ChE book reviews

Chemical Plant Simulation, Crowe, Hamielec, Hoffman, Johnson, Shannon, Woods, xiv+368 pp., Prentice-Hall, Englewood Cliffs, N. J., 1971.

Process engineers have long used computers to provide refined, detailed studies of individual process equipment. But the real virtue of large, high-speed computers is the ability to classify, file, and analyze masses of data. With a sufficiently powerful computer system, we are able to analyze complete processes. This attractive prospect has led to many attempts to build up special systems for chemical analysis. In a recent survey, I was able to identify 31 distinct systems; many more undoubtedly exist in proprietary situations. Most of these are directed towards "simulation,' but this differs greatly from the stochastic simulation of the systems engineers. For chemical plants, simulation means the generation and calculation of the many material, heat, and pressure balances needed to relate the flows, temperatures, pressures, and compositions in a complex process. Simulation can be applied to the material balance studies of a process under design; it can be used to provide cases for scheduling an operating process; or it can be used for control studies of an existing plant.

Of course, a simulation really evaluates only one operating condition or one design. The job of the process engineer is to make decisions; for him, simulation is just a first step, — he must explore many possible solutions, changing the simulation variables through changes in input data. This is really optimization, but optimization systems seem to be either too specialized or unable to accommodate efficiently the general building-block units of the process simulators. In any event, the recent widespread use of simulation systems in industry indicates that these systems do perform useful tasks. At the very least they provide an improved, up-to-date way of assembling and retaining the data needed for complex processes. To be efficient and competitive, all process engineering groups today must be facile in their use. Thus, the young engineer's first process assignment often involves computer simulation.

How do we take account of this in the chemical engineering curriculum? One solution,—fully demonstrated in a number of universities in the U.S. and Canada, — is to have students work realistic process simulations using a well-maintained computer system. The group at McMaster University, headed for many years by Prof. Ab Johnson, built up an expertise in this area through joint cooperative effort of students and faculty in several full-scale simulation studies. This effort was based on the PACER system first developed at Purdue by Prof. Paul Shannon and his student, Mosler, in 1964. The Important results of this collaboration are now available in a well-constructed and carefully edited book. The preliminary paper-bound version has been in use at McMaster and elsewhere since 1969. With so many tables, figures, and charts, the new edition is much easier to use.

Of course, the use of simulation studies in the undergraduate curriculum does require time. The student should not be asked to make such studies if it detracts from his ability to think about the process. If his major concern becomes one of getting the cards punched in the right places, rather than thinking about the effect of the numerical input values on the properties and flows, then the simulation study is not really worthwhile. Adequate time must be provided to evaluate carefully the significance of the process behavior underlying the simulation. However, if the system is properly used, simulations supply a good idea of the nature of real processes. Simple examples may give the student a clear understanding of process structure, but may also mislead him, through oversimplification of complex relationships.

The book is oriented to, and illustrated with, a specific system, PACER (and in particular the McMaster version, MACSIM), but it is a suitable introduction to many of the general ideas and principles of simulation. In spite of differences in programming and data handling, all of these simulation systems rely on the same basic ideas:

1. The existence of general-purpose equipment modules interrelated by streams.
2. The use of equipment vectors to store the particular characteristics of the equipment involved in a particular process.
3. The use of stream vectors to describe the properties of the streams, and more generally, of the information flow.
4. The characterization of the information flowsheet in terms of a process matrix.
5. The use of numerical iteration to calculate systems with recycle.
6. The ability to develop and use in the

simulation system general-purpose prediction routines or data libraries for physical and chemical properties.

Many of these concepts are fundamentally simple and are illustrated in elementary courses in stoichiometry and thermodynamics through simple, clearly described examples. However, computer application to large, practical problems results in system complexity and in multiplicity of detail. It is difficult to impress the undergraduate with the nature of this complexity and at the same time keep him from complete confusion. The straightforward how-to-do-it approach in this text is a good solution. Careful study of the text, with a simultaneous application to a realistic example project should give the student a good appreciation of the value of computers in process analysis.

The first two chapters provide an elementary introduction of the basic ideas, using simple process flows and simple equipment modules for mixing, separation, etc. In these chapters, there is a description of the recycle problem and its solution by iteration, and a brief review of techniques for analyzing process structure. Chapter 3 introduces PACER and describes the many control elements needed for this specific system. Even though the reader may be using some other simulation system, the specific description supplied may be the best way to understand clearly the nature and extent of control information required by large systems.

The central portion of the book is a detailed description, section by section, of the classic McMaster example, the contact sulphuric acid plant simulation. After a general description of the plant (Chapter 4), the two major decisions about modelling are described (Chapter 5). This is one of the most important chapters in the book since it emphasizes the way in which the engineer can control the sophistication, adaptability, and accuracy of the simulation at the expense of greater development time, more knowledge of basic data, and greater demands on the computer. Then, (Chapters 6-10), the various types of equipment modules are developed in some detail, using those for the sulphuric acid plant as basic examples. Here, the need for various levels of sophistication is described and illustrated. In spite of the specific nature of the examples, the discussion covers all the major types of equipment. Moreover, the problems at the end of each chapter are often oriented to other systems which have been studied by the McMaster group. In Chapter 11, the authors describe the use of the simulation, and the results obtained in some particular studies of the sulphuric acid plant. With a thorough study of these chapters, the reader should be able to apply PACER to other chemical processes with which he is familiar. And he would probably find it helpful even with another simulation system. Often, the users' manual is written for skilled or experienced engineers. Here, the descriptions and illustrations are definitely oriented to use as a text, or basic reference. In addition to the bare details, the book also includes a full description of some of the tricks which are essential for efficient simulation of real processes. For example, the sulphuric acid plant simulation uses a special pressure module to handle the pressure balances in the system without excessive information recycle.

In the closing chapters, several more general ideas are covered. Chapter 12 briefly describes optimization, using small-dimension direct-search techniques. Of course, optimization is the only efficient way to make decisions in large, multivariable problems, yet the need for optimization is not always recognized. In the survey mentioned earlier, only CHEOPS (which does not take advantage of the new developments in computers) and RPMS (which is limited to linear models) are truly oriented to optimization. The other systems, like PACER, require excessive duplication in the computation of each case. Optimization calls for several thousand cases in a typical direct search of ten to fifteen variables. Early versions of PACER are much too clumsy and slow to make such computations efficiently, since each case is treated as a complete simulation. There has recently been some recognition of this handicap, and it is possible that some of the proprietary systems now short-cut duplicated computation. But the description in Chapter 12 is little more than an introduction to basic ideas which can only be applied in a limited way to PACER models.

Chapter 13 is much more successful and important. This is a critique and summary of the strategy of tackling a simulation. It includes a detailed and complicated flowchart of simulation procedures which is well worth careful study. The authors are among the most experienced users of simulation. Their comments about their past experience are intelligent and significant. Finally, Chapter 14 provides a look ahead to possible future developments in the use of simu-

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With this unusual student-faculty ratio, classes at Caltech are generally small, interpersonal relations are fostered, and course programs and research activities tend to be closely interwoven.

logically complex two-phase polymer systems. A study was also made of terminal chains and their entanglements in triblock-diblock blends in which the proportion, length, and distribution of the terminal chains could be controlled. A study of rubbers consisting of two interpenetrating networks is expected to begin in the Fall of 1972.

Research activities are not restricted to the Polymer Laboratory. Thus, within Chemical Engineering, Professors W. H. Corcoran and N. W. Tschoegl collaborate in an effort to assess the effect of mechanical deformations on diffusion through membranes. A joint effort on segmental motion by NMR techniques is being planned with Professor R. W. Vaughan. Outside of Chemical Engineering, the Polymer Laboratory has maintained close contact with Professor W. G. Knauss's group in Aeronautics whose interests lies in the field of crack propagation and fracture in elastomers. Close liaison is also maintained with the Materials Science group at the Institute. Because of its small size, such interdepartmental contacts are easy to maintain at Caltech.

In the past, both Materials and Chemistry students have received Ph.D. or M.S. degrees for thesis work done in the Polymer Laboratory. Chemistry and Chemical Engineering form a single division at Caltech, and the polymer courses attract an increasing number of chemistry students. Chemistry undergraduates receive credit for undergraduate research performed in the Laboratory.

SEMINARS

During the academic year, the polymer group meets weekly for an informal luncheon seminar held in Professor N. W. Tschoegl's office. These seminars have the character of a special topics course for which, however, no credit is given. Approximately half of the seminar speakers come from outside Caltech. An effort is made to invite speakers who do research which is different from that of the group or who can supplement the expertise of the lecturers presenting the regular courses. Since it is recognized that many of the group's graduates will go into industry, a special effort is made to invite speakers from industrial R&D laboratories to acquaint group members with the directions and values of high-level industrial research and development work. Through the seminars the members of the group meet the many well-known polymer scientists who regularly pass through Caltech. The seminars contribute to the broadening of the group's concept of polymer research beyond the study of mechanical properties and rubbers.

The seminars also serve as a forum for periodic reporting by members of the group on the progress of their research. A graduate student is expected to present an average of three to four talks per year and in this manner gains valuable experience in the art of oral expression and communication. Every group member is expected to be sufficiently familiar with everybody else's research to be able to interact and such interaction is encouraged. This had led to intensive mutual reinforcement of interest and to cohesion within the group, and has sensitized group members to the demands and advantages of the team work so often essential to successful work in industry.

The seminar program has been very successful and has attracted interest from other groups at Caltech and also from outside the Campus. A major advantage of the seminars is, however, that they are normally restricted to a small group of about 15 people to encourage freewheeling and uninhibited discussion. □

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lation: the extension to design; the relationship of process simulation to the stochastic simulation of the systems engineer; and the strong dependence of simulation systems on new hardware developments.

In summary, this book is recommended as a basic source reference on simulation systems. The reader should find it valuable either as an undergraduate text or for self-study. With its use he should be able to understand the fundamental elements of a simulation, and have less confusion as to the application of simulation systems to large complex processes.

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