BOOKS

Mass Transfer in Engineering Practice, by Aksel L. Lydersen, Published by John Wiley & Sons, April 1983, 321 pp., $39.95.

The book provides for practicing engineers a short refresher treatment of principles of mass transfer, distillation, gas absorption and desorption, liquid-liquid extraction, leaching, humidification, drying of solids, adsorption and ion exchange, and crystallization. Many worked examples are given on each topic. References are given to more in-depth treatments of each subject.

The book would be suitable for an introductory course on separations in chemical engineering where the curriculum combined mass transfer and separations into one course. The treatment of multicomponent distillation is very limited.

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Chemical Reaction Equilibrium Analysis: Theory and Algorithms by William R. Smith and Ronald W. Missen, 364 pp., John Wiley, 1983, $42.95.

With the expansion of computing technology, many algorithms are being proposed for the computation of chemical and phase equilibrium. New machines from pocket calculators to main-frame computers and applications from rocketry to sour-water stripping, involving just one reaction in one phase or complex reaction systems in multiple phases, are leading to new specialized and generalized algorithms. In this setting, Smith and Missen and John Wiley deserve much credit for introducing this first survey and analysis of a fine selection of algorithms.

The manuscript is required reading for algorithm developers and an excellent primer for those planning equilibrium computations. It is well-written, contains numerous examples and exercises, and is an appropriate text for advanced and specialized undergraduate and graduate courses that emphasize thermodynamics and numerical methods.

Chapter 1, the first of nine chapters, presents a brief description and history of the chemical equilibrium problem (including phase equilibrium). Chapter 2 contains an excellent and thorough treatment of stoichiometry, with several algorithms to determine a complete and independent set of mass balances. Chapter 3 adds the thermodynamic conditions at equilibrium, formulated with extents of reaction or mole numbers as independent variables. The former (stoichiometric formulation) requires a stoichiometry matrix for an independent set of chemical reactions (or "chemical equations"), eliminating the need for extraneous mass balance constraints. The latter (non-stoichiometric formulation) involves a direct minimization of Gibbs free energy (G) subject to the element abundance constraints (atom balances). The mathematical equivalence of these two formulations is illustrated, but the computational distinctions are not examined quantitatively here or elsewhere in the book. Chapter 3 continues with methods of stability analysis, which at a stationary point in G are intended to determine whether an additional phase exists at equilibrium. These are well-established for phases involving a single species, but for solutions the discussion here (and subsequently in Chapter 9) is incomplete. The chapter concludes with a valuable presentation of the sources of free energy data and their utilization.

Chapter 4 presents numerous algorithms (accompanied by HP41C and BASIC programs) intended to solve simple equilibrium problems (few reactions, elements or both). The discussions are more didactic than in other chapters and, considering the limited scope and applicability of the algorithms, are over-emphasized. Chapter 5 provides a cursory review of numerical methods for constrained minimization and the solution of nonlinear algebraic equations. The emphasis is appropriately placed on second-order methods since the derivatives of the chemical potentials usually can be evaluated easily and exactly.

Chapter 6 presents general algorithms for computing equilibrium compositions of ideal solutions. The authors first discuss non-stoichiometric algorithms, focusing on second-order methods. The BNR (Brinkley-NASA-Rand) algorithm is derived and small differences among its parent algorithms are considered. Next the authors present their stoichiometric algorithm, VCS (introduced by Villars and first extended by Cruise, then by Smith). The BNR and VCS algorithms are compared qualitatively and applied to the combustion of hydrazine in a vapor phase containing 10 species and 3 elements. FORTRAN computer programs for both algorithms are provided. However, the reader is forewarned that more sophisticated software is available from other sources.

Chapter 7 adds the complication of non-ideal solutions. Expressions for the excess Gibbs free energy, equations of state, and Pitzer's theory of corresponding states are briefly reviewed. An indirect method to modify the algorithms of Chapter 6 (for ideal solutions) is contrasted with accurate evaluation of the derivatives of the chemical potentials. Chapter 8 presents an extensive discussion of sensitivity analysis and Chapter 9 focuses on practical considerations such as the sources of singularities, rank deficiency in the matrix of formula vectors, and specifications other than temperature and pressure.

We applaud the emphasis on the equilibrium model, with many fine examples involving special cases (e.g., singular matrices), but are critical of the failure to consider some of the more important computational aspects; for example, (1) use of the Helmholtz function to avoid shifts between one and three real roots with cubic equations of state, (2) use of approximate physical property models which are periodically tuned, (3) dependence of the rate of convergence on approximations to the elements of the Hessian matrix, and (4) the advantage of maximizing the entropy given the pressure and enthalpy.

While multiphase systems are considered, we must criticize the incomplete discussion of the methods to locate the correct phase distribution at equilibrium. This is especially difficult in the critical region, which is overlooked in this book.

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