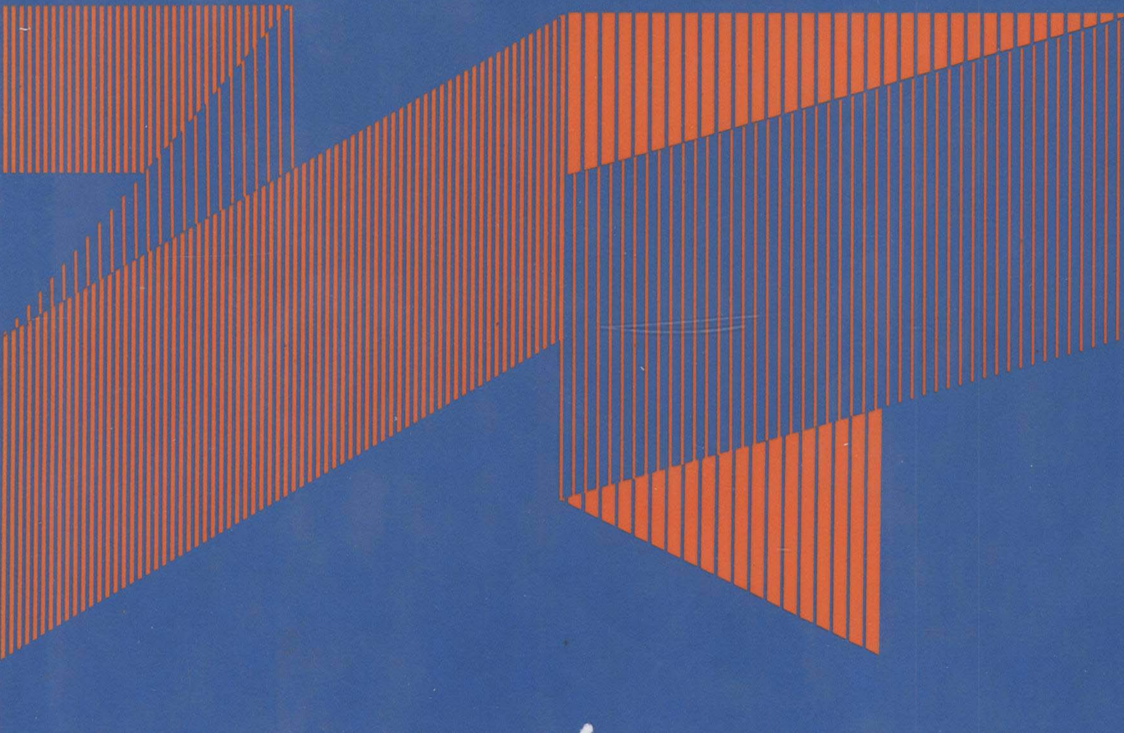
OPTIMIZATION OF CHEMICAL PROCESSES



T.F. EDGAR
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OPTIMIZATION OF CHEMICAL PROCESSES

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OPTIMIZATION OF CHEMICAL PROCESSES

BUILDING THE LITERATURE OF A PROFESSION

Fifteen prominent chemical engineers first met in New York more than 60 years ago to plan a continuing literature for their rapidly growing profession. From industry came such pioneer practitioners as Leo Baekeland, Arthur D. Little, Charles L. Reese, John V. N. Dorr, M. C. Whitaker, and R. S. McBride. From the universities came such eminent educators as William H. Walker, Alfred H. White, D. D. Jackson, J. H. James, Warren K. Lewis, and Harry A. Curtis. H. C. Parmelee, then editor of *Chemical and Metallurgical Engineering*, served as chairman and was joined subsequently by S. D. Kirkpatrick as consulting editor.

After several meetings, this committee submitted its report to the McGraw-Hill Book Company in September 1925. In the report were detailed specifications for a correlated series of more than a dozen texts and reference books which have since become the McGraw-Hill Series in Chemical Engineering and which became the cornerstone of the chemical engineering curriculum.

From this beginning there has evolved a series of texts surpassing by far the scope and longevity envisioned by the founding Editorial Board. The McGraw-Hill Series in Chemical Engineering stands as a unique historical record of the development of chemical engineering education and practice. In the series one finds the milestones of the subject's evolution: industrial chemistry, stoichiometry, unit operations and processes, thermodynamics, kinetics, and transfer operations.

Chemical engineering is a dynamic profession, and its literature continues to evolve. McGraw-Hill and its consulting editors remain committed to a publishing policy that will serve, and indeed lead, the needs of the chemical engineering profession during the years to come.

THE SERIES

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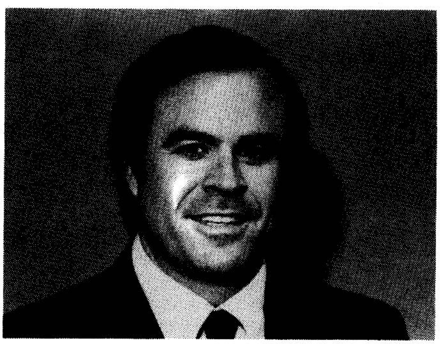
ABOUT THE AUTHORS



Thomas F. Edgar is professor and chairman of chemical engineering at the University of Texas at Austin. He earned his B.S. in chemical engineering from the University of Kansas and received his Ph.D. from Princeton University. Before receiving his doctorate, he was employed by Continental Oil Company. He is General Editor of the technical journal *In Situ* and a consultant to a number of companies in the field of process control. Professional honors include selection as the 1980 winner of the AIChE Colburn Award, Outstanding AIChE Student Chapter Counselor in 1974, and Katz Lecturer at the University of Michigan in 1981. He is listed in *Who's Who in America.*

He has published over 100 papers in the fields of process control, optimization, and mathematical modeling of processes such as separations and combustion. He is coauthor of the book *Chemical Process Control* (John Wiley, 1988) and author of *Coal Processing and Pollution Control Technology*, published by Gulf Publishing Company in 1983. Dr. Edgar has also been Chairman of the CAST Division of AIChE in 1986 and President of the CACHE Corporation from 1981 to 1984.

David M. Himmelblau is the Bob R. Dorsey Professor of Chemical Engineering at the University of Texas at Austin. He received his B.S. degree from the Massachusetts Institute of Technology and M.S. and Ph.D. degrees from Washington University. He has taught at the University of Texas at Austin for over 25 years. Prior to that time he worked for companies such as the International Harvester Company, Simpson Logging Company and Excel Battery Company.

Among his more than 160 publications are 11 books including one of the most widely used introductory books in chemical engineering, books on process analysis and simulation, decomposition, fault detection in chemical processes, and applied nonlinear programming. He has served in a number of positions in the AIChE including Chairman of the Educational Projects Committee, the Student Chapters Committee, and the CAST Division. From 1974 to 1976 he was a Director of the AIChE. His principal areas of research are in fault detection and diagnosis, process analysis and simulation, and optimization, and he also has been extensively involved in the development of computer-aided instructional materials for chemical engineers.

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.

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CONTENTS