

Section 4
Computer-integrated Approaches in CAPE

Section 4 presents a review on actual trends and shows new advances in the integration of software tools and process data. The material in this section is organized in five chapters.

Chapter 1 sets the goals for an integrated process and product design, possibly including the product application process in the analysis. Functions to be met by the product are the specifications. However, identifying a feasible chemical product is not enough, it needs to be produced through a sustainable process. Chapter 1 defines the general integrated chemical product-process design problem. The important issues and needs are identified with respect to their solution and illustrated through examples. Any CAPE method/tool needs to organize the scales and complexity levels so that the events at different scales can be described and understood: from property prediction at the nanoscale to phenomena occurring at the equipment scale. Integrated product-process design where modeling and supply chain issues play an important role is also highlighted.

Chapter 2 shows where, why, and how models of various types are used throughout the life of an industrial or manufacturing process. This justifies the need for tool and data integration across the process life cycle. Modeling addresses a diversity of goals, and relies on a range of forms, approaches, and tools. Models differ widely in the detail level, time, and length scale. Several industrial case studies help illustrate the challenges of modeling throughout the life cycle, since there is a huge range of models used to help answer vital sociotechnical questions through the life cycle of the process or product.

The last chapter of Section 3 has already presented the elementary principles and systematic methods of supply chain modeling and optimization. Chapter 3 shows how the practical implementation of supply chain management software suffers from several deficiencies, due to a limited focus or a lack of integration. To overcome these deficiencies and respond better to industrial demands facing a more dynamic environment, there is a need to explore new strategies for supply chain management. Integrated solutions are required for the next generation of software tools given the number and complex interactions present among main components in the global supply chain: financial flows, negotiation and environmental aspects need to be considered simultaneously along with a number of operating and design constraints. Agent-based systems are considered as a promising architecture for integration.

Reliable and consistent thermophysical property data for pure components and mixtures are essential for CAPE calculations. Chapter 4 reviews the data needed and the quality requirements. Major sources for physical properties and phase equilibrium data collections are compared. The text also provides up to date references to information sources available on the Internet.

The major issue in CAPE tools integration is to ensure software component interoperability and to allow seamless data exchange between tools. This issue is discussed in Chapter 5

that focuses on operational standards in the domain of CAPE, namely the CAPE-OPEN. Promising software interoperability standards, leading to service-oriented architectures and the emerging Semantic Web are also described. The organizational and economic consequences of the trend towards interoperability and standards in CAPE are also shortly described.