

---

# **Self-Organization in Nonequilibrium Systems**

**From Dissipative Structures to  
Order through Fluctuations**

---

***G. Nicolis***

*Université Libre de Bruxelles  
Belgium*

***I. Prigogine***

*Université Libre de Bruxelles  
Belgium*

*and*

*University of Texas at Austin  
Texas*

**A Wiley-Interscience Publication**

**JOHN WILEY & SONS**

**New York • Chichester • Brisbane • Toronto • Singapore**

---

# *Contents*

<b>General Introduction</b>	<b>1</b>
-----------------------------	----------

## **PART I. THE THERMODYNAMIC BACKGROUND**

<b>1. Introduction</b>	<b>19</b>
1.1. General Comments,	19
1.2. Open Systems,	24
<b>2. Conservation Equations</b>	<b>26</b>
2.1. Open Systems at Mechanical Equilibrium,	26
2.2. The Mass-balance Equations,	27
<b>3. Thermodynamics of Irreversible Processes: The Linear Region</b>	<b>31</b>
3.1. Gibbs's Formula: Entropy Production,	31
3.2. Phenomenological Relations: The Linear Range of Irreversible Processes,	36
3.3. Symmetry Properties of the Phenomenological Coefficients,	39
3.4. Stationary Nonequilibrium States,	41
3.5. Theorem of Minimum Entropy Production,	42
3.6. Impossibility of Ordered Behavior in the Linear Range of Irreversible Processes,	45
3.7. Diffusion,	46
<b>4. Nonlinear Thermodynamics</b>	<b>49</b>
4.1. Introduction,	49
4.2. The General Evolution Criterion,	50
4.3. Evolution Criterion and Kinetic Potential,	51
4.4. Stability of Nonequilibrium States. Dissipative Structures,	55

**PART II. MATHEMATICAL ASPECTS OF SELF-ORGANIZATION: DETERMINISTIC METHODS**

- 5. Systems Involving Chemical Reactions and Diffusion-Stability** **63**
- 5.1. General Formulation, 63
  - 5.2. Lyapounov Stability, 65
  - 5.3. Orbital Stability, 66
  - 5.4. Structural Stability, 68
- 6. Mathematical Tools** **70**
- 6.1. Introduction, 70
  - 6.2. Theory of Bifurcations, 70
  - 6.3. Stability Theory, 71
  - 6.4. Theory of Catastrophes, 74
  - 6.5. Homogeneous Systems Involving Two Variables, 76
  - 6.6. Branchings, Bifurcations, and Limit Cycles, 83
- 7. Simple Autocatalytic Models** **90**
- 7.1. Two Intermediates, 90
  - 7.2. The Trimolecular Model (the "Brusselator"), 93
  - 7.3. Scaling, Steady States, and Boundary Conditions, 94
  - 7.4. Linear Stability Analysis, 96
  - 7.5. Bifurcation of Steady-state Dissipative Structures: General Scheme, 106
  - 7.6. Bifurcation: Fixed Boundary Conditions, 109
  - 7.7. Bifurcation: No-flux Boundary Conditions, 113
  - 7.8. Qualitative Properties of Dissipative Structures in Vicinity of First Bifurcation, 115
  - 7.9. Successive Instabilities and Secondary Bifurcations, 120
  - 7.10. Comparison with Computer Simulations, 124
  - 7.11. Localized Steady-state Dissipative Structures, 131
  - 7.12. Bifurcation of Time-periodic Dissipative Structures, 140
  - 7.13. Qualitative Properties of Time-periodic Dissipative Structures, 147
  - 7.14. Traveling Waves in Periodic Geometries, 153
  - 7.15. The Brusselator as a Closed System, 156
  - 7.16. Concluding Remarks, 158

<b>8. Some Further Aspects of Dissipative Structures and Self-organization Phenomena</b>	<b>160</b>
8.1. Introduction,	160
8.2. Conservative Oscillations,	160
8.3. Simple Models Giving Rise to Limit Cycles,	165
8.4. Multiple Steady States and All-or-none Transitions,	169
8.5. Two-dimensional Problems,	178
8.6. Systems Involving More than Two Chemical Variables,	192
8.7. Coupled Oscillators,	195
8.8. Heterogeneous Catalysis and Localized Transitions,	197
8.9. Systems Involving Photochemical Steps,	200
8.10. Some Further Methods of Analysis of Reaction-Diffusion Equations,	202
8.11. Thermodynamic Aspects of Dissipative Structures,	212

### **PART III. STOCHASTIC METHODS**

<b>9. General Comments</b>	<b>223</b>
9.1. Introduction,	223
9.2. Stochastic Formulation,	224
9.3. Markovian Processes,	228
9.4. Equilibrium Limit,	232
9.5. Fluctuations in Nonequilibrium Systems: An Historical Survey,	236
<b>10. Birth-and-death Description of Fluctuations</b>	<b>239</b>
10.1. Master Equation for Birth-and-death Processes,	239
10.2. Limitations of Birth-and-death Formalism,	241
10.3. Some Methods of Analysis of Birth-and-death Master Equations,	242
10.4. Moment Equations,	252
10.5. Simple Examples,	257
10.6. Systems Involving Two Stochastic Variables: The Lotka-Volterra Model,	264
10.7. Concluding Remarks,	272

- 11. Effect of Diffusion: Phase-space Description and Multivariate Master Equation** 273
- 11.1. Necessity for a Local Description of Fluctuations, 273
  - 11.2. Phase-space Description of Fluctuations, 274
  - 11.3. A Simple Model, 276
  - 11.4. Approximate Solution of Master Equation, 280
  - 11.5. Molecular Dynamics Studies of Fluctuations, 283
  - 11.6. Discussion, 284
  - 11.7. Reduction to a Multivariate Master Equation in Concentration Space, 285
  - 11.8. The Multivariate Master Equation in a Model System, 289
  - 11.9. Spatial Correlations in the Trimolecular Model, 297
  - 11.10. Critical Behavior, 302
  - 11.11. Concluding Remarks, 309
- 12. A "Mean-field" Description of Fluctuations: Nonlinear Master Equation** 313
- 12.1. Introduction, 313
  - 12.2. Derivation of Nonlinear Master Equation, 314
  - 12.3. Further Properties and Moment Equations, 317
  - 12.4. Onset of a Limit Cycle, 319
  - 12.5. Onset of a Spatial Dissipative Structure, 324
  - 12.6. Multiple Steady-state Transitions and Metastability, 327
  - 12.7. Asymptotic Solutions of Nonlinear Master Equation, 331
  - 12.8. Concluding Remarks, 334
- PART IV. CONTROL MECHANISMS IN CHEMICAL AND BIOLOGICAL SYSTEMS**
- 13. Self-organization in Chemical Reactions** 339
- 13.1. Introduction, 339
  - 13.2. Belousov-Zhabotinski Reaction: Experimental Facts, 339
  - 13.3. Mechanism, 343
  - 13.4. The "Oregonator", 345
  - 13.5. Oscillatory Behavior, 347
  - 13.6. Spatial Patterns, 351
  - 13.7. Briggs-Rauscher Reaction, 352

<b>14. Regulatory Processes at the Subcellular Level</b>	<b>354</b>
14.1. Metabolic Oscillations,	354
14.2. The Glycolytic Cycle,	354
14.3. Allosteric Model for Glycolytic Oscillations,	358
14.4. Limit-cycle Oscillations,	369
14.5. Effect of External Disturbances on Limit-cycle Oscillation,	371
14.6. Patterns of Spatiotemporal Organization in Allosteric Enzyme Model,	375
14.7. Periodic Synthesis of cAMP,	379
14.8. Reactions Involving Membrane-bound Enzymes,	382
14.9. Physiological Significance of Metabolic Oscillations,	384
<b>15. Regulatory Processes at Cellular Level</b>	<b>387</b>
15.1. Introduction,	387
15.2. <i>Lac</i> Operon,	388
15.3. Mathematical Model for Induction of $\beta$ -Galactosidase,	389
15.4. All-or-none Transitions,	391
15.5. Catabolite Repression: Sustained Oscillations and Threshold Phenomena,	394
15.6. Control of Cellular Division,	402
15.7. Quantitative Model,	404
<b>16. Cellular Differentiation and Pattern Formation</b>	<b>409</b>
16.1. Introductory Remarks,	409
16.2. Positional Information,	410
16.3. Mechanisms Involved in Positional Information,	413
16.4. Dissipative Structures and Onset of Polarity,	415
16.5. A Quantitative Model,	416
16.6. Positional Differentiation,	421
16.7. Applications,	424

## **PART V. EVOLUTION AND POPULATION DYNAMICS**

<b>17. Thermodynamics of Evolution</b>	<b>429</b>
17.1. The Notion of Competition,	429
17.2. Prebiotic Evolution: General Presentation,	429
17.3. Prebiotic Polymer Formation,	430
17.4. Biopolymer Competition and Hypercycles,	434

17.5. Evolution Viewed as a Problem of Stability,	438
17.6. Evolutionary Feedback,	441
17.7. Energy Dissipation in Simple Reaction Networks,	442
17.8. A Biochemical Illustration,	446
<b>18. Thermodynamics of Ecosystems</b>	<b>448</b>
18.1. Introduction,	448
18.2. Basic Equations,	448
18.3. Example of Ordered Behavior: Organization in Insect Societies,	452
18.4. Evolution of Ecosystems,	455
18.5. Structural Instabilities and Increase of Complexity: Division of Labor,	459
18.6. Stability and Complexity,	462
<b>Perspectives and Concluding Remarks</b>	<b>464</b>
1. Introduction,	464
2. Fluctuation Chemistry,	464
3. Neural and Immune Networks,	466
4. Immune Surveillance against Cancer,	469
5. Social Systems and Epistemological Aspects,	472
<b>References</b>	<b>475</b>
<b>Addendum: Mathematical Problems</b>	<b>487</b>
<b>Index</b>	<b>489</b>