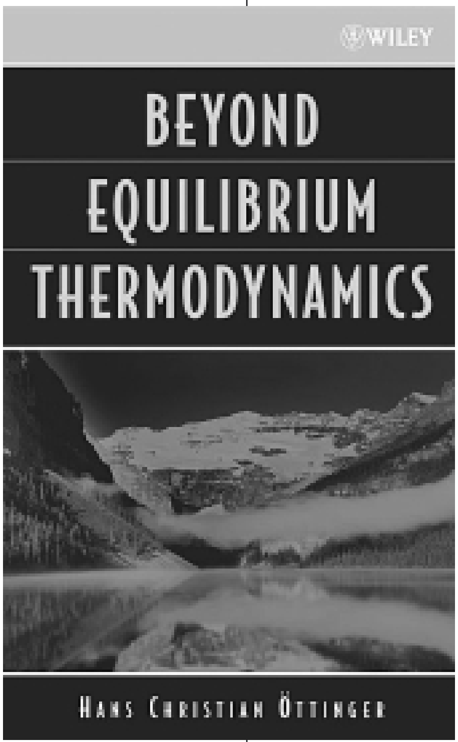
Book Review

Beyond Equilibrium Thermodynamics

Hans Christian Öttinger



While linear irreversible thermodynamics is fully developed and available in textbooks like the well known monograph of de Groot and Mazur [1] nonlinear nonequilibrium thermodynamics or as the author calls it 'beyond-equilibrium thermodynamics' is still in a state of rapid development. Apparently not the right condition to write a textbook on this subject. Fortunately, Hans Christian Öttinger, one of the prominent researchers in this field, still undertook the effort with the present quite remarkable result. The book offers a clear, well structured and complete treatment with emphasize on the GENERIC approach, a framework first proposed in 1997 by the author and Grmela, in two well known publications [2, 3] and still one of the major approaches in nonlinear nonequilibrium thermodynamics.

The appearance of this book is very important for at least two reasons. First, probably for the first time it offers scientist and engineers who want to master and apply contemporary nonlinear nonequilibrium thermodynamics a complete and self contained resource. Second, it will be of great value for specialists in the field. The very complete and thorough treatment provides an excellent platform for analyzing and discussing the fundamentals and prospects of the GENERIC approach. The book is divided in two parts, one on the phenomenological and one on the statistical approach, preceded by an introductory section and completed by six appendices. This very broad and thorough coverage reflects not only the author's authoritative knowledge and experience with the field but offers the readers also the possibility to acquire not only a working knowledge but also a deep understanding of beyond-equilibrium thermodynamics.

Chapter 1 plays a very special role. It contains a fairly complete and self-contained introduction to the phenomenological approach and in particular the famous GENERIC expression:

$$\frac{dx}{dt} = L(x) \cdot \frac{\delta E(x)}{\delta x} + M(x) \cdot \frac{\delta S(x)}{\delta x}$$

with x representing the state variables and the so called GENERIC building blocks E(x) and S(x), the energy and entropy functionals and the operators L(x) and M(x) representing reversible and dissipative properties [Note by editor: An introduction to GENERIC and nonequilibrium thermodynamics as a tool for applied rheologists is available in Appl. Rheol. 9 (1999) 17 - 26]. A thorough understanding of this chapter is needed for a proper understanding of the rest of the book. The presentation is very clear and the historical and conceptual background of the framework is explained carefully. Still I fear that readers will be disappointed by the fact the above equation is merely proposed instead of derived. A kind of axiomatic framework (cf. Callen's [4] postulates) leading to this result would be preferable but seems however not yet available. Appendix B is a step in that direction, but certainly not suitable as an introduction.

After the simple examples discussed in Chapter 1, Part I starts in Chapter 2 with an application of the formalism to a real-live system: three-dimensional hydrodynamics. The analysis illustrates many aspects of the analysis and the reader will note that even in this relatively simple case the determination of a suitable variables x and the associated building blocs E, S, L and M is far from trivial. Hydrodynamic systems are typically open and driven, this provides a challenge for the GENERIC framework, which is designed for isolated systems. In this case the analysis appears to work if no attention is payed at all to the boundary conditions. On page 55 we see that this is even required to remove an ambiguity in the Poisson bracket. An extended GENERIC treatment for open and driven systems with a more careful treatment of the boundary conditions would be preferable in such cases (see also the author's remarks on page 8).

Chapter 3 on linear irreversible thermodynamics (LIT) will be of great interest to the readers with a classical thermodynamic background since here the connection between GENERIC and LIT is explained. I am afraid, however, that the treatment will not be very satisfactory for those readers. The well known thermodynamic forces and fluxes of LIT are indeed readily obtained, but the GENERIC treat-

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ment, based upon an isolated system is very different from the common LIT analysis of open systems using balance equations and a local equilibrium hypotheses. The further discussion on transformation behavior and symmetry properties, however, is again very complete and clear.

For the readers of the journal Applied Rheology Chapter 4 on complex fluids will be of primary interest. Indeed it shows the GENERIC engine working at full power, providing many interesting results, including a beautiful classification of admissible rheological models, models for dilute polymer solutions, the pompon model and dumbbell and reptation models. The collection of many known results in a common setting opens a perspective to further improvement of the modelling.

Chapter 5 deals with a somewhat exotic subject: Relativistic Hydrodynamics. Even for readers with no particular affinity with this subject the treatment is of interest since it shows the power and the universality of the approach. Moreover, some non-trivial results in bulk viscous cosmology are reported.

Part II on the statistical approach starts after a brief introduction on 'bridging of scales' with Chapter 6 on the projection-operator method. Here it is shown in great detail – with interesting discussions on separation of time scales and levels of coarse graining - how atomistic expressions and properties of the GENERIC building blocks E, S, L and M are obtained by a projection-operator procedure. These important results lay a firm basis under the GENERIC framework.

As an illustration on the coarse graining procedure of Chapter 6, Chapter 7 deals with the kinetic theory of rarefied gases. After a brief introduction where also Boltzmann's equation, the Chapman-Enskog expansion and Grad's moment method are described, the GENERIC building blocks for the Boltzmann equation and a GENERIC version of Grad's expansion are presented. These results illustrate once more the power and generality of the approach.

The final chapter, Chapter 8 is on simulations, in particular thermodynamically guided simulations, defined in terms of some coarse grained level of description. The goal is to find the GENERIC building blocks for that level of description and to use the coarse grained model for solving problems of practical interest. The role of various simulation techniques, including Monte Carlo simulations, molecular dynamics, Brownian dynamics and some representative examples are discussed in detail.

Of the six appendices at the end of the book I would like to mention in particular Appendix B, where some abstract geometrical objects and their role in the GENERIC framework are discussed. This provides a foundation for the phenomenological theory introduced in Chapter 1. The appendix also discusses the use of body tensors in relation to the admissibility of the particular kinds of convection.

Finally Appendix F is of exceptional importance for anyone who wants to use the book for a thorough study of the subject. Unlike many other textbooks not only the answers or partial solutions but detailed solutions of all exercises are provided. Also for the reader who just want to look up the solutions this is a valuable source of information and very welcome, in view of the rather abstract nature of much of the main text.

It is really very fortunate that Hans Christian Öttinger, one of the few people who presently is able to write a book at this level on this difficult subject, has faced the challenge and produced the present book. I am convinced that it will be of use for many readers and also will have a big impact on future developments in the field.

[1] SR Groot, P Mazur: Non-equilibrium Thermodynamics, North-Holland, Amsterdam (1969).
[2] M Grmela, HC.Öttinger: Dynamics and thermodynamics of complex fluids. I. Development of a general formalism, Phys. Rev. E 56 (1997) 6620-6632.
[3] HC Öttinger, M Grmela: Dynamics and thermodynamics of complex fluids. II. Illustrations of a general formalism, Phys. Rev. E 56 (1997) 6633-6655.
[4] HB Callen: Thermodynamics and an Introduction to Thermostatistics, John Wiley & Sons, New York (1985).

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Bibliography:
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