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

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 dotriacotane 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 chemical engineers concerned with 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

The author attempts to cover all aspects 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 multicomponent 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

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