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# PREFACE

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THE CHEMICAL INDUSTRY has undergone significant changes during the past 25 years due to the increased cost of energy, increasingly stringent environmental regulations, and global competition in product pricing and quality. One of the most important engineering tools for addressing these issues is optimization. Modifications in plant design and operating procedures have been implemented to reduce costs and meet constraints, with an emphasis on improving efficiency and increasing profitability. Optimal operating conditions can be implemented via increased automation at the process, plant, and company levels, often called computer-integrated manufacturing, or CIM. As the power of computers has increased, following Moore's Law of doubling computer speeds every 18 months, the size and complexity of problems that can be solved by optimization techniques have correspondingly expanded. Effective optimization techniques are now available in software for personal computers—a capability that did not exist 10 years ago.

To apply optimization effectively in the chemical industries, both the theory and practice of optimization must be understood, both of which we explain in this book. We focus on those techniques and discuss software that offers the most potential for success and gives reliable results.

The book introduces the necessary tools for problem solving. We emphasize how to formulate optimization problems appropriately because many engineers and scientists find this phase of their decision-making process the most exasperating and difficult. The nature of the model often predetermines the optimization algorithm to be used. Because of improvements in optimization algorithms and software, the modeling step usually offers more challenges and choices than the selection of the optimization technique. Appropriate meshing of the optimization technique and the model are essential for success in optimization. In this book we omit rigorous optimization proofs, replacing them with geometric or plausibility arguments without sacrificing correctness. Ample references are cited for those who wish to explore the theoretical concepts in more detail.

The book contains three main sections. Part I describes how to specify the three key components of an optimization problem, namely the

1. Objective function
2. Process model
3. Constraints

Part I comprises three chapters that motivate the study of optimization by giving examples of different types of problems that may be encountered in chemical engineering. After discussing the three components in the previous list, we describe six steps that must be used in solving an optimization problem. A potential user of optimization must be able to translate a verbal description of the problem into the appropriate mathematical description. He or she should also understand how the problem formulation influences its solvability. We show how problem simplification, sensitivity analysis, and estimating the unknown parameters in models are important steps in model building. Chapter 3 discusses how the objective function should be developed. We focus on economic factors in this chapter and present several alternative methods of evaluating profitability.

Part II covers the theoretical and computational basis for proven techniques in optimization. The choice of a specific technique must mesh with the three components in the list. Part II begins with Chapter 4, which provides the essential conceptual background for optimization, namely the concepts of local and global optima, convexity, and necessary and sufficient conditions for an optimum. Chapter 5 follows with a brief explanation of the most commonly used one-dimensional search methods. Chapter 6 presents reliable unconstrained optimization and methods. Chapter 7 treats linear programming theory, applications, and software, using matrix methods. Chapter 8 covers recent advances in nonlinear programming methods and software, and Chapter 9 deals with optimization of discrete processes, highlighting mixed-integer programming problems and methods. We conclude Part II with a new chapter (for the second edition) on global optimization methods, such as tabu search, simulated annealing, and genetic algorithms. Only deterministic optimization problems are treated throughout the book because lack of space precludes discussing stochastic variables, constraints, and coefficients.

Although we include many simple applications in Parts I and II to illustrate the optimization techniques and algorithms, Part III of the book is exclusively devoted to illustrations and examples of optimization procedures, classified according to their applications: heat transfer and energy conservation (Chapter 11), separations (Chapter 12), fluid flow (Chapter 13), reactor design (Chapter 14), and plant design (Chapter 15), and a new chapter for the second edition on planning, scheduling, and control using optimization techniques (Chapter 16). Many students and professionals learn by example or analogy and often discover how to solve a problem by examining the solution to similar problems. By organizing applications of optimization in this manner, you can focus on a single class of applications of particular interest without having to review the entire book. We present a spectrum of modeling and solution methods in each of these chapters. The introduction to Part III lists each application classified by the technique employed. In some cases the

optimization method may be an analytical solution, leading to simple design rules; most examples illustrate numerical methods. In some applications the problem statement may be so complex that it cannot be explicitly written out, as in plant design and thus requires the use of a process simulator. No exercises are included in Part III, but an instructor can (1) modify the variables, parameters, conditions, or constraints in an example, and (2) suggest a different solution technique to obtain exercises for solution by students.

An understanding of optimization techniques does not require complex mathematics. We require as background only basic tools from multivariable calculus and linear algebra to explain the theory and computational techniques and provide you with an understanding of how optimization techniques work (or, in some cases, fail to work).

Presentation of each optimization technique is followed by examples to illustrate an application. We also have included many practically oriented homework problems. In university courses, this book could be used at the upper-division or the first-year graduate levels, either in a course focused on optimization or on process design. The book contains more than enough material for a 15-week course on optimization. Because of its emphasis on applications and short case studies in Chapters 11–16, it may also serve as one of the supplementary texts in a senior unit operations or design course.

In addition to use as a textbook, the book is also suitable for use in individual study, industrial practice, industrial short courses, and other continuing education programs.

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