

Contents

Foreword	v
<i>by Robert D. Forger</i>	
Preface to the Series	vii
<i>by Ernest C. Bernhardt</i>	
Preface to this Volume	ix
<i>by Charles L. Tucker III</i>	
1 Introduction to Process Modeling	1
<i>by Charles L. Tucker III</i>	
1.1 Why Models Are Useful	2
1.2 How to Build a Model	3
1.3 The Plan of the Book	5
References	6
2 Models of Material Behavior	7
<i>by Musa R. Kamal and Michael E. Ryan</i>	
2.1 Introduction	8
2.2 Types of Polymeric Systems	8
2.2.1 Thermoplastics and Thermosets	8
2.2.2 Amorphous and Crystalline Polymers	9
2.2.3 Blends and Composites	10
2.3 Properties Required for Modeling of Polymer Processing	10
2.3.1 Analysis of the Transport Equations	10
2.3.2 Identification of the Required Properties	11
2.3.3 Nature and Range of the Information Needed	11
2.3.4 Numerical Data versus Models and Equations	12
2.4 Rheological Behavior	13
2.4.1 Definition and Requirements of Rheological Material Parameters	13
2.4.2 Observed Types of Rheological Behavior	16
2.4.3 Experimental Techniques, Typical Data, Limitations	18
2.4.4 Rheological Constitutive Equations	21
2.4.5 Relationships Between Constitutive Equations	27
2.4.6 Molecular Weight Effects	28
2.4.7 Time-Temperature Superposition: WLF Equation	29
2.4.8 Blends and Composites	29
2.5 Equations of State and PVT Behavior	31
2.5.1 Available Data and Limitations	32
2.5.2 Theoretically-Based Equations of State	34
2.5.3 Empirical Equations of State	36
2.6 Glass Transition, Crystallinity and Crystallization	38
2.6.1 The Glass Transition Temperature	38
2.6.2 Crystallinity and Morphology	39
2.6.3 Experimental Determination of the Degree of Crystallinity	40
2.6.4 Nucleation and Growth of Polymer Crystals	41
2.6.5 Isothermal Crystallization Rates	43
2.6.6 Non-Isothermal Crystallization Rates	43

2.7	Thermal Conductivity and Diffusivity	44
2.7.1	Experimental Techniques	45
2.7.2	Effect of Temperature and Degree of Crystallinity	45
2.7.3	Effect of Molecular Weight	46
2.7.4	Effect of Orientation	47
2.7.5	Effect of Pressure	47
2.8	Thermoset Cure and Kinetics	48
2.8.1	Experimental Techniques to Study Cure Kinetics	48
2.8.2	Models of Cure Kinetics	49
2.8.3	Specific Heat and Heat Generation During Cure	52
2.8.4	Thermal Conductivity and Diffusivity Variation During Cure	53
2.8.5	Rheological Behavior of Reactive Polymer Systems	55
2.9	Microstructure Description and Measurement	57
2.9.1	Orientation Functions	58
2.9.2	Effect of Microstructure on Optical and Mechanical Properties	59
2.10	Concluding Remarks	60
	References	61
3	Model Simplification	69
	<i>by Ching-Chih Lee and Jose M. Castro</i>	
3.1	Introduction	70
3.2	Dimensional Analysis	70
3.2.1	Non-Dimensionalization of the General Equations	71
3.2.2	Examples	72
3.2.3	List of Dimensionless Groups Commonly Used in Polymer Processing	84
3.3	Common Assumptions in Polymer Processing Analysis	87
3.3.1	Quasi-Steady State	87
3.3.2	Fully Developed Flow	88
3.3.3	Lubrication Approximation	89
3.3.4	Membrane Problems	93
3.4	Building Models from Simplified Geometries	95
3.4.1	Pressure Flow in Simple Geometries	95
3.4.2	Drag Flow (Couette Flow) in Simple Geometries	98
3.4.3	Model Construction Based on Simple Geometries	99
3.5	Mathematical Manipulations	101
3.5.1	Special Coordinate Systems	102
3.5.2	Variable Transformations	104
3.5.3	Decoupling or Partial Decoupling of Equations	107
3.5.4	Superposition	107
3.5.5	Analogy	109
3.6	Concluding Remarks	110
	References	110
4	Simplified Geometry Models	113
	<i>by Stephen M. Richardson</i>	
4.1	Introduction	114
4.2	Governing Equations and Boundary Conditions	114
4.3	Pressure-Induced Flows in Geometrically Simple Units	119

4.3.1	Flows without freezing	119
4.3.2	Flows with freezing	128
4.4	Combined Pressure- and Drag-Induced Flows in Geometrically Simple Units	132
4.4.1	Flows without melting	133
4.4.2	Flows with melting	134
4.5	Flows in Networks of Geometrically Simple Units	134
4.6	Conclusion	137
	References	137
5	Finite Difference Solution of Field Problems	141
	<i>by Selçuk I. Güçeri</i>	
5.1	Introduction	142
5.2	Basic Formulations	143
5.2.1	Taylor Series Expansion	143
5.2.2	Example: Two-Dimensional Newtonian Fluid Flow	146
5.3	Steady-State Solution Procedures	151
5.3.1	Direct Methods	152
5.3.2	Iterative Methods	152
5.3.3	Block-Iterative Methods	155
5.3.4	Recommendations	157
5.4	Transient Solution Procedures	157
5.4.1	Explicit Methods	157
5.4.2	Implicit Methods	158
5.4.3	Alternating Direction Methods	160
5.4.4	Recommendations	161
5.5	Alternate Formulations for Finite Difference Equations	161
5.5.1	Control Volume Formulations	161
5.5.2	Upwind Differencing	164
5.5.3	Integration Cell Approach	165
5.6	Multigrid Schemes	171
5.7	Grid Generation Methods	173
5.7.1	Simply-Connected Domains	175
5.7.2	Multiply-Connected Domains	177
5.7.3	Non-Cartesian Coordinates	179
5.7.4	Three-Dimensional Grids	180
5.7.5	Pre-Specified Grid Control	182
5.7.6	Orthogonality and Adaptive Grid Control	184
5.7.7	Algebraic and Composite Grid Generation	188
5.8	Mapping Equations to the Computational Domain	190
5.8.1	Two-Dimensional Transformations	190
5.8.2	Three-Dimensional Transformations	193
5.8.3	Example: Two-Dimensional Newtonian Fluid Flow	195
5.9	Application to Injection Mold Filling	198
5.9.1	Governing Equations	198
5.9.2	Transformed Equations	204
5.9.3	Solution Procedures	207
5.9.4	Sample Results	212
5.10	Conclusion	216

5.A	Modified Strongly Implicit Method	217
5.B	Interchanging the Dependent and Independent Variables	230
	References	232
6	Finite Elements for Field Problems	237
	<i>by John F.T. Pittman</i>	
6.1	Introduction, Scope and Approach	238
6.2	Some Basic Ideas of Finite Elements	239
6.2.1	Elements, Nodes and Shape Functions	239
6.2.2	The Finite Element Galerkin Method	241
6.2.3	Weak Forms, Natural and Essential Boundary Conditions	241
6.2.4	The Finite Element Equation System	242
6.2.5	Global and Element Stiffness Matrices and Load Vectors	243
6.2.6	The Assembly Process	243
6.3	A Two-Dimensional Example	244
6.3.1	Poisson Equation with Essential or Natural Boundary Conditions	244
6.3.2	Linear Triangular Elements and Shape Functions	244
6.3.3	The Finite Element Equations	246
6.3.4	Element Stiffness Matrices and Load Vectors	246
6.3.5	Assembly and an Ordering Convention for Nodes	247
6.3.6	Application of Essential Boundary Conditions	247
6.3.7	The Form of the Global Stiffness Matrix	248
6.3.8	Application of Derivative Boundary Conditions	249
6.4	Shape Function Properties and Solution Convergence	249
6.4.1	Interpolation Within Elements	249
6.4.2	Inter-Element Continuity	250
6.4.3	Convergence	251
6.5	Extension of C^0 Elements to Higher Orders	251
6.5.1	Element Coordinates	251
6.5.2	Higher Order Elements in One Dimension	252
6.5.3	Rectangular Elements	253
6.5.4	Triangular Elements	255
6.5.5	Mapping and Parametric Elements	256
6.6	Element Calculations Carried out in Local Coordinates	258
6.6.1	Transformations to Local Coordinates	258
6.6.2	Numerical Integration	259
6.6.3	Integration Order	260
6.7	Finite Element Solution of Temperature-Independent Generalized Newtonian Flow	261
6.7.1	Scope	261
6.7.2	Governing Equations and Constitutive Relations	261
6.7.3	Formulation Options	262
6.7.4	The Primitive Variable Formulation	263
6.7.5	Penalty Function Formulation	269
6.7.6	Iterative and Mixed Methods	272
6.7.7	Divergence-Free Elements	273
6.7.8	Boundary Conditions	277
6.8	Steady State Heat Transfer	279

6.8.1	Scope	279
6.8.2	Governing Equation	279
6.8.3	Finite Element Equations	279
6.8.4	Upwinding	280
6.9	Strongly Coupled Flow and Heat Transfer	283
6.9.1	Scope	283
6.9.2	Iterative Solution of Non-Linear Equations	284
6.10	Post-Processing	285
6.10.1	Quantities Depending on Material Integrals	285
6.10.2	Quantities Depending on Local Derivatives	290
6.10.3	Evaluation of the Stream Function	292
6.10.4	Graphics	293
6.11	Transient Non-Linear Heat Conduction, Including Phase Change	293
6.11.1	Scope	293
6.11.2	Governing Equations for Non-Linear Conduction	294
6.11.3	Spatial Discretization by Finite Elements	294
6.11.4	Time Stepping	295
6.11.5	The Inclusion of Phase Change	298
6.11.6	Initial Conditions, Mesh Design, Integration Order	300
6.12	Solution of Systems of Linear Equations	301
6.12.1	Elimination Methods	301
6.12.2	Iterative Methods	303
6.13	Finite Element Packages	305
6.14	Illustrative Applications	306
6.14.1	Melt Thermocouple Performance	306
6.14.2	High-Speed Wire Coating	311
6.14.3	Design of Runner Systems for Multi-Cavity Molds	317
6.14.4	Material Deformation and Alignment in Center-Gated Disc Flow	319
6.14.5	Blow-Mold Cooling	322
6.15	Conclusion	324
	References	325
7	Boundary Element Solution of Field Problems	333
	<i>by Martin R. Barone and Tim A. Osswald</i>	
7.1	Introduction	334
7.2	Formulation	335
7.2.1	Steady Heat Conduction	335
7.2.2	Transient Heat Conduction	337
7.2.3	Creeping Flow	338
7.3	Equations for Special Geometry	339
7.3.1	Heat Conduction with Circular Holes	340
7.3.2	Fluid Flow Near Sharp Corners	341
7.4	Numerical Implementation	343
7.4.1	Discretization	343
7.4.2	Numerical Integration	347
7.4.3	Matrix Assembly and Solution	348
7.4.4	Substructuring and Vector Processing	350
7.5	Examples in Polymer Processing	351

7.5.1	Optimal Thermal Design of Molds	351
7.5.2	Mold Filling in Thin Cavities	355
7.5.3	Die Swell	363
7.6	Discussion	364
	References	365
8	Numerical Techniques for Free and Moving Boundary Problems	369
	<i>by H.P. Wang and H.S. Lee</i>	
8.1	A Representative Free Boundary Problem	370
8.2	Free Boundary Techniques	372
8.2.1	Iterative Streamlines (Kinematic Boundary Condition)	372
8.2.2	Normal Stress Balance	373
8.2.3	Spines: Finite Element Formulation for the Kinematic Boundary Condition	373
8.2.4	Transient Lagrangian Description	374
8.2.5	Comparison	375
8.3	Representative Moving Boundary Problems	375
8.3.1	Generalized Hele-Shaw (GHS) Model	375
8.4	Moving Boundary Techniques	379
8.4.1	Fixed Mesh Schemes	379
8.4.2	Moving Mesh Schemes	381
8.4.3	Boundary Element Methods	383
8.4.4	Graphical Method	384
8.5	Finite Element/Control Volume Approach for Injection Mold Filling	385
8.5.1	Finite Element Formulation for Pressure	385
8.5.2	Front Tracking Algorithm	387
8.5.3	Global/Local Coordinate Transformation for 3-D Parts	389
8.5.4	Finite Difference Approximation for Temperature	390
8.5.5	Numerical Stability and Time Step Selection	391
8.5.6	Influence of Viscosity Models	393
8.5.7	Outline of Numerical Procedure	394
8.5.8	Results Display	395
8.5.9	Further Development in Mold Filling Analysis	398
8.6	Conclusions	398
	References	399
9	Simulation of Viscoelastic Fluid Flow	403
	<i>by Roland Keunings</i>	
9.1	Introduction	404
9.2	Mathematical Models	405
9.2.1	Preliminaries	405
9.2.2	Conservation Equations	406
9.2.3	Differential Constitutive Models	407
9.2.4	Single-Integral Constitutive Models	408
9.2.5	Mathematical Analysis	409
9.2.6	Boundary Conditions	411
9.3	A Method Classification	413
9.4	Coupled Techniques for Differential Models	415

9.4.1	Preliminaries	415
9.4.2	Conventional Mixed Galerkin/Finite Element Formulations	415
9.4.3	Extension to Transient Flows	418
9.4.4	Mixed Finite Element Interpolations	420
9.4.5	Numerical Problems with Conventional Mixed Techniques	421
9.4.6	Stable Schemes for Viscoelastic Stress Computation	422
9.4.7	A Mixed Technique Based on Renardy's Formulation	424
9.4.8	Hybrid Techniques Based on Spectral Methods	424
9.5	Coupled Techniques for Integral Models	425
9.5.1	Preliminaries	425
9.5.2	Eulerian Formulation	425
9.5.3	Streamline Finite Elements	427
9.5.4	Lagrangian Formulation	428
9.6	Decoupled Techniques	429
9.6.1	Preliminaries	429
9.6.2	Basic Procedure	429
9.6.3	Solution of the Perturbed Newtonian Problem	430
9.6.4	Streamline Integration of Differential Models	431
9.6.5	Integral Models	432
9.7	Selected Numerical Simulations	435
9.7.1	Review of Published Simulations	435
9.7.2	Flow Through an Abrupt Contraction	436
9.7.3	Extrudate Swell	439
9.7.4	Breakup of Viscoelastic Jets	442
9.8	The High Weissenberg Number Problem	444
9.8.1	Preliminaries	444
9.8.2	Possible Causes for the Divergence of Conventional Iterative Schemes	445
9.8.3	Tracking Irregular Points and Stability Changes	447
9.8.4	A First Fact about the HWNP with Coupled Methods	448
9.8.5	Spurious Irregular Points	449
9.8.6	A Second Fact about the HWNP with Coupled Methods	450
9.8.7	A Plausibly True Turning Point with the Maxwell fluid	451
9.8.8	Causes for Excessive Approximation Errors	452
9.8.9	Boundary Layers and Singularities	453
9.8.10	Hyperbolicity, Change of Type, and Loss of Evolution	456
9.8.11	The HWNP with Decoupled Methods	458
9.9	Conclusions	
	References	459
10	Computer Implementation of Process Models	471
	<i>by Charles L. Tucker III</i>	
10.1	Coding	472
10.1.1	Portability	473
10.1.2	Control Structure	474
10.1.3	Names	476
10.1.4	Comments	479
10.1.5	Appearance on the Page	480
10.1.6	An Example	481

10.2	Program Design and Documentation	490
10.2.1	Problem Definition	490
10.2.2	Documentation	491
10.2.3	Module Design	492
10.2.4	Control Structure	494
10.2.5	Integration with Other Programs	495
10.2.6	Graphics	496
10.2.7	Research Programs	498
10.3	The User Interface	499
10.3.1	User Interface Design	499
10.3.2	Robust Interactive Input	502
10.4	Testing and Validation	504
10.4.1	Development Testing	504
10.4.2	Validation	505
10.5	Large Programs	506
10.5.1	Dynamic Memory Allocation in Fortran	506
10.5.2	Reducing Execution Time	509
10.6	Conclusion	514
10.6.1	Summary	514
10.6.2	Further Reading	514
	References	515
11	Advanced Computational Techniques	517
	<i>by Richard N. Ellson</i>	
11.1	Supercomputing	518
11.1.1	Supercomputer Architecture	518
11.1.2	Coding for Supercomputers	521
11.2	Visualization of Results	527
11.2.1	Glyphs	527
11.2.2	Applications	528
11.2.3	Graphics Hardware and Software	531
11.3	Conclusions	532
	References	532
12	Knowledge-Based Expert Systems for Materials Processing	535
	<i>by Stephen C.-Y. Lu</i>	
12.1	Introduction	536
12.2	Fundamentals of Expert Systems	538
12.2.1	Basic Components of an Expert System	538
12.2.2	Expert Systems vs. Conventional Programs	539
12.3	Inside an Expert System	541
12.3.1	Knowledge Representation	541
12.3.2	The Inference Engine	546
12.3.3	Reasoning Methods	547
12.3.4	Reasoning about Reasoning	549
12.3.5	Reasoning with Uncertainties	550
12.4	Knowledge Engineering	552
12.4.1	Expert System Development Stages	553

12.4.2	Knowledge Acquisition	556
12.4.3	Expert System Tools	558
12.5	Applications to Materials Processing	561
12.5.1	Present Applications	562
12.5.2	Existing Opportunities	563
12.5.3	Future Potentials	568
12.6	Conclusion	569
	References	570
13	An Overview of Computer Modeling	575
	<i>by Charles L. Tucker III</i>	
13.1	A Comparison of Numerical Methods	576
13.2	The Future of Computer Modeling	579
A	Summary of Vector and Tensor Operations	
	<i>by Charles L. Tucker III</i>	
A.1	Vectors and Tensors: Definition and Notations	582
A.1.1	Scalars and Vectors	582
A.1.2	Tensors	584
A.1.3	Cartesian Tensor Notation	584
A.1.4	Vector and Tensor Transformation	585
A.1.5	The Unit Tensor and the Kronecker Delta	585
A.1.6	Transposes, Symmetry and Anti-Symmetry	586
A.2	Vector and Tensor Algebra	586
A.2.1	Addition and Subtraction	586
A.2.2	Multiplication	586
A.2.3	The Trace and Scalar Invariants	587
A.2.4	The Inverse of a Tensor	588
A.3	Differential Operations	588
A.3.1	The Gradient Operator	588
A.3.2	Gradients of Scalar and Vector Fields	588
A.3.3	Divergence of Vector Fields and the Laplacian	589
A.3.4	Curl	589
A.3.5	Differential Operations in Cylindrical and Spherical Coordinates	589
A.4	The Material Derivative	590
	References	591
B	Transport and Kinematic Equations	593
	<i>by Charles L. Tucker III</i>	
B.1	Continuity	594
B.2	Stress	594
B.3	Kinematics	595
B.4	The Newtonian Fluid	597
B.5	The Equation of Motion	597
B.6	The Energy Equation	598
B.7	Other Transport Equations	600
B.8	Time Derivatives of Tensors	601
	Tables of Transport and Kinematic Equations	603
	References	611
Index		613