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ChE book reviews

MOLECULAR THERMODYNAMICS FOR NONIDEAL FLUIDS

by L. L. Lee
Butterworths, 80 Montvale Ave., Stoneham, MA 02180; $52.95 (1988)

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This is a graduate level book aimed at presenting modern statistical mechanical methods to engineers and applied scientists. Until the early 1970's these rigorous methods were only applicable to gases, crystalline solids, and simple liquids such as argon, and so are of limited value to engineers. Over the last fifteen years or so they have been extended to include nonspherical and polar molecules, electrolytes, nonideal solutions, and most recently, a wide variety of surface phenomena. There have been rapid developments in perturbation and integral equation theories, in computer simulation methods, and in scattering experiments that provide information about the molecular or atom-atom correlations functions. These powerful methods are gradually replacing the more empirical methods that engineers have traditionally used, and so a book of this sort is welcome. The only other books aimed at engineers of which I am aware are Reed and Gubbins' *Applied Statistical Mechanics* (now out of print and in some respects out of date) and Lucas' *Angewandte Statische Thermodynamik* (so far only available in the original German, although an English translation is planned for late 1989 or early 1990).

The coverage of the book is good. The first three chapters deal with introductory material–classical and quantum mechanics, the ensembles, and ideal gases. The remainder of the book covers more recent developments in the theory of liquids (Chapters 4-12, 14), the molecular dynamics simulation method (Chapter 13), and adsorption of solids (Chapter 15). There are useful appendices dealing with intermolecular forces, and giving computer programs for the solution of integral equations and molecular dynamics calculations. The parts dealing with liquids are thorough and well done. They cover the distribution functions and integral equations for fluids of polar and nonspherical molecules and not just spherical molecules as in many other books. There are quite detailed accounts of the integral equation and perturbation theory methods, including chapters on hard body fluids, Lennard-Jones fluids, polar fluids, electrolytes, and site-site model fluids.

As a teaching text the book has some drawbacks. The introduction to the ensembles is quite brief and lacks illuminating examples, figures, or much in the way of physical interpretation, so most students experiencing this material for the first time will find it hard going. There is a similar problem with the treatment of the distribution functions in Chapter 4. The chapter on molecular dynamics is well done, but for students it would be helpful to have some simpler examples or programs, and some discussion of the Monte Carlo method, which is easier to program for a beginner. It would have been helpful to have had more illustrative examples and well thought out questions at the end of chapters. The layout of the book is rather poor, with too much print on each page and poorly reproduced figures, making it somewhat difficult to read.

In conclusion, this is an up-to-date summary of a rapidly developing field that is aimed at an engineering audience. It will be especially useful to graduate students and other researchers as an introduction to the subject, but will need to be supplemented if it is used as a teaching text. ❐