Section 2
Computer-aided Process and Product Design

Section 2 presents a state-of-the-art review on methods and computer tools currently available to support engineering design activities. The material in this section is organized in five chapters covering the use of models is the development and improvement of processes and products. This activity relies on tools that integrate knowledge from many disciplines, since it has to take care of all the constraints of process and product design, such as equipment and plant flexibility and operability, raw materials and energy usage, economy, health and safety.

Feedstock and product purification are among the critical components of a chemical process. This is why Chapter 1 addresses the synthesis of separation systems, with emphasis on distillation, one of the most energy-intensive unit operations in the chemical process industry. Besides the optimization of a single column, improved sequencing in the case of multiple separations, heat integration and thermal coupling offer perspectives for significant energy savings and are reviewed. All potential solutions of the synthesis problem are considered by generating a superstructure to be optimized using mathematical programming techniques.

Chapter 2 covers process intensification. The design of more efficient and compact processing equipment, usually combining several functions, has long been realized by drawing on intuition and expertise. Now systematic design procedures based on modeling the fundamental principles underlying the process intensification technologies are being developed. Significant achievements are reported in the design of single and multiphase reactors, of reaction-separation systems and of hybrid separation processes by using computer-aided methods for process intensification.

The performance of a process is not only related to the proper design of the main equipment. All processes require utilities: water, solvents, waste treatment, and most of all, energy. Chapter 3 presents computer-aided methods for solving the optimal integration of processes with utility networks; it compares several formulations proposed to optimize the integration of different types of utility subsystems (e.g., combined heat and power, heat pumps and refrigeration, water circuit).

CAPE tools now allow the development, evaluation and optimization of new units and processes. Chapter 4 documents five industrial case studies that illustrate how a combination of rigorous models has been used to produce innovative designs meeting multiobjective targets besides economy: environment conservation, safety, operational flexibility, controllability. They required the use of commercial tools but were enhanced with detailed models of the units that were not routinely available. An efficient design relies on accurate bench and pilot plant data combined with 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.

The process industries undergo a move from the process-oriented to the product-centered businesses. A consequence of this switch is a growing interest in product development. Chapter 5 addresses this issue, with special emphasis on the product definition phase: how to translate customers' needs into product properties and how to foster the generation of novel product concepts. Applications of computer-aided techniques, such as data mining or case-based reasoning, are also illustrated by practical examples.