Intelligent Systems in Process Engineering: Paradigms from Design and Operations

Edited by George Stephanopoulos and Chonghun Han, Academic Press, New York, 1996, 625 pp., $69.95.

Are there "intelligent systems" or not? There are, if we understand them as software artifacts with an algorithm to "model and emulate," and thus automate, an engineering task that used to be carried out *informally* by a human.

Intelligent Systems in Process Engineering: Paradigms for Design and Operations uses this working definition and presents the results of ten years of research started at the Laboratory for Intelligent Systems in Process Engineering (LISPE) in the Chemical Engineering Department at MIT.

The book is divided into two sections with five chapters each. The first five chapters are related to process and product design, and the rest focus on process operations. Each chapter is centered around two themes: a process engineering problem and a set of techniques used to solve it. In each chapter one or more of these techniques are drawn from artificial intelligence, and the rest from more traditional areas such as systems and control theory, mathematical programming, and statistics. The following list summarizes techniques and applications covered in each chapter.

1. Modeling languages/descriptions of chemical reactions and processes
2. Automation in design/conceptual synthesis of chemical processes
3. Symbolic and qualitative reasoning/design of reaction pathways
4. Inductive and deductive reasoning/identification of potential hazards
5. Searching spaces of discrete solutions/design of molecules
6. Nonmonotonic reasoning/synthesis of operating procedures.
7. Inductive and analogical learning/improvement of process operations
8. Neural networks/functional estimation
9. Reasoning in time/modeling of temporal process trends
10. Explanation-based learning/improving batch scheduling algorithms.

It is not a textbook or a review but a showcase of several paradigms for some applications of artificial intelligence in process engineering. While it is not an introductory book, it provides the reader with a good overview of the area. It can also be read as an interesting and well written account of how some previously unsolved problems were tackled with the integrated approach, ingenuity and open mindedness of a new breed of chemical engineers and computer scientists. The contributors of the book should be commended for their efforts in demystifying artificial intelligence and intelligent systems and for their attempt to formalize and provide mathematical proof and analysis (in terms of complexity and combinatorics) wherever possible.

Although some of the original work described in the book was carried out at the end of the 80s, most chapters have an updated set of references to related work. Two exceptions are the chapters on Conceptual Synthesis of Chemical Processes and on Identification of Potential Hazards in Chemical Processes, which do not provide updated references to related research elsewhere in the U.S. and Europe.

In the integration of artificial intelligence and numerical techniques, their relative contribution is a continuum. This is clearly reflected in the book structure, which moves from the traditional artificial intelligence, i.e., "soft" (but not easy!) tasks of modeling and design, to the application of artificial intelligence techniques for improved understanding and manipulation of numerical results and procedures. In the former case numerical calculations are auxiliary, such as the one used in evaluating design decisions, while in the latter the numerical calculation is the core task.

Despite the variety of techniques and applications, each chapter exemplifies the following:

- Capture, articulation and utilization of various forms of knowledge (be it numerical or symbolic) within a framework that requires interaction and/or integration of complementary methodologies
- Hierarchical modeling (of molecules, reaction systems, processes and operations) to reduce the complexity of systems; this confirms the observation of H. A. Simon (*The Sciences of the Artificial*, MIT Press, Cambridge, MA, 1969) that hierarchical systems are easier to analyze, describe, understand, and develop than nonhierarchical systems.

As has been mentioned, however, there are many possible combinations of artificial intelligence and traditional techniques. A generic pattern emerges in their interaction, namely, that in most cases artificial intelligence techniques should be applied at the first stages where the problem is less formalized to prune the solution space. Numerical techniques can then be better exploited at the final stages for evaluation and optimization tasks.

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Polymer Science and Technology

By J. R. Fried, Prentice Hall PTR, Englewood Cliffs, NJ, 1995, 509 pp., $70.00.

During the past few years, a number of new textbooks have appeared for introductory courses in polymer science. Most of these are improvements over the first generation of polymer textbooks simply because more recent developments have been included. One of the latest additions to this area is *Polymer Science and Technology* by Joel R. Fried at the University of Cincinnati. Fried's reasons for writing this book are stated clearly in the Preface: "The decision was based on my belief that none of the available texts fully addressed the needs of students of chemical engineering. It is not that chemical engineers are a rare breed, but rather that they have special training in areas of thermodynamics and transport phenomena that is seldom challenged by texts designed primarily for students of chemistry or materials science." As a chemical engineer with research interests that overlap with polymer science, I reviewed this book with the author's objectives in mind.

The book is intended for advanced undergraduates and graduate students in chemical engineering. The book contains a total of 12 chapters, the first seven of which are described by the author as fundamental principles appropriate for an introductory course for chemistry or materials science students. Chapters 8–10 cover the major classifications of commercial polymers. These chapters could easily be included for chemistry or materials science students. Chapter 11 deals with polymer processing and basic rheology, and Chapter 12 introduces more recent applications of polymers in separation processes, in controlled release devices and as electronic materials. The last two chapters represent areas in which chemical engineers have made significant contributions to polymer science.

Chapter 1 is typical of any textbook in this field as it introduces the student to definitions, polymer classifications, chemical structure, molecular weight and its distribution, and nomenclature. Chapter 2 covers the basic expressions for polymerization rate and molecular weight for the two major mechanisms of step-growth and chain-growth (including copolymers) polymerization. The presentation given in this textbook is very similar to that in other introductory textbooks. I was somewhat surprised, however, that there was little discussion of the effect of kinetics on molecular weight and polydispersity. The instantaneous molecular weight distribution for chain growth was not presented at all. Also not covered in this book is the cumulative molecular weight distribution. The effect of conversion on the instantaneous distribution and, subsequently, the cumulative distribution are important from an industrial perspective. Given that the book has been written for chemical engineering students who have a background in reaction engineering as well as thermodynamics and transport phenomena, this material would have demonstrated how very broad distributions occur in practice.

Chapter 2 also discusses briefly ionic polymerization, coordination mechanisms, reactions on polymers, ring-opening polymerization and the use of macromers. Polymerization techniques such as bulk, suspension, and gas phase were treated qualitatively. A nice section was included on the use of spectroscopy (IR, Raman, and NMR) for chemical structure elucidation.

Chapter 3 covers the thermodynamics of polymer solutions and molecular weight determination. Few introductory textbooks go beyond Flory-Huggins theory for the thermodynamics of polymer solutions. Fried, however, does a good job in this book of discussing equation-of-state (EOS) theories using Flory's as an example. Since chemical engineers are exposed to equations of state in undergraduate thermodynamics courses, this section fulfills the author's objective very well. Two sections are worth noting here that are not often found in other textbooks. One is on the use of inverse gas chromatography to experimentally determine interaction parameters, and the other is on predicting activity from a group contribution method. The chapter ends with the requisite discussion of molecular weight determination with a short description of low-angle light scattering as the only topic not found in other texts at this level.

Chapter 4 covers solid-state properties such as the glass transition, secondary relaxations, crystallinity (including measurement techniques), and the melting point. An excellent section on thermal transitions is included with definitions of first- and second-order transitions and descriptions of dilatometry and calorimetry. In the area of mechanical property testing, both static and dynamic methods are covered at a level entirely appropriate for an advanced undergraduate student.

Chapter 5 is divided into two parts. The first part covers viscoelasticity using dynamic mechanical analysis as the framework. This is followed by a discussion on how parameters such as loss modulus, storage modulus, and tan δ are measured. Mechanical models common to other textbooks, based on combinations of Maxwell and Voight elements, are presented here. Also covered are the viscoelastic properties of polymer solutions and melts and dielectric relaxation, topics often neglected in other books. The second section focuses on rubber elasticity with a nice treatment of the thermodynamics. With the author's objective of expanded thermodynamic topics for chemical engineering students, I was surprised that the thermodynamics of elastomers in swelling solvents, the Flory-Rehner equation for example, was not covered.

Chapter 6 covers topics that can best be described under the heading "Fate of Polymers." Included are thermal, oxidative, UV, chemical, and hydrolytic stability. These topics have been included elsewhere, but Fried has added a section on plastics in the environment that addresses recycling, incineration, and biodegradation. I found the combination of topics in this chapter interesting. Using environmental fate could be an excellent way of motivating students to learn about stability issues in general.

Chapter 7 emphasizes the fact that commercial plastics are actually multicomponent mixtures. Sections are devoted to additives (plasticizers, fillers, and stabilizers), polymer blends, interpenetrating networks, and composites. The thermodynamic treatment of blends is minimal and would actually fit better in the chapter on polymer solution thermodynamics. Given the importance of phase separation on blend processing and subsequent properties, I expected more discussion here. There was also no general discussion of blend morphologies. On a related topic, block copolymers are mentioned only briefly in two or three places in the book with little or no discussion of their morphologies and properties.

Chapters 8, 9 and 10 cover commodity thermoplastics/fibers, elastomers and thermosets, and engineering/specialty plastics, respectively. Structures are given for many of the polymers along with physical properties, applications, and production levels. These chapters are, in effect, updated versions of similar chapters found in Billmeyer (1984). This information is often minimal in newer polymer texts, but its inclusion here provides the student with an appreciation of the breadth of polymer usage commercially. These chapters should be very beneficial to practicing engineers as well.

Chapter 11 begins with a description of the unit operations of polymer processing, followed by an introduction to rheology. In my opinion, the latter section utilizes a chemical engineering background better than any of the other topics up to this point in the book. All chemical engineering students are exposed to fluid mechanics or momentum transport, but rarely is there time to cover non-Newtonian fluids in great depth. Fried does a commendable job of motivating these advanced topics and introducing the students to elastic properties within the context of processing operations.

Chapter 12, the last chapter, covers the application of polymers in new technologies such as membrane separations, biotechnology, electronics, photonics, and drag reduction. The only topic detailed is the use of polymers as separation membranes. As with rheology and polymer processing, the use of polymers as separation membranes relies on transport phenomena, particularly diffusion in nonporous membranes and convection through porous membranes. Chemical engineering students with a knowledge of transport phenomena and a course in separation processes will be able to grasp this material readily.

In summary, I found *Polymer Science and Technology* to be worthy of consideration as a textbook for a polymer science elective for chemical engineering undergraduates. Problems are included at the end of each chapter, but not as many as in the latest edition of Rosen (1993) or in the new textbook by Grulke (1994). In terms of meeting the needs of undergraduates with a chemical engineering background, it is useful to compare Fried with Rosen and Grulke since all three books are written by chemical engineering faculty members. In the area of thermodynamics, both Fried and Grulke provide depth beyond the traditional Flory-Huggins treatment. Fried develops equation-of-state theories, while Grulke spends more time with the phase behavior of solutions and blends. In incorporating transport phenomena principles, both Rosen and Grulke provide more in-depth treatments of rheology, viscoelasticity, and processing than does Fried. On the other hand, Rosen does not cover diffusion in polymers, while Grulke does so within the context of devolatilization and drying and Fried uses membrane separations to discuss the topic. Lastly, in the area of reaction engineering, Rosen examines cumulative molecular weight distribution as a function of conversion, and Grulke covers different reactor types for polymerization in great detail. Fried describes polymerization techniques only briefly. The content of an introductory polymer course is certain to vary from instructor to instructor. Before adoption as a textbook, I recommend that this book be examined to determine if its coverage of topics is suitable for a given course.

Literature cited

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Thermodynamics

By K. S. Pitzer, 3rd ed., McGraw-Hill, New York, 1995, xvi + 626 pp.

The book on thermodynamics by Gilbert N. Lewis and Merle Randall published in 1923 had a major impact in both chemistry and chemical engineering. It made such convenient concepts as fugacity and activity coefficient accessible and became popular with those who dealt with the real world of mixtures. Its usefulness has been demonstrated by its widespread use today. The success of this book led to a major revision and updating in 1961 by Kenneth S. Pitzer and Leo Brewer, the so-called second edition. Much of the original material in Lewis and Randall was kept, but much valuable new work was added. Among this was the work of Pitzer on corresponding states, which has proved so useful to chemical engineers and remains the basis of many of the most trusted correlations at the present time. Now, more than 30 years later, Pitzer has revised and updated the 1961 version of Pitzer and Brewer's book.

The early chapters of the book cover the standard material needed for students of chemistry or engineering: the thermodynamic laws, state functions and their interrelationships, entropy, chemical potential, fugacity, etc. There is a useful chapter in this early material on statistical thermodynamics, with emphasis on the interpretation of entropy and on properties of gases and crystalline solids. After this basic material, there are chapters on properties of real gases, followed by five chapters on solutions of various kinds. The remaining chapters, Chapters 15–28, are perhaps the most interesting to the teacher of thermodynamics, since they include topics not often found in other books. Reflecting the interest of the author, there are five chapters dealing with the thermodynamics of electrolytes, electrodes and electrochemical cells. There are also very useful chapters on: surface properties; statistical thermodynamics; low-temperature gases (hydrogen, helium, methane); systems in the presence of gravitational, centrifugal, electrical and magnetic fields; multicomponent solutions; biochemical systems; multicomponent solid-vapor systems; and irreversible processes. There are also 17 appendices, several of which will be of particular interest to chemical engineers. They include an appendix on property estimation, most of which details the Pitzer acentric factor and its use in the generalized corresponding states correlations of thermodynamic properties. Other useful appendices include those on equations of state, property behavior near the critical point (the scaling laws), and equations for mixtures (Wilson, NRTL and UNIQUAC equations).

This book will be of great value to most academic and industrial practitioners, as well as to students. It explains clearly not only the rudiments of the subject, but many applications that are not easily available in other books. The inclusion of elementary statistical thermodynamic treatments of many of the important concepts is also an attractive feature not present in standard chemical engineering texts.

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