TABLE OF CONTENTS

AUTHORS . v

ACKNOWLEDGMENTS vii

I ADSORPTION AS A TREATMENT PROCESS 1
Introduction 1
Process Configuration 8
Regeneration 11
Practical Guidelines 12
Moving Bed 13
Safety Consideration 15
Experimental Design and Testing 16

II ADSORPTION THEORY 21
Principles of Adsorption 21
Adsorption : Interaction Forces 22
Dispersion Forces 22
Surface Tension 23
Porosity 25
Surface Function Groups 27
The Polanyi Theory 29
Isostere and Isobar 30
Classification of Adsorption Isotherms 32
Equilibrium Models 34
Single Component Adsorption 34
Multicomponent Adsorption 37
Adsorption Kinetics 39
External Diffusion 40
Internal Diffusion 41
Diffusion Models 43
Surface Diffusion Model 43
Pore Diffusion Model 44
Combined Diffusion Model 44

III THE CONCEPT OF THE DIFFERENTIAL REACTOR . . . 49
Introduction 49
Theoretical Considerations 49

Experimental Results and Discussion . . . 50
Materials 50
Equilibrium Studies 51
Kinetic Studies 52
Conclusions 68

IV GRAVIMETRIC DIFFERENTIAL REACTOR FOR GAS ADSORPTION STUDIES 72
Introduction 72
Experimental Results and Discussion 72
Materials 72
Procedure 73
Equilibrium Isotherm 74
Kinetic Rate Studies 77
Conclusions 81

V GRAVIMETRIC DIFFERENTIAL REACTOR FOR WATER ADSORPTION STUDIES 86
Introduction 86
Experimental Results and Discussion 86
Experimental Procedure 86
Buoyancy Determination 88
Equilibrium Study 92
Kinetic Analysis 93
Conclusions 97

VI COMBINED DIFFUSION DIFFERENTIAL REACTOR MODELS 100
Introduction 100
Liquid-Solid System 100
Method and Results 100
Sensitivity Analysis 104
Gas-Solid Systems 107
Ds, Dp Determination 108
Conclusions 114

VII KINETIC STUDIES OF MULTICOMPONENT ADSORPTION USING DIFFERENTIAL REACTOR TECHNIQUE 118
Introduction 118
Analytical Results and Discussion 118
Adsorption Equilibrium 119

Modeling Comparison 119
Modeling Simulation 122
Conclusions 129

VIII FIXED BED MODELING AND DESIGN FOR WATER ADSORPTION SYSTEMS. 132
Introduction 132
Experimental Results and Discussion 132
Mathematical Model 132
Experimental Procedure 134
Adsorption Equilibrium and Kinetic Parameters 136
Sensitivity Analysis 136
Modeling Comparison 140
Breakthrough Curves 141
Empirical Method 148
Conclusions 150

IX FIXED BED MODELING AND DESIGN FOR GAS ADSORPTION SYSTEMS 157
Introduction 157
Theory and Numerical Analysis 157
Combined Diffusion Model 157
Effective Diffusion Model 159
Experimental Results and Discussion 160
Experimental Procedure 160
Sensitivity Analysis 163
Modeling Comparison 164
Conclusions 169

X MODELING OF MULTICOMPONENT WATER ADSORPTION SYSTEMS. 177
Introduction 177
Experimental Results and Discussion 178
Mathematical Model 178
Experimental Procedure 180
Adsorption Equilibrium 180
Sensitivity Analysis 182
Modeling Comparison 184
Adsorption Breakthrough Curves 192
Empirical Model 199
Conclusions 201

XI COMPARISON OF AIR AND WATER ADSORPTION SYSTEMS. 208
Introduction 208
Method and Results 208
Adsorption of Benzene in Liquid-Solid System 208
Comparison of Benzene Adsorption in Water and Air Systems 213
Breakthrough Curve Comparison 213
Comparison of the Intraparticle Diffusivity in Both Systems . 218

XII THERMODYNAMIC ANALYSIS OF ADSORPTION SYSTEMS. 229
Introduction 229
Method and Results 229
Models and Methods 229
Experimental Procedure 231
Method of Approach 231
Results 232
Conclusions 253

XIII APPLICATION OF POTENTIAL THEORY FOR GAS ADSORPTION SYSTEMS. 256
Introduction 256
Method and Results 256
Theory 257
Demonstration of the Method 260
Limitations of the Method 263
Conclusions 274

XIV EVALUATION OF HUMIDITY EFFECTS FOR GAS ADSORPTION SYSTEMS 278
Introduction 278
Sorptive Behavior of Water 279
Okazaki's Model 279
Application and Limitations of Okazaki's Model 289
Water-Organic Adsorbate Interaction 291

XV A METHOD FOR NON-IDEAL ADSORBED PREDICTION FOR LIQUID-SOLID SYSTEMS 298
Introduction 298

Theory Development 298
Adsorbed Phase and Liquid Phase Surface Excess 298
Prediction Model for Ternary Liquid Solutions 301
Experimental Method 304
Results and Conclusions 306
Calculation of Activity Coefficient in the Bulk Phase 306
Calculation of Activity Coefficient in the Adsorbed Phase . . . 307
Conclusions 318

APPENDIX : MODEL PROGRAM 323

INDEX 345