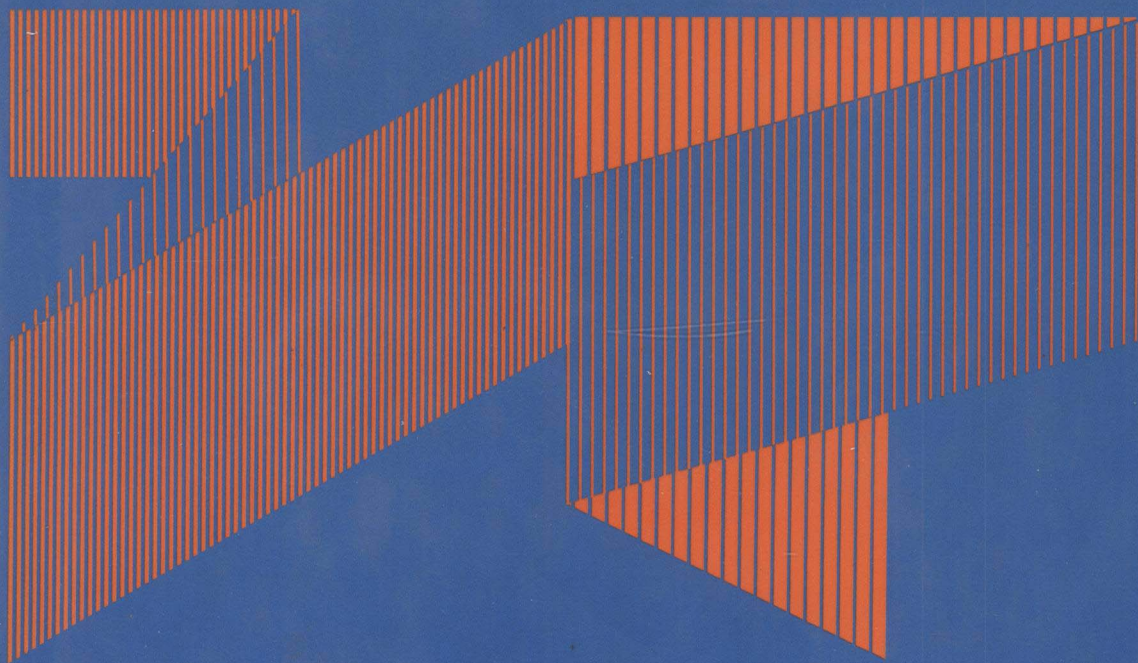

OPTIMIZATION OF CHEMICAL PROCESSES



T.F. EDGAR

D.M. HIMMELBLAU

OPTIMIZATION OF CHEMICAL PROCESSES

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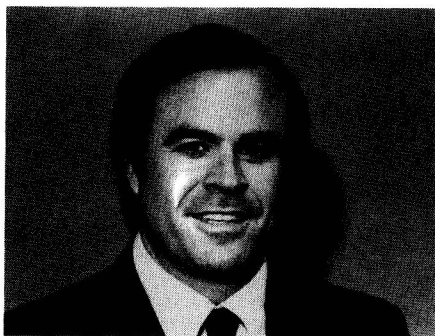
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PREFACE

The chemical industry has undergone significant changes during the past 15 years due to the increased cost of energy and increasingly stringent environmental regulations. Modification of both plant design procedures and plant operating conditions have been implemented in order to reduce costs and meet constraints. Most industry observers believe that the emphasis in the near future will be on improving efficiency and increasing profitability of existing plants rather than on plant expansion. One of the most important engineering tools that can be employed in such activities is optimization. As computers have become more powerful, the size and complexity of problems which can be solved by optimization techniques have correspondingly expanded.

To be able to make the most effective applications of optimization in the chemical process industries, you must understand both the theory *and* the practice of optimization, both of which are explained in this book. Optimization algorithms have reached a degree of maturity in recent years due to the extensive evaluation of proposed optimization techniques on a wide range of problems. We have chosen to focus on only the few superior techniques that offer the most potential for success and give reliable results, rather than on an extensive coverage of algorithms proposed in the optimization literature.

The book is intended to be introductory in nature in presenting the necessary tools for problem solving. We have placed more emphasis on how to formulate optimization problems appropriately than on the theory underlying optimization algorithms because many engineers and scientists find this phase of their decision-making process the most exasperating and difficult. In the book rigorous proofs are omitted, being replaced by 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. Because of the importance of problem formulation, Part I of the book presents the methodology of

how to specify the three key components of an optimization problem, namely,

1. The objective function
2. The process model
3. The constraints

Part I, comprised of three chapters, motivates the study of optimization by giving examples of different types of problems that may be encountered in chemical engineering. After discussing the three essential features of every optimization problem, we provide a list of six steps that must be used to varying degrees in solving an optimization problem. It is important that a potential user of optimization techniques be able to translate a verbal description of the problem into the appropriate mathematical description. It is also important for a user to understand how the problem formulation has a major impact on the ease of problem solution. We show how problem simplification and sensitivity analysis are important steps in analysis of model-building and estimating the unknown parameters in models. 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 listed above. Part II begins with a chapter (Chap. 4) that provides the essential conceptual background for optimization, namely the concepts of convexity, concavity, necessary and sufficient conditions for an extremum, and the Hessian matrix. Chapter 5 follows with a brief explanation of one-dimensional search methods. We choose to describe only a few effective ones. Chapter 6 presents reliable unconstrained optimization and methods. Chapter 7 treats linear programming theory and applications using both graphical and matrix methods to illustrate and emphasize the concepts involved. Chapter 8 covers modern nonlinear programming methods, mainly the generalized reduced gradient method, augmented Lagrange method, and successive quadratic programming. We conclude Part II with a chapter on optimization of staged and discrete processes, highlighting mixed-integer programming problems and methods. Only deterministic optimization problems are treated throughout the book as lack of space precludes 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 and examples classified according to their applications: heat transfer and energy conservation (Chap. 10), separations (Chap. 11), fluid flow (Chap. 12), reactor design (Chap. 13), and plant design (Chap. 14). Many students and professionals learn by example or analogy and often find out 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 requiring extensive review of the book. We present a spectrum of different methods in each of these chapters rather than overemphasize a few selected techniques. The Introduction to Part III lists each application classified by the technique employed. In some cases the optimization method may be analytical, leading to simple design rules; other 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 (a) modify the variables, parameters, conditions, or constraints in an example, and (b) suggest a different technique of solution, to obtain exercises for solution by students.

An understanding of optimization techniques does not require complex mathematics. We require as background only a few tools from 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). We have included two appendices in the book as supplementary reading for those without the necessary mathematical background.

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, and the material has been used for such courses at the University of Texas. The book contains more than enough material for a 15-week course on optimization, and, because of its emphasis on applications, it may also serve as one of the supplementary texts in a senior design course.

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

We wish to acknowledge the helpful suggestions of several colleagues in developing this book, especially Yaman Arkun, Georgia Institute of Technology; Lorenz T. Biegler, Carnegie-Mellon University; James R. Couper, University of Arkansas; James Fair, University of Texas-Austin; Ignacio Grossman, Carnegie-Mellon University; K. Jayaraman, Michigan State University; I. Lefkowitz, Case Western Reserve University; Leon Lasdon, University of Texas; and Mark Stadtherr, University of Illinois-Urbana Champaign. Several of the examples in Chap. 10 through 14 were provided by friends in industry and in universities and are acknowledged there. We also recognize the help of many graduate students in developing solutions to the examples.

T. F. Edgar
D. M. Himmelblau

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