Polymer Processing

Tim A. Osswald, Juan P. Hernandez-Ortiz

Modeling and Simulation

ISBN 3-446-40381-7

Inhaltsverzeichnis

Weitere Informationen oder Bestellungen unter http://www.hanser.de/3-446-40381-7 sowie im Buchhandel
TABLE OF CONTENTS

Preface vii

INTRODUCTION xvii

I.1 Modeling and Simulation xvii
I.2 Modeling Philosophy xx
I.3 Notation xxiv
I.4 Concluding Remarks xxvi
References xxvii

PART I BACKGROUND 1

1 POLYMER MATERIALS SCIENCE 1

1.1 Chemical Structure 1
1.2 Molecular Weight 4
1.3 Conformation and Configuration of Polymer Molecules 9
1.4 Morphological Structure 12
1.4.1 Copolymers and Polymer Blends 16
1.5 Thermal Transitions 18
1.6 Viscoelastic Behavior of Polymers 24
1.6.1 Stress Relaxation 24
1.6.2 Time-Temperature Superposition (WLF-Equation) 26
1.7 Examples of Common Polymers
   1.7.1 Thermoplastics
   1.7.2 Thermosetting Polymers
   1.7.3 Elastomers

Problems
References

2 PROCESSING PROPERTIES

2.1 Thermal Properties
   2.1.1 Thermal Conductivity
   2.1.2 Specific Heat
   2.1.3 Density
   2.1.4 Thermal Diffusivity
   2.1.5 Linear Coefficient of Thermal Expansion
   2.1.6 Thermal Penetration
   2.1.7 Measuring Thermal Data

2.2 Curing Properties

2.3 Rheological Properties
   2.3.1 Flow Phenomena
   2.3.2 Viscous Flow Models
   2.3.3 Viscoelastic Constitutive Models
   2.3.4 Rheometry
   2.3.5 Surface Tension

2.4 Permeability properties
   2.4.1 Sorption
   2.4.2 Diffusion and Permeation
   2.4.3 Measuring $S$, $D$, and $P$
   2.4.4 Diffusion of Polymer Molecules and Self-Diffusion

2.5 Friction properties

Problems
References

3 POLYMER PROCESSES

3.1 Extrusion
   3.1.1 The Plasticating Extruder
   3.1.2 Extrusion Dies

3.2 Mixing Processes
   3.2.1 Distributive Mixing
   3.2.2 Dispersive Mixing
   3.2.3 Mixing Devices

3.3 Injection Molding
3.3.1 The Injection Molding Cycle 141
3.3.2 The Injection Molding Machine 144
3.3.3 Related Injection Molding Processes 149
3.4 Secondary Shaping 150
  3.4.1 Fiber Spinning 151
  3.4.2 Film Production 151
  3.4.3 Thermoforming 157
3.5 Calendering 158
3.6 Coating 160
3.7 Compression Molding 163
3.8 Foaming 164
3.9 Rotational Molding
  References 167

PART II PROCESSING FUNDAMENTALS

4 DIMENSIONAL ANALYSIS AND SCALING 171
  4.1 Dimensional Analysis 172
  4.2 Dimensional Analysis by Matrix Transformation 174
  4.3 Problems with non-Linear Material Properties 192
  4.4 Scaling and Similarity
    Problems 203
    References 206

5 TRANSPORT PHENOMENA IN POLYMER PROCESSING 207
  5.1 Balance Equations 207
    5.1.1 The Mass Balance or Continuity Equation 208
    5.1.2 The Material or Substantial Derivative 209
    5.1.3 The Momentum Balance or Equation of Motion 210
    5.1.4 The Energy Balance or Equation of Energy 217
  5.2 Model Simplification 220
    5.2.1 Reduction in Dimensionality 222
    5.2.2 Lubrication Approximation 223
  5.3 Simple Models in Polymer Processing 225
    5.3.1 Pressure Driven Flow of a Newtonian Fluid Through a Slit 225
    5.3.2 Flow of a Power Law Fluid in a Straight Circular Tube (Hagen-Poiseuille Equation) 227
    5.3.3 Flow of a Power Law Fluid in a Slightly Tapered Tube 228
    5.3.4 Volumetric Flow Rate of a Power Law Fluid in Axial Annular Flow 229
    5.3.5 Radial Flow Between two Parallel Discs — Newtonian Model 230
    5.3.6 The Hele-Shaw model 232
5.3.7 Cooling or Heating in Polymer Processing 239
Problems 243
References 245

### 6 ANALYSES BASED ON ANALYTICAL SOLUTIONS 247

6.1 Single Screw Extrusion—Isothermal Flow Problems 248
   6.1.1 Newtonian Flow in the Metering Section of a Single Screw Extruder 249
   6.1.2 Cross Channel Flow in a Single Screw Extruder 251
   6.1.3 Newtonian Isothermal Screw and Die Characteristic Curves 255

6.2 Extrusion Dies—Isothermal Flow Problems 258
   6.2.1 End-Fed Sheeting Die 258
   6.2.2 Coat Hanger Die 261
   6.2.3 Extrusion Die with Variable Die Land Thicknesses 263
   6.2.4 Pressure Flow of Two Immiscible Fluids with Different Viscosities 264
   6.2.5 Fiber Spinning 266
   6.2.6 Viscoelastic Fiber Spinning Model 269

6.3 Processes that Involve Membrane Stretching 271
   6.3.1 Film Blowing 271
   6.3.2 Thermoforming 277

6.4 Calendering — Isothermal Flow Problems 278
   6.4.1 Newtonian Model of Calendering 278
   6.4.2 Shear Thinning Model of Calendering 285
   6.4.3 Calender Fed with a Finite Sheet Thickness 287

6.5 Coating Processes 289
   6.5.1 Wire Coating Die 289
   6.5.2 Roll Coating 291

6.6 Mixing — Isothermal Flow Problems 295
   6.6.1 Effect of Orientation on Distributive Mixing — Erwin's Ideal Mixer 295
   6.6.2 Predicting the Striation Thickness in a Couette Flow System — Shear Thinning Model 296
   6.6.3 Residence Time Distribution of a Fluid Inside a Tube 300
   6.6.4 Residence Time Distribution Inside the Ideal Mixer 301

6.7 Injection Molding — Isothermal Flow Problems 303
   6.7.1 Balancing the Runner System in Multi-Cavity Injection Molds 303
   6.7.2 Radial Flow Between Two Parallel Discs 306

6.8 Non-Isothermal Flows 309
   6.8.1 Non-Isothermal Shear Flow 309
   6.8.2 Non-Isothermal Pressure Flow Through a Slit 311

6.9 Melting and Solidification 312
   6.9.1 Melting with Pressure Flow Melt Removal 317
   6.9.2 Melting with Drag Flow Melt Removal 319
   6.9.3 Melting Zone in a Plasticating Single Screw Extruder 324
## TABLE OF CONTENTS

6.10 Curing Reactions During Processing 330
6.11 Concluding Remarks 331

Problems 331
References 339

### PART III NUMERICAL TECHNIQUES

#### 7 INTRODUCTION TO NUMERICAL ANALYSIS 343

7.1 Discretization and Error 344
7.2 Interpolation 344

7.2.1 Polynomial and Lagrange Interpolation 345
7.2.2 Hermite Interpolations 352
7.2.3 Cubic Splines 354
7.2.4 Global and Radial Interpolation 357

7.3 Numerical Integration 360

7.3.1 Classical Integration Methods 362
7.3.2 Gaussian Quadratures 364

7.4 Data Fitting 367

7.4.1 Least Squares Method 368
7.4.2 The Levenberg-Marquardt Method 369

7.5 Method of Weighted Residuals 376

Problems 381
References 383

#### 8 FINITE DIFFERENCE METHOD 385

8.1 Taylor-Series Expansions 387
8.2 Numerical Issues 392
8.3 The Info-Travel Concept 393
8.4 Steady-State Problems 395
8.5 Transient Problems 409

8.5.1 Higher Order Approximation Techniques 422

8.6 The Radial Flow Method 428
8.7 Flow Analysis Network 439
8.8 Predicting Fiber Orientation — The Folgar-Tucker Model 443

8.9 Concluding Remarks 445

Problems 448
References 450

#### 9 FINITE ELEMENT METHOD 453

9.1 One-Dimensional Problems 453

9.1.1 One-Dimensional Finite Element Formulation 454
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.1.2</td>
<td>Numerical Implementation of a One-Dimensional Finite Element Formulation</td>
<td>458</td>
</tr>
<tr>
<td>9.1.3</td>
<td>Matrix Storage Schemes</td>
<td>464</td>
</tr>
<tr>
<td>9.1.4</td>
<td>Transient Problems</td>
<td>466</td>
</tr>
<tr>
<td>9.2</td>
<td>Two-Dimensional Problems</td>
<td>470</td>
</tr>
<tr>
<td>9.2.1</td>
<td>Solution of Poisson’s equation Using a Constant Strain Triangle</td>
<td>470</td>
</tr>
<tr>
<td>9.2.2</td>
<td>Transient Heat Conduction Problem Using Constant Strain Triangle</td>
<td>474</td>
</tr>
<tr>
<td>9.2.3</td>
<td>Solution of Field Problems Using Isoparametric Quadrilateral Elements</td>
<td>474</td>
</tr>
<tr>
<td>9.2.4</td>
<td>Two Dimensional Penalty Formulation for Creeping Flow Problems</td>
<td>479</td>
</tr>
<tr>
<td>9.3</td>
<td>Three-Dimensional Problems</td>
<td>487</td>
</tr>
<tr>
<td>9.3.1</td>
<td>Three-dimensional Elements</td>
<td>487</td>
</tr>
<tr>
<td>9.3.2</td>
<td>Three-Dimensional Transient Heat Conduction Problem With Convection</td>
<td>489</td>
</tr>
<tr>
<td>9.3.3</td>
<td>Three-Dimensional Mixed Formulation for Creeping Flow Problems</td>
<td>491</td>
</tr>
<tr>
<td>9.4</td>
<td>Mold Filling Simulations Using the Control Volume Approach</td>
<td>493</td>
</tr>
<tr>
<td>9.4.1</td>
<td>Two-Dimensional Mold Filling Simulation of Non-Planar Parts (2.5D Model)</td>
<td>493</td>
</tr>
<tr>
<td>9.4.2</td>
<td>Full Three-Dimensional Mold Filling Simulation</td>
<td>497</td>
</tr>
<tr>
<td>9.5</td>
<td>Viscoelastic Fluid Flow</td>
<td>502</td>
</tr>
<tr>
<td></td>
<td>Problems</td>
<td>507</td>
</tr>
<tr>
<td></td>
<td>References</td>
<td>508</td>
</tr>
</tbody>
</table>

**10 BOUNDARY ELEMENT METHOD**

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.1</td>
<td>Scalar Fields</td>
<td>512</td>
</tr>
<tr>
<td>10.1.1</td>
<td>Green’s Identities</td>
<td>512</td>
</tr>
<tr>
<td>10.1.2</td>
<td>Green’s Function or Fundamental Solution</td>
<td>515</td>
</tr>
<tr>
<td>10.1.3</td>
<td>Integral Formulation of Poisson’s Equation</td>
<td>516</td>
</tr>
<tr>
<td>10.1.4</td>
<td>BEM Numerical Implementation of the 2D Laplace Equation</td>
<td>518</td>
</tr>
<tr>
<td>10.1.5</td>
<td>2D Linear Elements</td>
<td>522</td>
</tr>
<tr>
<td>10.1.6</td>
<td>2D Quadratic Elements</td>
<td>525</td>
</tr>
<tr>
<td>10.1.7</td>
<td>Three-Dimensional Problems</td>
<td>528</td>
</tr>
<tr>
<td>10.2</td>
<td>Momentum Equations</td>
<td>533</td>
</tr>
<tr>
<td>10.2.1</td>
<td>Green’s Identities for the Momentum Equations</td>
<td>534</td>
</tr>
<tr>
<td>10.2.2</td>
<td>Integral Formulation for the Momentum Equations</td>
<td>534</td>
</tr>
<tr>
<td>10.2.3</td>
<td>BEM Numerical Implementation of the Momentum Balance Equations</td>
<td>536</td>
</tr>
<tr>
<td>10.2.4</td>
<td>Numerical Treatment of the Weakly Singular Integrals</td>
<td>539</td>
</tr>
<tr>
<td>10.2.5</td>
<td>Solids in Suspension</td>
<td>544</td>
</tr>
<tr>
<td>10.3</td>
<td>Comments of non-Linear Problems</td>
<td>553</td>
</tr>
<tr>
<td>10.4</td>
<td>Other Boundary Element Applications</td>
<td>554</td>
</tr>
<tr>
<td></td>
<td>Problems</td>
<td>560</td>
</tr>
<tr>
<td></td>
<td>References</td>
<td>563</td>
</tr>
</tbody>
</table>
# 11 RADIAL FUNCTIONS METHOD

11.1 The Kansa Collocation Method 568
11.2 Applying RFM to Balance Equations in Polymer Processing 570
   11.2.1 Energy Balance 570
   11.2.2 Flow problems 577
Problems 594
References 596

# INDEX

597