incorporate CAPE as a guideline for the reunion of the flexible production, the technical and administrative data processing and the complete penetration of all enterprise activities with data processing (Westkämper 1992).

During this last decade these trends have consolidated and expanded. Thus, CAPE is a network with separate functions which are linked to each other and/or integrated by using common data and information. CAPE systems are used in the development and design, operations planning and production equipment planning departments. Otherwise, order processing is carried out by process control systems (materials resource planning). Both systems deliver data to an information system, which is the basis for the operation of the production with its flexible and control systems. Moreover, as the system boundaries have expanded, CAPE contribution and opportunities are present in the integrated product-process design and decision support to the complex management of the entire enterprise.

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This book aims to present and review the state of the art and latest developments in process systems engineering. It seeks to highlight the use of information technology tools in the development of new products and processes, in the optimal operation of complex equipment found in the process industries, and in the complex management of the whole business.

The book is intended as a valuable reference to the scientific and industrial community, and should contribute to the progress in computer-aided process and product engineering. This work should be also useful for teachers of postgraduate courses in these areas.

Following this introduction, the book consists of 27 chapters organized into five major sections:

Section 1 Computer-aided Modeling and Simulation,
Section 2 Computer-aided Process and Product Design,
Section 3 Computer-aided Process Operation,
Section 4 Computer-integrated Approaches in CAPE,
Section 5 Applications

Section 1 presents a review on actual trends and shows new advances in mathematical modeling and digital simulation techniques that permit practitioners to solve the complex scenario that describes real engineering systems. Basic techniques needed to develop and solve models are reviewed: this extends from applied mathematics to model validation and tuning, model checking and initialization, and to the estimation of physical properties.

In *Chapter 1* steady state process simulation is introduced, which involves large-scale algebraic systems. The most known solving algorithms are first presented. Alternative methods of the quasi-Newton family are then described and some issues such as convergence, ill-conditioned and singular Jacobian matrices are also discussed. Then, it focuses on large and sparse algebraic systems, how to work with bounds, constraints and discontinuities as well as how to deal with the stopping criteria to be adopted. Finally, a short introduction to continuation methods is provided.

Chapter 2 deals with distributed dynamic models, that is, partial differential equations (PDEs) or partial differential algebraic equations (PDAEs) incorporating convection, diffusion, reaction and/or thermodynamic property terms.

Numerical methods for solving PDEs are reviewed in three sections treating first semidiscretized (method of lines) and fully discretized methods before discussing adaptive and moving mesh methods. Some applications are discussed, such as preparative chromatography, fixed-bed reactors, slurry bubble columns, crystallizers and microbial cultivation processes. Finally, an approach for combining computational fluid dynamic (CFD) technology with process simulation is discussed.

Process and product design studies rely on good knowledge of materials behavior and physical properties. *Chapter 3* deals with estimation methods based on molecular modeling, describing the behavior of atomic and molecular systems subject to energetic interactions. It allows running numerical experiments and as any experiment, it can provide not only accurate physicochemical data but also increase the knowledge on the system studied. Molecular modeling concepts are presented so as to demystify them and stress their interests for chemical engineers. Multiscale approach including molecular modeling is not illustrated due to restricted space. Rather, routine examples on the use of several molecular techniques suitable to get accurate vapor-liquid equilibrium data when no data is available are provided.

Chapter 4 presents a critical review of modeling frameworks for complex processing systems with emphasis not only on the models themselves but also on specialized techniques for the efficient solution of these models. More specifically, due to their increased industrial interest a general modeling framework for adsorption-diffusion-based gas separation processes is presented in detail with focus on pressure-swing adsorption and membrane-based processes for gas separations. For subsequent sections of this chapter, a critical review of models and specialized solution techniques for crystallization and grinding processes is made. Finally, concluding remarks are drawn up and future research challenges are discussed.

Process models are of increasing size and complexity, therefore the methods and tools for their tuning, discrimination and verification are of great importance. The widespread use of process models for design, simulation and optimization requires the proper documentation, re-use and retrofit of already existing models, which also need the above techniques. Thus, *Chapter 5* deals with computer-aided approaches and methods of model tuning, discrimination and verification that are based on a formal structured description of process models.

Besides the length and time scales, a *detail* scale could also be considered which seeks to develop models with varying degrees of fidelity in relation to the real world phenomena. This is the subject of *Chapter 6*, which presents coverage of multiscale modeling through a discussion of the origins of such phenomena in process and product engineering, as well as discussing the approaches to the modeling of systems that seek to capture multiscale phenomena. The chapter discusses the development of the partial models that make up the multiscale model particularly focusing on the characteristics of those models. The issue of partial model integration is also developed through the use of integrating frameworks. Those frameworks are analyzed to understand the important implications of model coupling and computational behavior. Throughout the chapter reference is made to granulation processing that helps to illustrate the concepts and challenges in this important area.

Finally, *Chapter 7* of Section 1 addresses one of the current challenges facing the modeling community: the description of regulatory networks in micro-organisms. Micro-organisms constitute examples of entire autonomous chemical plants, which are able to produce and reproduce despite shortage of raw materials and energy supplies. Understanding the intracellular regulatory networks of micro-organisms is important to process systems engineering for several reasons: microbial systems still constitute relatively simple biological systems, the study and understanding of which may enable better understanding of higher biological systems such as human beings. Furthermore, microbial systems are used, often following genetic manipulation, to produce relatively complex organic molecules in an energy efficient manner. Understanding how to couple the microbial regulatory functions and the higher level process and production control functions is a prerequisite for process engineering.

Section 2 of this book brings together process engineering and product design. One major use of models is the development and improvement of processes and products. This is a multidisciplinary approach, and it requires consideration of many aspects of the behavior of a production plant: equipment design, steady state and dynamic operation of integrated processes, raw materials and energy usage, economy, health and safety. Section 2 reviews the methods currently available to integrate knowledge from different disciplines, and presents tools available to assist in the conception of new products, and in the design of plants able to manufacture them in a competitive and sustainable way.

Section 2 starts with a comprehensive review of the process separation synthesis problem with emphasis on complex distillation systems (*Chapter 1*). First, a critical overview of the synthesis of simple column sequences is presented with emphasis on the novel generalized modular representation framework developed at Imperial College London. Then, the synthesis problem of heat-integrated distillation trains is thoughtfully reviewed. Current state-of-the-art methodologies and algorithmic frameworks for the synthesis of complex distillation sequencing are also critically discussed.

The term process intensification is associated mainly with more efficient and compact processing equipment that can potentially replace large and inefficient units commonly used in chemical processing but also includes methodologies, such as process synthesis methods, that enable the systematic development of efficient processing units. *Chapter 2* provides an overview over current process intensification technologies and presents a number of recently developed systematic computer-aided process intensification methods and tools. They enable the systematic screening and scoping of large numbers of alternative processing options and can identify novel options of phenomena exploitation that may lead to higher efficiencies. Such tools provide the basis for systematic approaches to novelty in process intensification and have the potential to identify processing options, which can easily be missed in design activities that rely on intuition and past experiences.

Industrial processes require the use of energy, other utilities such as water and solvents, and produce wastes that need to be treated. The system performances rely not only on the efficiency of the process but also on the quality of its integration considering the energy conversion technologies, the possible combined heat and power production, the water usage and the waste treatment techniques. *Chapter 3* presents computer-aided methods for solving the optimal integration of utility systems. Graphical representations support the engineer's creativity; they are used to define the characteristics of a utility system, to analyze the potential of combined heat and power production and to analyze the quality of subsystems integration. From the requirement analysis, a utility system superstructure can be developed, to be later optimized using mathematical programming techniques. Several formulations are presented and discussed in order to integrate the different types of utility subsystems (e.g., combined heat and power, heat pumps and refrigeration) and optimize their integration with the processes. The problem of the water circuit integration can be addressed using similar concepts.

The computational basis for equipment and process design in the chemical manufacturing industries is introduced in *Chapter 4*. Problems encountered are discussed through the use of case studies that range from modeling, simulation and optimization of existing and proposed processes. The work described in the case studies represents recent developments and trends in the industry in the area of Computer Aided Process Engineering (CAPE). The applications focus on the use of optimization techniques for obtaining optimal designs and better approaches for controlling the processes close to or at the optimal point of operation. Designs use rigorous models based on thermodynamics, conservation laws and accurate models of transport and fluid flow, with particular emphasis on dynamic behavior and uncertainty in market conditions.

Product development and design starts to be a third paradigm in chemical engineering. This emerging field of research undergoes a phase of defining its scope and methods as well as the generalization of the existing industrial experience. *Chapter 5* introduces the main phases of product development and the classes of the applicable methods. The special attention is given to the definition phase: methods for translation of the consumer requirements into the product parameters and approaches to generation of the product ideas. Also given is an introduction to the experimental and knowledge-based methods and tools for product design. Finally, the challenges that face CAPE in the field of product development and design are presented.

Section 3 reviews the current problems facing process operations. It presents the state of relevant methods and technology, and needed advances to combat ever-increasing complexity. The scope covers resource planning and production scheduling, extending to the analysis of supply chain. Process monitoring and measurement validation are described, as being preliminary steps for real-time process optimization and model-based process control.

This section starts with a comprehensive review of state-of-the-art models, algorithms, methodologies and tools for the resource planning problem covering a wide range of manufacturing activities (*Chapter 1*). First, the long-range planning problem in the process industries is considered including a detailed critical discussion on the effect of uncertainty, the planning of refinery operations and offshore oilfields, the campaign planning problem and the integration of scheduling and planning. Then, the planning problem for new product development in pharmaceutical industries is discussed in some detail. Next, the tactical planning problem is briefly presented followed by a description of the resource planning problem in the power market and construction projects. Recent computational solution approaches to the planning problem are reviewed, while available software tools are outlined in the penultimate section of this chapter. Finally, concluding remarks are drawn and future challenges in this area are proposed.

The complex problem of what to produce and where and how to produce it best is considered through an integrated hierarchical approach. *Chapter 2* deals with production scheduling, focussing on the single site problem. Problem solution using heuristics is described, before presenting solution methods based on mathematical programming. Hybrid solutions are also mentioned, as well as the combined solution of scheduling and optimal operation. The state of the art for industrial applications is described, before concluding with new application domains and future challenges.

Measurements are needed to monitor process efficiency and equipment condition, but also to take care that operating conditions remain within acceptable ranges to ensure good product quality, avoid equipment failure and any hazardous conditions. However, measurements are never error free. Model-based data reconciliation techniques allow the detection and correction of random experimental errors, taking profit of redundant measurements. *Chapter 3* deals with process monitoring and online estimation of performance indicators. This includes also fault detection capability, and is required as part of a model-based control system, since model tuning should be based on validated plant data. The design of effective redundant sensor network is also addressed.

Operating a real plant at its optimal design conditions does not guarantee optimal operation. Some plant-model mismatch cannot be avoided, nor the effect of disturbances, this is why some sort of feedback control is needed. *Chapter 4* deals with model-based control, i.e., the use of rigorous process models for feedback control by model-based on-line optimization. Several implementations with increasing level of complexity are discussed. Some plant inputs can be fixed by an off-line optimization while other inputs are controlled to keep some key process parameters on target. When nonlinear process models are available this leads to nonlinear model predictive control (NMPC) where the future values of the controlled variables are predicted over a finite horizon (the prediction horizon) using the model, and the future inputs are optimized over a certain horizon (the control horizon).

As an extension of this concept, feedback control can be combined with model adaptation and re-optimization. Such a control scheme is presented for the example of batch chromatographic separations, including experimental results.

Structural plant-model mismatch is a major problem also addressed. A solution is the use of optimization strategies that incorporate feedback directly; this idea is presented in detail and the application to batch chromatography is used to demonstrate its potential.

To conclude, the problem of controlling quasicontinuous chromatographic separations is formulated as an on-line optimization problem where the measured outputs have to meet the constraints on the product purities but the optimization goal is not tracking of a pre-computed trajectory but optimal process operation.

With the increasing fundamental understanding of the underlying physicochemical phenomena of various processes and strict environmental, safety and energy consumption constraints the need for efficient real time optimization tools has reached unprecedented levels. A better understanding of the processes is leading to high-fidelity but complex mathematical models that can not always be solved efficiently in real time. The computation of the best operating or control strategy, given these models, is further complicated by the presence of constraints on control variables. In *Chapter 5* a parametric programming approach is presented, which moves real time computational effort off-line. This is achieved by *a priori* computing the optimal control variables as a set of explicit functions of the current state of the plant, where these functions are valid in certain polyhedral regions in the space of the state variables. This reduces real-time optimization to simple function evaluations.

Actually, many production facilities constitute large hybrid systems, making it necessary to consider the continuous-discrete interactions taking place within an appropriate framework for plant and process simulation and optimization. The next chapter of Section 3 (*Chapter 6*) briefly discusses existing modeling frameworks for discrete/hybrid production systems embodying different approaches. A very recent framework for process recipe initialization that integrates a recipe model into the batch plant-wide model is introduced. The on-line and off-line recipe adaptation from real-time plant information is presented. Finally, a model-based integrated advisory system is described. This system gives on-line advice to operators on how to react in case of process disturbances. This way, an enhanced overall process flexibility and productivity is achieved. Application of this promising approach is illustrated through examples of increasing complexity.

Process operation management and business competitiveness cannot be understood without considering supply chain activities. The main aim of *Chapter 7* is to provide a comprehensive review of recent work on supply chain management and optimization mainly focused on the process industry. The first part describes the key decisions and performance metrics required for efficient supply chain management. The second part critically reviews research work on enhancing the decision-making for the development of the optimal infrastructure (assets and network) and planning. Next, different frameworks are presented, which capture the dynamic behavior of the supply chains by establishing efficient replenishment inventory management strategies. Finally, available software tools for supply chain management are outlined and future research needs for the process systems engineering community are identified.

Section 4 focuses on recent developments aiming at the integration of different components in the CAPE world that offer a different degree of practical implementation. Supporting databases and a presentation of the necessary emergent standards in the CAPE domain are also included here.

As chemical product design involves different disciplines, different types of data and tools, different solution strategies, etc., the need for a framework for integrated chemical product-process design becomes a subject of paramount importance.

Moreover, there are chemical products where the reliability of the manufactured chemical product is more important than the cost of manufacture, while there are those where the cost of manufacture of the product is at least as important as the reliability of the product. Thus, product-centred process design is also very important. Identifying a feasible chemical product, however, is not enough; it needs to be produced through a sustainable process. The objective of *Chapter 1* of Section 4 is first to define the general integrated chemical product-process design problem, then to identify the important issues and needs with respect to their solution and finally to illustrate through examples, the challenges and opportunities for CAPE/PSE methods and tools. Integrated product-process design where modeling and supply chain issues play an important role is also highlighted.

Chapter 2 deals with the important issues of where, why and how models of various types are used throughout the life of an industrial or manufacturing process. The chapter does not deal specifically with the modeling of the life cycle process but concentrates on the use of models to address a plethora of important issues that arise during the many stages of a process' life, from the cradle to the grave.

In this chapter, the life cycle concept is first discussed in relation to a "cradle to the grave" viewpoint, and then in subsequent sections consideration is made to specific issues related to the modeling goals and realizations. Some important issues are discussed which surround model development, reuse, integration, model documentation and archiving. Consideration is also made to the future needs of such modeling approaches and the important implications of life cycle modeling for corporations.

Throughout this chapter the authors refer to several specific industrial case studies that help illustrate the importance of modeling throughout the life cycle as well as the challenges of doing so. What is evident in the following sections of this chapter is that there is a huge range of modeling used to help answer vital sociotechnical questions through the life cycle of the process or product.

It is important to appreciate that process and product engineering have vital links to social and human factors within a holistic approach to modeling. Major infrastructure projects continually reinforce a more complete view than that which is often taken by process and product engineers. In this chapter the vision of modeling within the process or product life cycle is expanded to see just what has been achieved and where the challenges lie for the future.

An introductory chapter (Section 3, Chapter 7) on the supply chain (SC) network has already presented the elementary principles and systematic methods of supply chain modeling and optimization. In *Chapter 3* of Section 4, the need for and integrated management of the SC is further emphasized and novel challenging solutions are presented.

As seen, supply chain management (SCM) comprises the entire range of activities related to the exchange of information and materials between costumers and suppliers involved in the execution of product and/or service orders in an extremely dynamic environment.

A successful management of the supply chain management requires direct visibility of the global results of a planning decision in order to include this global perspective. This requires significant integration across multiple dimensions of the planning problem for nonconventional manufacturing networks and multi-site facilities over their entire supply chain. Objectives such as resources management, minimum environmental impact, financial issues, robust operation and high responsiveness to continuous needs must be simultaneously considered along with a number of operating and design constraints.

All integrated applications needed to design and operate a plant during its whole life cycle need to access reliable physical properties for all chemicals and materials occurring in the process. *Chapter 4* presents an overview of the thermophysical properties needed for CAPE calculations and describes the major sources of such data currently available. Several databases for pure component physical properties are described. Phase equilibrium data collections are also reviewed. The quality of data inside the data calculation modules is essential: inaccurate data may lead to very expensive misjudgements whether it is to proceed with a new process or modification of it. Inadequate or unavailable data may cause a promising and profitable process can be delayed or in the worst case be rejected, only for the reason that it was not properly modelled in a simulation. The text provides also up-to-date references to information sources available on the Internet.

The lack of software standards in computer-aided process and product engineering has been a subject of concern for years, as a source of unnecessary costs, delays and inconsistencies between data produced and consumed by different nonintegrated systems using different bases, different calculation principles, different units of measurements, running on different computers under different operating systems and written in different languages. *Chapter 5* introduces software standards intended to remove these problems by providing the desired interoperability between software tools, platforms and databases. With appropriate machine-to-machine interface standards, using the best available tools together becomes a matter of plug-and-play, supposedly as easy as connecting USB devices or hi-fi systems. Moreover, not only do these standards enable the putting together of several software pieces available on your local PC, but they allow interoperating heterogeneous software modules available on your organisations' intranet, or on the Internet. The chapter starts with a discussion on the concepts of openness and of open standards; then some of the most significant operational standards in computer-aided process and product engineering are examined. Following this, the authors look at some of the current software interoperability technologies that will power future systems, namely web services, service-oriented architectures and ontologies for the Semantic Web. The chapter concludes with a brief look at the organisational and economic consequences of the trend towards interoperability and standards in CAPE.

Section 5 presents tutorial examples and case studies aiming to illustrate typical problems that can be solved using state of the art computer-aided tools. The goal is not only to show the benefits of using CAPE methods, but also to indicate what are some current limitations and point out areas where future research and developments should be directed.

Chapter 1 analyses the increased use of computers in chemical engineering education. The authors present a set of computer-aided educational modules that have been specially developed with the aim to avoid the dangers of misuse of the software. The motivation is to help the students to not only understand the concepts but also to appreciate how the theory can be applied to solve chemical engineering.

The computer-aided educational modules presented here involve property prediction (suitable for a course on thermodynamics or product design), extractive distillation-based separation (suitable for courses on separation processes, distillation, or process design) and model derivation and solution (suitable for courses on modeling, simulation and/or numerical methods).

The students are encouraged to first assemble modules for corresponding calculation steps into their own software for simple problems and then use specialized software for larger more complex problems. At this stage, an integrated computer-aided system also becomes very useful and data transfer between the various calculation steps and the corresponding software options take place automatically, thereby saving considerable time, which can be spent instead to understand the problem better and to analyze the results.

Chapter 2 describes industrial case studies in plant operation and process monitoring. The application and benefits of data validation is illustrated by several examples, taken in a range of industrial environments: oil and gas, chemicals, power plants. Besides plant monitoring and fault detection, the on-line evaluation of key performance indicators is also illustrated. It is shown how the use of more detailed models (e.g., starting with component mass balance, adding energy balances, and later equilibrium constraints) contributes to improving the result quality.

Chapter 3 describes the application of a production planning method for a multiproduct manufacturing plant, which optimizes profit under uncertainties in product demands.

Flexibility refers exclusively to the planning problem here and it is not coupled with a plant re-design. The development and the application of the method have been highlighted by means of a case study taken from a food additives plant.

This method is considered practical for plant management, because the required input data for the demand and process models and the profit function is easy to get by the users of the method. The generated output facilitates an easy interpretation of sensitivities of the optimized production planning in terms of common economic and product demand specification parameters.

Overall, the theoretical and practical aspects of the computer-aided process engineering covered in this book should find wide use in libraries and research facilities, and a direct impact in the chemical industry, particularly in production automation, utility networks, supply chain and business management with embedded computer integrated process engineering.

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