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CAPE

Computer Aided Process and Product Engineering

Edited by
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Preface

Computer Aided Process and Product Engineering (CAPE): Its Pivotal Role for the Future of Chemical and Process Engineering

Chemical and related industries are at the heart of the great number of scientific and technological challenges involving computer-aided processes and product engineering.

Chemical and related industries including process industries such as petroleum, pharmaceutical and health, agriculture and food, environment, textile, iron and steel, bitumous, building materials, glass, surfactants, cosmetics and perfume, and electronics are evolving considerably due to unprecedented market demands and constraints stemming from public concern over environmental and safety issues.

To respond to these demands, the following challenges faced by these process industries involve complex systems, both at the process-scale and at the product-scale:

1. Processes are no longer selected on a basis of economic exploitation alone. Rather, compensation resulting from the increased selectivity and savings linked to the process itself is sought after. Innovative processes for the production of commodity and intermediate products need to be researched where patents usually do not concern the products but the processes. The problem becomes more and more complex as factors such as safety, health, environment aspects including nonpolluting technologies, reduction of raw materials and energy losses, and product/by-product recyclability are considered. The industry, with large plants, must supply bulk products in large volumes and the customer will buy a process that is nonpolluting and perfectly safe, requiring computer-aided process engineering (CAPE).
2. New specialities, active material chemistry, and related industries involve the chemistry/biology interface of agriculture, food, and health industries. Similarly, it involves upgrading and conversion of petroleum feedstock and intermediates, conversion of coal-derived chemicals or synthesis gas into fuels, hydrocarbons or oxygenates. This progression from traditional chemistry is driven by the new market objectives where sales and competitiveness are dominated by the end-use properties of a product as well as its quality. It is important to underline that today, 60 % of all products sold by chemical companies are crystalline, polymer, or

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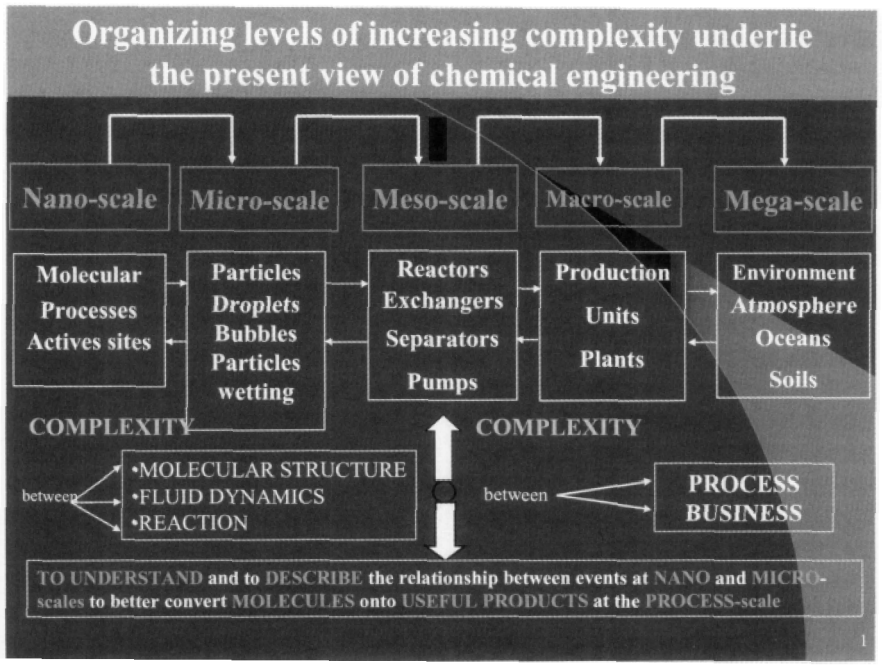
amorphous solids. These complex and structured materials have a clearly defined physical shape in order to meet the designed and the desired quality standards. This also applies to plastics, ceramics, soft solids, paste-like products, and emulsions. New developments require increasingly specialized materials, active compounds, and special effects chemicals. The chemicals are much more complex in terms of molecular structure than traditional, industrial chemicals. Control of the end-use property (size, shape, color, aesthetics, chemical and biological stability, degradability, therapeutic activity, solubility, touch, handling, cohesion, rugosity, taste, succulence, sensory properties, etc.), expertise in the design of the process, continual adjustments to meet changing demands, and speed to react to market conditions are the dominant elements. For these specialities and active materials the client buys the product that is the most efficient and first on the market. He will have to pay high prices and expect a large benefit from these short life-time and high-margin products, requiring most often computer-aided process and product engineering.

The triplet molecular processes-product-process engineering (3PE) approach requires the tools of CAPE.

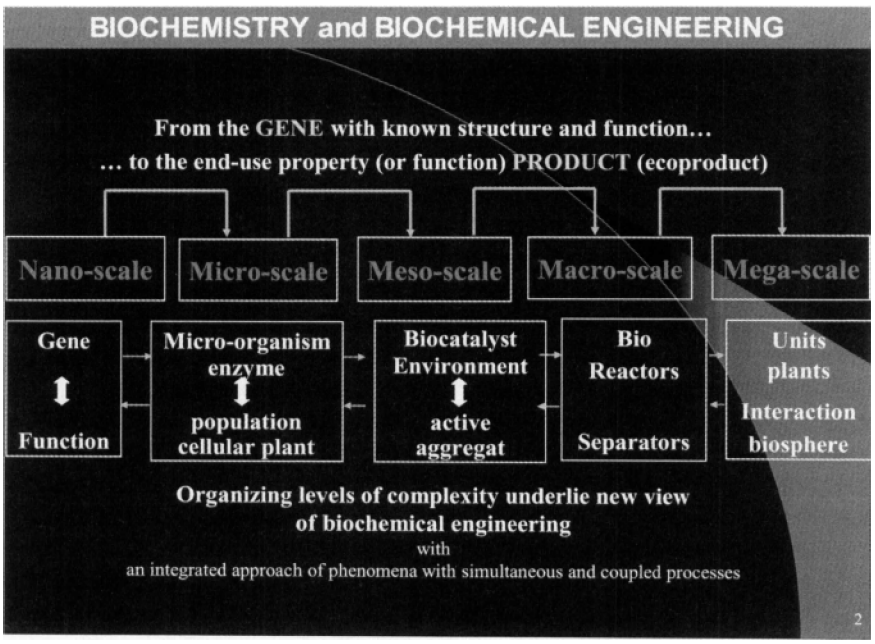
Today, chemical and process engineering are concerned with understanding and developing systematic procedures for the design and optimal operation of process systems, ranging from nano and microsystems to industrial-scale continuous and batch processes; this is illustrated by the chemical supply chain concept. In the supply chain, it should be emphasized that product quality is determined at the micro and nanolevel and that a product with a desired property must be investigated for both structure and function. A comprehension of the structure-property relationship at the molecular (e.g., surface physics and chemistry) and microscopic level is required. The key to success is to obtain the desired end-use property of a product, and thus control product quality by controlling complexity in the microstructure formation. This will help to make the leap from the nanolevel to the process level. Moreover, most chemical and biological processes are nonlinear, belonging to the so-called complex systems for which multiscale structure is common nature. Therefore, an integrated system approach for a multidisciplinary and multiscale modeling of complex, simultaneous, and often coupled momentum, heat and mass transfer processes is required:

- Different time scales (10^{-15}–10^{8} s) are used from femto and picoseconds for the motion of atoms in a molecule during a chemical reaction, nanoseconds for molecular vibrations, hours for operating industrial processes, and centuries for the destruction of pollutants in the environment.
- Different length scales (10^{-8}–10^{6} m) are used from nanoscale for molecular kinetic processes; microscale for bubbles, droplets, particles, and eddies; mesoscale for unit operations dealing with reactors, columns and exchangers; macroscale for production units; and megascale for environment and dispersion of emissions (see the following figure):



Therefore, organizing scales and complexity levels in process engineering is necessary in order to understand and describe the events at the nano and microscales, and to better convert molecules into useful products at the process scales.

This multiscale approach is now also encountered in biotechnology, bioprocesses, and product engineering, to manufacture products and to better understand and control biological tools such as enzymes and micro-organisms. In such cases, it is necessary to organize the levels of increasing complexity from the gene with known properties and structures, up to the product-process relation, by modeling coupled mechanisms and processes at different length scales: the nanoscale is used for molecular and genomic processes and metabolic transformations; pico and microscales are used for enzyme and integrated enzymatic systems, and biocatalyst and active aggregates; mesoscale is used for bioreactors, exchangers, separators; and macro and megascales are used for production units and interactions with the biosphere. Thus, organizing levels of complexity at different length scales, associated with an integrated approach to phenomena and simultaneous and coupled processes, are the heart of the new view of biochemical engineering (see next figure). Indeed this capability offers the opportunity to apply genetic-level controls to make better biocatalysts, novel products, or developing new drugs, new therapies, and biomimetic devices. Understanding an enzyme at the molecular level means that it may be tailored to produce a particular end-product. Also, the ability to think across length scales makes chemical engineers particularly well poised to elucidate the mechanistic understanding of molecular and cell biology and its large-scale manifestation, i.e., decoding communications between cells in the immune systems.



These examples are at the center of the new view of chemical and process engineering: organizing levels of complexity, by translating molecular processes into phenomenological macroscopic laws to create and control the required end-use properties and functionality of products manufactured by a continuous or batch process. I have defined this approach as the triplet molecular processes-product-process engineering (3PE): an integrated system approach of complex pluridisciplinary nonlinear and nonequilibrium processes and phenomena occurring on different length and time scales, involving a strong multidisciplinary collaboration between physicists, chemists, biologists, mathematicians, computer-aided specialists, and instrumentation specialists.

Today's tools are wide-ranging for the success of chemical and process engineering for modeling, complex systems at different scales encountered in the process and product engineering.

It's possible to understand and describe events on the nano and microscale in order to convert molecules into useful products on process and unit scales thanks to significant simultaneous breakthroughs in three areas: molecular modeling (both theory and computer simulation), scientific instrumentation and noninvasive measurement techniques, and powerful computational tools and capabilities for information collection and processing.

At the nanoscale, molecular modeling assists in maintaining better control of surface states of catalysts and activators, obtaining increased selectivity and facilitating asymmetrical synthesis, e.g., chiral technologies. Molecular modeling also assists in explaining the relationship between structure and activity at the molecular scale in order to control crystallisation, coating and agglomeration kinetics.

At the microscale, computational chemistry is very useful for understanding complex media and all systems whose properties are controlled by rheology and interfacial phenomena.

At the meso and macroscales, computer fluid dynamics (CFD) is required for scaling up new equipment, or for the design of new operation modes for existing equipment such as reversed flow, cyclic processes, and unsteady operations. It is especially useful when rendering multifunctional processes with higher yields in chemical or biological reactions coupled with separation or heat transfer. It also provides a considerable economic benefit.

At the production unit and multiproduct plant scale, dynamic simulation and computer tools for simulation of entire processes are needed more and more. These tools analyze the operating conditions of each piece of equipment in order to simulate the whole process in terms of time and energy costs. New performances (product quality and final cost) resulting from any change due to a blocking step or a bottleneck in the supply chain will be predicted in a few seconds. It is clear that such computer simulations enable the design of individual steps, the structure of the whole process at the megascale, and place individual processes in the overall context of production, emphasizing the role and the place of computer assistance in process and product engineering.

The previous considerations on the necessary multidisciplinary and multiscale integrated approach for managing complex systems encountered by chemical and related process industries in order to meet market demands led to the proposal of four main parallel objectives involving the tools of CAPE.

The first objective concerns a total multiscale control of the process to increase selectivity and productivity by the nanotailoring of materials. The nanotailoring can be produced with controlled structure, or by supplying the process with a local "informed" flux of energy and materials, or by increasing information transfer in the reverse direction, from process to man, requiring close computer control, relevant models, and arrays of local sensors and actuators.

The second objective concerns the process intensification by the design of novel equipment based on scientific principles, new operating modes, and new methods of production. Process intensification with multifunctional equipment that couples or uncouples elementary processes (transfer-reaction-separation), involving the reduction in the number of equipment units leads to reduced investment costs and significant energy recovery or savings. Cost reduction between 10 % and 20 % are obtained by optimizing the process. But the use of such hybrid technologies is limited by the resulting problems with control and simulation leading to interesting but challenging problems in dynamic modeling, design, operation and strong nonlinear control. Also, process intensification using microengineering and microtechnology will be used more and more for high-throughput and formulation screening. Indeed microengineered reactors have some unique characterictics that create the potential for high-performance chemicals and information processing on complex systems. Moreover, scale-up to production by replication of microreactor units used in the laboratory eliminates costly redesign and pilot plant experiments, thus accelerating the transfer from laboratory to commercial-scale production.

The third objective concerns the extension of chemical engineering methodology to product-focussed design and engineering in using the multiscale modeling of the above-mentioned approach, 3PE. Indeed to be able to design and control the product quality of structured materials, and make the leap from the nanolevel to the process level, chemical and process scientists and engineers face many challenges in fundamental concepts (structure-activity relationships on molecular level, interfacial phenomena, adhesive forces, molecular modeling, equilibria, kinetics, and product characterization techniques); in product design (nucleation growth, internal structure, stabilization, additive); in process integration (simulation and design tools based on population balance); and in process control (sensors and dynamic models). It should be underlined that much progress has been made in product-oriented engineering and in process control using the scientific methods of chemical engineering. The methods include examination of thermodynamic equilibrium states, analysis of transport processes and kinetics when they are separate and linked by means of models with or without the help of molecular simulation, and by means of computer tools of simulation, modeling and extrapolation at different scales for the whole supply chain up to the laboratory-scale. But how can operations be scaled up from laboratory to plant? Will the same product be obtained and will its properties be preserved? What is the role of the equipment design in determining product properties?

This leads to the fourth main objective, which is to implement the multiscale application of computational chemical engineering modeling and simulation to real-life situations from the molecular scale to the overall production scale in order to understand how phenomena at a smaller length scale relate to properties and behavior at a longer length scale. The long-term challenge is to combine the thermodynamics and physics of local structure-forming processes like network formation, phase separation, agglomeration, nucleation, crystallization, sintering, etc., with multiphase computer fluid dynamics. Indeed through the interplay of molecular theory, simulation and experimentation measurements a better quantitative understanding of structure-property relations evolves, which, when coupled with macroscopic chemical engineering science, form the basis for new materials and process design (CAPE). Turning to the macroscopic scale, dynamic process modeling and process synthesis are also increasingly developed. Moreover, integration and opening of modeling and event-driven simulation environments in response to the current demand for diverse and more complex models in process engineering is currently taking a more important place. The aim is to promote the adoption of a standard of communication between simulation systems at any time and length-scale level (thermodynamic, unit operations, numerical utilities for dynamic, static, batch simulations, fluid dynamics, process synthesis, energy integration, process control) in order to simulate processes and allow the customers to integrate the information from any simulator into another one. Thus expanding and developing interface specification standards to ensure interoperability of CAPE software components justifies the creation of a standardization body (CAPE-OPEN Laboratories Network, CO-LAN) to maintain and disseminate the software standards in the CAPE domain that have been developed in several international projects.

The CAPE Present Book: a Vade Mecum in Process Systems Engineering

It is clear and I have shown that chemical and process industries have to overcome challenges linked to the complexity. They need to master phenomena in order to produce products "first on the market" with "zero pollution, zero accident, and zero defects" processes. Therefore, never before have enterprises invested so much in information processing and computer-controlled production, which proved in many cases that it was capable of reducing the costs and greatly increasing the flexibility than any other technology in past decades. Moreover, information and communication technology offered a great number of standardized but also specific possibilities of applications and solutions as never before. Therefore, a strategy aiming at the strengthening of 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 the enterprise activities with date processing.

Within the European Federation of Chemical Engineering, the CAPE Working Party has been very active in this area since the end of the 1960s, as shown by the success of the ESCAPE series of symposia. The activity of the Working Party is also shown by the publication of this book, which aims to present and review the state-of-the-art and latest developments in process systems engineering. Its contents illustrates the modern day multidisciplinary and multiscale integrated approach for the integrated product-process design and decision support to the complex management of the entire enterprise. It also highlights the use of information technology tools in the development of new products and processes, in the optimal operation of complex and/or new equipment found in the chemical and process industries, and in the complex management of the supply chain.

Actually, this book, based on the competences of scientists and engineers confronted with industrial practice, is a reference tool. Its ensuing and clear objectives in the topic of process systems engineering are:

- the necessary multidisciplinary bases required for understanding and modeling the phenomena occurring at the different scales from molecular range up to the global supply chain and extended enterprise;
- the experimental and knowledge-based methods and tools available to assist in the conception of new processes and products design, and in the design of plants able to manufacture the products in a competitive and sustainable way;
- the presentation of needed advances to fight ever-increasing complexity involved within the product-process life cycle;
- some tutorial examples and cases studies aiming to the state-of-the-art computer-aided tools.

The theoretical and practical aspects of the computer-aided process engineering covered in this book, involving computer-aided modeling and simulation, computer-aided process and product design, computer-aided process operation, and computer integrated approaches in CAPE should find use in libraries and research facilities and make a direct impact in the chemical and related process industries.

This book judiciously titled "Computer Aided Process and Product Engineering – CAPE" is a vade mecum in process systems engineering. It is a valuable and indispensable reference to the scientific and industrial community and should be useful for engineers, scientists, professors and students engaged in the CAPE topic.

Bravo and many congratulations to our collegues Prof. Puigjaner and Prof. Heyen for this publication and to the many authors involved in the CAPE Working Party of the European Federation of Chemical Engineering that have made this vade mecum a reality.

Prof. Dr. Ing. *Jean-Claude Charpentier*
President of the European Federation of Chemical Engineering

Foreword

The European Working Party on Computer Aided Process Engineering has been an important and highly effective stimulus for and promoter of research and educational advances in process systems engineering for over 40 years. The 1991 redirection of the Working Party from the broad and all inclusive scope of embracing "the use of computers in chemical engineering", which was its theme for some thirty years, to its present emphasis on product and process engineering has had important consequences. It has reenergized the organization, sharpened its focus and promoted higher levels of technical achievement. Indeed over the past decade, the ESCAPE series of annual conferences sponsored by the Working Party has become a vital world forum for disseminating, discussing and analyzing progress in state-of-the-art methodologies to support product and process design, development, operation and management. This volume represents a well-directed effort by the Working Party to capture the current status of developments in this field and thus to give that field its current definition.

To be sure, the volume is an ambitious undertaking because the process systems engineering field has expanded enormously from its traditional primary focus on the design, control, and operations of continuously operated commodity chemical processes and its secondary concern with the design and control of batch unit operations. That expansion has included methodologies to support product design and development, increases in both scope and complexity of the processing systems under consideration, and approaches to quantify the risks resulting from technical and market uncertainties and incorporate risk-reward trade-offs in design and operational decisions. The scope of systems encompassed by process systems engineering now ranges from the molecular, biomolecular and nanoscale to the enterprise-wide arena. The levels of complexity include self-assembly processes at the nanoscale, self regulating processes at the cellular level, the combination of mechanical, electrical and surface energetic phenomena in heterogeneous particulate systems, the interplay between thermodynamic, reaction and transport phenomena in integrated reaction/separation operations, and even the decentralized and semiautonomous interactions of customers, suppliers, partners, competitors and government regulators at the enterprise level. Certainly, these developments have been greatly facilitated by remarkable advances in computing and information technologies. However, at least as important has been the expanded scope of the models that underpin design and operational decisions as well as key advances in the tools for creating, analyzing, solving and maintaining these models over the life cycle of the associate product/pro-

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cess. The models of interest are now defined not just in terms of the traditional algebraic and differential equations, but also include systems of partial differential and integral equations, graphs/networks, logical relations/conditions, hybrids of logical conditions/relations and continuous equations, and even object-oriented representations of information, decision and work flows.

Has this volume succeeded in addressing the expanded role of models, the thrusts in product design and development, the much enlarged scope and complexity of applications, and the innovative approaches to addressing uncertainty and risk? While it is impossible to address the full scope of these developments within the limited pages of a single volume, the editors and authors, all active contributors of the Working Party, have indeed done remarkably well in capturing and highlighting many of the most important developments.

In Section 1, we find coverage of fundamental issues such as the development of modeling frameworks, model parameter estimation and verification methods, approaches to treatment of multiscale models, as well as numerical methods for solution of algebraic, differential and partial differential systems. The applications to particulate-based processes such as crystallization, grinding, and granulation are of continuing special interest. Computational fluid dynamics and molecular modeling tools, which have become integrated into the process systems engineering toolbox are reviewed and the state of methods for the modeling and analysis of microorganisms are presented. The computational biology domain is receiving a high level of attention by the systems engineering community and will certainly receive even more extensive coverage in future reviews. The second section, which principally treats process design, reviews current developments in overall process synthesis as well as synthesis of reaction, separation and utility subsystems. The area of process intensification, which seeks to capture the potential synergies from exploiting the complex interactions of reaction-separation phenomena, is noted, discussed and recognized as an important direction for further research in process systems engineering. The third section on process operations covers important developments in the well-established functional levels of the process operations hierarchy: monitoring and data reconciliation, model based control, real-time optimization, scheduling, planning, and supply chain management. Additionally, issues related to the operation of flexible batch plants are reviewed. Key to progress in developments in scheduling, planning, supply chain and flexible batch plant operations have been advances in the formulation and solution of large-scale mixed integer optimization problems. The importance of these and need for continuing advances cannot be overemphasized.

The fourth section treats three key integration issues as well as two supporting technology developments. While the basic features of product design are reviewed in Section 3, the progress in meeting the challenges of integrating product and process design are addressed in Section 4. As noted in that chapter, to date most of the progress has been in applications such as structured or formulated products in which the linkage between product and process is very close but further developments are on the horizon. The modeling technology required to support the product/process lifecycle raised in one of the chapters is a key issue facing many industry sectors. This

issue is not yet as intensively addressed in the process systems community as it should be, given its importance in capturing product/process knowledge and managing corporate risk. The chapter on integrated supply chain management at roots deals with strategic and tactical enterprise-wide decisions. Uncertainty and risk are critical components of such decisions requiring more attention and intense future study. The sections on physical property estimation and databases, as well as open standards for CAPE software, discuss components that comprise an essential infrastructure for CAPE developments. The importance of tools for physical property prediction/estimation is evident in domains such as pharmaceutical products, in which the absence of such predictive tools has significantly retarded CAPE efforts in product and process design. The volume concludes with several enlightening case studies spanning the technologies reviewed in the preceding sections that are well chosen to make these technologies, their strengths and weaknesses more concrete.

Given the limitations of a single volume, there necessarily are additional topics that will in the future require more intensive review and discussion. These include process intensification research at the micro and even nanoscales. While there have been research on microscale process design and control, the essential complexity of the phenomena that occurs at micro and nanoscales makes work in this area both challenging and of potential high impact. There has been progress in rigorous treatment of the full range of external and internal parameter uncertainties and promising computational methods for generating risk-reward frontiers that deserves notice, including the integration of discrete event simulation and discrete optimization methods. Algorithms and strategies for addressing multistage stochastic decision problems and incorporating the full valuation of the decision flexibility in multistage decision frameworks are receiving increased attention. Finally, large-scale optimization methods for attacking enterprise level decision problems of industrial scope are emerging and will become even more prominent in the near future.

In summary, this volume is remarkably thorough in capturing the current state of development of the process systems engineering field and representing its broad scope. It will serve this field well in stimulating further research and in encouraging students to learn and contribute to a vital and growing body of knowledge that has important applications in broad sectors of the chemical, petrochemical, specialty, pharmaceuticals, materials, electronics and consumer products industries. The editors and authors are to be congratulated for a job well done.

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