
Contents

Part I Illustrations & Applications

1	Simple Models for Polymeric and Anisotropic Liquids	3
1.1	Section-by-Section Summary	7
2	Dumbbell Model for Dilute and Semi-Dilute Solutions	13
2.1	FENE-PMF Dumbbell in Finitely Diluted Solution	15
2.2	Introducing a Mean Field Potential	16
2.3	Relaxation Equation for the Tensor of Gyration	16
2.4	Symmetry Adapted Basis	18
2.5	Stress Tensor and Material Functions	21
2.6	Reduced Description of Kinetic Models	23
3	Chain Model for Dilute Solutions	25
3.1	Hydrodynamic Interaction	25
3.2	Long Chain Limit, Cholesky Decomposition	27
3.3	NEBD Simulation Details	27
3.4	Universal Ratios	29
4	Chain Model for Concentrated Solutions and Melts	33
4.1	NEMD Simulation Method	34
4.2	Stress Tensor	35
4.3	Lennard–Jones (LJ) Units	35
4.4	Flow Curve and Dynamical Crossover for Polymer Melts	35
4.5	Characteristic Lengths and Times	36
4.6	Linear Stress-Optic Rule (SOR) and Failures	39
4.7	Nonlinear Stress-Optic-Rule	42
4.8	Stress-Optic Coefficient	44
4.9	Interpretation of Dimensionless Simulation Numbers	48

5	Chain Models for Transient and Semiflexible Structures	49
5.1	Conformational Statistics of Wormlike Chains (WLC)	49
5.1.1	Functional Integrals for WLCs	50
5.1.2	Properties of WLCs	51
5.2	FENE-C Wormlike Micelles	53
5.2.1	Flow-Induced Orientation and Degradation	54
5.2.2	Length Distribution	56
5.2.3	FENE-C Theory vs Simulation, Rheology, Flow Alignment	57
5.3	FENE-B Semiflexible Chains	61
5.3.1	Actin Filaments	61
5.4	FENE-B Liquid Crystalline Polymers	66
5.4.1	Static Structure Factor	69
5.5	FENE-CB Transient Semiflexible Networks, Ring Formation	72
6	Primitive Path Models	77
6.1	Doi-Edwards Tube Model and Improvements	77
6.2	Refined Tube Model	
	with Anisotropic Flow-Induced Tube Renewal	79
6.2.1	Linear Viscoelasticity of Melts and Concentrated Solutions	80
6.3	Nonlinear Viscoelasticity, Particular Closure	84
6.3.1	Example: Refined Tube Model, Stationary Shear Flow	84
6.3.2	Example: Transient Viscosities for Rigid Polymers	85
6.3.3	Example: Doi-Edwards Model as a Special Case	85
6.4	Nonlinear Viscoelasticity without Closure	86
6.4.1	Galerkin's Principle	87
7	Elongated Particle Models	91
7.1	Director Theory	92
7.2	Structural Theories of Suspensions	93
7.2.1	Semi-Dilute Suspensions of Elongated Particles	95
7.2.2	Concentrated Suspensions of Rod-Like Polymers	95
7.3	Uniaxial Fluids, Micro-Macro Correspondence	96
7.3.1	Concentrated Suspensions of Disks, Spheres, Rods	97
7.3.2	Example: Tumbling	97
7.3.3	Example: Miesowicz Viscosities	98
7.4	Uniaxial Fluids: Decoupling Approximations	99
7.4.1	Decoupling with Correct Tensorial Symmetry	102
7.5	Ferrofluids: Dynamics and Rheology	103
7.6	Liquid Crystals: Periodic and Irregular Dynamics	105
7.6.1	Landau – de Gennes Potential	108
7.6.2	In-Plane and Out-of-Plane States	109

8	Connection between Different Levels of Description	111
8.1	Boltzmann Equation	111
8.2	Generalized Poisson Structures	112
8.3	GENERIC Equations	112
8.3.1	Building Block \mathbf{L}	113
8.3.2	Building Block \mathbf{M}	115
8.4	Dissipative Particles	117
8.5	Langevin and Fokker–Planck Equation, Brownian Dynamics	117
8.5.1	Motivation	117
8.5.2	Interpretation, and Langevin Equation	118
8.6	Projection Operator Methods	119
8.7	Stress Tensors: Giesekus – Kramers – GENERIC	121
8.8	Generalized Canonical Ensemble and Friction Matrix	123
8.9	Beyond-Equilibrium Molecular Dynamics (BEMD)	124
8.9.1	Multiplostated Equations	128
8.9.2	Applicability of BEMD	130
8.9.3	DOLLS/SLLOD Analogy with Multiplostated Equations	132
8.10	Examples for Coarse-Graining	134
8.10.1	From Connected to Primitive Path	134
8.10.2	From Disconnected to Primitive Path	136

Part II Theory & Computational Recipes

9	Equilibrium Statistics: Monte Carlo Methods	145
9.1	Expectation Values, Metropolis Monte Carlo	146
9.2	Normalization Constants, Partition Function	148
9.2.1	Standard Monte Carlo	149
9.2.2	Direct Importance Sampling	150
9.2.3	Path Sampling	150
9.3	Density of States Monte Carlo (DSMC)	151
9.4	Quasi Monte Carlo	153
10	Irreducible and Isotropic Cartesian Tensors	155
10.1	Notation	155
10.2	Anisotropic (Irreducible) Tensors	156
10.3	Differential Operators (∇ , \mathcal{L} etc.)	158
10.4	Isotropic Tensors	159
10.4.1	Construction of the Isotropic Tensors $\mathbf{\Delta}^{(l)}$	160
10.4.2	Generalized Cross Product $\mathbf{\Delta}^{(l,1,l)}$	160
10.4.3	Generalized Tensor $\mathbf{\Delta}^{(l,k,l)}$	161
10.4.4	Implications (Summary)	161
10.5	Differential Operations (Tabular Form)	162
10.6	Nematic Order Parameters	163
10.6.1	Uniaxial Phase	163

10.6.2	Biaxial Phase	164
10.7	Tensor Invariants	165
10.8	Solutions of the Laplace Equation	167
10.9	The Reverse $\Delta^{(t)}$ Operation	168
10.10	Integrating Irreducible Tensors	168
11	Nonequilibrium Dynamics of Anisotropic Fluids	169
11.1	Orientational Distribution Function	169
11.1.1	Alignment Tensors	170
11.1.2	Uniaxial Distribution Function	170
11.2	Fokker–Planck Equation, Smoluchowski Equation	170
11.2.1	Spatial Inhomogeneous Distribution	172
11.2.2	Flow Field	172
11.2.3	Spatial Homogeneous Distribution, N th Order Potential	173
11.2.4	Examples for Potentials and Applications	174
11.3	Coupled Equations of Change for Alignment Tensors	174
11.3.1	Dynamical Closures	176
11.3.2	Equations of Change for Order Parameters	176
11.4	Langevin Equation	178
11.4.1	Brownian Dynamics Simulation	179
12	Simple Simulation Algorithms and Sample Applications	181
12.1	Index of Programs	182
12.2	Recipes	182
12.2.1	Random Vectors, Random Paths (2D, 3D)	182
12.2.2	Periodic and Reflecting Boundary Conditions (nD)	183
12.2.3	Useful Initial Phase Space Coordinates (nD)	184
12.2.4	Visualization, Animation & Movies (nD)	184
12.3	Monte Carlo	185
12.3.1	Standard Monte Carlo Integration (nD)	185
12.3.2	Ising Model via Metropolis Monte Carlo (2D)	186
12.4	Molecular Dynamics	187
12.4.1	Molecular Dynamics of a Lennard–Jones System (nD)	187
12.4.2	Associating Equilibrium FENE Polymers (2D,3D)	188
12.5	NonEquilibrium Molecular Dynamics	190
12.5.1	NonEquilibrium Molecular Dynamics (nD)	190
12.5.2	Flow through Nanopore (3D)	191
12.6	Brownian Dynamics	194
12.6.1	Brownian Dynamics of a Lennard–Jones System (nD)	194
12.6.2	Hydrodynamic Interaction via Chebyshev Polynomials (3D)	194
12.7	Coarse-Graining	195
12.7.1	Coarse-Graining Polymer Chains (nD)	195

Concluding Remarks	197
13.1 Acknowledgement	198
Notation	199
14.1 Special Symbols	199
14.2 Tensor Symbols	199
14.3 Upper Case Roman Symbols	200
14.4 Lower Case Roman Symbols	201
14.5 Greek Symbols	202
14.6 Caligraphic Symbols	202
14.7 FENE Models	203
14.8 Gaussian Integrals	204
References	205
Author Index	217
Index	223