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# OPTIMIZATION OF CHEMICAL PROCESSES

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SECOND EDITION

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## OPTIMIZATION OF CHEMICAL PROCESSES, SECOND EDITION

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# CONTENTS

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|                   |     |
|-------------------|-----|
| Preface           | xi  |
| About the Authors | xiv |

## **PART I Problem Formulation**

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|  |               |
|--|---------------|
| <b>1 The Nature and Organization of Optimization Problems</b>                                    | <b>3</b>      |
| 1.1 What Optimization Is All About   | 4             |
| 1.2 Why Optimize?  | 4             |
| 1.3 Scope and Hierarchy of Optimization  | 5             |
| 1.4 Examples of Applications of Optimization   | 8             |
| 1.5 The Essential Features of Optimization Problems  | 14            |
| 1.6 General Procedure for Solving Optimization Problems  | 18            |
| 1.7 Obstacles to Optimization  | 26            |
| References   | 27            |
| Supplementary References   | 27            |
| Problems   | 28            |
| <br><b>2 Developing Models for Optimization</b>  | <br><b>37</b> |
| 2.1 Classification of Models   | 41            |
| 2.2 How to Build a Model   | 46            |
| 2.3 Selecting Functions to Fit Empirical Data  | 48            |
| 2.3.1 <i>How to Determine the Form of a Model</i> / 2.3.2 <i>Fitting Models by Least Squares</i> |               |
| 2.4 Factorial Experimental Designs   | 62            |
| 2.5 Degrees of Freedom   | 66            |
| 2.6 Examples of Inequality and Equality Constraints in Models                                    | 69            |
| References   | 73            |
| Supplementary References   | 73            |
| Problems   | 74            |

|          |  |           |
|----------|--|-----------|
| <b>3</b> | <b>Formulation of the Objective Function</b>   | <b>83</b> |
| 3.1      | Economic Objective Functions                   | 84        |
| 3.2      | The Time Value of Money in Objective Functions | 91        |
| 3.3      | Measures of Profitability                      | 100       |
|          | References                                     | 104       |
|          | Supplementary References                       | 104       |
|          | Problems                                       | 105       |

## Part II Optimization Theory and Methods

---

|          |   |            |
|----------|---|------------|
| <b>4</b> | <b>Basic Concepts of Optimization</b>   | <b>113</b> |
| 4.1      | Continuity of Functions   | 114        |
| 4.2      | NLP Problem Statement   | 118        |
| 4.3      | Convexity and Its Applications  | 121        |
| 4.4      | Interpretation of the Objective Function in Terms of its Quadratic Approximation  | 131        |
| 4.5      | Necessary and Sufficient Conditions for an Extremum of an Unconstrained Function  | 135        |
|          | References  | 142        |
|          | Supplementary References  | 142        |
|          | Problems  | 142        |
| <b>5</b> | <b>Optimization of Unconstrained Functions: One-Dimensional Search</b>  | <b>152</b> |
| 5.1      | Numerical Methods for Optimizing a Function of One Variable   | 155        |
| 5.2      | Scanning and Bracketing Procedures  | 156        |
| 5.3      | Newton and Quasi-Newton Methods of Unidimensional Search  | 157        |
|          | 5.3.1 <i>Newton's Method</i> / 5.3.2 <i>Finite Difference Approximations to Derivatives</i> / 5.3.3 <i>Quasi-Newton Method</i>  |            |
| 5.4      | Polynomial Approximation Methods  | 166        |
|          | 5.4.1 <i>Quadratic Interpolation</i> / 5.4.2 <i>Cubic Interpolation</i>   |            |
| 5.5      | How One-Dimensional Search Is Applied in a Multidimensional Problem   | 173        |
| 5.6      | Evaluation of Unidimensional Search Methods   | 176        |
|          | References  | 176        |
|          | Supplementary References  | 177        |
|          | Problems  | 177        |
| <b>6</b> | <b>Unconstrained Multivariable Optimization</b>   | <b>181</b> |
| 6.1      | Methods Using Function Values Only  | 183        |
|          | 6.1.1 <i>Random Search</i> / 6.1.2 <i>Grid Search</i> / 6.1.3 <i>Univariate Search</i> / 6.1.4 <i>Simplex Search Method</i> / 6.1.5 <i>Conjugate Search Directions</i> / 6.1.6 <i>Summary</i> |            |
| 6.2      | Methods That Use First Derivatives  | 189        |
|          | 6.2.1 <i>Steepest Descent</i> / 6.2.2 <i>Conjugate Gradient Methods</i>   |            |

|            |  |            |
|------------|--|------------|
| <b>6.3</b> | <b>Newton's Method</b>   | <b>197</b> |
|            | <i>6.3.1 Forcing the Hessian Matrix to Be Positive-Definite /</i>    |            |
|            | <i>6.3.2 Movement in the Search Direction / 6.3.3 Termination /</i>  |            |
|            | <i>6.3.4 Safeguarded Newton's Method / 6.3.5 Computation of</i>      |            |
|            | <i>Derivatives</i>   |            |
| <b>6.4</b> | <b>Quasi-Newton Methods</b>  | <b>208</b> |
|            | References   | 210        |
|            | Supplementary References   | 211        |
|            | Problems   | 211        |
| <b>7</b>   | <b>Linear Programming (LP) and Applications</b>                      | <b>222</b> |
| 7.1        | Geometry of Linear Programs  | 223        |
| 7.2        | Basic Linear Programming Definitions and Results                     | 227        |
| 7.3        | Simplex Algorithm  | 233        |
| 7.4        | Barrier Methods  | 242        |
| 7.5        | Sensitivity Analysis   | 242        |
| 7.6        | Linear Mixed Integer Programs  | 243        |
| 7.7        | LP Software  | 243        |
| 7.8        | A Transportation Problem Using the EXCEL Solver                      |            |
|            | Spreadsheet Formulation  | 245        |
| 7.9        | Network Flow and Assignment Problems                                 | 252        |
|            | References   | 253        |
|            | Supplementary References   | 253        |
|            | Problems   | 254        |
| <b>8</b>   | <b>Nonlinear Programming with Constraints</b>                        | <b>264</b> |
| 8.1        | Direct Substitution  | 265        |
| 8.2        | First-Order Necessary Conditions for a Local Extremum                | 267        |
|            | <i>8.2.1 Problems Containing Only Equality Constraints /</i>         |            |
|            | <i>8.2.2 Problems Containing Only Inequality Constraints /</i>       |            |
|            | <i>8.2.3 Problems Containing both Equality and Inequality</i>        |            |
|            | <i>Constraints</i>   |            |
| 8.3        | Quadratic Programming  | 284        |
| 8.4        | Penalty, Barrier, and Augmented Lagrangian Methods                   | 285        |
| 8.5        | Successive Linear Programming  | 293        |
|            | <i>8.5.1 Penalty Successive Linear Programming</i>                   |            |
| 8.6        | Successive Quadratic Programming                                     | 302        |
| 8.7        | The Generalized Reduced Gradient Method                              | 306        |
| 8.8        | Relative Advantages and Disadvantages of NLP Methods                 | 318        |
| 8.9        | Available NLP Software   | 319        |
|            | <i>8.9.1 Optimizers for Stand-Alone Operation or Embedded</i>        |            |
|            | <i>Applications / 8.9.2 Spreadsheet Optimizers / 8.9.3 Algebraic</i> |            |
|            | <i>Modeling Systems</i>  |            |
| 8.10       | Using NLP Software   | 323        |
|            | <i>8.10.1 Evaluation of Derivatives: Issues and Problems /</i>       |            |
|            | <i>8.10.2 What to Do When an NLP Algorithm Is Not "Working"</i>      |            |

|  |            |
|--|------------|
| References   | 328        |
| Supplementary References   | 329        |
| Problems   | 329        |
| <b>9 Mixed-Integer Programming</b>   | <b>351</b> |
| 9.1 Problem Formulation  | 352        |
| 9.2 Branch-and-Bound Methods Using LP Relaxations  | 354        |
| 9.3 Solving MINLP Problems Using Branch-and-Bound Methods  | 361        |
| 9.4 Solving MINLPs Using Outer Approximation   | 369        |
| 9.5 Other Decomposition Approaches for MINLP   | 370        |
| 9.6 Disjunctive Programming  | 371        |
| References   | 372        |
| Supplementary References   | 373        |
| Problems   | 374        |
| <b>10 Global Optimization for Problems with Continuous and Discrete Variables</b>  | <b>381</b> |
| 10.1 Methods for Global Optimization   | 382        |
| 10.2 Smoothing Optimization Problems   | 384        |
| 10.3 Branch-and-Bound Methods  | 385        |
| 10.4 Multistart Methods  | 388        |
| 10.5 Heuristic Search Methods  | 389        |
| 10.5.1 Heuristic Search / 10.5.2 Tabu Search / 10.5.3 Simulated Annealing / 10.5.4 Genetic and Evolutionary Algorithms / 10.5.5 Using the Evolutionary Algorithm in the Premium Excel Solver / 10.5.6 Scatter Search |            |
| 10.6 Other Software for Global Optimization  | 411        |
| References   | 412        |
| Supplementary References   | 413        |
| <br><b>Part III Applications of Optimization</b>   |            |
| <b>11 Heat Transfer and Energy Conservation</b>  | <b>417</b> |
| Example 11.1 Optimizing Recovery of Waste Heat   | 419        |
| Example 11.2 Optimal Shell-and-Tube Heat Exchanger Design  | 422        |
| Example 11.3 Optimization of a Multi-Effect Evaporator   | 430        |
| Example 11.4 Boiler/Turbo-Generator System Optimization  | 435        |
| References   | 438        |
| Supplementary References   | 439        |
| <b>12 Separation Processes</b>   | <b>441</b> |
| Example 12.1 Optimal Design and Operation of a Conventional Staged-Distillation Column   | 443        |

|                     |  |     |
|---------------------|--|-----|
| <b>Example 12.2</b> | Optimization of Flow Rates in a Liquid–Liquid Extraction Column  | 448 |
| <b>Example 12.3</b> | Fitting Vapor–Liquid Equilibrium Data Via Nonlinear Regression   | 451 |
| <b>Example 12.4</b> | Determination of the Optimal Reflux Ratio for a Staged-Distillation Column   | 453 |
|                     | References   | 458 |
|                     | Supplementary References   | 458 |
| <b>13</b>           | <b>Fluid Flow Systems</b>  | 460 |
| <b>Example 13.1</b> | Optimal Pipe Diameter  | 461 |
| <b>Example 13.2</b> | Minimum Work of Compression  | 464 |
| <b>Example 13.3</b> | Economic Operation of a Fixed-Bed Filter   | 466 |
| <b>Example 13.4</b> | Optimal Design of a Gas Transmission Network   | 469 |
|                     | References   | 478 |
|                     | Supplementary References   | 478 |
| <b>14</b>           | <b>Chemical Reactor Design and Operation</b>   | 480 |
| <b>Example 14.1</b> | Optimization of a Thermal Cracker Via Linear Programming   | 484 |
| <b>Example 14.2</b> | Optimal Design of an Ammonia Reactor   | 488 |
| <b>Example 14.3</b> | Solution of an Alkylation Process by Sequential Quadratic Programming  | 492 |
| <b>Example 14.4</b> | Predicting Protein Folding   | 495 |
| <b>Example 14.5</b> | Optimization of Low-Pressure Chemical Vapor Deposition Reactor for the Deposition of Thin Films                    | 500 |
| <b>Example 14.6</b> | Reaction Synthesis Via MINLP   | 508 |
|                     | References   | 513 |
|                     | Supplementary References   | 514 |
| <b>15</b>           | <b>Optimization in Large-Scale Plant Design and Operations</b>   | 515 |
| <b>15.1</b>         | Process Simulators and Optimization Codes  | 518 |
| <b>15.2</b>         | Optimization Using Equation-Based Process Simulators   | 525 |
| <b>15.3</b>         | Optimization Using Modular-Based Simulators  | 537 |
|                     | <i>15.3.1 Sequential Modular Methods / 15.3.2 Simultaneous Modular Methods / 15.3.3 Calculation of Derivatives</i> |     |
| <b>15.4</b>         | Summary  | 546 |
|                     | References   | 546 |
|                     | Supplementary References   | 548 |
| <b>16</b>           | <b>Integrated Planning, Scheduling, and Control in the Process Industries</b>                                      | 549 |
| <b>16.1</b>         | Plant Optimization Hierarchy   | 550 |
| <b>16.2</b>         | Planning and Scheduling  | 553 |
|                     | <i>16.2.1 Planning / 16.2.2 Scheduling</i>   |     |

|                   |   |     |
|-------------------|---|-----|
| <b>16.3</b>       | Plantwide Management and Optimization   | 565 |
| <b>16.4</b>       | Unit Management and Control   | 567 |
|                   | <i>16.4.1 Formulating the MPC Optimization Problem</i>  |     |
| <b>16.5</b>       | Process Monitoring and Analysis   | 575 |
|                   | References  | 579 |
|                   | Supplementary References  | 581 |
| <b>Appendixes</b> |   | 583 |
| <b>A</b>          | Mathematical Summary  | 583 |
|                   | <i>A.1 Definitions / A.2 Basic Matrix Operations / A.3 Linear Independence and Row Operations / A.4 Solution of Linear Equations / A.5 Eigenvalues, Eigenvectors / References / Supplementary References / Problems</i> |     |
| <b>B</b>          | Cost Estimation   | 603 |
|                   | <i>B.1 Capital Costs / B.2 Operating Costs / B.3 Taking Account of Inflation / B.4 Predicting Revenues in an Economic-Based Objective Function / B.5 Project Evaluation / References</i>                                |     |
|                   | Nomenclature  | 631 |
|                   | Name Index  | 637 |
|                   | Subject Index   | 643 |



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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.

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 R. Fair, University of Texas-Austin; Christodoulos Floudas, Princeton University; Fred Glover, University of Colorado; Ignacio Grossmann, Carnegie-Mellon University; K. Jayaraman, Michigan State University; I. Lefkowitz, Case Western Reserve University; Tom McAvoy, University of Maryland; János Pintér, Pintér Consulting Services; Larry Ricker, University of Washington; and Mark Stadtherr, University of Notre Dame. Several of the examples in Chapters 11–16 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, especially Juergen Hahn and Tyler Soderstrom for this edition.

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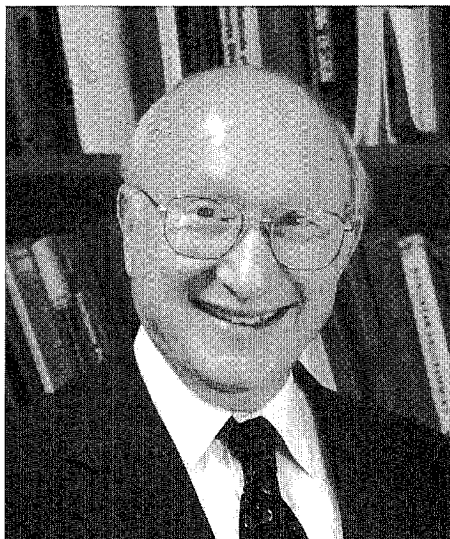
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