

# SYSTEMATIC METHODS OF CHEMICAL PROCESS DESIGN

L.T. Biegler, I.E. Grossmann,  
and A.W. Westerberg  
*Carnegie Mellon University*

To join a Prentice Hall PTR Internet mailing list, point to:  
<http://www.prenhall.com/register>



Prentice Hall PTR  
Upper Saddle River, New Jersey 07458  
<http://www.prenhall.com>

# CONTENTS

Preface xiii  
Foreword xvii

<b>1</b>	<b>Introduction to Process Design</b>	<b>1</b>
1.1	The Preliminary Design Step for Chemical Processes	1
1.2	A Scenario for Chemical Process Design	3
1.3	The Synthesis Step	6
1.4	Design in a Team	8
1.5	Converting Ill-Posed Problems to Well-Posed Ones	10
1.6	A Case Study Process Design Problem	13
1.7	A Roadmap for This Book	18
	References	20
	Exercises	21
<b>I</b>	<b>PRELIMINARY ANALYSIS AND EVALUATION OF PROCESSES</b>	<b>23</b>
<b>2</b>	<b>Overview of Flowsheet Synthesis</b>	<b>25</b>
2.1	Introduction	25
2.2	Basic Steps in Flowsheet Synthesis	26
2.3	Decomposition Strategies for Process Synthesis	36
2.4	Synthesis of an-Ethyl Alcohol Process: A Case Study	39
2.5	Summary	50
	References	51
	Exercises	51
<b>3</b>	<b>Mass and Energy Balances</b>	<b>55</b>
3.1	Introduction	55
3.2	Developing Unit Models for Linear Mass Balances	57

3.3	Linear Mass Balances	85	
3.4	Setting Temperature and Pressure Levels from the Mass Balance	94	
3.5	Energy Balances	98	
3.6	Summary	104	
	References	104	
	Exercises	105	
<b>4</b>	<b>Equipment Sizing and Costing</b>		<b>110</b>
4.1	Introduction	110	
4.2	Equipment Sizing Procedures	111	
4.3	Cost Estimation	132	
4.4	Summary	138	
	References	139	
	Exercises	139	
<b>5</b>	<b>Economic Evaluation</b>		<b>142</b>
5.1	Introduction	142	
5.2	Simple Measures to Estimate Earnings and Return on Investment	144	
5.3	Time Value of Money	147	
5.4	Cost Comparison after Taxes	155	
5.5	Detailed Discounted Cash Flow Calculations	162	
5.6	Inflation	169	
5.7	Assessing Investment Risk	170	
5.8	Summary and Reference Guide	173	
	Exercises	174	
<b>6</b>	<b>Design and Scheduling of Batch Processes</b>		<b>180</b>
6.1	Introduction	180	
6.2	Single Product Batch Plants	180	
6.3	Multiple Product Batch Plants	184	
6.4	Transfer Policies	186	
6.5	Parallel Units and Intermediate Storage	187	
6.6	Sizing of Vessels in Batch Plants	190	
6.7	Inventories	193	
6.8	Synthesis of Flowshop Plants	195	
	References	199	
	Exercises	199	
<b>II</b>	<b>ANALYSIS WITH RIGOROUS PROCESS MODELS</b>		<b>205</b>
<b>7</b>	<b>Unit Equation Models</b>		<b>207</b>
7.1	Introduction	208	
7.2	Thermodynamic Options for Process Simulation	210	

- 7.3 Flash Calculations 217
- 7.4 Distillation Calculations 224
- 7.5 Other Unit Operations 232
- 7.6 Summary and Future Directions 239
- References and Further Reading 240
- Exercises 242

## **8 General Concepts of Simulation for Process Design 243**

- 8.1 Introduction 243
- 8.2 Process Simulation Modes 245
- 8.3 Methods for Solving Nonlinear Equations 254
- 8.4 Recycle Partitioning and Tearing 271
- 8.5 Simulation Examples 285
- 8.6 Summary and Suggestions for Further Reading 289
- References 291
- Exercises 292

## **9 Process Flowsheet Optimization 295**

- 9.1 Description of Problem 295
- 9.2 Introduction to Constrained Nonlinear Programming 297
- 9.3 Derivation of Successive Quadratic Programming (SQP) 307
- 9.4 Process Optimization with Modular Simulators 314
- 9.5 Equation-Oriented Process Optimization 321
- 9.6 Summary and Conclusions 331
- References 332
- Exercises 334

## **III BASIC CONCEPTS IN PROCESS SYNTHESIS 339**

### **10 Heat and Power Integration 341**

- 10.1 The Basic Heat Exchanger Network Synthesis (HENS) Problem 342
- 10.2 Refrigeration Cycles 373
- References 382
- Exercises 382

### **11 Ideal Distillation Systems 387**

- 11.1 Separating a Mixture of *n*-Pentane, *n*-Hexane, and *n*-Heptane 387
- 11.2 Separating a Five-Component Alcohol Mixture 395
- References 401
- Exercises 401

<b>12</b>	<b>Heat Integrated Distillation Processes</b>	<b>408</b>
12.1	Heat Flows in Distillation	408
	References	425
	Exercises	425
<b>13</b>	<b>Geometric Techniques for the Synthesis of Reactor Networks</b>	<b>429</b>
13.1	Introduction	430
13.2	Graphical Techniques for Simple Reacting Systems	432
13.3	Geometric Concepts for Attainable Regions	438
13.4	Reaction Invariants and Reactor Network Synthesis	447
13.5	Chapter Summary and Guide to Further Reading	450
	References	452
	Exercises	453
<b>14</b>	<b>Separating Azeotropic Mixtures</b>	<b>455</b>
14.1	Separating a Mixture of <i>n</i> -Butanol and Water	456
14.2	Separating a Mixture of Acetone, Chloroform, and Benzene	464
14.3	Sketching Distillation and the Closely Related Residue Curves	475
14.4	Separating a Mixture of <i>n</i> -Pentane, Water, Acetone, and Methanol	482
14.5	More Advanced Work	488
	References	490
	Exercises	490
<b>IV</b>	<b>OPTIMIZATION APPROACHES TO PROCESS SYNTHESIS AND DESIGN</b>	<b>495</b>
<b>15</b>	<b>Basic Concepts for Algorithmic Methods</b>	<b>497</b>
15.1	Introduction	497
15.2	Problem Representation	498
15.3	Solution Strategies for Tree Representations	503
15.4	Models and Solution Strategies for Network Representations	507
15.5	Alternative Mathematical Programming Formulations	509
15.6	Summary of Mathematical Models	513
15.7	Modeling of Logic Constraints and Logic Inference	514
15.8	Modeling of Disjunctions	519
15.9	Notes and Further Reading	521
	References	521
	Exercises	523
<b>16</b>	<b>Synthesis of Heat Exchange Networks</b>	<b>527</b>
16.1	Introduction	527
16.2	Sequential Synthesis	528

- 16.3 Simultaneous MINLP Model 551
- 16.4 Comparison of Sequential and Simultaneous Synthesis 559
- 16.5 Notes and Further Reading 561
  - References 562
  - Exercises 563

## **17 Synthesis of Distillation Sequences**

**567**

- 17.1 Introduction 567
- 17.2 Linear Models for Sharp Split Columns 567
- 17.3 Example of MILP Model for Four-Component Mixture 571
- 17.4 MILP Model for Distillation Sequences 575
- 17.5 Heat Integration and Pressure Effects 576
- 17.6 MILP Model with Continuous Temperatures 578
- 17.7 MILP Model with Discrete Temperatures 581
- 17.8 Design and Synthesis with Rigorous Models 587
- 17.9 Notes and Further Reading 590
  - References 591
  - Exercises 592

## **18 Simultaneous Optimization and Heat Integration**

**595**

- 18.1 Introduction 595
- 18.2 Sequential versus Simultaneous Optimization and Heat Integration 596
- 18.3 Linear Models 601
- 18.4 Nonlinear Models 604
- 18.5 Notes and Further Reading 613
  - References 614
  - Exercises 615

## **19 Optimization Techniques for Reactor Network Synthesis**

**618**

- 19.1 Introduction 618
- 19.2 Reactor Network Synthesis with Targeting Formulations 620
- 19.3 Reactor Network Synthesis in Process Flowsheets 645
- 19.4 Summary and Further Reading 656
  - References 658
  - Exercises 660

## **20 Structural Optimization of Process Flowsheets**

**663**

- 20.1 Introduction 663
- 20.2 Flowsheet Superstructures 663
- 20.3 Mixed-Integer Optimization Models 666
- 20.4 MILP Approximation 667
- 20.5 MILP Model for the Synthesis of Utility Plants 669

20.6	Modeling/Decomposition Strategy	672
20.7	Notes and Further Reading	686
	References	686
	Exercises	687
<b>21</b>	<b>Process Flexibility</b>	<b>690</b>
21.1	Motivating Example	691
21.2	Mathematical Formulations for Flexibility Analysis	697
21.3	Flexibility Test Problem	698
21.4	Flexibility Index Problem	699
21.5	Vertex Solution Methods	701
21.6	Example with Nonvertex Critical Point	702
21.7	Active Set Method	704
21.8	Active Set Method for Nonvertex Example	707
21.9	Special Cases for Flexibility Analysis	709
21.10	Optimal Design under Uncertainty	712
21.11	Notes and Further Reading	713
	References	714
	Exercises	715
<b>22</b>	<b>Optimal Design and Scheduling for Multiproduct Batch Plants</b>	<b>719</b>
22.1	Introduction	719
22.2	Horizon Constraints for Flowshop Plants—Single-Product Campaigns	719
22.3	MINLP Design Model for Flowshop Plants—Single-Product Campaigns	722
22.4	MILP Reformulation for Discrete Sizes	725
22.5	NLP Design Model—Mixed-Product Campaigns (UIS)	728
22.6	Cyclic Scheduling in Flowshop Plants	729
22.7	NLP Design Model—Mixed Product Campaigns	735
22.8	State-Task Network for the Scheduling of Multiproduct Batch Plants	736
22.9	Notes and Further Reading	743
	References	743
	Exercises	745
<b>Appendix A</b>	<b>Summary of Optimization Theory and Methods</b>	<b>748</b>
<b>Appendix B</b>	<b>Smooth Approximations for <math>\max \{0, f(x)\}</math></b>	<b>771</b>
<b>Appendix C</b>	<b>Computer Tools for Preliminary Process Design</b>	<b>773</b>
<b>Author Index</b>		<b>781</b>
<b>Subject Index</b>		<b>786</b>