

BOOK REVIEWS

Theory of Molecular Fluids, Vol. 1: Fundamentals

By C. G. Gray and K. E. Gubbins, Oxford Univ. Press, 1985, 626 pp., \$79.00.

This book represents the results of a major undertaking to review and codify the research to date on intermolecular forces and fundamental statistical mechanics for fluids composed of small, nearly-rigid molecules with more than one atom. The treatment is restricted to equilibrium properties of classical, non-reacting, nonelectrolyte fluids, with particular emphasis on liquids. Intermolecular potential models are discussed in great detail, especially the generalized Stockmayer potential and the site-site potential. The fundamental statistical mechanics presentation focuses on the pertinent molecular distribution functions and correlation functions. Both perturbation theories and integral equation theories for the pair correlation function, needed to calculate equilibrium properties, are discussed in much detail, with appropriate historical descriptions. Extensive appendices provide much useful background material for the less sophisticated reader, including information on spherical harmonics and related quantities, mathematical results, molecular polarizabilities, and the virial and hypervirial theorems. In addition, there is a rather complete table of multipole moments and polarizabilities for use in applications.

Since the fluids for which the theories are developed include many species dealt with in chemical processing, the potential applications in chemical engineering are of a much greater magnitude than previous theories of monatomic fluids. Direct applications would be in such areas as phase equilibria, dielectric phenomena, and surface effects. For the immediate future, this work will be useful to advanced graduate students and certain research workers in chemical engineering thermodynamics, with Volume 1 of interest primarily to theorists. A good knowledge of quantum mechanics, statistical mechanics, and other physical chemistry topics will be needed to comprehend the material without extended self study or tutelage—probably a level of knowledge

well beyond that obtained by most undergraduate chemical engineers.

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Adsorption Technology: A Step-by-Step Approach to Process Evaluation and Application (Chemical Industries Series, Vol. 19).

Edited by Frank L. Slejko, Marcel Dekker, Inc., 1985, 240 pp., \$55.00 (U.S. and Canada); \$66.00 (all other countries).

This book promises in the preface that it will fill a void in the existing literature on adsorption—it is meant to be an introductory text that “will carry [the novice] through the tortuous path of applying adsorption technology.” In order to accomplish this, the text contains four large chapters, each written by different authors. The first chapter deals with the theory and models of adsorption. The second describes methods available for testing adsorbents. The third chapter is a summary of some of the practical design considerations for large-scale adsorption systems, and the fourth treats specific applications of industrial wastewater treatment using adsorption. Only the first chapter is written by an academic, and the book has a definite industrial, technological flavor, heavy on examples and empirical observations and somewhat light on fundamental principles. There are a reasonable number of references at the end of all chapters except the second. The index is fairly complete and the nomenclature is consistent from chapter to chapter. There are no example problems or homework problems, and this of course reduces its suitability as a text for a course.

The first chapter on adsorption theory is the shortest of the four. After a brief introduction to the various types of adsorption isotherms for solutes on to solid surfaces (BET, Langmuir, Gibbs, Freundlich), it presents a correlation for mass transfer coefficients from the fluid to the particle surface due to Williamson et al. (1963). Since the governing equation for the fluid phase solute concentra-

tion is not written, the reader is assumed to be able to derive this on his own. A little more space is devoted to the transport of solute in the particles by bulk and surface diffusion. However, the reactor models section gives only curves of final results with no details, and refers the reader to a computer program called MADAM written at the University of Michigan. In this reviewer's opinion, this chapter should have been much more comprehensive.

The second chapter on the testing of adsorbents provides physical data for granular carbons, activated carbons, and synthetic adsorbents (surface area, density, etc.). It also describes in detail the procedures that should be followed to measure the adsorption capacity for a particular compound. This chapter is replete with good technical hints and very practical comments on how to make adsorption measurements and the chemical and physical factors that can influence them. Unfortunately, there are no references given for the source of any of the information. The third chapter is a very thorough summary of the various operating modes, regeneration methods, pretreatment techniques, etc. commonly used industrially. There are also good descriptions of the available batch processes, moving bed processes and fixed bed processes. There is also some good information about scale-up and hydraulics of fixed bed absorbers. The final chapter deals with the treatment of wastewater by adsorption. Examples are given of various pesticides and other organic molecules (phenolics, chlorinated hydrocarbons, aromatic hydrocarbons) that have been removed by adsorption methods. It also specifies some of the differences between activated carbon and polymeric adsorbents, and the advantages and disadvantages of each.

In summary, I think this book would be of great value to readers wishing an introduction to adsorption technology, together with some very helpful practical hints as to choice of adsorbents, methods of characterization, and techniques for design and operation. Because of the rather superficial treatment of the fundamentals of transport phenomena and

physical chemistry of adsorption, and the lack of worked out examples and homework problems, I would not use it as a text at the graduate or undergraduate level. However, this book should be read by anyone faced with the problem of implementing an adsorption process to remove organic materials from wastewater.

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Proceedings of the Second International Conference on Foundations of Computer-Aided Process Design

Edited by Arthur W. Westerberg and Henry H. Chien, CACHE, Ann Arbor, 1984, 1042 pp., \$37.50.

This volume contains the proceedings of FOCAPD-83, the second in a series of international conferences on process design. Like the first such conference held three years earlier, this meeting was designed as a forum for academic and industrial experts with interests in both re-

search and applications. The intense week-long conference was organized into nine sessions, each containing one or two rather detailed, invited presentations followed by a lengthy and often lively discussion period. The proceedings contain all 22 papers presented at the conference, four additional discussion papers, and summaries of the discussion sessions.

In comparison with the first conference, which was review-oriented and emphasized numeric analysis, thermodynamics, process synthesis, and other somewhat theoretical aspects of design and simulation, the subject areas chosen for FOCAPD-83 were more applied. Topics covered included expert systems for design, computer-aided systems engineering, database technology applications, equation-oriented and simultaneous modular alternatives to sequential modular flowsheet simulation and optimization, operability, resiliency, and flexibility, and batch design and scheduling, as well as recent research on specific modeling techniques including collocation, differential homotopy-continuation, hybrid fixed-point algorithms, algorithm

synthesis, nonlinear algebraic solution techniques, two-phase reactor modeling, and the structure and efficient use of thermodynamic models within design calculations. The proceedings are organized into sessions exactly as the conference was, even including the spill-over eighth session at which additional papers had been presented from several topics covered in other sessions. For clarity in the proceedings, these papers might have been better grouped with the topics to which they were related.

Within the defined scope of FOCAPD-83, the detailed presentations from this highly successful conference will provide researchers, practitioners, and educators with a good assessment of the current state of the art in a number of important process design areas. These papers, broadened further by the discussion summaries, should give readers an understanding of the problems now being faced and solved, and an outlook of challenging directions for continued research.

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