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Optimization in Chemical Engineering

Optimization is used to determine the most appropriate value of variables under given conditions. The primary focus of using optimization techniques is to measure the maximum or minimum value of a function depending on the circumstances. Any engineering discipline involving design, maintenance and manufacturing requires certain technical decisions to be taken at different stages. The primary outcome of taking these decisions is to maximize the profit with minimum utilization of resources.

This book presents a detailed explanation of problem formulation and problem solving with the help of algorithms such as secant method, Quasi-Newton method, linear programming and dynamic programming. It covers important chemical processes such as fluid flow systems, heat exchangers, chemical reactor and distillation systems with the help of solved examples.

It begins by explaining the fundamental concepts followed by an elucidation of various modern techniques including trust-region methods, Levenberg-Marquardt algorithms, stochastic optimization, simulated annealing and statistical optimization. It studies multi-objective optimization technique and its applications in chemical engineering. The knowledge of such a technique is necessary as most chemical processes are multiple input and multiple output systems.

The book also discusses theory and applications of various optimization software tools including LINGO, MATLAB, MINITAB and GAMS. It is designed as a coursebook for undergraduate and postgraduate students of chemical engineering and allied branches including biotechnology, food technology, petroleum engineering and environmental science.

Suman Dutta is Assistant Professor at the Department of Chemical Engineering, Indian School of Mines, Dhanbad. He was a visiting researcher at the Centre for Water Science in Cranfield University, UK. He teaches courses on chemical engineering thermodynamics, chemical reaction engineering, fluid mechanics, process modeling and optimization and process instrumentation and control. His areas of research include wastewater treatment, membrane technology, advanced oxidation process, photocatalysis, process simulation and optimization.

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To my father
Late Sukumar Dutta
and
God almighty

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978-1-107-09123-8 - Optimization in Chemical Engineering
Suman Dutta
Frontmatter
More information

Contents

List of Figures *xiii*
List of Tables *xvii*
Preface *xix*

1. A Brief Discussion on Optimization
1.1 Introduction to Process Optimization 1
1.2 Statement of an Optimization Problem 2
1.3 Classification of Optimization Problems 3
1.4 Salient Feature of Optimization 8
1.5 Applications of Optimization in Chemical Engineering 9
1.6 Computer Application for Optimization Problems 10
Summary 10
Review Questions 10
References 11

2. Formulation of Optimization Problems in Chemical and Biochemical Engineering
2.1 Introduction 12
2.2 Formulation of Optimization Problem 12
2.3 Fluid Flow System 13
2.3.1 Optimization of liquid storage tank 13
2.3.2 Optimization of pump configurations 14
2.4 Systems with Chemical Reaction 17
2.4.1 Optimization of product concentration during chain reaction 18
2.4.2 Optimization of gluconic acid production 20
2.5 Optimization of Heat Transport System 21
2.5.1 Calculation of optimum insulation thickness 21
2.5.2 Optimization of simple heat exchanger network 24
2.5.3 Maximum temperature for two rotating cylinders 26
2.6 Calculation of Optimum Cost of an Alloy using LP Problem 28

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CAMBRIDGE

Cambridge University Press
978-1-107-09123-8 - Optimization in Chemical Engineering
Suman Dutta
Frontmatter
More information

2.7 Optimization of Biological Wastewater Treatment Plant 30
2.8 Calculation of Minimum Error in Least Squares Method 31
2.9 Determination of Chemical Equilibrium 33
Summary 35
Exercise 35
References 39

3. Single Variable Unconstrained Optimization Methods
3.1 Introduction 40
3.2 Optimization of Single Variable Function 41
3.2.1 Criteria for optimization 41
3.2.2 Classification of unconstrained minimization methods 47
3.3 Direct Search Methods 48
3.3.1 Finding a bracket for a minimum 48
3.3.2 Unrestricted search method 49
3.3.3 Exhaustive search 51
3.3.4 Dichotomous search 53
3.3.5 Interval halving method 56
3.3.6 Fibonacci method 59
3.3.7 Golden section method 62
3.4 Direct Root Methods 64
3.4.1 Newton method 65
3.4.2 Quasi-Newton method 66
3.4.3 Secant method 67
3.5 Polynomial Approximation Methods 68
3.5.1 Quadratic interpolation 69
3.5.2 Cubic interpolation 70
Summary 72
Exercise 72
References 73

4. Trust-Region Methods
4.1 Introduction 74
4.2 Basic Trust-Region Method 75
4.2.1 Problem statement 75
4.2.2 Trust-Region radius 76
4.2.3 Trust-Region subproblem 78
4.2.4 Trust-Region fidelity 78

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CAMBRIDGE

Cambridge University Press
978-1-107-09123-8 - Optimization in Chemical Engineering
Suman Dutta
Frontmatter
More information

4.3 Trust-Region Methods for Unconstrained Optimization 79
4.4 Trust-Region Methods for Constrained Optimization 80
4.5 Combining with Other Techniques 82
4.6 Termination Criteria 83
4.7 Comparison of Trust-Region and Line-Search 83
Summary 84
Exercise 84
References 84

5. Optimization of Unconstrained Multivariable Functions
5.1 Introduction 86
5.2 Formulation of Unconstrained Optimization 87
5.3 Direct Search Method 87
5.3.1 Random search methods 87
5.3.2 Grid search method 90
5.3.3 Univariate method 93
5.3.4 Pattern search methods 94
5.4 Gradient Search Method 99
5.4.1 Steepest descent (Cauchy) method 100
5.4.2 Conjugate gradient (Fletcher–Reeves) method 102
5.4.3 Newton's method 104
5.4.4 Marquardt method 106
5.4.5 Quasi-Newton method 109
5.4.6 Broydon–Fletcher–Goldfrab–Shanno method 113
5.5 Levenberg–Marquardt Algorithm 114
Summary 116
Review Questions 116
References 117

6. Multivariable Optimization with Constraints
6.1 Formulation of Constrained Optimization 119
6.2 Linear Programming 122
6.2.1 Formulation of linear programming problems 122
6.2.2 Simplex method 127
6.2.3 Nonsimplex methods 133
6.2.4 Integer linear programming 139
6.3 Nonlinear Programming with Constraints 144
6.3.1 Problems with equality constraints 144

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CAMBRIDGE

Cambridge University Press
978-1-107-09123-8 - Optimization in Chemical Engineering
Suman Dutta
Frontmatter
More information

6.3.2 Problems with inequality constraints 149
6.3.3 Convex optimization problems 151
Summary 154
Review Questions 154
References 156

7. Optimization of Staged and Discrete Processes
7.1 Dynamic Programming 157
7.1.1 Components of dynamic programming 158
7.1.2 Theory of dynamic programming 159
7.1.3 Description of a multistage decision process 160
7.2 Integer and Mixed Integer Programming 166
7.2.1 Formulation of MINLP 167
7.2.2 Generalized Benders Decomposition 169
Summary 176
Exercise 176
References 178

8. Some Advanced Topics on Optimization
8.1 Stochastic Optimization 180
8.1.1 Uncertainties in process industries 180
8.1.2 Basic concept of probability theory 182
8.1.3 Stochastic linear programming 186
8.1.4 Stochastic nonlinear programming 191
8.2 Multi-Objective Optimization 193
8.2.1 Basic theory of multi-objective optimization 197
8.2.2 Multi-objective optimization applications in chemical engineering 202
8.3 Optimization in Control Engineering 206
8.3.1 Real time optimization 206
8.3.2 Optimal control of a batch reactor 208
8.3.3 Optimal regulatory control system 212
8.3.4 Dynamic matrix control 214
Summary 218
Review Questions 218
References 219

9. Nontraditional Optimization
9.1 Genetic Algorithm 222
9.1.1 Working principle of GAs 223

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CAMBRIDGE

Cambridge University Press
978-1-107-09123-8 - Optimization in Chemical Engineering
Suman Dutta
Frontmatter
More information

9.1.2 Termination 228
9.2 Particle Swarm Optimization 229
9.2.1 Working principle 230
9.2.2 Algorithm 231
9.2.3 Initialization 231
9.2.4 Variants of PSO 232
9.2.5 Stopping criteria 235
9.2.6 Swarm communication topology 236
9.3 Differential Evolution 241
9.3.1 DE algorithm 241
9.3.2 Initialization 242
9.3.3 Mutation 243
9.3.4 Crossover 244
9.3.5 Selection 245
9.4 Simulated Annealing 245
9.4.1 Procedure 246
9.4.2 Applications of SA in chemical engineering 253
Summary 253
Exercise 254
References 255

10. Optimization of Various Chemical and Biochemical Processes
10.1 Heat Exchanger Network Optimization 258
10.1.1 Superstructure 259
10.1.2 Problem statement 260
10.1.3 Model formulation 260
10.2 Distillation System Optimization 263
10.3 Reactor Network Optimization 267
10.4 Parameter Estimation in Chemical Engineering 271
10.4.1 Derivation of objective function 271
10.4.2 Parameter estimation of dynamic system 273
10.5 Environmental Application 276
Summary 281
Review Questions 281
References 282

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CAMBRIDGE

Cambridge University Press
978-1-107-09123-8 - Optimization in Chemical Engineering
Suman Dutta
Frontmatter
More information

11. Statistical Optimization

11.1 Design of Experiment 284
11.1.1 Stages of DOE 285
11.1.2 Principle of DOE 286
11.1.3 ANOVA study 289
11.1.4 Types of experimental design 291
11.2 Response Surface Methodology 296
11.2.1 Analysis of a second order response surface 301
11.2.2 Optimization of multiple response processes 303
Summary 305
Review Questions 305
References 305

12. Software Tools for Optimization Processes

12.1 LINGO 307
12.2 MATLAB 316
12.3 MINITAB® 323
12.4 GAMS 333
Summary 342
Review Questions 342
References 342

Multiple Choice Questions – 1 343
Multiple Choice Questions – 2 349
Multiple Choice Questions – 3 355
Index 359

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CAMBRIDGE

Cambridge University Press
978-1-107-09123-8 - Optimization in Chemical Engineering
Suman Dutta
Frontmatter
More information

List of Figures

1.1	Convex function	4
1.2	Concave function	5
1.3	Local and global optimum points	6
1.4	Classification of optimization problem	7
1.5	Conversion of $f(x)$ to $-f(x)$	8
1.6	Plot of objective function vs. decision variable	8
2.1	Liquid storage tank	13
2.2	Configuration of an L level pump network	15
2.3	Concentration vs. time plot for a series reaction in PFR	18
2.4	Objectives used during optimization of gluconic acid production	21
2.5	Changes of heat flux with insulation thickness	22
2.6	Heat exchanger network with three heat exchangers	24
2.7	Rotating cylinder (with temperature and velocity profile)	26
2.8	Biological wastewater treatment plant	30
2.9	Least square method	31
3.1	Global and relative optimum points	41
3.2	Undefined derivative at x^*	43
3.3	Inflection or saddle point	44
3.4	Unimodal functions	47
3.5	Work done vs. intermediate pressure graph	51
3.6	Exhaustive search (see Example 3.3)	52
3.7	Interval halving method	57
3.8	Convergence process of Newton method	66
3.9	Convergence process of secant method	67
3.10	Quadratic interpolation	70
4.1	Trust region	77
5.1	Contour representation for random jumping method	88
5.2	Contour representation for grid search method	91
5.3	Contour representation for Cr(VI) removal	92
5.4	Contour for quadratic function	94
5.5	Pattern search method	94
5.6	Gradient search method	99

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CAMBRIDGE

Cambridge University Press
978-1-107-09123-8 - Optimization in Chemical Engineering
Suman Dutta
Frontmatter
More information

5.7	Direction of movement of any point	100
6.1	Graphical representation of feasible region	120
6.2	Constrained optimization problem	120
6.3	Unbounded feasible region	121
6.4	Graphical representation of problem 6.12a–6.12d	127
6.5	Ellipsoid method	135
6.6	Interior point method	136
6.7	Karmarkar's region inversion	137
6.8	Integer linear programming	140
7.1	Single-stage decision process	161
7.2	Multi-stage decision process	161
7.3	The annual net profit vs. time plot	163
7.4	Representation of 5 stage dynamic programming	164
7.5	Generalized Benders Decomposition method	175
8.1	Fluidization column	181
8.2	Multi-objective optimization	195
8.3	Pareto optimal set	195
8.4	Utopia point	196
8.5(a)	Convex objective space	199
8.5(b)	Non-convex objective space	199
8.6	Flowchart for evolutionary algorithm	201
8.7	Utopia-tracking approach	202
8.8	PID controller as MOO problem	205
8.9	Plant decision hierarchy	207
9.1	Parent chromosomes	226
9.2	Single point crossover	226
9.3	Multipoint crossover	226
9.4	Mutation operation	227
9.5	Flowchart of genetic algorithm	228
9.6	Movement of particles in PSO	230
9.7(a)	von Neumann topology	236
9.7(b)	Star topology	236
9.7(c)	Wheel topology	237
9.7(d)	Circle topology	237
9.7e	Pyramid topology	237
9.8	Flowchart for differential algorithm	242
9.9	Flowchart of simulated annealing	247
9.10	Probability of accepting vs temperature plot	253
10.1	HEN superstructure	259
10.2	Continuous distillation column	264
10.3	Reactor network superstructure	269
11.1	Full factorial design with three variables	292
11.2	Fractional factorial design with three variables	292

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CAMBRIDGE

Cambridge University Press
978-1-107-09123-8 - Optimization in Chemical Engineering
Suman Dutta
Frontmatter
More information

11.3	Central composite design	294
11.4	Box–Behnken design	295
11.5(a)	Response surface formed from Eq. 11.22a	298
11.5(b)	Contour representation of Fig. 11.5a	299
11.6(a)	Response surface formed from Eq. 11.22b	299
11.6(b)	Contour representation of Fig. 11.6a	300
11.7(a)	Response surface formed from Eq. 11.22c	300
11.7(b)	Contour representation of Fig. 11.7a	301
12.1	LINGO main window	308
12.2	Lingo Model-Lingo1 window with a maximization model	309
12.3	Toolbar of LINGO	309
12.4	LINGO error message box	309
12.5	Solver status window	310
12.6	LINGO solution report window	311
12.7	LINGO solver status window	315
12.8	Plot of objective 1 and objective 2	321
12.9	Pareto front for obj1 and obj2	322
12.10	MINITAB main window	324
12.11	MINITAB window for selecting DOE	325
12.12	MINITAB window with B–B design	326
12.13	MINITAB window with data for B–B design	327
12.14	MINITAB window for analyzing the response surface design	328
12.15	MINITAB window for selecting “response”	328
12.16	MINITAB window with results	329
12.17(a)	Response surface of Eq. 12.2 at pH = 0	330
12.17(b)	Response surface of Eq. 12.2 at TiO2 = 0	331
12.17(c)	Response surface of Eq. 12.2 at Time = 0	331
12.18(a)	Contour of the response Eq. 12.2 at pH = 0	332
12.18(b)	Contour of the response Eq. 12.2 at TiO2 = 0	332
12.18(c)	Contour of the response Eq. 12.2 at Time = 0	333
12.19	Main window of GAMS	334

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978-1-107-09123-8 - Optimization in Chemical Engineering
Suman Dutta
Frontmatter
More information

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CAMBRIDGE

Cambridge University Press
978-1-107-09123-8 - Optimization in Chemical Engineering
Suman Dutta
Frontmatter
More information

List of Tables

2.1	Composition and cost of copper alloys	29
3.1	Values of stationary points	46
3.2	Values of successive iterations with accelerated step size	50
3.3	The available interval of uncertainty after different trials	52
3.4	Work done with different intermediate pressure (Exhaustive search method)	53
3.5	Final intervals of uncertainty for different pairs of experiments	54
3.6	Final interval of uncertainty by golden section method	63
5.1	Value of objective function at different grid points	92
6.1	Subproblems for branch and bound method	143
6.2	Results of the subproblems in Table 6.1	143
7.1	Values of the decision variables (as per Eq. 7.14)	164
7.2	Values of the decision variables (as per Eq. 7.15)	165
7.3	Values of the decision variables (as per Eq. 7.16)	165
7.4	Values of the decision variables (as per Eq. 7.17)	165
7.5	Values of the decision variables (as per Eq. 7.18)	166
8.1	Number of worker present with probability	185
9.1	Decimal to binary conversion	224
9.2	Single and multiple point crossover	227
9.3	Chromosomes after crossover	227
9.4	Calculated values of different iteration	252
11.1	Single factor experiment with 5 level of the factor and 5 replicates	287
11.2	Arrangement of experimental run after randomization	288
11.3	Reaction rate data at different pH	288
11.4	Three variable B–B design	295
11.5	Values of the coefficient (Anupam *et al.*)	302
12.1	Widget capacity data	313
12.2	Vendor widget demand	313
12.3	Shipping cost per widget ($)	313
12.4	Description of MATLAB function used for optimization	317
12.5	Levels of independent variables for B–B design	325
12.6	Matrix of B–B design	326
12.7	ANOVA for percentage dye removal	329

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CAMBRIDGE

Cambridge University Press
978-1-107-09123-8 - Optimization in Chemical Engineering
Suman Dutta
Frontmatter
More information

12.8	Different variable type and their GAMS keyword	335
12.9	Different relational operator in GAMS	335
12.10	Available solution procedure in GAMS	335
12.11	Availability and cost of petroleum stocks	338
12.12	Specification and selling price	339

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CAMBRIDGE

Cambridge University Press
978-1-107-09123-8 - Optimization in Chemical Engineering
Suman Dutta
Frontmatter
More information

Preface

Optimization in the field of chemical engineering is required to utilize the resources in an efficient way as well as to reduce the environmental impact of a process. Application of optimization processes helps us achieve the most favorable operating conditions. Maximum profit is achievable if a process plant runs at optimum conditions. Knowledge of optimization theory as well its practical application is essential for all engineers.

The idea of this book came to my mind long back, perhaps six years ago. Then I started working on it; selecting topics to be included, collecting research papers, and preparing the manuscript. Many people helped me during this process, especially while collecting research articles from different sources: Sudip Banerjee, Arindam Chatterjee, D.K. Sandilya to name a few. I received very useful suggestions from reviewers of this manuscript.

This book contains detailed theory and applications of optimization in chemical engineering and related fields. Prerequisites for this book include some understanding of chemical engineering, biotechnology and mathematics. This book has been divided into twelve chapters. It contains various classical methods for optimization; it also introduces some of the recently developed topics in optimization. Examples from the field of chemical engineering and biochemical engineering are discussed throughout the book.

Chapter 1 discusses the classification and fundamentals of optimization methods. It also includes the salient features of optimization. This chapter also lists different types of objective functions and conditions for optimization. Chapter 2 gives emphasis to different chemical engineering processes and problem formulation procedures for optimization application. This chapter includes objective function formulation of fluid flow system, heat transfer equipments, mass transfer equipments, and reactors. One dimensional unconstrained problem formulation and optimization have been discussed in Chapter 3. This chapter includes different methods like Newton's method, Quasi-Newton method, Secant method etc. Chapter 4 discusses the Trust-Region methods for both constrained and unconstrained optimization problems. An overview of optimization of multivariable unconstrained functions is given in Chapter 5. This chapter comprises various search methods (i.e. random search, grid search), gradient method, Newton's method etc. Chapter 6 discusses the optimization methods for multivariable functions with constraints. This chapter contains both linear programming and non-linear programming. Optimization of staged and discrete processes has been discussed in Chapter 7. This includes dynamic programming, integer and mixed integer programming. Chapter 8 contains some advanced topics on optimization. This chapter discusses stochastic optimization, multiobjective optimization and optimization problems related to control systems. Most chemical process involve highly nonlinear equations that are difficult to optimize using simple and traditional optimization techniques. Chapter 9 discusses some nontraditional optimization methods like Genetic Algorithm (GA), Particle Swarm optimization, Simulated annealing etc. Chapter 10 elucidates the practical application of optimization theory in various chemical and biochemical processes. Chapter 11 describes different statistical optimization methods. This chapter contains response surface methodology with examples from chemical engineering and biotechnology. Chapter 12 gives an overview of different optimization software tools. This chapter elucidates software for optimization such as LINGO, MATLAB, MINITAB and GAMS. A large number of multiple-choice questions are included at the end of this book. I hope this book will be helpful

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Suman Dutta
Frontmatter
More information

for students at undergraduate and graduate levels. Students will benefit if they go through the theories and solved examples side by side.

I am grateful to LINDO Systems Inc., MathWorks Inc., Minitab Inc., and GAMS for giving permission to include material and screenshots in this book. I am thankful to Gauravjeet Singh Reen for his support during the preparation of the manuscript. I must convey my gratitude to all members of Cambridge University Press for their kind cooperation. I am indebted to my family members for their kind cooperation. I am also thankful to all my colleagues, friends, and well-wishers.

Readers of this book are requested to send their comments and suggestions for further improvement.

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