

heterogeneous catalysis and does an excellent job of capturing the essential elements and tools required. This book is a valuable reference guide and is highly recommended for anyone working in the field of heterogeneous catalysis and in particular those interested in catalytic modeling. This book could also serve as a useful supplemental text for both basic and advanced courses in catalysis.

Matthew Neurock
Dept. of Chemical Engineering
University of Delaware
Newark, DE 19716

Applied Statistical Thermodynamics

By Klaus Lucas, Springer-Verlag, Berlin Heidelberg, 514 pp., 1991

This text takes the reader from the foundations of statistical and quantum mechanics, through the theory of intermolecular forces, and to the prediction of fluid-phase behavior of real systems. It is intermediate in level between Prausnitz et al.'s *Molecular Thermodynamics of Fluid Phase Equilibria* and Gray and Gubbins' *Molecular Theory of Fluids*. Like these texts, *Applied Statistical Thermodynamics* does not address complex fluids or other applications of statistical thermodynamics, such as adsorption. However, it more than adequately fulfills its stated objectives.

While many of the existing texts on statistical thermodynamics and computer simulation emphasize theory and technique above application, Lucas is clearly motivated by the description of real fluids. According to the author, the book could form the basis for a two-semester senior or first-year graduate course. The text covers a broad range of topics from elementary molecular theory to advanced aspects of liquid-state perturbation theory. Although the author claims that the text is suitable for newcomers to the field, it would certainly help if the reader had some previous knowledge of quantum and statistical mechanics.

A most appealing feature of the book is the remarkably clear and convincing argument for the use of molecular approaches in the evaluation of thermodynamic properties of fluids. The interpolation and extrapolation of ex-

perimental thermodynamic data and the prediction of mixture properties from properties of the pure components are, of course, topics of considerable importance for chemical engineers. Lucas notes that even the most complex empirical equation is likely to give poor estimates outside the fitting range. This is well illustrated in the text by the Bender equation of state with 20 adjustable parameters. For mixtures, the problem is still more acute. The remedy for this situation is to use equations which have a sound physical basis. If the interaction parameters cannot be obtained accurately from first principles (which is often the case), it is still possible to fit the theoretically derived equations over a relatively narrow range of experimental data and extrapolate with confidence. Numerous examples in the text demonstrate the success of this approach over the empirical route.

Chapter 1 presents a succinct review of classical and molecular thermodynamics. Chapter 2 deals with the tools for the calculation of the intermolecular forces—quantum mechanics—and the evaluation of macroscopic thermodynamic functions from these interactions—statistical mechanics. Chapter 3 is devoted to the ideal gas. Various thermodynamic functions are evaluated as well as the reaction equilibrium constants. Most of this is standard material which is also well treated in other texts, such as McQuarrie's *Statistical Mechanics*.

Chapter 4 presents a thorough discussion of intermolecular forces, beginning with a useful overview. The later sections emphasize the derivation of working formula for pair and three body potentials at long and short range. Some of the multipole expansions are extremely complex. For example, that for interaction between carbon monoxide and methane occupies nearly one page. If induction and dispersion forces are included, the expressions are even more forbidding. One has to wonder, in these days of symbolic computation programs, if it is really necessary to present all the gory details. For practical applications, the author suggests using the Maitland-Smith-Kihara potential for isotropic interactions and the site-site repulsion—multipole approximation (SSR-MPA) for anisotropic interactions. Chapter 5 concentrates on the application of the material developed in the previous chapters to real

gases. The properties of real gas mixtures are accurately described with pure component data. Transport properties are also briefly discussed.

Chapter 6 begins with a short discussion of the ideas behind Monte Carlo and molecular dynamics simulation. The reader would need to consult other texts, such as Allen and Tildesley's *Computer Simulation of Liquids*, for detailed information on how to write simulation programs. It is unfortunate that *Applied Statistical Thermodynamics* does not mention a number of powerful new techniques, including the Gibbs Ensemble and Gibbs-Duhem integration, which have revolutionized molecular-based phase equilibria calculations. Other topics considered in Chapter 6 include the corresponding states principle for liquids, distribution functions and their use in evaluating thermodynamic properties, and fluids of spherical and nonspherical hard bodies. Building on this material, the chapter continues with an extended discussion of perturbation theories. Finally, semiempirical models, such as the BACK and COR equations of state, are considered within the framework of generalized van der Waals theory. In Chapter 7, the concepts developed for pure liquids are extended to mixtures.

In general, the book is very well written. The author maintains a sharp focus on the more important issues. A helpful feature is the inclusion of a summary at the end of each chapter. The example problems are also welcome. However, *Applied Statistical Thermodynamics* would be even more attractive as a course text, if it included additional (exercise) problems after each chapter.

Julian Talbot
School of Chemical Engineering
Purdue University
West Lafayette, IN 47907

Handbook of Industrial Crystallization

Edited by A. S. Myerson, Butterworth-Heinemann, Boston, 242 pp., 1993

The editor of the handbook points out in the Preface that the literature on crystallization is scattered, and that this book will correct the situation "by providing a means for scientists or engineers to de-