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.
Optimization in Chemical Engineering

Suman Dutta
To my father
Late Sukumar Dutta
and
God almighty
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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...
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.