ChE book reviews

Principles of Quantum Chemistry
By D. V. George
Pergamon Press, 1972

Reviewed by Phillip Certain,
University of Wisconsin

The first thing one notices about this book is the unusual photograph on the dustjacket. A careful reading of the book gives absolutely no information about what the subject of the photograph (an electron micrograph of a mitochrondria membrane?) might be. Instead one discovers that this text is a straightforward presentation of the fundamentals of quantum chemistry, pitched at a level appropriate to advanced (and bright!) undergraduates.

It is a very compact presentation, requiring only 260 pages to cover most of the topics normally treated in a course on quantum chemistry and spectroscopy. The book begins with a brief historical introduction to quantum mechanics, including a "derivation" of the Schrödinger equation based on de Broglie's wave hypothesis. After the particle-in-a-box is treated, the postulational approach to quantum mechanics is presented in a very nice way. There is a good discussion of the significance of the commutator of two operators with respect to the uncertainty principle; and a simple introduction to Dirac notation is included.

As simple applications of quantum mechanics, George considers the usual rigid rotator, harmonic oscillator, and hydrogen atom. He presents the ladder-operator approach to the eigenvalues of the angular momentum operator, and develops the eigenfunctions from the differential equations approach.

Two additional chapters are invluded to provide necessary background for quantum chemistry. One is a very brief discussion of variation and perturbation methods and the other is an introduction to group theory.

This basic material constitutes the first half of the book. The remaining half is devoted to discussions of many-electron atoms, molecular orbital and valence bond theory, Hückel molecular orbital theory, ligand field theory and spectroscopy. These subjects receive an average of 20 pages each, so that it is evident the author maintains his concise presentation throughout.

Given the limited space available, George treats his subject clearly and concisely. There are some very attractive features of the book. Not a great deal of mathematical background is assumed for the student. Although the presentation is distinctly mathematical, the math is carefully done and more advanced techniques are discussed separately before applications are presented. There is a concise summary and set of exercises at the end of each chapter. The style of writing is informal and readable.

The essentials are in the book, but detailed applications and explanations in general have been sacrificed to conserve space. The instructor who chooses this book as a text should be prepared to provide a fair amount of supplementary material to the students. The book might be most useful in a free-wheeling course in which the instructor wants a text for the students which is a concise reference on the fundamentals.

The book is similar in length and level of presentation to M. W. Hanna's *Quantum Mechanics in Chemistry* [Benjamin (1969)]. The experience of our undergraduate students with this latter book is that, without substantial initial help, its conciseness is a real barrier to understanding. □

Optimization by Variational Methods

By Morton M. Denn
McGraw-Hill Book Company, New York, 1969
Reviewed by E. Stanley Lee, University of Southern California

Many books on optimization have been published. But, unfortunately, most books are not written for chemical engineers and do not use chemical engineering systems as examples. This book fulfills this gap in the variational approach. Furthermore, it is well written and has many useful examples.

Variational methods cover many different areas and frequently involve fairly sophisticated mathematics. Professor Denn did an excellent job in presenting the material and in avoiding the requirement of more sophisticated mathematical background. However, the user of this book must be cautioned about the fact that many chemical engineering students do not have the mathematical maturity and the teacher must present the material in great detail during the initial period. More homework and problem solv-

ing periods in class also help the situation.

Chapter 1 presents the basic concepts of optimization by differential calculus, also known as single stage optimization by differential calculus. It provides a useful and easy transition from differential calculus for the optimization of finite number of variables to the variational calculus for the optimization of functionals. The latter is treated in Chapters 3 to 6 for continuous systems and in Chapter 7 for staged systems. Computational problems are treated in Chapter 9 and Chapter 10 treats nonserial processes. An introductory coverage on feedback control and distributed-parameter systems is given in Chapters 8 and 11. In Chapter 12, an introduction to dynamic programming is given together with a demonstration of the interconnections between dynamic programming and the variational approaches.

In teaching a typical chemical engineering optimization course at the graduate level, this reviewer has found that it is useful to divide this course into two parts: the variational approaches and the programming approaches. The latter category includes all the linear and nonlinear programming techniques, and dynamic programming. As a foundation to these two categories, the various search techniques and numerical methods for solving algebraic and differential equations are introduced. Since practical chemical engineering problems are usually nonlinear problems; numerical solution, not analytical solution, should be emphasized.

Viewed from the above concept, this book can be used as a textbook for the variational approaches. If optimization is a one-year course, the variational approaches should be covered in a semester. The second semester is more appropriate with the first semester covering the programming techniques and the search techniques.

If the variational techniques are to be covered in one semester, fairly detailed discussions should be given to Chapters 1 and 3. The derivations in Chapters 4 and 5 can be omitted except to summarize the results to provide a transition from Chapters 3 to 6. Chapters 6, 7, 9 and 10 should, again, be covered completely. Since Chapter 2 is only an introductory chapter on search techniques which should be covered in the previous semester, this chapter can be omitted. Greater emphasis should be placed on Chapters 9 and 10. Furthermore, the material in these two chapters can be supplemented with recent publications in the literature. □