BOOK REVIEWS

Fluidization and Fluid-Particle Systems

By F. A. Zenz, Pemm-Corp Publications, Vol. II, Draft-1989, 665 pp., $60.

As indicated in the Preface, this is the first draft of a volume sequel to an earlier one published by the author with D. F. Othmer in 1960 by Reinhold in a series titled *Fluidization and Fluid-Particle Systems*. The author is one of the most well recognized industrial consultants worldwide in the field of fluidization. This volume addresses a number of important design problems associated with fluidization equipment. It unveils some myths concerning the design know-how which is of practical use for design engineers or practitioners working on fluidized bed systems. Thus, it is a welcome contribution to this important practical field.

The volume consists of 13 chapters. It starts with the author's long-standing perceptions regarding the analogies of physical and thermodynamic properties among vapors, liquid and particulate solids. For example, in analogy, the "boiling points" for gas-liquid-phase transition corresponds to the "terminal velocity" of the solid particle for gas-solid fluidization, and the "temperature" for gas-liquid mixing corresponds to the "interstitial fluid velocity" for gas-solid fluidization. It is interesting to note that in recent efforts, the approach of using the molecular analogy in numerical computation for gas-solid transport by employing the gas kinetic theory bears a similarity to that attempted earlier from a practical viewpoint by the author. The volume goes on to discuss various topics pertaining to fluidization equipment design and correlations. These topics include correlations on incipient fluidization, distributor and plenum region design, solids mixing and segregation, particle elutriation, cyclone performance, design and prediction, particle attrition, internals effects, heat-transfer correlations, granular bed filter performance, ejectors, and particle feeding systems into pressurized vessels. The volume contains valuable detailed design strategies and ideas for equipment varying from wagon wheel and multilevel grids, and inbed spiral platecoil internals to internal cyclone support and bracing and cyclone dipleg eductor. A large number of design problems and calculations and numerical examples are given in the volume.

As noted, this is presented in a draft form. The present volume does not contain complete information on nomenclature, figure captions, references, subject index and so on. Thus, considerable editorial work will be needed before it can be in a publishable book form. The materials presented, however, are very unique reflecting the extensive practical experience and knowledge of the author in this field. It is noted that almost all the references cited in this volume were published before 1980. Information on more recent developments in the design of fluidized systems such as in the areas of high-pressure fluidized bed combustion, fine powder processing, and bioprocessing would be helpful.

With some technical updates and editorial improvements, this volume in a final book form will be a very valuable addition to the fluidization literature. It will provide a very useful and much needed design guide for many types of fluidization equipment which would be most appreciated by practitioners. Academic researchers may also find the volume useful in gaining insight into the complexity of fluidization equipment design.

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Molecular Dynamics Simulation —Elementary Methods

By J. M. Haile, John Wiley and Sons, 1992, 489 pp., $59.95.

The two basic techniques for the molecular-based study of matter by computer simulation were introduced 40 and 36 years ago, respectively (Monte Carlo in 1953; molecular dynamics in 1957). Today, simulations are an indispensable tool of materials science, statistical mechanics, and liquid, solid state and polymer physics. It is only within the last six years or so that an expository literature aimed at educating new practitioners of simulations has started to emerge. This pedagogical literature has now been enriched by Jim Haile's *Molecular Dynamics Simulation—Elementary Methods*. The author aims at providing the novice simulator with a core of fundamental concepts that can eventually be used to tackle a wide variety of problems. In his words, this a book about principles, not applications. Its premise is that fundamentals are best transmitted by concentrating, in depth, on a small number of topics. Accordingly, the book deals exclusively with the deterministic simulation of isolated atomic systems.

Chapter 1 is introductory. Chapter 2, Fundamentals, discusses Newtonian and

Hamiltonian dynamics, phase space, elements of dynamical systems, sampling theory, periodic boundary conditions, and the effect of periodicity on the conservation of energy, linear momentum and angular momentum. Chapter 3, Hard Spheres, addresses the kinematics of hard-sphere collisions, the Alder-Wainwright algorithm for hard sphere simulations, the initialization and equilibration of hard body simulations, unpredictability due to multibody or simultaneous binary encounters, the hard sphere solid-fluid transition, and the assessment of the reliability of simulation results. Chapter 4, Finite Difference Methods, treats numerical algorithms used to integrate Newton's equations of motion for multibody systems whose constituents interact via continuous potentials. Topics addressed here include truncation and round-off errors, algorithmic stability, the Verlet and predictor-corrector algorithms, and the subtleties of assessing and comparing finite difference algorithms. Chapter 5, Soft Spheres, discusses the Lennard-Jones potential exclusively, its shifting and truncation, the use of neighbor lists to speed up code execution, the initialization and equilibration of soft sphere simulations, and the assessment of the reliability of simulation results. Having explained how constant-energy molecular dynamics works, the author devotes the final two chapters to explaining how the technique can be used to calculate physical properties. Chapter 6, Static Properties, addresses the calculation of simple properties (temperature, configurational energy, pressure, and mean square force); thermodynamic derivatives (heat capacity, compressibility, and thermal pressure coefficient); entropy and chemical potential (via thermodynamic integration, particle insertion, and coupling parameter routes); and the radial distribution function. Finally, Chapter 7, Dynamic Properties, treats time correlation functions, the generalized Einstein and Green-Kubo routes to transport coefficients (with emphasis on diffusion coefficients and shear viscosity), and the calculation of the self and distinct space-time correlation functions.

There are 13 appendices. The three most important ones are a discussion of statistical mechanics in the microcanonical ensemble and molecular dynamics Fortran programs (executable under Fortran 77 compilation) for hard and soft spheres, respectively. The programs are thoroughly commented and even explained with convenient text and diagrams. Each of the seven chapters contains between 20 and 40 problems (most very instructive, many quite challenging) on a miscellany of topics, including, among others, thermodynamics, statistical mechanics, dynamics, kinetic theory, and Monopoly. Each chapter has its own reference section; in addition, there is a general bibliography. In line with the book's overall objective, these literature citations are illustrative and are not intended to be all-inclusive.

Molecular Dynamics Simulation—Elementary Methods is, overall, a very well written book. Future practitioners of the technique will benefit from the author's expository clarity, attention to detail, and emphasis on fundamentals. Frequent quotations from Lord Kelvin's Baltimore lectures of 1884 are interspersed throughout the text, providing interesting historical counterpoint and reminding readers that ".... the way we tackle problems is not at all modern—it's merely the computer that's new and that allows us to push an established methodology farther than ever before." The discussion of collisions and the stability of trajectories (Chapter 2) is particularly enlightening: the two-dimensional motion of a confined hard disk is used here to illustrate how both quasi-periodic and chaotic motion can result from slight changes in the nature of the disk's collisions with the confining boundaries. Equally noteworthy are the sections on sampling theory (Chapter 2), and on algorithmic errors, accuracy, and stability (Chapter 4). Chapter 7 deals with material that is probably less familiar to chemical engineers than most other topics in the book. It is also, because of the excellent discussion of correlation functions, of generalized Einstein expressions, and of the Green-Kubo relations, the most instructive and best written portion of the book. On the other hand, one very much hopes (given the quality of what follows), that readers will not be deterred by Chapter 1, the book's weakest. The author's otherwise lucid style is replaced here by rather vague discussions on the relationship between modeling and simulation, theory and experiment, and on reductionism and simulation.

This book is an important and welcome addition to the simulation literature, especially for practitioners of molecular dynamics who are interested not just in applying the technique, but in understanding it in depth. The author's rather reticent choice of topics (deterministic simulations of isolated, atomic, spherically symmetric systems) excludes the entire field of stochastic techniques and therein lies the work's chief limitation. Occasionally this also leads to unnecessary complications, as in Chapter 6, where the fluctuation route to the isothermal compressibility in an isolated (microcanonical) system calls for the calculation of the adiabatic compressibility, the thermal pressure coefficient, and the isochoric heat capacity. Still, it is deep appreciation for what Jim Haile has written, much more than regret for what he hasn't, that best describe this reviewer's reaction to this fine book.

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Mixing in the Process Industries

Edited by N. Harnby, M. F. Edwards, and A. W. Nienow, 2nd ed., 1992, Butterworth-Hinemann, Oxford, 414 pp.

This is the second edition of an edited book, first published in 1985 based "on a long-running post-experience course [...] at the University of Bradford." The stated territory of the work is a broad coverage of subjects in mixing and is touted as now reflecting "the balance of interest shown in the topic by industrialists from both the United States and western Europe." As such, this book deals with inherently interesting and important problems, including mixing of powders (solid-solid), characterization of powder mixtures, mixing in fluidized beds, mixing of cohesive powders, dispersion of fine particles in liquids, descriptions of liquid mixing equipment, mixing of liquids in stirred tanks, jet mixing, mixing in single-phase and multiphase chemical reactors, mixing in laminar flows, static mixers, mechanical aspects of mixing equipment sizing and design, dynamics of emulsification, gas-liquid dispersion, and suspension of solid particles. Intrinsically, there is much in these chapters which should be of interest to practitioners, dispersed throughout a