

volume are only that it had to stop somewhere. What is provided will surely serve to stimulate advances in fundamental aspects of corrosion and its allied fields of science and engineering.

Richard Alkire
Department of Chemical Engineering
University of Illinois
Urbana, IL 61801

Molecular Connectivity in Structure-Activity Analysis

By L. B. Kier and L. H. Hall, Research Studies Press (a division of John Wiley and Sons), Letchworth, Herefordshire, England.

Kier and Hall have extended and elucidated a different method for correlating the physical and thermodynamic properties of organic substances using the concept of molecular connectivity. In this formalism, the molecule is treated as a mathematical graph whose vertices are the atoms and whose edges are the bonds of the molecule. Connectivity indices, χ , are defined from the number of paths of various lengths (number of bonds) in the molecule, the degree of branching, and the types of atoms. Kier and Hall have shown high correlations among some of these indices and many properties of organic substances such as critical properties, densities, solubility in water, and even the effectiveness of nonspecific anesthetics. An interesting feature of this method is that connectivity indices can be related to structural features of the molecules under consideration.

This book contains nine chapters. Chapter 1, Origins of Molecular Connectivity, gives background information, briefly discusses methods for describing molecular structure, and describes in detail the molecular connectivity method that enables one to calculate connectivity indices. Neither the concept nor the mathematics is difficult at this level, and a computer program for calculating the indices is available from Hall.

Chapter 2, Physical Properties, describes a number of correlations of physical properties such as molar refraction, water solubility, molar volume, heat of vaporization, magnetic susceptibility, and the various molecular connectivity indices for different classes of compounds. For example, the molar volumes of 37 linear and branched chain paraffins from pentane to dotriacontane have been correlated with three connectivity indices, giving a correlation coefficient of 0.9999 and a standard error of 1.17. The actual molar volumes range from about 116 to

about 566, so this standard error represents an error of about 1% for the lightest paraffin and about 0.2% for the heaviest. This chapter will be most interesting for property estimations.

In Chapter 3, Topological Information, the relationships between the molecular connectivity indices and the structural features of molecules are discussed. This chapter illustrates which indices are likely to be significant in correlating various properties.

The relationship of the χ 's to electronic structure is treated in Chapter 4, Electronic Information. This includes types of bonding (single, double and triple), electrons in π and lone pair orbitals, and the effects of heteroatoms. Electronegativity and solvent polarity are also discussed.

Chapter 5, Statistical Considerations, is a reasonably simple treatment of many aspects of statistics that are important in developing correlations discussed elsewhere in the book.

Chapter 6, Strategies for the Use of Molecular Connectivity, gives guidelines for using the molecular connectivity method. Topics such as selection of the indices to be used, nonlinear correlating equations, and molecular symmetry are discussed.

Chapter 7 gives several examples of the use of the method in quantitative structure activity relation (QSAR) studies of biologically active substances. Chapter 8 is a bibliography of published studies using molecular connectivity. Chapter 9 contains some thoughts about future directions for molecular connectivity. References are given at the end of each chapter. Author and subject indices are at the end of the book.

This book is well written and quite easy to read. Its main focus is on the correlation and prediction of physical and thermodynamic properties as well as correlating properties with structure. It not only describes the theory behind the method and presents results which have been obtained by using it, but also explains how readers can apply the method to their own problems.

George Thomson
356 Fleetwood Dr.
Bartlesville, OK 74006

Chemical Process Simulation

By Asghar Husain, A Halstead Press Book, John Wiley & Sons, New Delhi, 1986, 376 pp., \$34.95.

The author attempts to cover all as-

pects of simulation as applied to chemical process engineering. The material is divided into four topics: general-purpose steady-state process simulation, specific-purpose simulation, dynamic simulation, and process synthesis. The author states that the book will "be of great interest to students, R&D scientists and practising engineers."

The book is basically an extensive literature survey with over 400 references published up to 1984, which will be of considerable value. Practical applications are inadequate since many systems and techniques described are obsolete. Little guidance is given as to what is current.

The features to be found in general-purpose sequential modular simulators are described and illustrated through reference to ASPEN and the author's program, PROSIM. Unfortunately, little direction is given would-be users on the use of such simulators, particularly the pitfalls which might be encountered. Related chapters cover the simultaneous equations approach, decomposition of networks, convergence promotion, and physical properties.

Specific-purpose simulations, many of which the author has done himself, employ more detailed models (particularly of reactors) than are found in most general-purpose simulators. The examples include many familiar processes and multi-component distillation. This chapter is the best in the book and of most use to potential users because the process modeling is covered in considerable detail.

The topic of dynamic simulation covers continuous system simulation languages such as CSMP, some of the simulators which have been developed specifically for chemical processes, and the simulation of batch processes and distillation systems. In the chapter on process synthesis, all of the basic problems that have been studied over the years are reviewed: heat-exchanger network synthesis, separation system sequencing, etc. But most of the material in both chapters is a rehash of the literature. Neither is recommended since many important concepts are glossed over or omitted entirely.

L. H. Rinard
City College of New York
New York, NY 10031

Advanced Biochemical Engineering

By H. R. Bungay and Georges Belfort, Eds., John Wiley and Sons, New York, 1987

This book begins with a preface that proclaims its uniqueness with the basis

largely on the summer course in biochemical engineering presented at RPI. The objectives of the book, other than to complement other textbooks in biochemical engineering, are not clearly defined, however, so one is left to assume that it is intended as either a teaching text for advanced students of biochemical engineering or as a reference source for practicing biochemical engineers. It is difficult to endorse the book strongly as either. There are no problems or other pedagogical exercises that distinguish the book as a textbook; in only a few instances, do the contents qualify as advanced reference material for biochemical engineers. Instead, the book can best be described as a compilation of review articles, some of which serve only to acquaint the unfamiliar reader with basic concepts, others of which examine topics in greater detail.

These points are demonstrated throughout the book. Chapters 1 and 2, a breakdown of biochemical product categories and an introductory chapter on cells and enzymes, respectively, seem to be directed toward an audience with no prior background in either the commercial or scientific aspects of biochemical engineering. Evidence of this claim ranges from the anthropomorphic representations of microbial cells in Figure 2.1 (inappropriate for any serious text) to the rudimentary coverage of enzyme kinetics at the end of the chapter. Likewise, Chapter 1 is a rather uninspiring synopsis of what biotechnology has produced in the past and can be expected to offer in the future.

Chapter 3 on the analysis of biological reactors adopts more of an advanced flavor by reviewing modeling concepts and by presenting results from selected computer simulation studies, but this chapter could benefit from less emphasis on computational analyses and greater attention to novel problems encountered in the operation of real systems. Nonideal reactors are not covered at all, nor is there discussion of reactor design strategies for alleviating problems associated with the likes of plasmid instability, cell recycle, filamentous organisms, or shear-sensitive mammalian cells.

Subsequent chapters generally follow one of two patterns: the chapters most relevant to biochemical processing (e.g., Chapter 4 on biomass refining and Chapter 8 on product recovery) are similar in form and content to review articles that have appeared elsewhere, and the chapters covering more fundamental topics (e.g., Chapter 5 on recombinant DNA and Chapter 9 on sorption) are overviews of material covered more extensively in other monographs.

This is not to say that the book is without some merit. The chapters on molecular enzyme engineering and on the molecular biology of industrial microorganisms contain many interesting and relevant examples, and the final chapter is an excellent survey of membrane separation technology. Moreover, the book is of general value in that it assembles timely information on several topics in a single source. But on the whole, the book lacks a strong identity and is inconsistent in its depth of coverage. Thus, those seeking an introduction to various topics pertinent to biotechnology (as opposed to the more specialized field of biochemical engineering) will find this text useful, although some chapters are much better in this regard than others. On the other hand, those expecting an advanced treatise on biochemical engineering, as promised by the title, will not be entirely satisfied.

D. S. Clark
Dept. of Chemical Engineering
University of California
Berkeley, CA 94720

Polymer Science

By V. R. Gowariker, N. V. Viswanathan and J. Sreedhar, John Wiley & Sons, Inc., 505 pp., 1986, \$39.95

Polymer Science contains 15 chapters; a bibliography and an appendix consisting of a list of universities/institutions offering courses on polymer science and technology. The chapters include the traditional sections on chemistry of polymerization, molecular weight and size, kinetics of polymerization, copolymerization, a list of individual polymers, polymer reactions and polymer degradation. The book also contains sections on the structure of macromolecules, the glass transition tem-

perature, crystallinity, polymer solutions and processing.

The book jacket claims that these "15 chapters are aimed to raise the reader to a level where he/she can easily assimilate other specialized and exhaustive treatises on the subject." After reading the text this reviewer has come to the conclusion that the authors have not reached their goal. This book is too superficial particularly with the physico-chemical and physics aspects of polymer science. There is no mention of rubber elasticity, rheology, chain stiffness and liquid crystals, crystalline unit cells, crystallization rates, etc. The section on physical methods does not include melting behavior. No section deals with the important issue of structure/property relations in polymer materials. A better title for this book would be *An Introduction to Polymer Chemistry*.

A number of erroneous statements are made. Examples are: the useful range of degrees of polymerizations (claimed to be only 200–300), remarks on polymer dissolution, and polymer crystallinity. Some of the values of melting points and crystallinities are highly misleading. High-density polyethylene, for example, is thought to have typical values of 144–150°C and 90% for the melting point and crystallinity, respectively. The book certainly will not serve, contrary to the authors' hope, as a "Handbook on important polymer-related properties."

The language used in the book is unusual. The printing is of moderate quality and the reproduction of photographs is poor.

Many of the existing textbooks listed in the bibliography cover the topic in a better way. Finally, the list in the appendix of universities and institutes with polymer-related programs fails to mention important centers such as, Leeds and Bristol in Great Britain, Freiburg and Mainz in the Federal Republic of Germany, for France and the USSR, only one entry each, and Dutch institutes are ignored.

Paul Smith
University of California
Materials Program and Department
of Chemical & Nuclear Engineering
Santa Barbara, California 93106