Contents

Foreword by George E. Keller, II *xi*
Preface *xiii*
Software Selection and Copyright Notice *xvii*
Acknowledgments *xix*
About the Authors *xxi*
List of Computer Files *xxiii*

1 Simulation of Adsorption Processes *1*
1.1 Introduction to Gas-phase Adsorption Technologies *1*
1.2 Core Concepts in Gas Adsorption *2*
1.2.1 The Adsorption Process *2*
1.2.2 How the Driving Forces Achieve Separation *3*
1.3 Isotherms *4*
1.3.1 The Langmuir Isotherm (1918) *5*
1.3.2 The Linear Isotherm *5*
1.3.3 The Brunauer–Emmett–Teller (BET) Isotherm (1938) *5*
1.3.4 The Freundlich Isotherm (1906) *6*
1.3.5 The Sips (Langmuir–Freundlich) Isotherm (1948) *6*
1.3.6 The Toth Isotherm (1971) *6*
1.3.7 Summary *6*
1.4 The Properties of Packed Beds *6*
1.4.1 Void Fractions *7*
1.4.2 External Voids *8*
1.4.3 Internal Voids *8*
1.4.4 Densities *8*
1.4.4.1 Bulk Density *8*
1.4.4.2 Skeletal or Solid Density *9*
1.4.4.3 Envelope or Particle Density *10*
1.4.4.4 Caveats *10*
1.4.5 Relationships *10*
1.4.6 Gas-phase Behavior *10*
1.4.6.1 Pressure Drop *10*
1.4.6.2 Compressibility *11*

1.5 PSA and TSA Implementation Details *12*
1.5.1 Common Adsorbent Characteristics *12*
1.5.2 Common Process Configurations *12*
1.6 Introduction to Aspen Adsorption *13*
1.7 PSA Workshop: Aspen Adsorption Modeling for Air Separation *15*
1.7.1 Adding Components to an Aspen Adsorption Simulation *17*
1.7.2 Creating a Flowsheet in Aspen Adsorption *22*
1.7.3 Specifying Operating Conditions: Tables and Forms *33*
1.7.4 Scheduling Events with the Cycle Organizer *42*
1.7.5 Running an Aspen Simulation *51*
1.7.6 Viewing and Exporting Simulation Results *51*
1.8 PSA Workshop: Hydrogen Separation in Aspen Adsorption *57*
1.8.1 Define the Components and Property Model *58*
1.8.2 Creating a Flowsheet in Aspen Adsorption *63*
1.8.3 Run a Breakthrough Simulation *65*
1.8.4 Create the PSA Flowsheet *77*
1.9 PSA Workshop: Modeling Hydrogen Separation using gCSS *87*
1.9.1 Define the Components and Property Models *91*
1.9.2 Working with Model Libraries: Advanced Flowsheet Options *95*
1.9.3 Introduction to Scripting: Set Repeated Values and Initialize Blocks *108*
1.9.4 Inspecting Blocks: Advanced Operating Conditions *112*
1.9.5 Defining the Cycle Organizer *119*
1.9.6 Viewing Results *127*
1.10 TSA Workshop: Temperature Swing Adsorption for Air Drying *128*
1.11 Conclusions *140*
1.12 Practice Problems *143*
1.12.1 Introducing a gas_interaction Unit into Workshop 1 *143*
1.12.2 Naphtha Upgrading Using Adsorption *145*
1.13 Nomenclature *149*
Bibliography *150*

2 Simulation of SMB Chromatographic Processes *155*
2.1 Introduction to Chromatography *155*
2.1.1 Mathematical Differences from Gas Adsorption *155*
2.1.1.1 The Trace Liquid Assumption *155*
2.1.1.2 Concentration Versus Partial Pressure *156*
2.1.2 Thermodynamic Differences from Gas Adsorption *156*
2.1.2.1 Isotherms *156*
2.1.2.2 Physical Property Models *156*
2.2 Introduction to SMB Chromatography *156*
2.3 SMB Implementation Details *157*
2.3.1 Common Process Configurations *157*
2.3.2 M-Values *160*
2.3.3 Scale-Up Concerns *161*
2.3.4 Pressure Drop Limitations *162*
2.3.5 Introduction to Operational Modes *163*

2.4 SMB Workshop: Simulate a Four-Zone SMB in Aspen Chromatography for the Separation of Tröger's Base Enantiomers *163*
2.4.1 Creating a Flowsheet in Aspen Chromatography *163*
2.4.2 Adding Components to an Aspen Chromatography Simulation *164*
2.4.3 The Chrom_CCC_separator2 Block *165*
2.4.4 Viewing Results *188*
2.5 Tandem SMB Workshop: Simulate a Separation with Dual SMB Columns *192*
2.6 Practice Problems *194*
2.6.1 Run Workshop 2.4 as a Steady-State Simulation *194*
2.6.2 Simulation of an Industrial-Scale Xylene Separation Using Literature Data *200*
2.6.3 Simulate a Five-Zone SMB System for Separating Phenylalanine, Tryptophan, and Methionine *202*
Bibliography *206*

3 Shortcut Design of SMB Systems *213*
3.1 General Concepts *213*
3.1.1 Mass Balances *215*
3.1.2 Differential Equations *217*
3.1.3 The Method of Characteristics *218*
3.2 Triangle Theory *219*
3.2.1 Notations *219*
3.2.2 Introduction *219*
3.2.3 Constraints on the System *222*
3.3 Triangle Theory Workshop: Design of a System for the Separation of Amino Acids *224*
3.4 Exercise 1: Calculating Transitions in a Fixed Bed Using Mathematica *230*
3.4.1 Differential Equations – Analysis *232*
3.4.2 Constructing the Solution from Eigenvectors and Eigenvalues *238*
3.4.3 Use the Steady-State Information to Constrain Operating Conditions *239*
3.4.4 Calculate the Curves Defined by the Eigenvectors *241*
3.4.5 Calculate the Eigenvalues along the Transition *244*
3.4.6 Calculate the Concentrations in Time and Space *246*
3.4.7 Account for Shock Waves *246*
3.5 Exercise 2: Constructing the Constraints on the TMB System in Mathematica *249*
3.6 Standing Wave Design *253*
3.6.1 Standing Wave Design in a Nonlinear Ideal System *254*
3.6.2 Standing Wave Design in a System with Nonlinear Isotherm and Significant Mass Transfer Effects *261*
3.7 Standing Wave Design Workshop: Calculating the Operating Conditions for an Ideal and a Nonideal System *265*
3.8 Conclusions *271*

3.9 Practice Problems *272*
3.9.1 Use the Triangle Theory Tool and the Standing Wave Design Tool to Create an Aspen Simulation of the Separation of 1-phenol-1-propanol on Tribenzoate *272*
Bibliography *274*

4 Operational Modes of SMB Processes *283*
4.1 Overview *283*
4.2 Selection of Operational Modes *284*
4.3 Varicol *284*
4.3.1 Design Heuristics and Examples *286*
4.3.2 Workshop 1: Apply Varicol to the 4-Zone SMB Model *287*
4.4 PowerFeed *293*
4.4.1 Design Heuristics and Examples *294*
4.4.2 Workshop 2: Apply PowerFeed to the Four-Zone SMB Model *297*
4.5 ModiCon *309*
4.5.1 Design Heuristics and Examples *309*
4.5.2 Workshop 3: Apply ModiCon to the 4-Zone SMB Model *315*
4.6 Combined Modes *323*
4.6.1 Workshop 4: Extend Previously Created Flowsheets *323*
4.7 Parallel Two Zones *330*
4.7.1 Introduction to Parallel Two Zones *330*
4.7.2 Specification Analysis *334*
4.7.3 Importing Flowsheets *337*
4.8 Conclusions *345*
4.9 Practice Problems *345*
4.9.1 Simulation of a Five-Zone SMB Unit Using the ModiCon Operational Mode *345*
4.9.2 Compare Parallel Two-Zone Results with SMB Results *345*
Bibliography *347*

5 Parameter Estimation, Regression, and Sensitivity of Adsorptive and Chromatographic Processes *349*
5.1 Empirical Correlations for Physical Properties *349*
5.1.1 Axial Dispersion Coefficient *349*
5.1.2 Mass Transfer Coefficient *350*
5.1.3 Caveats *351*
5.2 Parameter Workshop: Regressing against Steady-State Experiments *351*
5.2.1 Introduction to "Experiments" In Aspen Software *351*
5.2.2 Experimental Data *352*
5.2.3 Parameter Regression in Excel *352*
5.2.4 Parameter Regression in Aspen Chromatography *363*
5.2.4.1 Defining an Estimation Flowsheet *363*
5.2.4.2 Entering Experimental Data *364*
5.2.4.3 Estimation Settings *368*
5.2.4.4 Running an Estimation *370*

5.2.5 Parameter Regression In Mathematica *370*
5.2.5.1 Defining the Functions *371*
5.2.5.2 Entering the Data *372*
5.2.5.3 Regression *375*
5.3 Parameter Workshop: Regressing Against Dynamic Experiments *376*
5.3.1 Problem Description *376*
5.3.2 Dynamic Estimation Settings *376*
5.3.3 Performance Concerns *380*
5.4 Xylene Parameter Regression *380*
5.5 Conclusions *386*
5.6 Practice Problems *387*
5.6.1 Perform Dynamic Parameter Estimation in Aspen Adsorption *387*
5.6.2 Sensitivity Analysis Using Scripts in Aspen Adsorption *389*
Bibliography *393*

Literature Cited in the Text *395*

Index *399*