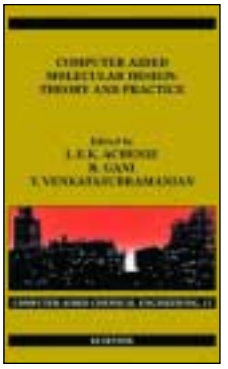
Books

Computer Aided Molecular Design: Theory and Practice

L. E. K. Achenie, R. Gani, and V. Venkatasubramanian (editors), Elsevier Science Inc. (www.elsevier.com), 407 pp., $220, 2003



Computer aided molecular design (CAMD) is a technique that is being used more frequently by researchers to design molecules with certain desirable properties. It is also finding increasing uses in industrial applications. CAMD is used to identify molecules that match a specified set of targeted properties, and their potential for application to chemical, biochemical and other material products.

This book mainly deals with macroscopic properties, and, therefore, does not cover molecular design of large, complex molecules, such as drugs. It focuses on the theoretical aspects related to CAMD, the different techniques that have been developed, and the different applications that have been reported (highlighted by case studies).

The book is divided into three main sections: Part I: Theory, Methods & Tools, (Chapters 1–7); Part II: Applications & Practices of CAMD (Chapters 8–15) ; and Part III: New Frontiers (Chapter 16). It also contains a glossary, a subject index and an author index.

Part I covers formulation and solution techniques. Chapter 1 introduces CAMD and discusses its important issues. Chapter 2 discusses methods on a generate-and-test approach, followed by two chapters on optimization methods involving mathematical programming. Evolutionary techniques based on genetic algorithms are presented in Chapter 5, while Chapter 6 describes a hybrid CAMD method. This part concludes with Chapter 7, where the application of CAMD to identify multistep reaction stoichiometries is presented.

Part II demonstrates the application and practice of some of the techniques described in Part I to different types of problems in CAMD. Chapters 8 and 9 describe the industrial application of CAMD methods for solvent design and selection. In particular, the use of the hybrid CAMD method is highlighted. In Chapter 10, the authors discuss the optimal design of a solvent, using the optimization-based CAMD method. Chapter 11 extends the application of CAMD from single solvent design to solvent mixture design, together with an application example. In Chapter 12, the authors provide an example of the application of the global optimization-based CAMD to optimal refrigerant design, while Chapter 13 discusses the application of genetic algorithm-based CAMD to polymer design. Chapter 14 presents a detailed case study of the application of CAMD to identify multistep reaction stoichiometries (using the method described in Chapter 7). The final chapter in this part of the book discusses the application of CAMD to the design of fuel additives employing the genetic algorithm-based CAMD method (as discussed in Chapter 5).

In Part III of the book, some of the new frontiers for computer aided product design (CAPD) are presented, and the outstanding issues and challenges are discussed.

The authors have targeted this book for a mixed audience, *i.e.*, scientists and engineers who would like to apply CAMD to solve their specific problems or would like to learn more about this topic, and educators who would like to use it as part of process/product design courses. In addition, it will serve as a handbook for software development and benchmarking of CAMD problem solutions. It is also intended for those who would like to use it as the starting point to further develop and extend the state-of-the-art in CAMD. The authors have done an excellent job of fulfilling their objective, and this book will be of great use to anyone interested in CAMD.

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Advances in Fluid Mechanics IV

M. Rahman, R. Verhoeven and C. C. Brebbla (editors), WIT Press (www.witpress.com), 760 pp., $382, 2002

This book contains edited versions of the papers presented at the Fourth International Conference on Advances in Fluid Mechanics, held in Ghent, Belgium in May 2002. It includes 67 papers, divided into 12 sections: 1. Biofluids; 2. Convection, heat and mass transfer; 3. Experimental vs. simulation methods; 4. Fluid structure interaction; 5. Hydrodynamics; 6. Industrial applications; 7. Material properties and fluids; 8. Multiphase flow; 9. Numerical methods in fluid mechanics; 10. Boundary layer flow and tidal dynamics; 11. Turbulence; and 12. Wave modeling. Section 9 is the longest with 14 papers, while sections 5 and 8 each include 9 papers.

These papers are intended to represent the state of current research in the respective areas, and hence are narrowly focused summaries of highly specific research studies. Because of the abbreviated scope of the papers, background information is severely limited so that most of the papers will be of interest only to those who are active or have a specific interest in the particular topic. The format is quite uniform, each beginning with an abstract and an introduction, and ending with a conclusion or summary and references.

The book provides an interesting perspective on the range and nature of current research topics related to fluid mechanics, but the high price will likely limit the "customers" primarily to libraries.

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