

CONTENTS

Chapter 1	The Chemical Industry	1
1.1	What Is the Chemical Industry?	1
1.2	The Chemical Industry as a Growth Industry	3
1.3	Product Classification	8
1.4	Role of Research and Development	9
1.5	Role of the Chemical Engineer	10
Chapter 2	The Generation and Screening of Alternatives	13
2.1	Analysis and Synthesis	13
2.2	Screening of Alternatives	15
2.3	Separation Sequences	19
2.4	Alternative Processing Routes	21
2.5	Alternative Processing Techniques	22
2.6	Analysis of Alternatives	23
2.7	Synthesis of a Process	q26
2.8	Concluding Remarks	29
Chapter 3	Estimation of Thermophysical Properties	32
3.1	Pure-Compound Properties	33
3.2	Critical Properties	33
3.3	Pressure-Volume-Temperature Relationships	35
3.4	Vapor Pressure	39
3.5	Latent Heat of Vaporization	40
3.6	Gas Heat Capacity	41
3.7	Enthalpy Charts	42
3.8	Standard Heat of Formation	43
3.9	Free Energy of Formation	46
3.10	Entropy of Formation	47
3.11	Other Physical Properties	48
3.12	Mixture Properties	51
3.13	Vapor-Liquid Equilibrium	52
3.14	Data Sources	54

Chapter 4	Reaction Equilibrium Analysis	56
4.1	Chemical Equilibrium	57
4.2	Effect of Data Inaccuracies	59
4.3	Effect of Operating Parameters on Equilibrium Conversion	62
4.4	Optimum Feed Composition	66
4.5	Overcoming Positive ΔG°	68
4.6	Adiabatic Reaction Path	74
4.7	Representation of Simultaneous Reactions	75
4.8	Equilibrium in Simultaneous Reactions	78
4.9	Free-Energy-Minimization Method	81
Chapter 5	Nonreacting Process Analysis	87
5.1	Lost-Work Concept	87
5.2	Availability Concept	90
5.3	Separation and Purification	95
5.4	Blending	98
Chapter 6	Reactor Design and Analysis	103
6.1	Reactor Material Balance	103
6.2	Chemical Kinetics	104
6.3	Types of Chemical Reactions	106
6.4	Effect of Temperature on Reaction Rates	109
6.5	Batchwise and Continuous Reactions	111
6.6	Types of Idealized Chemical Reactors	111
6.7	Basic Design Equations for a Batch Reactor	113
6.8	Basic Design Equations for a CSTR	114
6.9	Basic Design Equations for Tubular-Flow Reactors	118
6.10	Comparison of Reactors	119
6.11	Thermal Behavior of a CSTR	133
6.12	Thermal Behavior of a Tubular-Flow Reactors	135
6.13	Some Stability and Start-Up Considerations	136
6.14	Heterogeneous Reactions	138
6.15	Tubular-Reactor Stability	149
6.16	Final Comment	151
Chapter 7	Economic Analysis and Evaluation	155
7.1	Project Evaluation	156
7.2	Cash-Flow Diagram	156
7.3	Time Value of Money	157
7.4	Evaluation Criteria	165

7.5	Comparison between Present Worth and DCF Return	168
7.6	Realistic Economic Evaluation	174
7.7	Characteristics of Inflation	174
7.8	Allowing for Inflation	176
7.9	Effect of Inflation on Future Equipment Needs	178
7.10	Capital-Cost Estimates	181
7.11	Cost Indexes	182
7.12	Fixed-Capital Estimates	183
7.13	Total-Product-Cost Estimation	193
7.14	Direct Production Costs	193
7.15	Fixed Charges	195
7.16	Plant Overhead Costs	196
7.17	General Expenses	197
7.18	Gross-Earning Expenses	197
7.19	Preliminary Total-Product-Cost Estimation	197
Chapter 8 Forecasting the Future		202
8.1	How to Predict	203
8.2	Market Forecasting	203
8.3	Qualitative Methods	204
8.4	Quantitative Methods	206
8.5	Growth of the General Economy	212
8.6	Correlation Analysis	213
8.7	Historical Analogy	214
8.8	Consumption Patterns	214
8.9	Market Simulation	215
8.10	A Word of Caution	215
8.11	Forecasting Plant Capacity	216
8.12	Chemical-Price Forecasting	219
8.13	Projecting Production Rates	220
8.14	Projecting Costs	221
8.15	Projecting Demand	221
8.16	Twaddle-Malloy Illustrative Example	222
8.17	Economic-Price Forecasting	223
Chapter 9 Dealing with Uncertainty		227
9.1	Dealing with Uncertainty in Economic Analysis	228
9.2	Sensitivity Analysis	228
9.3	Quantifying Uncertainty	229
9.4	The Decision Process	234

9.5	Decision Making	234
9.6	Design under Risk	241
9.7	Reliability and Redundancy	243
9.8	Process Availability and Redundancy	246
9.9	Evaluating the Profitability of Redundancy	247
9.10	Planing Production Capacity with Uncertain Demand	251
Chapter 10 Tactics and Strategy of Process Synthesis		260
10.1	Qualitative Approaches to Process Synthesis	261
10.2	Functional Analysis and Evolutionary Process Synthesis	265
10.3	Programmed Strategies for Process Synthesis	274
10.4	Optimization Methods for Process Synthesis	278
10.5	Optimum-Seeking Procedures	279
10.6	Mathematical Programming	279
10.7	Chemical-Process Simulation	283
10.8	Computer-Aided Process Synthesis	294
10.9	Concluding Remarks	297
Chapter 11 Case Studies		304
11.1	Methanol Production	304
11.2	Styrene Production	316
11.3	Ethylene Glycol	328
11.4	Taming the Runaway Reaction	335
11.5	Capacity-Expansion Project	342
References		352
Index		357