# Numerical Methods for Chemical Engineers with MATLAB Applications

Prentice Hall International Series in the Physical and Chemical Engineering Sciences



# Numerical Methods For Chemical Engineers With Matlab Applications

**Ensheng Dong** 

### **Numerical Methods For Chemical Engineers With Matlab Applications:**

Numerical Methods for Chemical Engineers with MATLAB Applications A. Constantinides, Navid Mostoufi, 1999 Master numerical methods using MATLAB today s leading software for problem solving This complete guide to numerical methods in chemical engineering is the first to take full advantage of MATLAB s powerful calculation environment Every chapter contains several examples using general MATLAB functions that implement the method and can also be applied to many other problems in the same category. The authors begin by introducing the solution of nonlinear equations using several standard approaches including methods of successive substitution and linear interpolation the Wegstein method the Newton Raphson method the Eigenvalue method and synthetic division algorithms With these fundamentals in hand they move on to simultaneous linear algebraic equations covering matrix and vector operations Cramer's rule Gauss methods the Jacobi method and the characteristic value problem Additional coverage includes Finite difference methods and interpolation of equally and unequally spaced points Numerical differentiation and integration including differentiation by backward forward and central finite differences Newton Cotes formulas and the Gauss Quadrature Two detailed chapters on ordinary and partial differential equations Linear and nonlinear regression analyses including least squares estimated vector of parameters method of steepest descent Gauss Newton method Marquardt Method Newton Method and multiple nonlinear regression The numerical methods covered here represent virtually all of those commonly used by practicing chemical engineers The focus on MATLAB enables readers to accomplish more with less complexity than was possible with traditional FORTRAN For those unfamiliar with MATLAB a brief introduction is provided as an Appendix Over 60 MATLAB examples methods and function scripts are covered and all of them are included on the book s CD **Applied Numerical Methods** for Chemical Engineers Navid Mostoufi, Alkis Constantinides, 2022-05-22 Applied Numerical Methods for Chemical Engineers emphasizes the derivation of a variety of numerical methods and their application to the solution of engineering problems with special attention to problems in the chemical engineering field These algorithms encompass linear and nonlinear algebraic equations eigenvalue problems finite difference methods interpolation differentiation and integration ordinary differential equations boundary value problems partial differential equations and linear and nonlinear regression analysis MATLAB is adopted as the calculation environment throughout the book because of its ability to perform all the calculations in matrix form its large library of built in functions its strong structural language and its rich graphical visualization tools Through this book students and other users will learn about the basic features advantages and disadvantages of various numerical methods learn and practice many useful m files developed for different numerical methods in addition to the MATLAB built in solvers develop and set up mathematical models for problems commonly encountered in chemical engineering and solve chemical engineering related problems through examples and after chapter problems with MATLAB by creating application m files Clearly and concisely develops a variety of numerical methods and

applies them to the solution of chemical engineering problems These algorithms encompass linear and nonlinear algebraic equations eigenvalue problems finite difference methods interpolation linear and nonlinear regression analysis differentiation and integration ordinary differential equations boundary value problems and partial differential equations Includes systematic development of the calculus of finite differences and its application to the integration of differential equations and a detailed discussion of nonlinear regression analysis with powerful programs for implementing multivariable nonlinear regression and statistical analysis of the results Makes extensive use of MATLAB and Excel with most of the methods discussed implemented into general MATLAB functions All the MATLAB language scripts developed are listed in the text and included in the book's companion website Includes numerous real world examples and homework problems drawn from the field of chemical and biochemical engineering **Numerical Methods for Chemical Engineering Kenneth J.** Beers, 2006-10-30 Suitable for a first year graduate course this textbook unites the applications of numerical mathematics and scientific computing to the practice of chemical engineering Written in a pedagogic style the book describes basic linear and nonlinear algebric systems all the way through to stochastic methods Bayesian statistics and parameter estimation These subjects are developed at a level of mathematics suitable for graduate engineering study without the exhaustive level of the theoretical mathematical detail The implementation of numerical methods in MATLAB is integrated within each chapter and numerous examples in chemical engineering are provided with a library of corresponding MATLAB programs This book will provide the graduate student with essential tools required by industry and research alike Supplementary material includes solutions to homework problems set in the text MATLAB programs and tutorial lecture slides and complicated derivations for the more advanced reader These are available online at www cambridge org 9780521859714 **Numerical Methods for Chemical Engineering** Kenneth J. Beers, 2007 Suitable for a first year graduate course this textbook unites the applications of numerical mathematics and scientific computing to the practice of chemical engineering Written in a pedagogic style the book describes basic linear and nonlinear algebric systems all the way through to stochastic methods Bayesian statistics and parameter estimation These subjects are developed at a level of mathematics suitable for graduate engineering study without the exhaustive level of the theoretical mathematical detail The implementation of numerical methods in MATLAB is integrated within each chapter and numerous examples in chemical engineering are provided with a library of corresponding MATLAB programs This book will provide the graduate student with essential tools required by industry and research alike Supplementary material includes solutions to homework problems set in the text MATLAB programs and tutorial lecture slides and complicated derivations for the more advanced reader These are available online at www cambridge org 9780521859714 Numerous applications specific to chemical engineering and MATLAB integrated into each chapter with an extensive library of example problems also located on the web It avoids theoretically detailed mathematics Contains numerous problems and homework exercises at the end of each chapter categorised according to difficulty with solutions

available on the resource site **MATLAB Numerical Methods with Chemical Engineering Applications** Kamal I. M. Al-Malah, 2013-07-31 A practical professional guide to MATLAB computational techniques and engineering applications MATLAB Numerical Methods with Chemical Engineering Applications shows you step by step how to use MATLAB to model and simulate physical problems in the chemical engineering realm Written for MATLAB 7 11 this hands on resource contains concise explanations of essential MATLAB commands as well as easy to follow instructions for using the programming features graphical capabilities and desktop interface Every step needed toward the final solution is algorithmically explained via snapshots of the MATLAB platform in parallel with the text End of chapter problems help you practice what you ve learned Master this powerful computational tool using this detailed self teaching guide COVERAGE INCLUDES MATLAB basics Matrices MATLAB scripting language M file Image and image analysis Curve fitting Numerical integration Solving differential equations A system of algebraic equations Statistics Chemical engineering applications MATLAB Graphical User Interface Design Environment GUIDE **Chemical Engineering Computation with MATLAB®** Yeong Koo Yeo, 2020-12-15 Chemical Engineering Computation with MATLAB Second Edition continues to present basic to advanced levels of problem solving techniques using MATLAB as the computation environment The Second Edition provides even more examples and problems extracted from core chemical engineering subject areas and all code is updated to MATLAB version 2020 It also includes a new chapter on computational intelligence and Offers exercises and extensive problem solving instruction and solutions for various problems Features solutions developed using fundamental principles to construct mathematical models and an equation oriented approach to generate numerical results Delivers a wealth of examples to demonstrate the implementation of various problem solving approaches and methodologies for problem formulation problem solving analysis and presentation as well as visualization and documentation of results Includes an appendix offering an introduction to MATLAB for readers unfamiliar with the program which will allow them to write their own MATLAB programs and follow the examples in the book Provides aid with advanced problems that are often encountered in graduate research and industrial operations such as nonlinear regression parameter estimation in differential systems two point boundary value problems and partial differential equations and optimization This essential textbook readies engineering students researchers and professionals to be proficient in the use of MATLAB to solve sophisticated real world problems within the interdisciplinary field of chemical engineering The text features a solutions manual lecture slides and MATLAB program files Numerical Methods with Chemical Engineering Applications Kevin D. Dorfman, Prodromos Daoutidis, 2017-01-11 This undergraduate textbook integrates the teaching of numerical methods and programming with problems from core chemical engineering subjects Numerical Methods with Chemical Engineering Applications Kevin D. Dorfman, 2017 **MATLAB** 

**Applications in Chemical Engineering** Chyi-Tsong Chen,2022-05-20 This book addresses the applications of MATLAB and Simulink in the solution of chemical engineering problems By classifying the problems into seven different categories the

author organizes this book as follows Chapter One Solution of a System of Linear Equations Chapter Two Solution of Nonlinear Equations Chapter Three Interpolation Differentiation and Integration Chapter Four Numerical Solution of Ordinary Differential Equations Chapter Five Numerical solution of Partial Differential Equations Chapter Six Process Optimization Chapter Seven Parameter Estimation Each chapter is arranged in four major parts In the first part the basic problem patterns that can be solved with MATLAB are presented The second part describes how to apply MAT LAB commands to solve the formulated problems in the field of chemical engineering In the third and the fourth parts exercises and summary of MATLAB instructions are provided respectively The description of the chemical engineering example follows the sequence of problem formulation model analysis MATLAB program design execution results and discussion In this way learners are first aware of the basic problem patterns and the underlying chemical engineering principles followed by further familiarizing themselves with the relevant MATLAB instructions and programming skills Readers are encouraged to do exercises to practice their problem solving skills and deepen the fundamental knowledge of chemical engineering and relevant application problems The table of contents is listed below Chapter 1 Solution of a System of Linear Equations 1 1 1 Properties of linear equation systems and the relevant MATLAB commands 1 1 2 Chemical engineering examples 10 1 3 Exercises 43 1 4 Summary of the MATLAB commands related to this chapter 48 Chapter 2 Solution of Nonlinear Equations 51 2 1 Relevant MATLAB commands and the Simulink solution interface 51 2 2 Chemical engineering examples 70 2 3 Exercises 103 2 4 Summary of MATLAB commands related to this chapter 122 Chapter 3 Interpolation Differentiation and Integration 125 3 1 Interpolation commands in MATLAB 125 3 2 Numerical differentiation 131 3 3 Numerical integration 153 3 4 Chemical engineering examples 157 3 5 Exercises 183 3 6 Summary of the MATLAB commands related to this chapter 195 Chapter 4 Numerical Solution of Ordinary Differential Equations 197 4 1 Initial value problems for ordinary differential equations 197 4 2 Higher order ordinary differential equations 222 4 3 Stiff differential equations 227 4 4 Differential algebraic equation system 232 4 5 Boundary valued ordinary differential equations 236 4 6 Chemical engineering examples 254 4 7 Exercises 285 4 8 Summary of the MATLAB commands related to this chapter 308 Chapter 5 Numerical Solution of Partial Differential Equations 311 5 1 Classifications of PDEs 311 5 2 The MATLAB PDE toolbox 316 5 3 Chemical engineering examples 341 5 4 Exercises 388 5 5 Summary of the MATLAB commands related to this chapter 397 Chapter 6 Process Optimization 399 6 1 The optimization problem and the relevant MATLAB commands 399 6 2 Chemical engineering examples 448 6 3 Exercises 481 6 4 Summary of the MATLAB commands related to this chapter 501 Chapter 7 Parameter Estimation 503 7 1 Parameter estimation using the least squares method 503 7 2 Chemical engineering examples 517 7 3 Exercises 549 7 4 Summary of the MATLAB commands related to this chapter 560 References 563 Index 569 Numerical Methods for Chemical Engineering Kenneth J. Beers, 2007 Applications of numerical mathematics and scientific computing to *Numerical Methods for Chemical Engineers Using Excel, VBA, and MATLAB Victor J.* chemical engineering

Law,2013-03-05 While teaching the Numerical Methods for Engineers course over the last 15 years the author found a need for a new textbook one that was less elementary provided applications and problems better suited for chemical engineers and contained instruction in Visual Basic for Applications VBA This led to six years of developing teaching notes that

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**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 INTRODUCTION TO NUMERICAL METHODS IN CHEMICAL **ENGINEERING, SECOND EDITION** AHUJA, PRADEEP, 2019-08-01 This book is an exhaustive presentation of the applications of numerical methods in chemical engineering Intended primarily as a textbook for B E B Tech and M Tech students of chemical engineering the book will also be useful for research and development process professionals in the fields of chemical biochemical mechanical and biomedical engineering The book now in its second edition comprises three parts Part I on General Chemical Engineering is same as given in the first edition of the book It explains solving linear and non linear algebraic equations chemical engineering thermodynamics problems initial value problems boundary value problems and topics related to chemical reaction dispersion and diffusion as well as steady and transient heat conduction Whereas Part II and Part III comprising two chapters and six chapters respectively are newly introduced in the present edition Besides three appendices covering computer programs have been included For practice the book provides students with numerous worked out examples and chapter end exercises including their answers NEW TO THE SECOND EDITION Part II on Fixed Bed Catalytic Reactor consists of solving multiple gas phase reactions in a PFR diffusion and multiple reactions in a catalytic pellet and fixed bed catalytic reactor with multiple reactions Part III on Multicomponent Distillation consists of solving vapour liquid liquid isothermal flash using NRTL model adiabatic flash using Wilson model bubble point method theta method and Naphtali Sandholm method for distillation using modified Raoult's law with Wilson activity coefficient model Numerical Methods in Biomedical Engineering Stanley Dunn, Alkis Constantinides, Prabhas V. Moghe, 2005-11-21 Numerical Modeling in Biomedical Engineering brings together the integrative set of computational problem solving tools important to biomedical engineers Through the use of comprehensive homework exercises relevant examples and extensive case studies this book integrates principles and techniques of numerical analysis Covering biomechanical phenomena and physiologic cell and molecular systems this is an essential tool for students and all those

studying biomedical transport biomedical thermodynamics ABET oriented pedagogical layout Extensive hands on homework exercises Numerical Methods for Scientists and Engineers Zekeriya Altac, 2024-10-15 Numerical Methods for Scientists and Engineers With Pseudocodes is designed as a primary textbook for a one semester course on Numerical Methods for sophomore or junior level students It covers the fundamental numerical methods required for scientists and engineers as well as some advanced topics which are left to the discretion of instructors. The objective of the text is to provide readers with a strong theoretical background on numerical methods encountered in science and engineering and to explain how to apply these methods to practical real world problems Readers will also learn how to convert numerical algorithms into running computer codes Features Numerous pedagogic features including exercises pros and cons boxes for each method discussed and rigorous highlighting of key topics and ideas Suitable as a primary text for undergraduate courses in numerical methods but also as a reference to working engineers A Pseudocode approach that makes the book accessible to those with different or no coding backgrounds which does not tie instructors to one particular language over another A dedicated website featuring additional code examples guizzes exercises discussions and more https github com zaltac NumMethodsWPseudoCodes A complete Solution Manual and PowerPoint Presentations are available free of charge to instructors at www routledge com 9781032754741 **Chemical Process Engineering Volume 1** Rahmat Sotudeh-Gharebagh, A. Kayode Coker, 2022-03-25 Written by two of the most prolific and respected chemical engineers in the world this groundbreaking two volume set is the new standard in the industry offering engineers and students alike the most up do date comprehensive and state of the art coverage of processes and best practices in the field today This first new volume in a two volume set explores and describes integrating new tools for engineering education and practice for better utilization of the existing knowledge on process design Useful not only for students professors scientists and practitioners especially process chemical mechanical and metallurgical engineers it is also a valuable reference for other engineers consultants technicians and scientists concerned about various aspects of industrial design The text can be considered as a complementary text to process design for senior and graduate students as well as a hands on reference work or refresher for engineers at entry level The contents of the book can also be taught in intensive workshops in the oil gas petrochemical biochemical and process industries The book provides a detailed description and hands on experience on process design in chemical engineering and it is an integrated text that focuses on practical design with new tools such as Excel spreadsheets and UniSim simulation software Written by two industry and university s most trustworthy and well known authors this book is the new standard in chemical biochemical pharmaceutical petrochemical and petroleum refining Covering design analysis simulation integration and perhaps most importantly the practical application of Microsoft Excel UniSim software this is the most comprehensive and up to date coverage of all of the latest developments in the industry It is a must have for any engineer or student s library Coupled CFD-DEM Modeling Hamid Reza Norouzi, Reza Zarghami, Rahmat

Sotudeh-Gharebagh, Navid Mostoufi, 2016-10-17 Discusses the CFD DEM method of modeling which combines both the Discrete Element Method and Computational Fluid Dynamics to simulate fluid particle interactions Deals with both theoretical and practical concepts of CFD DEM its numerical implementation accompanied by a hands on numerical code in FORTRAN Gives examples of industrial applications

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