

Section 3
Computer-aided Process Operation

Section 3 focuses on the application of computing technology to integrate and facilitate the key technical decision processes which arise in chemical manufacture. It comprises decision support systems at different levels of decision making. It discusses the problem of coordinated planning and scheduling of distributed plants at the top level, product sequencing, and precise allocation over time of detailed process operations resource constrained, coordination between units, process monitoring and regulatory control in a real-time environment extended to contemplate hybrid systems. An introduction to modeling the entire supply chain is also presented, which is further elaborated in Section 4.

Section 3 consists of seven chapters introducing the current problems facing process operations, the state of relevant methods and technology, and needed advances to combat ever-increasing complexity of computer-aided process operations in a business-wide context. Chapter 1 presents 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 and including a detailed critical discussion on the effect of uncertainty.

The emerging trend in the area of short-term scheduling is the development of efficient solution techniques and to render ever larger problems tractable. Chapter 2 deals with issues that must be resolved related mainly to problem scale. A sensible way forward is proposed by trying to capture the problem in all its complexity and then to explore rigorous or approximate solution procedures, rather than develop exact solutions to somewhat idealized problems. A final challenge relates to the seamless integration of the activities at different levels including data and functional fragmentation, inconsistencies between activities and datasets, and different tools being used for different activities, which are the subjects of subsequent chapters and sections.

The need for quality measurements to monitor process operations, evaluation of their efficiency and the equipment condition, thus avoiding equipment failure and any subsequent hazardous conditions is treated in Chapter 3. Recent progress in automatic data collection and current developments aiming at combining online data acquisition with data reconciliation are presented in detail. The measurement information can also be used in the control scheme in various ways. The weakest form of feedback is to use the measurements for parameter adaptation only, which requires a structurally correct model. Chapter 4 introduces model-based control techniques and points out new trends. The techniques use the combination of first principles-based and black-box models the parameters of which are estimated from operational data as a way to obtain sufficiently accurate models without excessive effort.

Online optimization using measurement information in many cases is an attractive alternative to the tracking of pre-computed references because the process can be

operated much closer to its real optimum, while still meeting hard bounds on the specifications. A rigorous treatment of real-time optimization problem is given in Chapter 5.

The last two chapters expand the concept of computer-aided process operations to also consider hybrid systems (Chapter 6) and the whole network of material procurement, material transformation to intermediates and final products, and distribution of these products to customers (Chapter 7). The need for integrated solutions will be further explored in Section 4.