Revised Edition

# MATLAB Applications in Chemical Engineering

**Chyi-Tsong Chen** 



# **Matlab For Chemical Engineers**

**Chyi-Tsong Chen** 

# **Matlab For Chemical Engineers:**

Chemical Engineering Computation with MATLAB® Yeong Koo Yeo, 2017-08-01 Most problems encountered in chemical engineering are sophisticated and interdisciplinary Thus it is important for today s engineering students researchers and professionals to be proficient in the use of software tools for problem solving MATLAB is one such tool that is distinguished by the ability to perform calculations in vector matrix form a large library of built in functions strong structural language and a rich set of graphical visualization tools Furthermore MATLAB integrates computations visualization and programming in an intuitive user friendly environment Chemical Engineering Computation with MATLAB presents basic to advanced levels of problem solving techniques using MATLAB as the computation environment The book provides examples and problems extracted from core chemical engineering subject areas and presents a basic instruction in the use of MATLAB for problem solving It provides many examples and exercises and extensive problem solving instruction and solutions for various problems Solutions are developed using fundamental principles to construct mathematical models and an equation oriented approach is used to generate numerical results A wealth of examples 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 This book also 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 **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 **Chemical Engineering Computation with MATLAB** Yeong Koo Yeo, 2021 This new edition continues to present basic to advanced levels of problem solving techniques using MATLAB It 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 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 **Programming for Chemical Engineers Using C, C++, and MATLAB** Jr. Raul Raymond NUMERICAL, SYMBOLIC AND STATISTICAL COMPUTING FOR CHEMICAL ENGINEERS A. Kapuno, 2010-12 **USING MATLAB** Ghosh, Pallab, 2018-09-01 Numerical analytical and statistical computations are routine affairs for chemical engineers They usually prefer a single software to solve their computational problems and at present MATLAB has emerged as a powerful computational language which is preferably used for this purpose due to its built in functions and toolboxes Considering the needs and convenience of the students the author has made an attempt to write this book which explains the various concepts of MATLAB in a systematic way and makes its readers proficient in using MATLAB for computing It mainly focuses on the applications of MATLAB rather than its use in programming basic numerical algorithms Commencing with the introduction to MATLAB the text covers vector and matrix computations solution of linear and non linear equations differentiation and integration and solution of ordinary and partial differential equations Next analytical computations using the Symbolic Math Toolbox and statistical computations using the Statistics and Machine Learning Toolbox are explained Finally the book describes various curve fitting techniques using the Curve Fitting Toolbox Inclusion of all these advanced level topics in the book stands it out from the rest KEY FEATURES Numerous worked out examples to enable the readers understand the steps involved in solving the chemical engineering problems MATLAB codes to explain the computational techniques Several snapshots to help the readers understand the step by step procedures of using the toolboxes Chapter end exercises including short answer questions and numerical problems Appendix comprising the definitions of some important and special matrices Supplemented with Solutions Manual containing complete detailed solutions to the unsolved analytical problems Accessibility of selected colour figures including screenshots and results outputs of the programs cited in the text at www phindia com Pallab Ghosh TARGET AUDIENCE BE B Tech Chemical Engineering ME M Tech Chemical Engineering Numerical, Symbolic and Statistical Computing for Chemical E Pallab Ghosh, 2018-10-30 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 Programming for Chemical Engineers Using C, C++, and MATLAB Raul Raymond Kapuno,2005\* Chemical Engineering Analysis and Optimization Using MATLAB Weiguo Xie, Sam Toan, Richard Davis, 2024-12-16 Tackle challenging optimization problems with MATLAB software Optimization techniques measure the minimum or maximum value of a given function depending on circumstances constraints and key factors Engineering processes pertaining to design or manufacture involve optimization techniques at every stage designed to minimize resource expenditure and maximize outcomes Optimization problems can be challenging and computationally intensive but the increasingly widely used MATLAB platform offers numerous tools enabling engineers to tackle these essential elements of process and industrial design Chemical Engineering Analysis and Optimization Using MATLAB introduces cutting edge highly in demand skills in computer aided design and optimization With a focus on chemical engineering analysis the book uses the MATLAB platform to develop reader skills in programming modeling and more It provides an overview of some of the most essential tools in modern engineering design Chemical Engineering Analysis and Optimization Using MATLAB readers will also find Case studies for developing specific skills in MATLAB and beyond Examples of code both within the text and on a companion website End of chapter problems with an accompanying solutions manual for instructors This textbook is ideal for advanced undergraduate and graduate students in chemical engineering and related disciplines as well as professionals with backgrounds in engineering design 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 **Introduction to Software for Chemical Engineers** Mariano Martín Martín, 2025-03-24 The field of chemical engineering and its link to computer science

is in constant evolution and engineers have an ever growing variety of tools at their disposal to tackle everyday problems Introduction to Software for Chemical Engineers Third Edition provides a quick guide to the use of various computer packages for chemical engineering applications It covers a range of software applications including Excel and general mathematical packages such as MATLAB MathCAD R and Python Coverage also extends to process simulators such as CHEMCAD HYSYS and Aspen equation based modeling languages such as gPROMS optimization software such as GAMS AIMS and Julia and specialized software like CFD or DEM codes The different packages are introduced and applied to solve typical problems in fluid mechanics heat and mass transfer mass and energy balances unit operations reactor engineering and process and equipment design and control This new edition is updated throughout to reflect software updates and new packages It emphasizes the addition of SimaPro due to the importance of life cycle assessment as well as general statistics software SPSS and Minitab that readers can use to analyze lab data The book also includes new chapters on flowsheeting drawing process control and LOOP Pro as well as updates to include Pyomo as an optimization platform reflecting current trends The text offers a global idea of the capabilities of the software used in the chemical engineering field and provides examples for solving real world problems Written by leading experts this handbook is a must have reference for chemical engineers looking to grow in their careers through the use of new and improving computer software Its user friendly approach to simulation and optimization as well as its example based presentation of the software makes it a perfect teaching tool for both undergraduate and graduate level readers **Introduction to MATLAB with Applications for Chemical** and Mechanical Engineers Daniel G. Coronell, 2015-03-26 Introduction to MATLAB with Applications for Chemical and Mechanical Engineers provides applications from chemical engineering and biotechnology such as thermodynamics heat transfer fluid mechanics and mass transfer The book features a section on input output and storage of data as well as a section on data analysis and parameter estimation that contains statistical analysis curve fitting optimization and error analysis Many applied case studies are included from the engineering disciplines It also offers instruction on the use of the MATLAB optimization toolbox With a CD ROM of MATLAB programs this text is essential for chemical engineers mechanical engineers applied mathematicians and students , **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 Software for Chemical Engineers, Second Edition Mariano Martín Martín, 2019-06-06 The field of Chemical Engineering and its link to computer science is in constant evolution and new engineers have a variety of tools at their disposal to tackle their everyday problems Introduction to Software for Chemical Engineers Second Edition provides a guick guide to the use of various computer packages for chemical engineering applications It covers a range of software applications from Excel and general mathematical packages such as MATLAB and MathCAD to process simulators CHEMCAD and ASPEN equation based modeling languages gProms optimization software such as GAMS and AIMS and specialized software like CFD or DEM codes The different packages are introduced and applied to solve typical problems in fluid mechanics heat and mass transfer mass and energy balances unit operations reactor engineering process and equipment design and control This new edition offers a wider view of packages including open source software such as R Python and Julia It also includes complete examples in ASPEN Plus adds ANSYS Fluent to CFD codes Lingo to the optimization packages and discusses Engineering Equation Solver It offers a global idea of the capabilities of the software used in the chemical engineering field and provides examples for solving real world problems Written by leading experts this book is a must have reference for chemical engineers looking to grow in their careers through the use of new and improving computer software Its user friendly approach to simulation and optimization as well as its example based presentation of the software makes it a perfect teaching tool for both undergraduate and master levels Exercises Solution Manual for MATLAB Applications in Chemical Engineering Chyi-Tsong Chen, 2022-06-30 This self study solution manual in accompany with the book MATLAB Applications in Chemical Engineering is designed to provide readers with the key points of solving exercise problems at the end of each chapter which therefore instructively guides readers to familiarize themselves with the related MATLAB commands and programming methods for various types of problems Additionally through the assistance of this solution manual the readers would profoundly strengthen the logical abilities problem solving skills and deepen the applications of MATLAB programming language to solve analysis design simulation and optimization problems arose in related fields of chemical engineering The preparation of this manual is not for directly providing solutions but through key guidance overview and analysis and instructional solution steps to gradually cultivate readers problem solving skills Numerical Techniques for Chemical and Biological Engineers Using MATLAB® Said S.E.H. Elnashaie, Frank Uhlig, 2007-03-12 This interdisciplinary book presents numerical techniques needed for chemical and biological engineers using Matlab The book begins by exploring general cases

and moves on to specific ones The text includes a large number of detailed illustrations exercises and industrial examples The book provides detailed mathematics and engineering background in the appendixes including an introduction to Matlab The text will be useful to undergraduate students in chemical biological engineering and in applied mathematics and Introduction to Matlab for Chemical & Petroleum Engineering Sam Toan, Bahareh Nojabaei, Hertanto Adidharma, 2016-08-17 The importance of using computer aided calculations for engineers is evident nowadays Several classes in universities are taught to help engineering students become comfortable in using computation tools The purpose of this book is to provide a useful reference for students specifically chemical and petroleum en gineering majors and learn computer programming using MATLAB MATLAB is a very good tool as it has various built in functions MATLAB also has very easy to use graphing tools These capabilities and features of MATLAB make it a perfect computational tool for undergraduate level engineering stu dents The book chapters are designed to cover most of the topics in chemical and pe troleum engineering required courses We first introduce the basics of program ing as well as plotting features in MATLAB The students learn how to solve linear and nonlinear equations and system of equations using MATLAB in Chapter 6 Curve fitting and interpolation are covered in Chapter 7 The focus of the last several chapters is mostly on differentiation integration and solving ordinary and partial differential equations We provide chemical and petroleum engineer ing related examples in each chapter Furthermore some numerical methods that can be utilized at both the undergraduate and graduate levels are also dis cussed We the authors hope that this book would be helpful for both engineer ing students and instructors

Introduction to Matlab for Chemical & Petroleum Engineering Sam Toan, Hertanto Adidharma, Bahareh Nojabaei, 2017-07-30 For engineers today the importance of mastering computer aided calculations is becoming increasingly evident Universities around the world recognize the discipline as essential to success as an engineer and in turn offer an array of courses to help engineering students become comfortable using computational methods The purpose of this book is to serve as a useful reference and guide as students specifically chemical and petroleum engineering majors learn computational programming using MATLAB MATLAB is a very robust program with various built in analytical functions and easy to use plotting tools MATLAB s capabilities features and intuitive design make it an exceptional computational tool for undergraduate level engineering students The chapters contained in this book cover most of the topics in required chemical and petroleum engineering courses In Chapters 1 through 5 we introduce the reader to the basics of programing and plotting in MATLAB In Chapter 6 students learn how to use MATLAB to solve linear and non linear equations and systems of equations We cover curve fitting and interpolation in Chapter 7 The focus of the final chapters shifts to differentiation integration and solving ordinary and partial differential equations We provide chemical and petroleum engineering related examples in each chapter Along the way we also discuss various numerical methods that can be applied at both the undergraduate and graduate levels We the authors hope that this book will be helpful to engineering students and instructors



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