# TABLE OF CONTENTS

**HANDBOOK OF POLYMER SOLUTION THERMODYNAMICS**

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>PREFACE</strong></td>
<td>i</td>
</tr>
<tr>
<td><strong>Chapter 1: INTRODUCTION</strong></td>
<td>1</td>
</tr>
<tr>
<td>A. OBJECTIVES OF THE HANDBOOK OF POLYMER SOLUTION THERMODYNAMICS</td>
<td>1</td>
</tr>
<tr>
<td><strong>Chapter 2: FUNDAMENTALS OF POLYMER SOLUTION THERMODYNAMICS</strong></td>
<td>3</td>
</tr>
<tr>
<td>A. PURE POLYMER PVT BEHAVIOR</td>
<td>3</td>
</tr>
<tr>
<td>B. PHASE EQUILIBRIA THERMODYNAMICS</td>
<td>4</td>
</tr>
<tr>
<td>C. MODELING APPROACHES TO POLYMER SOLUTION THERMODYNAMICS</td>
<td>6</td>
</tr>
<tr>
<td>D. LATTICE MODELS</td>
<td>8</td>
</tr>
<tr>
<td>1. Flory-Huggins Model</td>
<td>8</td>
</tr>
<tr>
<td>2. Solubility Parameters and the Flory-Huggins Model</td>
<td>9</td>
</tr>
<tr>
<td>3. Modifications of the Flory-Huggins Model</td>
<td>11</td>
</tr>
<tr>
<td>4. Sanchez-Lacombe Equation of State</td>
<td>12</td>
</tr>
<tr>
<td>5. Panayiotou-Vera Equation of State</td>
<td>13</td>
</tr>
<tr>
<td>6. Kumar Equation of State</td>
<td>13</td>
</tr>
<tr>
<td>7. High-Danner Equation of State</td>
<td>14</td>
</tr>
<tr>
<td>8. Oishi-Prausnitz Activity Coefficient Model</td>
<td>15</td>
</tr>
<tr>
<td>E. VAN DER WAALS MODELS</td>
<td>16</td>
</tr>
<tr>
<td>1. Flory Equation of State</td>
<td>17</td>
</tr>
<tr>
<td>2. Chen, Fredenslund, and Rasmussen Equation of State</td>
<td>18</td>
</tr>
<tr>
<td>F. LIQUID-LIQUID EQUILIBRIA OF POLYMER SOLUTIONS</td>
<td>18</td>
</tr>
<tr>
<td>1. Thermodynamics of Liquid-Liquid Equilibria</td>
<td>18</td>
</tr>
<tr>
<td>2. Types of Liquid-Liquid Equilibria</td>
<td>20</td>
</tr>
<tr>
<td>4. Computation of Liquid-Liquid Equilibria Compositions</td>
<td>26</td>
</tr>
<tr>
<td>5. Parameter Estimation from Liquid-Liquid Equilibria Data</td>
<td>26</td>
</tr>
<tr>
<td>6. Sample Correlations of Liquid-Liquid Equilibria Data</td>
<td>27</td>
</tr>
<tr>
<td>G. EFFECT OF POLYDISPERSSION</td>
<td>29</td>
</tr>
</tbody>
</table>
TABLE OF CONTENTS (Continued)

Chapter 3: RECOMMENDED PROCEDURES .............................................. 31

A. SELECTION OF MODELS ................................................................. 31
   1. Correlation of Pure Polymer PVT Behavior ............................... 31
   2. Prediction of Vapor-Liquid Equilibria .................................... 32

B. PROCEDURE: METHOD FOR ESTIMATING THE SPECIFIC VOLUME
   OF A PURE POLYMER LIQUID .................................................. 38
   1. Method ............................................................................. 38
   2. Procedure ...................................................................... 38
   3. Limitations and Reliability ............................................... 39
   4. Comments ..................................................................... 39
   5. Literature Sources ......................................................... 39
   6. Example ......................................................................... 39

C. PROCEDURE: OISHI-PRAUSNITZ METHOD FOR ESTIMATING
   THE ACTIVITY COEFFICIENTS OF SOLVENTS IN
   POLYMER SOLUTIONS .......................................................... 42
   1. Method ............................................................................. 42
   2. Procedure ...................................................................... 45
   3. Limitations and Reliability ............................................... 46
   4. Comments ..................................................................... 47
   5. Literature Sources ......................................................... 47
   6. Example ......................................................................... 48

D. PROCEDURE: CHEN-FREDENSLOM-RASMUSSEN EQUATION
   OF STATE FOR ESTIMATING THE ACTIVITY COEFFICIENTS
   OF SOLVENTS IN POLYMER SOLUTIONS ................................. 64
   1. Method ............................................................................. 64
   2. Procedure ...................................................................... 68
   3. Limitations and Reliability ............................................... 69
   4. Literature Source ............................................................ 69
   5. Example ......................................................................... 69

E. PROCEDURE: HIGH-DANNER EQUATION OF STATE FOR
   ESTIMATING THE ACTIVITY COEFFICIENT OF A SOLVENT
   IN A POLYMER SOLUTION ..................................................... 73
   1. Method ............................................................................. 73
   2. Procedure ...................................................................... 77
   3. Limitations and Reliability ............................................... 79
   4. Literature Sources ............................................................ 79
   5. Example ......................................................................... 79
TABLE OF CONTENTS (Continued)

F. PROCEDURE: FLORY-HUGGINS CORRELATION FOR VAPOR-LIQUID
   EQUILIBRIA OF POLYMER SOLVENT SYSTEMS ..................... 82
   1. Method ................................................. 82
   2. Procedure ............................................ 83
   3. Limitations and Reliability ............................. 83
   4. Literature Source ...................................... 83
   5. Example ............................................... 83

Chapter 4: POLYMER DATA BASE ................................... 85

A. INTRODUCTION ............................................. 85

B. EXPERIMENTAL METHODS ................................. 85
   1. Inverse Gas Chromatography (IGC) .................. 86
   2. Piezoelectric Sorption (PZS) ......................... 86
   3. Differential Vapor Pressure (DVP) ................. 87
   4. Gravimetric Sorption (GS) ............................ 87
   5. Light Scattering (LS) .................................. 88
   6. Ultracentrifuge (UC) .................................. 90
   7. Turbidimetry (TB) and Light Scattering Turbidimetry (LST) 91
   8. Microanalytical (MA) .................................. 92
   9. Ultraviolet Spectrometry (UVS) and Infrared Spectrometry (IRS) 92
  10. Size Exclusion Chromatography (SEC) ............... 92

C. DATA REDUCTION PROCEDURES .......................... 92
   1. Pure Polymer PVT Data .................................. 93
   2. Finite Dilution Flory Chi Parameter .................... 94
   3. Infinite Dilution Flory Chi Parameter ............... 95
   4. Differential Vapor Pressure, Gravimetric Sorption, and
      Piezoelectric Sorption Methods ......................... 96
   5. Gas Chromatograph Data at Infinite Dilution .......... 99
   6. Henry’s Law Constant ................................ 102
   7. Osmotic Pressure Data ................................ 102

D. LISTING OF SYSTEMS INCLUDED IN DATA BASES ....... 103
   1. Pure Polymer PVT Data .................................. 103
   2. Finite Concentration VLE Data ....................... 104
   3. Infinite Dilution VLE Data ............................ 106
   4. Binary Liquid-Liquid Equilibria Data ................ 117
   5. Ternary Liquid-Liquid Equilibria Data ............ 118
# TABLE OF CONTENTS (Concluded)

## Chapter 5: COMPUTER PROGRAMS

A. PHASE EQUILIBRIA CALCULATIONS - POLYPROG ........................................... 121
   1. Installation ........................................... 121
   2. Features ........................................... 121
   3. Tutorial Session .................................... 124

B. DATA RETRIEVAL - POLYDATA ................................................................. 129
   1. Installation ........................................... 129
   2. Features ........................................... 130
   3. Tutorial Session .................................... 132

C. FILE FORMATS USED BY POLYDATA ......................................................... 133
   1. Pure Polymers ........................................ 133
   2. Infinitely Dilute Solvent Weight Fraction Activity
      Coefficients (WFAC) .................................. 135
   3. Finite Concentration Solvent Weight Fraction Activity
      Coefficients (WFAC) .................................. 136
   4. Binary LLE ........................................... 137
   5. Ternary LLE ........................................... 138
   6. Bibliographic Sources ............................... 139
   7. Polymer Synonyms .................................... 140

## Chapter 6: APPENDICES

A. GLOSSARY OF TERMS ................................................................. 141

B. STANDARD POLYMER ABBREVIATIONS ............................................. 142

C. NOMENCLATURE ................................................................. 147

D. UNITS AND CONVERSION FACTORS .............................................. 150
   1. Units and Symbols .................................... 150
   2. Prefixes ........................................... 153
   3. Usage Format ........................................ 155
   4. Conversion ........................................... 156

E. TEXT REFERENCES ................................................................. 161

F. DATA REFERENCES ................................................................. 166