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Process Synthesis

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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.

Lorenz T. Biegler

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INDUSTRIAL APPLICATIONS OF CHEMICAL PROCESS SYNTHESIS

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Systematic approaches for the invention of conceptual chemical process designs have been proposed and discussed for more than twenty-five years. During that same time, the importance of front-end engineering, especially conceptual design, to product quality, health and safety, environmental impact, energy consumption, operability, capital and operating costs, and overall competitiveness has become

ever more apparent. A number of process synthesis frameworks, approaches, methods, and tools have now been developed to the point of industrial application. This chapter describes a framework for the industrial chemical plant innovation process, showing how process synthesis fits into that structure and how that framework has in turn influenced the development of systematic process synthesis methods. It also describes a number of industrial case studies in which process synthesis techniques have been successfully applied to the conceptual design of total process flowsheets, as well as to specific design subproblems including heat-integrated distillation trains, multiple-effect distillation, and the separation of azeotropic systems. Typical energy savings of 50% and net present cost reductions of 35% have been achieved in industrial practice using systematic process synthesis methodologies. Even greater benefits are expected to be realized as the next generation of approaches currently being developed is transferred to industry.

I. Introduction

The manufacturing sector of the chemical processing industry is generally in the business of making materials rather than making artifacts. This is done in response to perceived needs and the belief that the materials offered will satisfy these needs in a valuable manner.

In contrast with artifact-making, material-making tends to involve more conversion and transformation than assembly, and is generally more capital- and energy-intensive than labor-intensive. Material-making sometimes involves substances that are toxic or otherwise hazardous to the environment. Furthermore, since material-making equipment costs are often sublinear functions of capacity, material-making facilities tend to be large and aggregated to take advantage of economies of scale, integrated material and energy flows, and centralized environmental mitigation. Many material-making facilities have very long operating lives, much longer than the life of many artifacts and most artifact-making machinery.

Chemical manufacturing plants come into existence through a series of actions sometimes called the *innovation process*. This process leads from the identification of a need to the operation of a material-making facility. The characteristics of material-making—relatively few but fairly large manufacturing facilities, very long operating lives, high initial capital costs, high continuing operating costs, and potential environmental impacts—place special importance on sound implementation of the innovation process and, in particular, on making good engineering design decisions within that process.

All existing chemical process designs were somehow invented. Some, especially lower volume products involving complex chemistry, have been implemented by a rather straightforward extrapolation of the laboratory procedure used to experimentally demonstrate the transformation of available raw materials into the desired product. Larger volume products, on the other hand, are more often implemented as continuous processes that bear little resemblance to either the procedure or the equipment used in the laboratory. Generally there is a combinatorially very large number of alternative pieces of equipment and interconnections among these pieces of equipment that will feasibly implement the desired chemistry. Identifying better process alternatives is a key activity within the innovation process.

Successful design engineers seem to build and evolve conceptual process flowsheets from a rich repertoire of past experiences and design heuristics. Such an experience base generally includes an extensive knowledge of available equipment, simple and complex unit operations, standard tricks or patterns (for example, strategies for breaking azeotropes), encyclopedias of complete flowsheets for existing chemicals, and some sense of hierarchy of which process design problems to tackle in what order and at what level of detail. This wealth of background information is copied directly or modified as necessary to fit the situation at hand. Generally time and resource constraints limit the number of conceptual process alternatives that may be generated and evaluated by the designer to a tiny fraction of the total number feasible. The key to discovering alternatives with superior economics is the judicious use of modern methods and tools together with a little good luck.

Occasionally, process designs are produced that are conceded by those skilled in the art as being *clever.* Perhaps most, if not all, world-beating designs exhibiting superior economics exploit something clever. What is technically feasible, what is competent, and what is clever process design? Is there a *best* design that cannot be beaten? Can the invention of chemical process designs be organized, systematized, or even automated? How can more or better alternatives be generated? These questions have been the focus of process synthesis research over the last twenty-five years. It is not the intention of this chapter to discuss the latest advances in that research. Rather, it is to illustrate that some of these results are beginning to have a real impact on industrial practice.

II. Industrial Chemical Process Innovation

To understand chemical process synthesis in an industrial environment, it may be useful to first discuss the chemical innovation process. *Invention* is discovery. A new material composition may be invented. The chemistry to transform raw materials into this new composition may be invented. The process flowsheet to implement this chemistry on an industrial scale may also be invented. But the invention of a flowsheet does not guarantee that the chemistry will be reduced to practice in an economical manner. That is accomplished by *innovation,* an organized multistage goal-directed process, which leads from the identification of a customer's need to the operation of a facility to produce a material believed to address that need.

The innovation process may be implemented in a number of different ways. The specific details and emphasis within the innovation process may differ, depending on whether the objective is to build a pioneering facility for a new chemical or an improved facility for an existing chemical. But in general, a product that addresses the need must be (or has already been) identified; a chemical route must be found from available raw materials that produces this desired product; and a facility that implements this chemistry must be conceived, designed, constructed, started, operated, and maintained (Fig. 1). Of special interest in the context of conceptual process design are the stages *basic chemistry* (in which the fundamental reaction chemistry is selected), *detailed chemistry* (in which supporting chemical details of catalysis, solvents, and reaction conditions

- **Need Identification**
- **Manufacturing Decision**
- **Basic Chemistry**
- **Detailed Chemistry**
- **Task Identification**
- **Unit Operations**
- **Basic Plant Engineering**
- **Detailed Engineering**
- **Vendor Specifications**
- **Component Acquisition**
- **Construction Plan and Schedule**
- **Plant Construction**
- **Operating Procedures**
- **Commissioning and Start-up**
- **Production Plan and Schedule**
- **Plant Operation and Maintenance**

FIG. 1. Innovation process sequence.

are defined), *task identification* (in which the physical operations to prepare raw materials for reaction and isolate reaction products for sale are identified), *unit operations* (in which the chemical and physical operations previously identified are associated with actual pieces of equipment), and *basic plant engineering* (where the supporting utilities and other facilities infrastructure are defined).

Each stage of the innovation process is in a sense implemented by all of the stages that follow. Consequently, there is a great deal of interaction among the stages. For example, the choices that can be made at one stage are clearly limited by selections made during previous stages. At the same time, the optimal choice to be made among alternatives identified at any stage may well depend on costs associated with subsequent stages that implement that choice but have yet to be addressed. Earlier stages are both less well-defined and less constrained than later stages. However, decisions made in these earlier stages typically prove to have a greater impact on the overall economic outcome of the entire venture. Because of the interacting nature of the stages, it is often necessary to revisit stages or iterate among the stages in order to converge to an acceptable solution.

A. Multiple Levels of Detail

Because of the interacting nature of the innovation process stages, it is possible that each visit to a stage may be approached with a slightly different objective or even conducted at different levels of detail. For example, each stage of the innovation process might be visited four times (Fig. 2).

1. The first pass through any stage of the innovation process is at the lowest level of detail, which might be called the *targeting* level. Its purpose might be to get a rough indication of what is to be accomplished at that stage of the innovation process as well as to see what is likely to be feasible given the choices that have been made previously in the process. Targeting is already familiar in the context of heat-integration networks where fairly simple analytical procedures can give much information about what is technically and perhaps economically feasible by bounding the expected performance even before the generation of any heat-exchanger network alternatives.
2. The second pass through each innovation stage might be called the *preliminary* or *conceptual* level. Here, a tentative, not too detailed solution to the given innovation problem is conceived. One general design paradigm to accomplish this essentially consists of a four-block procedure, as shown in Fig. 3. In the first *formulation* block, the goals for the particular stage of the innovation process are specified. This is followed by an iteration of three blocks consisting of *synthesis* (generation of a solution

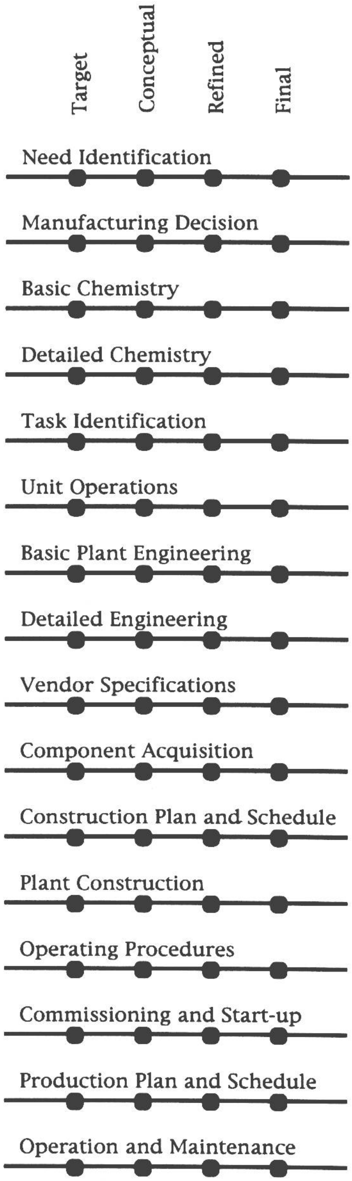

FIG. 2. Innovation process levels of detail.

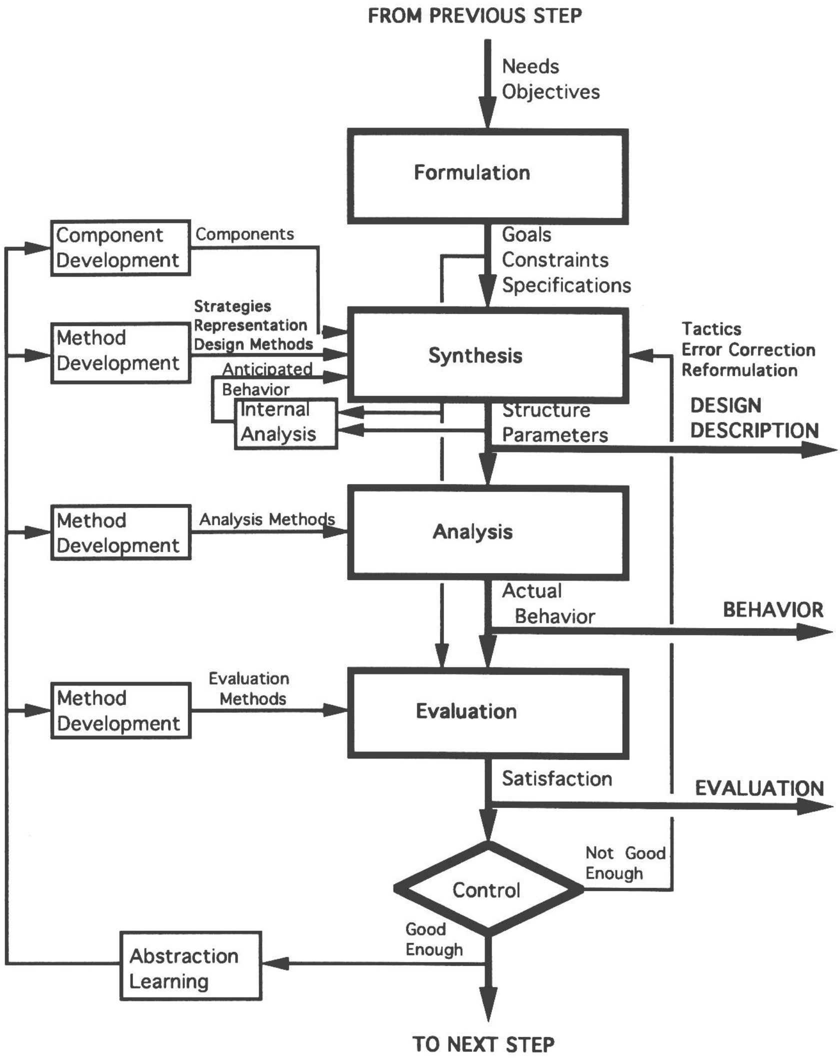

FIG. 3. General design paradigm.

alternative from available components), *analysis* (determination of the behavior of the alternative generated), and *evaluation* (comparison of the performance of the proposed alternative against the goals specified by the formulation block). If the performance of the proposed solution is judged to be satisfactory, the step is completed; otherwise, a new alternative must be generated, analyzed, and evaluated. In general, alternatives are not gen-