# Contents

Preface *ix* About the Authors *xi* 

- 1 Introduction 1
- 1.1 Chemical Product Engineering 1
- 1.2 Chemical Product Design 2
- Product Design and Computer-Aided Product Design 4 References 6

۱v

- 2 Some Typical Applications of Chemical Product Design and Intellectual Property 7
- 2.1 Natural Fiber Plastic Composites 7
- 2.2 Wheat Straw Polypropylene Composites 10
- 2.3 Modeling Natural Fiber Polymer Composites 12
- 2.4 Graphene Composites 14
- 2.5 Corrosion Protection Using Polymer Composites 15
- 2.6 Intellectual Property 17 References 19
- 3 Mathematical Principles for Chemical Product Design 23
- 3.1 Factorial and Fractional Factorial Design 23
- 3.2 Response Surface Methods and Designs 25
- 3.3 D-Optimal Designs 26
- 3.4 Bayesian Design of Fractional Factorial Experiments 27
- 3.5 Regression Analysis 27
- 3.6 Artificial Neural Networks 28
- 3.7 Mixture Design of Experiments 31
- 3.8 Multiway Principal Component Analysis 35
- 3.8.1 Model-based Principal Component Analysis (MB-PCA) 37
- 3.8.2 MPLS Analysis Using NIPALS 38 References 39

## 4 Disinfectant Formulation Design 41

- 4.1 Introduction 41
- 4.2 Disinfectants Characteristics 42

- vi Contents
  - 4.2.1 Antimicrobial Tests 42
  - 4.2.2 Stability Tests 43
  - 4.2.3 Corrosion Tests 43
  - 4.3 Toxicity of Disinfectants 44
  - 4.3.1 Harmful (Xn) 45
  - 4.3.2 Severe Eye Damage, Xi (R41) 45
  - 4.3.3 Eye Irritant, Xi (R36) 46
  - 4.3.4 Skin Irritant, Xi (R38) 46
  - 4.3.5 Respiratory Irritant, Xi (R37) 47
  - 4.4 Experimental Design for Antimicrobial Activity 47
  - 4.4.1 Prior Knowledge 48
  - 4.4.2 Historical Data Augmentation 49
  - 4.4.3 Linear Least Squares Regression Analysis 49
  - 4.4.4 Artificial Neural Networks 51
  - 4.5 Experimental Design for Stability of Hydrogen Peroxide 54
  - 4.5.1 Historical Data Analysis 54
  - 4.5.2 Historical Data Augmentation Using Bayesian D-optimality Approach 55
  - 4.6 Experimental Design for Corrosion *61*
  - 4.6.1 Preliminary Experimental Design 62
  - 4.6.2 Response Surface Methodology 63
  - 4.6.3 Artificial Neural Networks 64
  - 4.7 Final Formulation Optimization 66
  - 4.7.1 Optimization 67
  - 4.7.2 Optimized Formulation Verification 69
  - 4.7.3 Comparing the Optimized Formulations to an Available Product 70
  - 4.8 Conclusion 70 References 71
  - 5 Streptomyces Lividans 66 for developing a Minimal Defined Medium for Recombinant Human Interleukin-3 73
  - 5.1 Introduction 73
  - 5.2 Materials and Methods 74
  - 5.2.1 Microorganism and Medium 74
  - 5.2.2 Analytical Methods 74
  - 5.2.3 Experimental Design and Data Analysis 76
  - 5.3 Results and Discussion 78
  - 5.3.1 Starvation Trails 78
  - 5.3.2 Screening Mixture Experiments 80
  - 5.3.3 Defined Medium Optimization by Mixture Design Method 82
  - 5.4 Conclusion 87 References 87
  - 6 Multivariate Modeling of a Chemical Toner Manufacturing Process 91
  - 6.1 Introduction 91
  - 6.1.1 Process and Data Description 92
  - 6.1.2 Model Cross-Validation 93

#### Contents vii

- 6.2 Results and Discussion 97
- 6.3 Conclusion 101 References 102

#### 7 Wheat Straw Fiber Size Effects on the Mechanical Properties of Polypropylene Composites 105

- 7.1 Introduction 105
- 7.2 Materials and Methods 108
- 7.2.1 Materials 108
- 7.2.2 Fiber Preparation and Size Measurement 108
- 7.2.3 Fiber Thermal and Chemical Analysis 109
- 7.2.4 Composite Sample Preparation and Properties Measurement 109
- 7.3 Results and Discussions 110
- 7.3.1 Fiber Fractionation and Size Measurement 110
- 7.3.2 Fiber Thermal and Chemical Analysis 113
- 7.3.3 Fiber Size Reduction During Compounding Process 114
- 7.3.4 Composite Flexural Properties 117
- 7.3.5 Composite Impact Properties 118
- 7.3.6 Composite-Specific Properties 120
- 7.4 Conclusion 122 References 122
- 8 Framework for Product Design of Wheat Straw Polypropylene Composite 125
- 8.1 Introduction 125
- 8.2 Product Design Framework for WS-PP Composite 128
- 8.3 Response Surface Models 130
- 8.3.1 The Design of Mixture Experiment 131
- 8.3.2 Materials and Methods 133
- 8.3.3 Results and Discussion 134
- 8.3.3.1 Flexural Modulus 134
- 8.3.3.2 Izod Impact Strength 136
- 8.3.3.3 Other Properties 137
- 8.4 Case Study *138*
- 8.5 Conclusion 144 References 145

### 9 Product Design for Gasoline Blends to Control Environmental Impact Using Novel Sustainability Indices: A Case Study 147

- 9.1 Introduction 147
- 9.2 Methodology 148
- 9.2.1 The Impacts of Gasoline Blends on Octane Number (ON) 148
- 9.2.2 The Impacts of Blending Ethanol and Gasoline on Mileage 149
- 9.2.3 The Effects of Ethanol, Methanol, and Isooctane on the Octane Number of Gasoline Blends 150
- 9.2.4 The Impacts of E5, M5, and I5 on Heat Value, Mileage, and Price 150

| 9.2.5  | Impacts of E5, M5, and I5 on Environment in Potential Environmental<br>Impacts (PEIs) 152  |
|--|--|
| 9.2.6  | The Impacts of E5, M5, and I5 on Safety Risk 154   |
| 9.2.7  | Selecting the Best Blend Through the Analytic Hierarchy  |
|  | Process (AHP) 155  |
| 9.3  | Results 158  |
| 9.4  | Conclusion 160   |
| <i></i>  | References 161   |
| 10   | Corrosion Protection of Copper Using   |
| 10   | Polyetherimide/Graphene Composite Coatings 163   |
| 10.1   | Introduction 163   |
| 10.1   | Experimental 164   |
|  | Material 164   |
| 10.2.1   |  |
| 10.2.2   | Composite Preparation, Coating, and Curing 165   |
| 10.2.3   | Morphology Characterization 165  |
| 10.2.4   | Adhesion 165   |
| 10.2.5   | Electrochemical Measurement 166<br>Results and Discussion 167  |
| 10.3   |  |
| 10.3.1   | Morphology 167   |
| 10.3.2   | Adhesion 170<br>Potentia dumamia Magguramenta 170  |
| 10.3.3   | Potentiodynamic Measurements 170   |
| 10.3.4   | Impedance 174  |
| 10.4   | Conclusion 177   |
|  |  |
|  | References 177   |
| 11   |  |
| 11   | Optimization of Mechanical Properties of Polypropylene   |
| <b>11</b><br>11.1  | Optimization of Mechanical Properties of Polypropylene<br>Montmorillonite Nanocomposites 181   |
|  | <b>Optimization of Mechanical Properties of Polypropylene</b><br><b>Montmorillonite Nanocomposites</b> <i>181</i><br>Introduction <i>181</i>   |
| 11.1   | <b>Optimization of Mechanical Properties of Polypropylene</b><br><b>Montmorillonite Nanocomposites</b> 181<br>Introduction 181<br>Methodology 183  |
| 11.1<br>11.2<br>11.3   | <b>Optimization of Mechanical Properties of Polypropylene</b><br><b>Montmorillonite Nanocomposites</b> 181<br>Introduction 181<br>Methodology 183<br>Mathematical Models 183   |
| 11.1<br>11.2<br>11.3<br>11.4   | <b>Optimization of Mechanical Properties of Polypropylene</b><br><b>Montmorillonite Nanocomposites</b> 181<br>Introduction 181<br>Methodology 183<br>Mathematical Models 183<br>Optimization Mechanism 183   |
| 11.1<br>11.2<br>11.3<br>11.4<br>11.5   | <b>Optimization of Mechanical Properties of Polypropylene</b><br><b>Montmorillonite Nanocomposites</b> 181<br>Introduction 181<br>Methodology 183<br>Mathematical Models 183<br>Optimization Mechanism 183<br>Results and Discussion 185   |
| 11.1<br>11.2<br>11.3<br>11.4<br>11.5<br>11.5.1   | <b>Optimization of Mechanical Properties of Polypropylene</b><br><b>Montmorillonite Nanocomposites</b> 181<br>Introduction 181<br>Methodology 183<br>Mathematical Models 183<br>Optimization Mechanism 183<br>Results and Discussion 185<br>Minimizing the Cost of PP-OMMT 185   |
| 11.1<br>11.2<br>11.3<br>11.4<br>11.5<br>11.5.1<br>11.5.2   | <b>Optimization of Mechanical Properties of Polypropylene</b><br><b>Montmorillonite Nanocomposites</b> 181<br>Introduction 181<br>Methodology 183<br>Mathematical Models 183<br>Optimization Mechanism 183<br>Results and Discussion 185<br>Minimizing the Cost of PP-OMMT 185<br>Minimizing the Variance Between Desired Properties 187   |
| 11.1<br>11.2<br>11.3<br>11.4<br>11.5<br>11.5.1   | <b>Optimization of Mechanical Properties of Polypropylene</b><br><b>Montmorillonite Nanocomposites</b> 181<br>Introduction 181<br>Methodology 183<br>Mathematical Models 183<br>Optimization Mechanism 183<br>Results and Discussion 185<br>Minimizing the Cost of PP-OMMT 185<br>Minimizing the Variance Between Desired Properties 187<br>Conclusion 192   |
| 11.1<br>11.2<br>11.3<br>11.4<br>11.5<br>11.5.1<br>11.5.2   | <b>Optimization of Mechanical Properties of Polypropylene</b><br><b>Montmorillonite Nanocomposites</b> 181<br>Introduction 181<br>Methodology 183<br>Mathematical Models 183<br>Optimization Mechanism 183<br>Results and Discussion 185<br>Minimizing the Cost of PP-OMMT 185<br>Minimizing the Variance Between Desired Properties 187   |
| 11.1<br>11.2<br>11.3<br>11.4<br>11.5<br>11.5.1<br>11.5.2   | <b>Optimization of Mechanical Properties of Polypropylene</b><br><b>Montmorillonite Nanocomposites</b> 181<br>Introduction 181<br>Methodology 183<br>Mathematical Models 183<br>Optimization Mechanism 183<br>Results and Discussion 185<br>Minimizing the Cost of PP-OMMT 185<br>Minimizing the Variance Between Desired Properties 187<br>Conclusion 192   |
| 11.1<br>11.2<br>11.3<br>11.4<br>11.5<br>11.5.1<br>11.5.2<br>11.6   | <b>Optimization of Mechanical Properties of Polypropylene</b><br><b>Montmorillonite Nanocomposites</b> 181<br>Introduction 181<br>Methodology 183<br>Mathematical Models 183<br>Optimization Mechanism 183<br>Results and Discussion 185<br>Minimizing the Cost of PP-OMMT 185<br>Minimizing the Variance Between Desired Properties 187<br>Conclusion 192<br>References 193   |
| 11.1<br>11.2<br>11.3<br>11.4<br>11.5<br>11.5.1<br>11.5.2<br>11.6   | Optimization of Mechanical Properties of Polypropylene<br>Montmorillonite Nanocomposites 181<br>Introduction 181<br>Methodology 183<br>Mathematical Models 183<br>Optimization Mechanism 183<br>Results and Discussion 185<br>Minimizing the Cost of PP-OMMT 185<br>Minimizing the Variance Between Desired Properties 187<br>Conclusion 192<br>References 193<br>Product Selection and Business Portfolio for Long-Range  |
| 11.1<br>11.2<br>11.3<br>11.4<br>11.5<br>11.5.1<br>11.5.2<br>11.6   | Optimization of Mechanical Properties of Polypropylene<br>Montmorillonite Nanocomposites 181<br>Introduction 181<br>Methodology 183<br>Mathematical Models 183<br>Optimization Mechanism 183<br>Results and Discussion 185<br>Minimizing the Cost of PP-OMMT 185<br>Minimizing the Variance Between Desired Properties 187<br>Conclusion 192<br>References 193<br>Product Selection and Business Portfolio for Long-Range<br>Financial Stability: Case Study from the Petrochemical  |
| 11.1<br>11.2<br>11.3<br>11.4<br>11.5<br>11.5.1<br>11.5.2<br>11.6<br><b>12</b>  | Optimization of Mechanical Properties of Polypropylene<br>Montmorillonite Nanocomposites 181<br>Introduction 181<br>Methodology 183<br>Mathematical Models 183<br>Optimization Mechanism 183<br>Results and Discussion 185<br>Minimizing the Cost of PP-OMMT 185<br>Minimizing the Variance Between Desired Properties 187<br>Conclusion 192<br>References 193<br>Product Selection and Business Portfolio for Long-Range<br>Financial Stability: Case Study from the Petrochemical<br>Industry 195  |
| 11.1<br>11.2<br>11.3<br>11.4<br>11.5<br>11.5.1<br>11.5.2<br>11.6<br><b>12</b>  | Optimization of Mechanical Properties of PolypropyleneMontmorillonite Nanocomposites181Introduction181Methodology183Mathematical Models183Optimization Mechanism183Results and Discussion185Minimizing the Cost of PP-OMMT185Minimizing the Variance Between Desired Properties187Conclusion192References193Product Selection and Business Portfolio for Long-Range<br>Financial Stability: Case Study from the Petrochemical<br>IndustryIndustry195Introduction195  |
| <ul> <li>11.1</li> <li>11.2</li> <li>11.3</li> <li>11.4</li> <li>11.5</li> <li>11.5.1</li> <li>11.5.2</li> <li>11.6</li> </ul> 12 12.1 12.2  | Optimization of Mechanical Properties of PolypropyleneMontmorillonite Nanocomposites181Introduction181Methodology183Mathematical Models183Optimization Mechanism183Results and Discussion185Minimizing the Cost of PP-OMMT185Minimizing the Variance Between Desired Properties187Conclusion192References193Product Selection and Business Portfolio for Long-Range<br>Financial Stability: Case Study from the Petrochemical<br>IndustryIndustry195Introduction195Manufacturing Strategy and Product Selection Tools196   |
| <ul> <li>11.1</li> <li>11.2</li> <li>11.3</li> <li>11.4</li> <li>11.5</li> <li>11.5.1</li> <li>11.5.2</li> <li>11.6</li> </ul> 12 12.1 12.2 12.3   | Optimization of Mechanical Properties of Polypropylene<br>Montmorillonite Nanocomposites 181<br>Introduction 181<br>Methodology 183<br>Mathematical Models 183<br>Optimization Mechanism 183<br>Results and Discussion 185<br>Minimizing the Cost of PP-OMMT 185<br>Minimizing the Variance Between Desired Properties 187<br>Conclusion 192<br>References 193<br>Product Selection and Business Portfolio for Long-Range<br>Financial Stability: Case Study from the Petrochemical<br>Industry 195<br>Introduction 195<br>Manufacturing Strategy and Product Selection Tools 196<br>Model Development 199 |
| <ul> <li>11.1</li> <li>11.2</li> <li>11.3</li> <li>11.4</li> <li>11.5</li> <li>11.5.1</li> <li>11.5.2</li> <li>11.6</li> <li>12</li> <li>12.1</li> <li>12.2</li> <li>12.3</li> <li>12.4</li> </ul> | Optimization of Mechanical Properties of Polypropylene<br>Montmorillonite Nanocomposites 181Introduction 181Methodology 183Mathematical Models 183Optimization Mechanism 183Results and Discussion 185Minimizing the Cost of PP-OMMT 185Minimizing the Variance Between Desired Properties 187Conclusion 192References 193Product Selection and Business Portfolio for Long-Range<br>Financial Stability: Case Study from the Petrochemical<br>Industry 195Introduction 195Manufacturing Strategy and Product Selection Tools 196<br>Model Development 199<br>Illustrative Case Study 201                  |