

Ralph E. White  
Venkat R. Subramanian

# Computational Methods in Chemical Engineering with Maple



Springer

# Computational Methods In Chemical Engineering With Maple

**Asha Immanuel Raju Chaduvula**



## **Computational Methods In Chemical Engineering With Maple:**

*Computational Methods in Chemical Engineering with Maple* Ralph E. White, Venkat R. Subramanian, 2010-02-06 This book presents Maple solutions to a wide range of problems relevant to chemical engineers and others. Many of these solutions use Maple's symbolic capability to help bridge the gap between analytical and numerical solutions. The readers are strongly encouraged to refer to the references included in the book for a better understanding of the physics involved and for the mathematical analysis. This book was written for a senior undergraduate or a first year graduate student course in chemical engineering. Most of the examples in this book were done in Maple 10. However, the codes should run in the most recent version of Maple. We strongly encourage the readers to use the classic worksheet mws option in Maple as we believe it is more user friendly and robust. In chapter one you will find an introduction to Maple which includes simple basics as a convenience for the reader such as plotting, solving linear and nonlinear equations, Laplace transformations, matrix operations, do loop and while loop. Chapter two presents linear ordinary differential equations in section 1 to include homogeneous and nonhomogeneous ODEs, solving systems of ODEs using the matrix exponential and Laplace transform method. In section two of chapter two, nonlinear ordinary differential equations are presented and include simultaneous series reactions, solving nonlinear ODEs with Maple's dsolve command, stop conditions, differential algebraic equations and steady state solutions. Chapter three addresses boundary value problems.

*Advanced Transport Phenomena* P. A. Ramachandran, 2014-09-25 An integrated modern approach to transport phenomena for graduate students featuring traditional and contemporary examples to demonstrate the diverse practical applications of the theory. Written in an easy to follow style, the basic principles of transport phenomena and model building are recapped in Chapters 1 and 2 before progressing logically through more advanced topics including physicochemical principles behind transport models. Treatments of numerical, analytical and computational solutions are presented side by side, often with sample code in MATLAB to aid students' understanding and develop their confidence in using computational skills to solve real world problems. Learning objectives and mathematical prerequisites at the beginning of chapters orient students to what is required in the chapter, and summaries and over 400 end of chapter problems help them retain the key points and check their understanding. Online supplementary material including solutions to problems for instructors, supplementary reading material, sample computer codes and case studies complete the package.

*Glyconanotechnology* Tomáš Bertók, 2019-11-08 Glycomics, a comprehensive study of glycans, often denoted as the third alphabet of molecular biology, besides nucleic acids and proteins, relies on techniques that use heavy machinery such as mass spectrometry, liquid chromatography and capillary electrophoresis. The use of biosensors and biochips for glycan analysis offers the possibility of lower costs, lower time and sample consumption and ease of use. This highly interdisciplinary book introduces students, researchers and professionals to the broad scope of this area, including the basics of nanotechnology and materials science, glycomics and bioanalytical chemistry, as well as several historical facts and contexts.

and future perspectives The introductory chapters are utilized in the book later for the state of the art chapters on glycan based diagnostics and imaging enrichment techniques and therapy which makes this book unique and of great interest to a wide audience The authors are skilled specialists and research scientists with many years of experience in this area and former investigators on a prestigious European Research Council Starting Grant Recent Developments in Fractional Calculus: Theory, Applications, and Numerical Simulations Lakhveer Kaur,Pushpendra Kumar,2025-05-30 This book discusses recent developments in fractional calculus and fractional differential equations in a very elaborative manner and is of interest to research scholars academicians and scientists who want to enhance the knowledge in the context of new insights and mathematical ideas in fractional calculus and its emerging applications in various fields It focuses on strengthening the existing results along with identifying the practical challenges encountered The purpose of this collection is to provide comprehension of articles that reflect recent mathematical results as well as some results in applied sciences untouched by the tools and techniques of fractional calculus along with their modelling and computation having applications in diverse arenas

**Computational Techniques for Chemical Engineers** C. Storey,H. H. Rosenbrock,2013-10-22 Computational Techniques for Chemical Engineers offers a practical guide to the chemical engineer faced with a problem of computing The computer is a servant not a master its value depends on the instructions it is given This book aims to help the chemical engineer in the right choice of these instructions The text begins by outlining the principles of operation of digital and analogue computers and then discussing the difficulties which arise in formulating a problem for solution on such a machine This is followed by separate chapters on digital computers and their programming the use of digital computers in chemical engineering design work optimization techniques and their application in the selection of optimum designs the solution of sets of non linear algebraic equations via hill climbing and determination of equilibrium compositions by minimization of Gibbs free energy Subsequent chapters discuss the solution of partial or simultaneous differential equations parameter estimation in differential equations continuous systems and analogue computers Computational Methods in Chemical Engineering Owen T. Hanna,Orville C. Sandall,1995 Authors Owen Hanna and Orville Sandall include broad use of convergence acceleration techniques such as Pade approximation for series Shanks transformation for series linear and nonlinear systems of algebraic equations systematic use of global Richardson extrapolation for integrals and ODE systems to monitor the overall error and discussion of methods for the solution of stiff ODE

**Computational and Statistical Methods for Chemical Engineering** Wim P. Krijnen,Ernst C. Wit,2022-12-19 In the recent decades the emerging new molecular measurement techniques and their subsequent availability in chemical database has allowed easier retrieval of the associated data by the chemical analyst Before the data revolution most books focused either on mathematical modeling of chemical processes or exploratory chemometrics Computational and Statistical Methods for Chemical Engineering aims to combine these two approaches and provide aspiring chemical engineers a single comprehensive account of computational

and statistical methods The book consists of four parts Part I discusses the necessary calculus linear algebra and probability background that the student may or may not have encountered before Part II provides an overview on standard computational methods and approximation techniques useful for chemical engineering systems Part III covers the most important statistical models starting from simple measurement models via linear models all the way to multivariate non linear stoichiometric models Part IV focuses on the importance of designed experiments and robust analyses Each chapter is accompanied by an extensive selection of theoretical and practical exercises The book can be used in combination with any modern computational environment such as R Python and MATLAB Given its easy and free availability the book includes a bonus chapter giving a simple introduction to R programming This book is particularly suited for undergraduate students in Chemical Engineering who require a semester course in computational and statistical methods The background chapters on calculus linear algebra and probability make the book entirely self contained The book takes its examples from the field of chemistry and chemical engineering In this way it motivates the student to engage actively with the material and to master the techniques that have become crucial for the modern chemical engineer

**Nonparametric identification of nonlinear dynamic systems** Kenderi, Gábor, 2018-11-11 A nonparametric identification method for highly nonlinear systems is presented that is able to reconstruct the underlying nonlinearities without a priori knowledge of the describing nonlinear functions The approach is based on nonlinear Kalman Filter algorithms using the well known state augmentation technique that turns the filter into a dual state and parameter estimator of which an extension towards nonparametric identification is proposed in the present work

Problem Solving in Chemical Engineering with Numerical Methods Michael B. Cutlip, Mordechai Shacham, 1999 A companion book including interactive software for students and professional engineers who want to utilize problem solving software to effectively and efficiently obtain solutions to realistic and complex problems An Invaluable reference book that discusses and Illustrates practical numerical problem solving in the core subject areas of Chemical Engineering Problem Solving in Chemical Engineering with Numerical Methods provides an extensive selection of problems that require numerical solutions from throughout the core subject areas of chemical engineering Many are completely solved or partially solved using POLYMATH as the representative mathematical problem solving software Ten representative problems are also solved by Excel Maple Mathcad MATLAB and Mathematica All problems are clearly organized and all necessary data are provided Key equations are presented or derived Practical aspects of efficient and effective numerical problem solving are emphasized Many complete solutions are provided within the text and on the CD ROM for use in problem solving exercises

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Chemical Engineering Education, 2003

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