ADSORPTION CALCULATIONS AND MODELING

by Chi Tien

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Reviewed by
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A number of monographs began to appear in the mid-1980s on adsorption processes. Among them were *Principles of Adsorption and Adsorption Processes* (Ruthven, Wiley, 1984), *Large-Scale Adsorption and Chromatography* (Wankat, CRC Press, 1986), *Gas Separation by Adsorption Processes* (Yang, Butterworth, 1987), *Adsorption Engineering* (Suzuki, Elsevier, 1990), and *Pressure Swing Adsorption* (Ruthvan, Farooq, and Knaebel, VCH Publishers, 1994). A few others are currently in preparation. In addition, we have a collection of books on adsorption science with emphases on materials, thermodynamics and equilibrium, and rate behavior.

Adsorption Calculations and Modeling, by Tien, differs from the previous books in the adsorption process area. It is mainly concerned with laying the foundation for understanding isothermal, non-regenerative batch and fixed-bed processes, with emphasis on liquid-phase adsorption. Some computer programs on a diskette are included. The book is in large format and is part of the Butterworth-Heinemann Series in Chemical Engineering.

In the preface, Tien states that the book ". . . is not a treatise on adsorption nor a textbook on the subject of adsorption. Rather, it is a fairly narrowly focused and practically oriented book, aimed at giving an introductory, yet fairly complete presentation, on the calculation and analysis of adsorption processes. . . . some subjects have not been discussed in detail here, such as pressure- or thermal-swing adsorption . . . Instead, topics such as biological carbon adsorption, adsorption with impregnated adsorbents, and characterization of solutions of unknown composition, which had not been discussed in any previous texts, have been given fairly complete coverage. . . . The level is consistent with what is taught in an accredited B.S. degree program in chemical or civil (environmental) engineering. The book may be used as a textbook or part of a text for graduate courses dealing with separation technology, although as stated previously, the book was not written as a text."

The book begins generally before narrowing in focus to isothermal, liquid-phase applications. The introduction (Chapter 1) compares adsorption with other separation processes and gives examples involving wastewater treatment, air separation by PSA, and separation of hydrocarbons in a simulated moving bed. Chapter 2 on thermodynamics introduces the Gibbs adsorption isotherm. Equations for the various heats of adsorption are also developed, but are not used later.

Chapter 3 introduces various equations that can be used to describe single component isotherms. While the treatment is fairly broad, emphasis on liquid-phase adsorption, Polanyi potential theory-based models, and the Freundlich isotherm begins here. Numerous references to sources of data are provided, as are large tables of isotherm constants for liquid-phase adsorption.

Chapter 4 describes several methods for estimating multicomponent adsorption equilibrium. These include the extended Langmuir and Langmuir-Freundlich equations, the ideal adsorbed solution theory (used extensively later), the vacancy solution theory, potential theory-based methods, and methods for heterogeneous surfaces. In addition, some prior work on adsorption of organic vapors in the presence of water vapor and the adsorption of weak organic electrolytes from aqueous solutions is presented. Chapter 5 discusses rate behavior in adsorbent particles in various applications. Correlations are given for axial dispersion coefficients in fixed and fluidized beds, external mass transfer, and intraparticle mass transfer.

Development of equations for modeling various adsorption processes is contained in the next three chapters. Chapter 6 develops particle rate equations and various material balances (batch, continuous-flow through tanks, and fluidized, fixed, and moving beds). Then, batch processes and fixed-bed processes are discussed in detail in Chapters 7 and 8, respectively. Numerical methods based on finite differences and orthogonal collocation are introduced. For fixed beds, the discussion includes coverage of local equilibrium theory, constant pattern behavior, and the Thomas solution. Pressure swing adsorption is briefly covered.

Chapters 9, 10, and 11 treat applications on which the author has focused some of his research efforts—adsorption from solutions of unknown composition, adsorption with chemical reaction in impregnated adsorbents, and adsorption with biological growth.

An interesting feature of the book is the inclusion of more than twenty computer programs on diskette. These are in FORTRAN source code, carry a notice that they were developed by Hee Moon at Syracuse University in 1987, and are copyrighted by the publisher. The diskette is divided into directories for equilibrium, batch, and fixed beds. Programs are included for single and multicomponent adsorption. Within the equilibrium section, the initial program is for fitting data to either Langmuir, Freundlich, Sips (Langmuir-Freundlich), or Radke-Prausnitz isotherms. Then, programs are included for single and multicomponent calculations using the Polanyi potential theory with fits to Dubinin equations (D-R form for liquid-phase emphasized) and polynomial forms (gas phase emphasized). Programs are also included within the equilibrium directory for IAS calculations using Langmuir (with or without a first-order correction term) and Freundlich isotherm and programs for adsorption on heterogeneous surfaces. Programs within the batch directory allow single and multicomponent uptake data to be fit to models for surface and pore diffusion, including a branched network. Programs within the fixed-bed directory permit calculations for multicomponent liquid phase adsorption in fixed beds based on the linear driving force approximation with equilibria described by either Freundlich or D-R equations. All programs have a sample data file.

On the whole, this is a very nice book that achieves the goals that Tien set out to accomplish. My criticisms of the book are few and, for the most part, reflect my own views. The book complements other available books, many of which have a gas-phase orientation. If supplemented with problems and examples, this book would make an excellent textbook for a course emphasizing adsorption from the liquid phase. ❐