

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-Heinemann, 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

variety of industries, as well as workers in fluid mechanics, turbulence, including direct simulations of turbulent flows, rheology, both polymer and suspension, polymer processing, colloid science, reaction engineering, transport and polymer reactors.

Reviewing edited books is treacherous since there is always some unavoidable convergence toward the mean. Attention has to be paid to the whole but, generic comments, loosely interpreted in an average sense, might punish good chapters while at the same time appearing to needlessly encourage. However, in reading the book I could not avoid thinking which one of the chapters could possibly have been published as reviews in this journal. When viewed in this light the picture is not encouraging. Neither is the global picture, I am afraid.

The book consists of 17 chapters (one less than in the first edition) ranging in length from a well-used 17 pages (mixing in single-phase chemical reactors) to a rather long 43 pages (mechanical aspects of mixing); the average chapter is about 24 pages. The cast of authors is slightly different than in the first edition, with nine authors being common to both. The first edition had a total of 11 different authors, the new one two more. Of the 13, six are academics and the rest from industry. When counted by chapter there are 12 academic authors and 11 industrialists. This makes for balance, if only in a numerical sense. The only U.S.-based author is now deceased. The rest, with the exception of a lone chapter from Switzerland, are from the U.K. By whatever definition I could imagine, except the tautological one of who is doing really applied mixing work in the U.K., I could hardly call it representative of academic U.K.-based work.

The preface of this edition states: "We think and hope that this *highly-revised second edition* satisfies the demand by industry and academia." This might be a bit of both an overstatement and wishful thinking. The words in italics are the only change in the preface of this second edition and the overall updating is very light. Only 13% of the references are 1985-on, and four chapters have none. Let us further state that the whole thing does not begin on a foundation of greatness. Even in this second edition the whole thing looks a bit rushed and non-uniform; some chapters have end of chapter notations, others not. Not a few

chapters look a bit myopic as well. I could not avoid thinking that the contents could have been improved, had some of the authors examined literature in the immediate vicinity of their interests. Obvious references, even in the interest of providing a global picture, are missing; I could not find any reference to Tatterson's work in Chapter 8 (Mixing of Liquids in Stirred Tanks); the references to rheological work in p. 23 are a strange lot. Some chapters look decidedly old-fashioned: Chapter 11 (Laminar Flow and Distributive Mixing) could have been in the early 70s without being revolutionary, and Chapter 14 (Dynamics of Emulsification), while by far not the worst, could probably have been much better if more modern material had been considered. I estimate that between a third and a half of the chapters are in areas where I consider myself knowledgeable; the majority of these are either out of date, some by about a decade or so, or are hopelessly naive. It is nevertheless a good thing that all this material is under one roof, since, for better or for worse, this paints a picture of what is currently being used in a practical sense.

It is conceivable that this is what industry demands and needs. It is also conceivable that some industrial researchers might find ready-made answers here although I hope that some ideas are not taken too literally. I can speak with more authority regarding academic wants and needs. If you want an overview of what gets consumed by industry or if you seek topics and ideas for research proposals, then you should consult this book. If you want insight and understanding, then you should look elsewhere.

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### **Applied Digital Control, Theory, Design & Implementation**

*By J. R. Leigh, Prentice-Hall International, United Kingdom, Ltd., 1992, 524 pp.*

As the title suggests, the author of this book tries to give a balanced treatment of theory and practice of digital control. The scope is kept wide to cover many topics of interest. In doing so, however, certain areas naturally lack depth. In my opinion, what distinguishes this book

from others is its increased emphasis on practical issues regarding computer control implementation. In comparison with the first edition, the major changes include a more detailed discussion on available distributed control systems, seven additional case histories of industrial applications and a chapter on adaptive and robust control with its separate list of references. The book is probably most useful as a reference book for engineering students and practitioners. It can be used as a textbook both at the undergraduate and graduate (MS) levels. Background required is classical feedback control and a working knowledge of mathematics and computing.

The chapters can be categorized as follows:

1. Mathematical foundations (Chapters 2-4 and 8)
2. Design-oriented topics (Chapter 5)
3. Hardware implementation (Chapters 6 and 10)
4. Industrial applications, survey of commercial DCS systems (Chapters 7 and 11)
5. More survey-type chapters which are still in research stage (Chapters 9 and 12)

Chapters 6, 7, 10 and 11 particularly distinguish this book from others.

Chapter 1 summarizes the elements of a digital control loop and prompts the reader to question the issues to be addressed during design and implementation. Chapter 2 covers the classical material on discrete-time signals, sampling and reconstruction. Loss of information during sampling of continuous signals and aliasing are discussed together with Shannon's sampling theorem. This material which can be found in other texts is clearly presented, but there is no significant discussion on filtering. Z-transform techniques are introduced in Chapter 3 along with pulse transfer functions and difference equations. The treatment is again quite classical and clear. Some proofs are not as detailed as one might like to see. The rest of the mathematical exposition includes inverse Z-transforms, solution of difference equations, transformations between z- and s-planes and analysis of time response for different pole locations in the z-plane.

Chapter 4 discusses some of the traditional methods of analysis and design. Different methods of discretization (such as backward, forward and trapezoidal)