

Contents

1	Introduction	1
1.1	Everything Flows	1
1.1.1	The Maxwell model and the relaxation time	4
1.1.2	The Kelvin model and the retardation time	7
1.2	Non-Newtonian Fluids	8
1.2.1	Non-Newtonian fluids in shear flow	9
1.2.2	Non-Newtonian fluids in uniaxial extensional flow	14
1.3	Numerical Simulation of Non-Newtonian Flow	16
1.3.1	Early work	16
1.3.2	The high Weissenberg number problem	17
1.3.3	Numerical work since the mid 1980's	18
2	Fundamentals	19
2.1	Some Important Vectors	19
2.1.1	Fluid velocity and acceleration	19
2.1.2	Forces and the stress vector	20
2.2	Conservation Laws and the Stress Tensor	21
2.2.1	Conservation of mass	21
2.2.2	Conservation of linear momentum	21
2.2.3	Conservation of angular momentum	21
2.2.4	The stress tensor	22
2.2.5	Conservation of energy	23
2.3	The Newtonian Fluid	24
2.4	The Generalized Newtonian Fluid	25
2.4.1	Derivation of the stress tensor	26
2.5	The Order Fluids and the CEF Equation	27
2.5.1	Strain tensors	27
2.5.2	Order fluids	28
2.5.3	Limitations of order fluid models	30
2.5.4	The CEF equation.	32
2.6	More Complicated Constitutive Relations	33
2.6.1	Differential constitutive models	33
2.6.2	Integral constitutive models	45

3	Mathematical Theory of Viscoelastic Fluids	49
3.1	Introduction	49
3.2	Existence and Uniqueness	51
3.3	Properties of the Differential Systems	54
3.3.1	Loss of evolution and Hadamard instability	56
3.3.2	Classification	59
3.3.3	Change of type in steady flow	61
3.3.4	Characteristic variables	62
3.4	Boundary Conditions	64
3.5	Singularities	65
3.5.1	Elliptic problems	65
3.5.2	Viscoelastic flows	68
3.5.3	Numerical investigations	71
4	Parameter Estimation in Continuum Models	73
4.1	Introduction	73
4.2	Determination of Viscosity	76
4.2.1	Shear viscosity	76
4.2.2	Dependence of viscosity on temperature	79
4.2.3	Dependence of viscosity on pressure	81
4.2.4	Extensional viscosity	82
4.3	Determination of the Relaxation Spectrum	83
4.3.1	Dynamic experiments	84
4.3.2	Mathematical problems	85
4.3.3	Linear regression techniques	86
4.3.4	Nonlinear regression techniques	88
4.3.5	Examples	89
4.3.6	Sampling localization	91
5	From the Continuous to the Discrete	95
5.1	Introduction	95
5.2	Finite Difference Approximations	97
5.2.1	Finite differences for viscoelastic flows	100
5.3	Finite Element Approximations	104
5.3.1	Finite elements in one dimension	105
5.3.2	Finite elements in two dimensions	107
5.3.3	Finite elements for viscoelastic flows	110
5.4	Finite Volume Methods	113
5.4.1	Finite volumes for viscoelastic flows	117
5.5	Spectral Methods	121
5.5.1	Spectral methods in one dimension	121
5.5.2	Spectral methods in two dimensions	125
5.5.3	Spectral methods for viscoelastic flows	127
5.6	Spectral Element Methods	129
5.6.1	Spectral elements for viscoelastic flows	130

6	Numerical Algorithms for Macroscopic Models	135
6.1	Introduction	135
6.2	From Picard to Newton	136
6.3	Differential Models: Steady Flows	137
6.3.1	Direct methods	138
6.3.2	Iterative methods	140
6.4	Differential Models: Transient Flows	149
6.4.1	Projection methods	150
6.4.2	The influence matrix method	153
6.4.3	Taylor-Galerkin methods	155
6.4.4	The θ method	157
6.4.5	Lagrangian methods	160
6.5	Computing with Integral Models	163
6.6	Integral Models: Steady Flows	164
6.7	Integral Models: Transient Flows	167
6.7.1	Lagrangian techniques	167
6.7.2	Eulerian techniques	170
7	Defeating the High Weissenberg Number Problem	173
7.1	Introduction	173
7.2	Discretization of Differential Constitutive Equations	177
7.2.1	Streamline upwinding - SU and SUPG	177
7.2.2	Discontinuous Galerkin methods	182
7.3	Discretization of the Coupled Governing Equations	187
7.3.1	Compatible approximation spaces	187
7.3.2	EVSS-type methods	190
7.3.3	Change of type and loss of evolution	195
8	Benchmark Problems I: Contraction Flows	201
8.1	Vortex Growth Dynamics	202
8.1.1	Boger fluids - observed flow transitions	202
8.1.2	Boger fluids - effects of changes of geometry	206
8.1.3	Concentrated polymer solutions and melts - observed flow transitions	209
8.1.4	Concentrated polymer solutions and melts - effects of change of geometry	213
8.2	Vortex Growth Mechanisms	216
8.2.1	Experimental work	216
8.2.2	Numerical studies	222
8.3	Numerical Simulation	225
8.3.1	Comparisons with experiments	226
8.3.2	Benchmarking numerical methods	231
9	Benchmark Problems II	247
9.1	Flow Past a Cylinder in a Channel	247
9.1.1	Streamline patterns and drag: unbounded flows	247
9.1.2	Streamline patterns and drag: cylinders in channels	251
9.1.3	Comparison of numerical and experimental results	252

9.1.4	Purely elastic instabilities	254
9.1.5	Comparison of numerical methods	257
9.1.6	Mesoscopic calculations	263
9.2	Flow Past a Sphere in a Tube	267
9.2.1	Drag coefficient	268
9.2.2	Benchmarking numerical methods	274
9.2.3	Negative wakes: steady flow	277
9.2.4	Velocity overshoots - transient flow calculations	281
9.2.5	Comparison between experimental and numerical results	284
9.3	Flow between Eccentrically Rotating Cylinders	287
9.3.1	The Taylor-Couette problem	288
9.3.2	Lubrication theory	291
9.3.3	Statically loaded journal bearing	293
9.3.4	Dynamically loaded journal bearing	297
10	Error Estimation and Adaptive Strategies	305
10.1	Introduction	305
10.2	Problem Description	308
10.2.1	Weak formulation	308
10.3	Discretization and Error Analysis (Galerkin method)	311
10.3.1	An error indicator	315
10.4	Adaptive Strategies	316
10.4.1	Numerical example: flow past a sphere in a tube	317
11	Contemporary Topics in Computational Rheology	327
11.1	Advances in Mathematical Modelling	327
11.2	Dynamics of Dilute Polymer Solutions	330
11.2.1	The Rouse model	331
11.2.2	Dumbbell models	335
11.3	Closure Approximations	335
11.4	Stochastic Differential Equations	338
11.4.1	The CONNFFESSIT approach	341
11.4.2	Variance reduction techniques	343
11.4.3	Lagrangian particle method	345
11.4.4	Brownian configuration fields	346
11.5	Dynamics of Polymer Melts	347
11.5.1	The Doi-Edwards model	347
11.5.2	The pom-pom model	354
11.6	Lattice Boltzmann Methods	357
11.7	Closing Comments	359
A	Some Results about Tensors	361
A.1	Existence and Symmetry of the Stress Tensor	361
A.2	Small Displacement Gradient Limit of $\gamma^{[0]}(\mathbf{x}, t, t')$	364
A.3	Partial Time Derivative of the Deformation Gradient Tensor $\mathbf{F}(\mathbf{x}, t, t')$	364

B	Governing Equations in Orthogonal Curvilinear Coordinates	365
B.1	Differential Relations and Identities	365
B.2	Differential Operators in Orthogonal Curvilinear Coordinates . .	366
B.2.1	Rectangular coordinates $(x_1, x_2, x_3) = (x, y, z)$	366
B.2.2	Cylindrical polar coordinates $(\hat{x}_1, \hat{x}_2, \hat{x}_3) = (r, \theta, z)$	368
B.2.3	Spherical polar coordinates $(\hat{x}_1, \hat{x}_2, \hat{x}_3) = (r, \theta, \phi)$	369
B.3	Conservation Equations	371
B.3.1	Rectangular coordinates (x, y, z)	371
B.3.2	Cylindrical polar coordinates (r, θ, z)	371
B.3.3	Spherical polar coordinates (r, θ, ϕ)	372
B.4	Some Important Theorems in Vector and Tensor Calculus	373
B.4.1	The Reynolds transport theorem	373
B.4.2	The divergence theorem	373
B.4.3	Stokes's theorem	373