Computational Methods in Chemical Engineering

By Owen T. Hanna and Orville C. Sandall, Prentice-Hall, Upper Saddle River, NJ, 1995, 454 pp., $75.00.

This excellent book's strengths are the broad coverage of most relevant topics and the discussion of details that affect the *application* of numerical methods, even if they are not central to the method. For example, what do you do when evaluating an integral and the integrand goes to infinity? With a 50-page appendix, the book gives a handbook-like review of calculus: infinite series, convergence of series, numerical evaluation of derivatives, and other summaries which will prove helpful.

There are several themes that make the book pedagogically sound: analytic methods are discussed before numerical methods, thus allowing the reader to build on existing knowledge, while errors of the numerical method are always assessed.

The book includes: linear algebraic equations, nonlinear algebraic equations, series expansions, interpolation, least squares, optimization, quadrature, ordinary differential equations (initial and boundary value problems), and partial differential equations.

Its broad scope is illustrated by several topics that are important but seldom treated, such as Padé approximations, Shanks transformation, and continuation methods. Naturally things are left out: nothing on numerical evaluation of Laplace transforms, very little on stiff algorithms (making the reader think they have to generate their own), nothing on the Churchill and Usagi interpolation method to piece together correlations derived for large and small values of parameters (Churchill and Usagi, *AIChE J.*, November 1972, p. 1121), and nothing on orthogonal collocation method for solving boundary value problems. There is only one paragraph on the finite element method. In fact, nearly all the problems are one-dimensional. While it is unrealistic to include the details of the finite element method in a text for juniors, they shouldn't be ignorant of the possibilities, since in most of their jobs that is how many problems will be solved.

The title of this book suggests a strong orientation toward chemical engineering, which is inaccurate. Chapter 1 is an excellent discussion of the types of problems arising in chemical engineering, but most of the problems posed are mathematical ones rather than chemical engineering ones. For example, the computational methods used in process simulation are not discussed, despite the fact that chemical engineers probably use those computational methods most. The book stands as an excellent test for an engineering course on computational methods, not restricted to chemical engineers.

The book also comes with a computer diskette. The programs are in Fortran-77 and True Basic, and explanations abound throughout the book. However, many of the problems described in the book can be solved using spreadsheets (and since students know how to use them this would save them time), but spreadsheets are not mentioned. Also ignored are the programs MATLAB, Mathematica, Maple, and Math CAD, which can solve many of these same problems. Thus the authors put themselves firmly in the camp of those who insist on writing one's own code. In these days of "faster, better, cheaper," this reviewer feels those programs (languages?) permit the student-engineer to work "faster, cheaper" at least. However, the book, which says it is about computational methods, does an excellent job in that realm. It is focused on that subset of the class that is interested in details of the methods rather than the casual users of the methods (who are considerably more numerous). The text is perfect for an engineering-wide course on computational methods and useful for mathematically inclined chemical engineers, but less useful for the entire class of chemical engineering students.

Bruce A. Finlayson
Dept. of Chemical Engineering
University of Washington
Seattle, WA 98195

The Structure and Reaction Processes of Coal

By K. L. Smith, L. D. Smoot, T. H. Fletcher, and R. J. Pugmire, Plenum Press, New York, 1994, 471 pp., $75.00.

One standard exercise in economics is to define the characteristics of a resource and then to determine how each characteristic impacts its value. *The Structure and Reaction Processes of Coal* does a first-rate job of the first part of the exercise. Coal characteristics are clearly defined, and a huge database related to coal characteristics is organized and summarized. The book fails, however, to provide a satisfactory linkage between most coal characteristics and the value of coal for combustion, gasification or any other application.

The book begins with an excellent introduction to coal types and a long list of commonly measured properties of coal including chemical (e.g., proximate and elemental analysis), physical (e.g., density, surface area), mechanical (e.g., strength, grindability), thermal (e.g., calorific value), electrical and ash. Next, there is an introduction to the most important coal databases and coal "banks." Data in these databases include measures of many of the properties listed above (such as eighteen tests of basic composition) from more than 1,000 coals collected from all over the U.S. The banks contain a large number of carefully collected samples, available for scientific investigation. The authors then introduce the concept of basic coal-type categories and suggest that a "suite" of 11 coals, selected for detailed analysis in the remainder of the text, can serve to represent all the major ranks and geographic locales for U.S. coal.

The first topic covered in depth is the connection between the origins of coals and coal structure. It is noted that this topic is of great importance because the variability of coal history is responsible for the great variation in coal properties. Coverage of the topic has strengths and weaknesses similar to those found throughout the text. Major strengths include an impressively thorough review of the literature. This is accompanied by an impressive set of tables, figures and direct quotes. There is a demonstrated ability to succinctly explain the nature of competing hypotheses and to present evidence in support of one position. However, in places the detailed commentary on the literature overwhelms and dilutes the themes. Lengthy paragraphs containing dozens of briefly summarized literature references tend to force the reader to lose focus. In places the text simply reads like an annotated database. Also, based on the introductory chapters, one expects the discussion to be structured around the

"suite of coals" picked as representative. Yet, discussion of these coals is entirely segregated to less than three pages of a 40-page-long chapter.

The chapter on coal structure characterization provides an excellent accounting of the analytical tools used to study coals and the results of recent work in this field. Happily, this chapter is structured around the characterization of the selected suite of representative coals. Problems of context do persist. A discussion of "char evolution" is initiated without an introduction to the nature of char or any indication of the value of characterizing the "evolution" of this coal derivative. An explanation for the study of char evolution can be inferred only from discussion of coal utilization in later chapters. Moreover, only by reading figure captions carefully and jumping around in the text, does the reader gain some understanding of the means by which "evolution" was studied. Also, some of the figures and tables are not entirely satisfactory.

The discussions of the chemistry of devolatilization and the concomitant transformations of structure are thorough and well focused. A high point in this chapter is an excellent review of the wide variety of efforts to model the process of devolatilization during heating, and to link the nature of the coal devolatilization to the coal rank and type. The reader really understands the need to follow the dynamics of coal/char transformation in high-temperature environments. Once again, however, the link between this discussion and the selected suite of coals is tenuous.

The final chapter is on the conversion of chars, and is a little disappointing. The authors fail to make the critical link between coal characteristics and the value of different coals for combustion, gasification or any other application. The reader is left with the feeling that factors other than structure are rate-determining in real applications. Specifically it appears that residual mineral content (e.g., calcium) can have a very important catalytic impact, particle size can have an important impact in situations in which diffusion is rate-controlling, and even the type of burner and residence time in a high-temperature precombustion environment can all be factors more significant than structure. Perhaps, this is a correct understanding. The authors could have done more to help the reader with this vexing issue.

To sum up, this book is an excellent source of information on coal/char static and dynamic structures. It also provides a fascinating insight into modern methods for studying coal structure and for modeling its transformations. As an annotated database of the modern literature on many aspects of coal science, it is superb. However, one is a little disappointed at the end to discover no clear and simple link is made between the structure and uses of coal.

Jonathan Phillips
Chemical Engineering Dept.
The Pennsylvania State University
University Park, PA 16802

Plastics for Electronics: Materials, Properties and Design Applications

By William M. Alvino, McGraw-Hill, New York, 1995, 363 pp., $50.00.

This book is organized in four parts: fundamentals of plastics for electronics, design considerations for plastics, utilization of plastics in electronics, and reference sources on plastic materials. The first part constitutes the major portion of the book and reviews the usage of plastics in the electrical industry, basic polymer concepts, major thermoplastics and thermosets, elastomers, alloys and blends, polymer processing, high-performance polymers, and organic coatings. This diverse range of topics imparts almost a handbook-like feel to the book. A significant amount of information is covered, making this part a handy reference. A large number of industrially important plastics are discussed, with their performance characteristics summarized. The reader will therefore save a great deal of time and energy which would otherwise be needed for collecting and analyzing a large body of literature.

The second part discusses two general topics: engineering properties (and testing of such properties) and design considerations. Here, the properties under consideration include mechanical, electrical, thermal and environmental (e.g., chemical resistance) behavior. Concise definitions and testing methodologies are presented. Selected plastics and elastomers are reviewed in the context of their performance characteristics. The chapter on design considerations forms an extension of the property and testing discussions. Although informative, the text is cut-and-dry. Specific examples or case studies would have helped illustrate certain points.

The third part is focused on forms, particular applications and uses of plastics. Discussions center around sheets, films, flexible circuits, tapes, and adhesives. One chapter is devoted to polymers in microelectronics, where general concepts about resists and electronics packaging are examined. The final part lists several sources of information such as professional societies, databases, and business and government publications.

The overall contribution of this book is the compilation of industrially relevant information on plastics for electrical applications. Although it does not cover fundamental polymer principles extensively, it does fill a gap between textbooks and handbooks. While it does not delve into any given subject in great detail, it touches on a large number of topics. Hence, it can be relied on as one key reference for practitioners in the electrical industry. The book will be particularly useful for those already familiar with the basics of polymer science and engineering.

David S. Soane
Soane Technologies
Hayward, CA 94545
