Section 1
Computer-aided Modeling and Simulation

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 scenarios that describe real engineering systems.

The material in this section is organized in seven chapters covering basic methods and techniques needed to develop and solve models: these extend from large-scale algebraic systems found in steady-state process systems (Chapter 1) to partial differential equations (PDEs) or partial differential algebraic equations (PDAEs) encountered in distributed dynamic models (Chapter 2). In Chapter 1 a description of direct substitution gradient and Newton's basic methods is followed by the presentation of more elaborated alternative methods of the quasi-Newton family and continuation methods. Distributed dynamic models are dealt with in Chapter 2, which involve the solution of PDEs or PDAEs incorporating convection, diffusion, reaction and/or thermodynamic property terms. Since there only exist analytical solutions in few cases due to nonlinearity and complexity, computational methods (or numerical analyses) are in general required to solve such distributed dynamic models. This chapter ends with an approach for combining computational fluid dynamic (CFD) technology with process simulation, which is illustrated and discussed through motivating case studies.

Chapter 3 presents molecular modeling concepts involved in the multiscale modeling approach for process study in a broader framework that promotes computer-aided integrated product and process design. Molecular modeling is presented as an emerging discipline for the study of energetic interaction phenomena. A molecular simulation performs numerical experiments that obtain accurate physicochemical data provided sampling, and energy force field issues are addressed carefully. Still, computer-demanding molecular modeling tools will likely not be used "online" or be incorporated in process simulators. But, rather like computer fluid dynamics tools, they should be used in parallel with existing efficient simulation tools in order to provide information at the molecular scale on energetic interaction phenomena and increase the knowledge of processes that must manufacture ever more demanding end products.

Modeling frameworks for complex processing (specifically separation) systems with emphasis not only on the models themselves but also on specialized techniques for the efficient solution of these models are considered in Chapter 4. Specifically, modeling frameworks on pressure-swing adsorption and membrane-based processes for gas separations, crystallisation, and grinding processes are presented due to their increased industrial interestThe increased complexity and size of process models requires appropriate methods and tools for their tuning, discrimination, and verification. An extension to model validation and tuning, model checking and initialization is made in Chapter 5, followed by a 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 (Chapter 6). Finally, Chapter 7 of Section 1 addresses one of the current challenges facing the modeling community: the description of regulatory networks in micro-organisms as examples constituting entire autonomous chemical plants.