BOOK REVIEWS

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.

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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