PREFACE

Over the past thirty years, *process synthesis* has had a major impact on the development, design, and operation of chemical processes. This field exploits key physical and chemical phenomena in the process, as well as their interactions, and it requires a systematic approach to address these phenomena. Process synthesis strategies have been developed for the design of heat-exchanger networks, utility systems, separation sequences, reactor networks, and control systems. While many strategies consider the design of these homogeneous systems separately, a key research question is the interaction of these subsystems and exploitation of this synergy for the overall synthesis of process flowsheets.

Synthesis methods began with the application of *heuristics* gathered by specific process knowledge and experience. This led naturally to early application of artificial intelligence tools and expert systems. Rigorous and elegant approaches then evolved through *problem representations* (i.e., conceptual/graphical representations), which are generally geometric in nature and are based on physical insights in the process. Unlike heuristics, these representations allow the development of provable ways to synthesize a process and demonstrate its superiority over an *ad hoc* procedure. Finally, quantitative approaches are also needed, especially in assessing trade-offs among design criteria and interactions between subsystems that could not be addressed directly with simple rules or simple representations. As optimization strategies were developed and refined to handle larger and more difficult problems, *optimization-based* formulations of these problems led to powerful strategies for process synthesis.

Today it is recognized that all three approaches (heuristics-based selection, geometric representation, and optimization methods) are useful, and indeed required, for complex process synthesis strategies. This follows because different applications lend themselves to quite different representations. This volume addresses a variety of these synthesis strategies for process subsystems, but represents only a sampling of the state-of-the-art of process synthesis research. The five chapters in this volume address quite different process subsystems and application areas but still combine basic concepts related to a systematic approach.

The first chapter, by Siirola, reviews the impact of process synthesis in industry and shows how process synthesis fits into the innovation process within industrial manufacturing and research. It also highlights a number of industrial successes leading to substantial energy savings and overall cost reductions. Most of these savings are in the areas of distillation sequences, and examples include heat-integrated separation sequences and separation of azeotropic systems.

The second chapter, by Westerberg and Wahnschafft, further develops the synthesis of nonideal separation sequences through the use of physical insights, artificial intelligence, shortcut models, and geometric constructions. Using a combination of these approaches, as illustrated with a number of examples, the strategy in this chapter yields complex separation sequences that guarantee the separation of nonideal mixtures into desired products.

The third chapter, by Grossmann, develops an overall framework for algorithmic process synthesis. This framework is applied to heat-exchanger network synthesis, separation sequences, and superstuctures for total flowsheets. These examples are formulated and solved as mixed integer nonlinear programs (MINLP) which deal with the optimization of discrete (structural) and continuous decisions. Illustrated with numerous process synthesis formulations, the chapter reviews MINLP algorithms and also discusses the incorporation of logic constraints and heuristics in developing a qualitative/quantitative framework for process synthesis.

The fourth chapter, by Balakrishna and Biegler, deals with the difficult problem of reactor network synthesis. These systems are generally very nonlinear and nonconvex, and both heuristic- and optimization-based approaches can lead to nonunique and only locally optimal solutions—an undesirable situation. The paper combines geometric concepts from attainable regions (AR) of the reactor network with an optimization-based approach. The AR concepts, recently developed by Glasser and co-workers, lead to insights that offer smaller, simpler, and superior NLP (nonlinear programming) and MINLP formulations for this system. This approach is demonstrated on numerous examples, including some that interact with other flowsheet subsystems.

The last chapter, by Walsh and Perkins, deals with an optimization-based approach for operability and control in process synthesis and design. Process control is often performed after the design is completed, without considering control and operability at the design stage. This chapter shows strong interactions of design and control and develops a comprehensive strategy for these systems. Centered around the optimization of dynamic systems with uncertainty, a strategy is developed to guarantee good control structures over a large variety of disturbances. This approach is applied to an industrial wastewater treatment process with impressive results.

All of the chapters develop highly successful synthesis methods for their respective cutting-edge applications. Nevertheless, they also highlight many unresolved issues in process synthesis and give guidelines for future research. As a result, there are still many challenging research issues in this active field. It is our hope that this volume points these out and spurs future research in this area.

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